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A Collocation Method for the Solution of the Neutron Transport Equation With Both Symmetric and Asymmetric Scattering

Jim E. Morel

Prepared by Sandia National Laboratories, Albuquerque, New Mexico 87185
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A COLLOCATION METHOD FOR THE SOLUTION OF THE
NEUTRON TRANSPORT EQUATION WITH BOTH SYMMETRIC
AND ASYMMETRIC SCATTERING*

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ABSTRACT

A collocation method is developed for the solution of the one-dimensional neutron transport equation in slab geometry with both symmetric and polarly asymmetric scattering. In order to provide a method based on a standard approach to compare with the collocation method, the traditional discrete-ordinates method is extended to treat asymmetric scattering. For the symmetric scattering case, it is found that the collocation method offers a combination of some of the best characteristics of the finite-element and discrete-ordinates methods. For the asymmetric scattering case, it is found that the computational cost of cross-section data processing under the collocation approach can be significantly less than that associated with the discrete-ordinates approach.

A general diffusion equation treating both symmetric and asymmetric scattering is developed and used in a synthetic acceleration algorithm to accelerate the iterative convergence of collocation solutions. It is shown that a certain type of asymmetric scattering can radically alter the asymptotic behavior of the transport solution and is mathematically equivalent within the diffusion approximation to particle transport under the influence of an electric field.

The method easily extends to other geometries and higher dimensions. Applications exist in the areas of neutron transport with highly anisotropic scattering (such as that associated with hydrogenous media), charged particle transport, and particle transport in controlled-fusion plasmas.

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FORWARD

This report is a reprint of a dissertation submitted by the author in 1979 to the University of New Mexico in partial fulfillment of the requirements for the degree of Doctor of Philosophy in Engineering (Nuclear). Several typographical errors found in the original dissertation have been corrected in this report.

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CHAPTER 1

INTRODUCTION

1.1 Purpose and Scope

Our primary purpose is to develop a collocation technique for the numerical solution of the one-dimensional, one-speed, neutron transport equation in slab geometry. The technique is first developed for symmetric scattering and then extended to asymmetric scattering. Because it is consistent with a one-dimensional geometry, we consider scattering with polar but not azimuthal asymmetry. A general diffusion equation which is valid for both symmetric and asymmetric scattering is also derived, and a standard convergence acceleration algorithm is modified to accelerate the iterative convergence of the collocation solution. Finally, some numerical results are presented to illustrate the collocation technique.

1.2 Background and Motivation

In this section we present a brief historical discussion relating to the development of methods for the numerical solution of the neutron transport equation. In addition, we discuss our motivation for performing this research.

1.2.1 Discrete-Ordinates and Finite-Element Methods

There are basically two numerical methods presently used for the solution of the transport equation: discrete-ordinates and finite-element methods. The discrete-ordinates, or modern S_n method, was developed during the late 1950's and early 1960's by B. G. Carlson (1963) and his co-workers at the Los Alamos Scientific Laboratory. It evolved from Carlson's (1953) original S_n technique and Chandrasekar's (1950) semi-analytical discrete-ordinates method.

The finite-element technique was first introduced by Courant (1943) for solving certain structural mechanics problems. It represents a direct extension of the classical Rayleigh-Ritz technique and has been applied to a great variety of scientific and engineering problems in recent years (Prenter, 1975). Early applications of this method to the solution of the neutron transport equation were made by Kaper, et al. (1971) and Miller, et al. (1973).

The discrete-ordinates method is principally characterized by the use of finite-difference approximations and numerical quadrature formulae to treat the differential and integral terms appearing in the transport equation. It is applied to the first-order integro-differential form of the transport equation (as opposed to the second-

order even-parity or integral forms), yields discrete solutions, and generates equations which can be solved efficiently using iterative methods.

The finite-element technique is principally characterized by the use of a variational principle to determine an approximate solution constructed from a set of basis functions. The exact nature of the variational principle can vary widely. In order to utilize a Ritz procedure, early finite-element methods were restricted to the solution of the second-order even-parity form of the transport equation (Kaper, et al., 1971). There are several significant disadvantages associated with the use of this equation. However, Martin and Duderstadt (1977) have recently developed a finite-element procedure for the solution of the first-order integro-differential form of the transport equation.

The primary advantages of the finite-element method, relative to the discrete-ordinates method, are that continuous rather than discrete solutions are obtained and that the basis functions can be tailored to the problem. The main disadvantage is that the finite-element equations generally cannot be solved efficiently using iterative methods. Direct solution techniques requiring large amounts of computer storage must usually be employed. It is significant to note that finite-element methods can be more

accurate than discrete-ordinates methods with the same number of unknowns (Miller, et al., 1973). However, it is not clear as to what extent this increased accuracy can compensate for the necessity of using direct solution techniques.

Recently, several hybrid methods have been developed which utilize a low-order explicit finite-element treatment for the spatial variables with a discrete-ordinates treatment for the angular variables (Reed, et al., 1973), (Hill, 1975). Complicated spatial boundaries can be treated, and the equations can be efficiently solved using iterative methods.

1.2.2 The Collocation Method

Like the finite-element method, the method of collocation is a general approach to the solution of integral and differential equations. In recent years, it has primarily been applied to the solution of ordinary differential equations (Prenter, 1975). This method has been known for quite some time. References to it appear in the literature as early as 1938 (Lanczos). Surprisingly, this method has been largely ignored by the neutron transport community. The only related work of which we are aware is that of Reed (1972). Reed demonstrated a correspondence between a particular type of oblique projection technique and the

standard discrete-ordinates treatment of the angular variables. Although he did not specifically state it, this oblique projection technique is equivalent to a collocation technique. Thus, Reed effectively showed that discrete-ordinates and collocation methods are related. However, because he was interested only in exploiting this relationship to develop spherical harmonics-equivalent discrete-ordinates methods, it was only superficially investigated. The connection between discrete-ordinates and collocation methods is further investigated and discussed in Chapter 6.

Collocation methods are similar to finite-element methods in that basis functions are used to represent the solution. However, collocation solutions satisfy the exact equation in a pointwise rather than variational sense. A detailed comparison of finite-element and collocation methods is provided in Chapter 2.

A complete description of our collocation technique is contained in Chapter 6. However, for purposes of general comparison with discrete-ordinates and finite-element methods, it is briefly described as follows:

a) Only the angular directional variables are treated. When the collocation method is applied, the transport equation is reduced to a coupled system of differential equations with unknowns which are continuous functions of the spatial variable. In order to solve this system on a

computer, the spatial variable must be discretized in some way. Although any treatment can be used, we employ the standard discrete-ordinates spatial variable treatment in our calculations.

b) Because basis functions are used to represent the angular dependence of the flux solution, the method is versatile, and continuous solutions (normally associated with finite-element techniques) are obtained.

c) The collocation equations are identical in algebraic form to the standard discrete-ordinates equations and thus are similarly amenable to efficient iterative solution.

The collocation approach clearly has some of the best characteristics of both the discrete-ordinates and finite-element approaches.

1.2.3 Asymmetric Scattering

A scattering cross section is symmetric if it depends only upon the quantity $\vec{\Omega}_1 \cdot \vec{\Omega}_2$, where $\vec{\Omega}_1$ and $\vec{\Omega}_2$ denote the incident and scattered directions respectively. A cross section is asymmetric if it explicitly depends upon $\vec{\Omega}_1$ and $\vec{\Omega}_2$. The differential cross sections describing neutron scattering in reactor and shielding materials are generally symmetric. Hence, historically, little effort has been made to develop numerical methods which treat asymmetric scattering. However, neutron transport methods have recently been

applied to the transport of neutral particles in plasmas (Greenspan, 1974). Plasma media are often anisotropic. That is to say that the particles comprising the plasma are not isotropically distributed in their direction of movement. For instance, the charged particles in a TOKAMAK plasma tend to travel along the toroidal axis (along the magnetic field lines) rather than in the radial direction (across the magnetic field lines). Even though neutral particles entering the plasma scatter symmetrically in the center-of-mass frame, the anisotropy of the plasma gives rise to cross-section asymmetry in the laboratory frame. To date, this asymmetry has been neglected because present production discrete-ordinates codes can accept only symmetric cross sections. Thus there are applications for a method which can treat asymmetric scattering, but in searching the literature, we have been unable to find any previous development of one. Although most applications actually require two-dimensional calculations, we feel that the development of a one-dimensional method is a logical first step. In order to provide a method based upon a standard approach to compare with our collocation method, we extend the traditional S_n method to treat asymmetric scattering. This is done only for purposes of theoretical comparison. The asymmetric S_n method is not computationally tested.

1.2.4 The General Diffusion Equation and Convergence

Acceleration

We were unable to locate any references dealing with a diffusion equation valid for both symmetric and asymmetric scattering. The development of such a general equation is important for two reasons. First, it can yield qualitative (and possibly quantitative) information about the effect of cross section asymmetry. Second, it can be used in an algorithm to accelerate the iterative convergence of the collocation solutions.

The standard (symmetric) diffusion equation has been used in an algorithm known as diffusion-synthetic convergence acceleration to accelerate the iterative convergence of discrete-ordinates solutions (Alcouffe, 1977). This technique has been demonstrated to be the most effective of all convergence acceleration methods (Miller, 1978). We have modified the method to accelerate the iterative convergence of collocation solutions with both symmetric and asymmetric scattering.

1.3 Organization

A comparison of finite-element and collocation methods is given in Chapter 2. Chapter 3 is devoted to a discussion of generalized Lagrangian basis sets. These sets play a major role in our method. The transport

equation which is solved and the standard diffusion equation are described in Chapter 4. In Chapter 5, the standard discrete-ordinates angular variable treatment is briefly discussed. In addition, this treatment is extended to include asymmetric scattering. Discrete-ordinates methods for treating the spatial variables and the standard diffusion-synthetic convergence acceleration method are also briefly discussed. In Chapter 6 we develop our collocation technique and discuss its characteristics. The general diffusion equation is derived in Chapter 7. The qualitative effect of cross-section asymmetry is discussed and the analytic solutions to some particularly interesting problems are given. In addition, our adaptation of the diffusion-synthetic convergence acceleration algorithm is discussed. Computational results are presented in Chapter 8. Conclusions and recommendations for future work are given in Chapter 9.

CHAPTER 2

COLLOCATION AND FINITE-ELEMENT METHODS

2.1 Introduction

In this chapter we discuss and compare collocation and finite-element methods within the general context of projection methods. Projection methods encompass a wide variety of analytic and numerical techniques for solving integral and differential equations of all types. Even though many standard methods are projection methods, they are often not recognized as such. For instance, the spherical harmonics method for solving the neutron transport equation is a classic example of a projection technique.

2.2 Projection Operators

All projection methods are characterized by a space of trial functions and a projection operator which projects from a more general space of functions onto the trial space.

Definition 2.2.1

A projection operator, P , is an operator defined over a general space of functions, G , which maps every element of G to an element of a trial space,

T , where T is a subspace of G , and which maps every element of T to itself.

If $f \in G$ then $Pf \in T$ and we refer to Pf as the projection of f . Furthermore, $P(Pf) = Pf$. Thus it is clear that

$$P^2 = P. \quad (2.2.1)$$

Equation 2.2.1 expresses the so-called idempotent property. This property is an important one and can also be used as a definition for projection operators.

Collocation methods are constructed with collocation operators, and Galerkin methods, which are the most applicable and widely used finite-element methods, are constructed with Galerkin operators. Since Galerkin methods are representative of all finite-element methods, we restrict our discussion to collocation and Galerkin operators.

Definition 2.2.2

A projection operator P is a collocation operator if there exists a discrete set of points, $\{x_i\}_{i=1}^N$, such that for every $f \in G$, $Pf(x_i) = f(x_i)$, $i=1, N$.

To insure that P is well defined for our purposes, we require that given any two elements of T , $g(x)$ and $h(x)$, $g(x) = h(x)$ if, and only if, $g(x_i) = h(x_i)$, $i=1, N$.

Thus a collocation projection of f approximates f in a pointwise sense. Such projections are directly related to interpolation.

Definition 2.2.3

A projection operator P is a Galerkin operator if for every $f \in G$, Pf represents that element of T which minimizes the functional Γ , where

$$\Gamma = \int_{\vec{x}} [f(\vec{x}) - Pf(\vec{x})]^2 d\vec{x} .$$

To insure that P be well defined for our purposes, we require that T be finite-dimensional.

Thus a Galerkin projection of f approximates f in an integral least-squares sense. These projections are directly related to least-square fitting.

2.3 Application to the Solution of Equations

A projection operator can be used to map an exact equation defined over a general space of functions to an approximate equation defined over a trial space. This is the central theme of all projection methods.

For example, suppose that we wish to obtain an approximate solution for an equation of the form

$$Lf = q , \tag{2.3.1}$$

where L is a linear operator, and q is a known function.

Let P be a projection operator defined over the solution space of the equation. The approximate solution, $\tilde{f}$, is assumed to be an element of the trial space. The equation for $\tilde{f}$ can be succinctly expressed as follows:

$$PL\tilde{f} = Pq . \quad (2.3.2)$$

We refer to equation 2.3.2 as the projected equation.

If one makes a poor choice of trial space, it is possible that the projected equation will not have a unique solution. However, we shall ignore such complications as they are exceedingly rare in practice. The projected equation can assume different forms depending upon the nature of the trial space. For instance, suppose that $\tilde{f}$ can be represented in terms of a set of basis functions,

$$\{B_i(\vec{x})\}_{i=1}^N:$$

$$\tilde{f}(\vec{x}) = \sum_{i=1}^N \tilde{f}_i B_i(\vec{x}) . \quad (2.3.3)$$

Then the projected equation would be an $N \times N$ system of linear equations for the expansion coefficients, $\{\tilde{f}_i\}_{i=1}^N$. For multi-variable problems, trial spaces are often used where the expansion coefficients are functions of one or more variables:

$$\tilde{f}(\vec{x}, \vec{y}) = \sum_{i=1}^N \tilde{f}_i(\vec{y}) B_i(\vec{x}) . \quad (2.3.4)$$

If L were a differential operator in both the $\vec{x}$ and $\vec{y}$ variables, the projected equation would be an $N \times N$ system of differential equations for the expansion coefficients.

If the exact solution is actually an element of the trial space, then the solution of the projected equation (henceforth referred to as the projected solution) will be equal to the exact solution. This is, of course, a highly desirable characteristic. However, it should be noted that if the exact solution is not an element of the trial space, the projected solution is rarely equal to the projection of the exact solution.

Practical error bounds for the projected solution are generally quite difficult to obtain. However, we can easily obtain an error expression which is qualitatively useful.

Theorem 2.3.1

Let the residual of the projected solution be defined by $R = L\tilde{f} - q$. Then the error in the projected solution, $\xi = \tilde{f} - f$, satisfies

$$L\xi = R.$$

Proof: By assumption,

$$Lf = q,$$

and so

$$Lf - L\tilde{f} = g - L\tilde{f} ,$$

or

$$L(\tilde{f} - f) = R ,$$

or

$$L\xi = R .$$

If $\tilde{f}$ satisfies all boundary conditions imposed upon f , it follows directly from theorem 2.3.1 that

$$\xi = L^{-1}R . \quad (2.3.5)$$

Thus if the residual is identically equal to zero, $\tilde{f} = f$. Since R generally cannot be made identically equal to zero, a reasonable alternative is to try to make R "close" to zero. This is achieved in projection methods simply by choosing f so that the projection of its residual is identically zero. It is readily seen from equation 2.3.2 that this is the case:

$$PR = P(L\tilde{f} - q) , \quad (2.3.6)$$

$$= PL\tilde{f} - Pq ,$$

$$= 0 .$$

For the case of a collocation projection, it follows from definition 2.2.2 that the residual satisfies

$$R(\vec{x}_i) = 0, i=1, N. \quad (2.3.7)$$

Although it is hardly obvious, it can be shown (Prenter, 1975) that for the case of a Galerkin projection, the residual satisfies

$$\int_{\vec{x}} (R(\vec{x})t(\vec{x})) d\vec{x} = 0 \quad (2.3.8)$$

for every $t \in T$. A residual (or any arbitrary function) having the above property is said to be orthogonal to the trial space T .

Intuition suggests that Galerkin techniques might be more accurate in general than collocation techniques when the same trial space is used. This is in fact the case. It is important to note, however, that the computational effort expended in applying the Galerkin operator is significantly greater than that expended in applying a collocation operator. Thus in terms of accuracy per unit of computational cost, collocation methods can be quite competitive with Galerkin methods.

2.4 Galerkin-Equivalent Collocation Methods

It is well known that a Galerkin solution for a given equation is unique to the trial space. Conversely, collocation operators projecting onto the same trial space but having different collocation points generally yield different approximate solutions for the same equation. It is important to note that in certain instances, a collocation operator defined over a given trial space can produce the Galerkin solution corresponding to that space. This is ideal because high accuracy is obtained at low cost. In Chapter 6, we discuss a specific family of collocation operators which yield Galerkin solutions to the transport equation.

2.5 Examples

In order to make some of the concepts presented in this chapter more concrete, we use a collocation technique and a Galerkin technique, respectively, to obtain an approximate solution to a simple differential equation. In particular we solve

$$\frac{d}{dx} f(x) - f(x) = 1.0 \quad (2.5.1)$$

for $x \in (0,1)$, with the boundary condition $f(0) = 0$. The exact solution to this equation is

$$f(x) = e^x - 1.0 \quad (2.5.2)$$

For simplicity we wish to use a trial space of linear functions. However, with this type of equation, one must ensure that each element of the trial space meets the boundary condition. Thus we choose

$$\tilde{f}(x) = ax . \quad (2.5.3)$$

Substituting equation 2.5.3 into equation 2.5.1, we obtain

$$\frac{d}{dx} \tilde{f}(x) - \tilde{f}(x) = a - ax = 1.0. \quad (2.5.4)$$

Let x_0 be the collocation point associated with a collocation operator P_c defined over the trial space. Then it follows from definition 2.2.2 that given any $g(x) \in G$,

$$P_c g(x) = [g(x_0)/x_0]x . \quad (2.5.5)$$

Following expression 2.3.2, we obtain the projected equation:

$$[(a - ax_0)/x_0]x = [1.0/x_0]x . \quad (2.5.6)$$

It readily follows from this equation that

$$a = 1.0/(1.0 - x_0) . \quad (2.5.7)$$

Thus,

$$\tilde{f}_c(x) = [1.0/(1.0 - x_0)]x . \quad (2.5.8)$$

Let P_g denote the Galerkin operator defined over the trial space. Then it follows from definition 2.2.3 that given any $g(x) \in G$,

$$P_g g(x) = \left[3.0 \int_0^1 (g(x')x') dx' \right] x . \quad (2.5.9)$$

The projected equation takes the following form:

$$\left[3.0 \int_0^1 ((a - ax')x') dx' \right] x = \left[3.0 \int_0^1 (x') dx' \right] x . \quad (2.5.10)$$

After integration and some simplification, we find that

$$a = 3.0 , \quad (2.5.11)$$

and so

$$\tilde{f}_g(x) = 3.0x . \quad (2.5.12)$$

The optimum projected solution to this problem might be considered to be the Galerkin projection of the exact solution since it represents that element of the trial space which best fits the exact solution in an integral least-squares sense. It is easily shown that

$$P_g f(x) = (3.0/2.0)x \quad . \quad (2.5.13)$$

These examples demonstrate several points of interest:

- a) The Galerkin method requires greater computational effort than the collocation method because integrals must be performed rather than simple point function evaluations.
- b) A different collocation solution is obtained for each value of the collocation point. If $x_0 = 1.0/3.0$, the optimum solution is obtained. If $x_0 = 2.0/3.0$, the Galerkin solution is obtained. As $x \rightarrow 1.0$, the collocation solution becomes unbounded. This demonstrates that the accuracy of a solution can be strongly dependent upon the collocation points which are used. However, the possibility of an unbounded solution is not indicative of the general case. It is due to the crudeness of the linear approximation.

- 3) Since $P_c f(x) = [(e^{x_0} - 1.0)/x_0]x$, it follows from equation 2.5.8 that $\tilde{f}_c(x) \neq P_c f(x)$, except for the case $x_0 = 0$. Furthermore, $\tilde{f}_g(x) \neq P_g f(x)$. This lack of equality is indicative of the general case. However, the magnitudes of the differences are large again because of the crudeness of the linear approximation.

CHAPTER 3

GENERALIZED LAGRANGIAN BASIS SETS

3.1 Introduction

Generalized Lagrangian basis sets play a key role in our collocation method as they are used to define collocation operators. We now present the theory of these basis sets.

3.2 Interpolation Operators and Basis Set Construction

An interpolation scheme can be thought of as an operator which maps vectors to functions.

Definition 3.2.1

An interpolation operator H is an operator which is defined with respect to a set of abscissa values, $\{x_i\}_{i=1}^N$, contained in some domain X . Given any vector of ordinate values $\vec{y} = (y_1, y_2, \dots, y_N)$, H maps $\vec{y}$ to a function $Y(x)$, defined over X with

$$Y(x_i) = y_i, \quad i = 1, N.$$

It is required that H have an inverse; or equivalently, that distinct vectors be mapped to distinct functions.

Definition 3.2.2

An interpolation operator H is linear if given arbitrary vectors $\vec{y}_1$ and $\vec{y}_2$, and arbitrary scalars, c_1 and c_2 ,

$$H(c_1\vec{y}_1 + c_2\vec{y}_2) = c_1H\vec{y}_1 + c_2H\vec{y}_2 .$$

Any vector $\vec{y}$ can be expressed in terms of the standard orthonormal basis vectors, $\{\vec{e}_i\}_{i=1}^N$, as follows:

$$\vec{y} = \sum_{i=1}^N y_i \vec{e}_i , \quad (3.2.1)$$

where

$$\vec{e}_i = (e_{i1}, e_{i2}, \dots, e_{iN}) ,$$

$$e_{ij} = \delta_{ij} ,$$

and

$$\begin{aligned} \delta_{ij} &= 1.0 && \text{if } i = j , \\ &= 0.0 && \text{otherwise .} \end{aligned}$$

If H is a linear interpolation operator, then

$$Y(x) = H \left(\sum_{i=1}^N y_i \vec{e}_i \right) , \quad (3.2.2)$$

$$= \sum_{i=1}^N y_i H \vec{e}_i ,$$

$$= \sum_{i=1}^N y_i E_i(x) ,$$

where

$$E_i(x) = H(\vec{e}_i), \quad i = 1, N .$$

Thus we see that the range of a linear interpolation operator forms a linear space of functions. Furthermore, a basis set for the range can be obtained simply by applying the operator to a basis set of vectors.

Definition 3.2.3

A set of basis functions, $\{B_i(x)\}_{i=1}^N$, is a generalized Lagrangian basis set if there exists a linear interpolation operator, H , such that

$$B_i(x) = H(\vec{e}_i) , \quad i=1, N .$$

It is easily seen from definition 3.2.1 and expression 3.2.2 that

$$B_i(x_j) = \delta_{ij}, \quad i=1, N, \quad j=1, N. \quad (3.2.3)$$

This property alone can be used to define a generalized Lagrangian basis set. However, the definition which we have given is a constructive one and, hence, is more useful. Almost all of the commonly used interpolation schemes are linear, e.g., the global polynomial, cubic spline, and piecewise linear schemes. Thus a wide variety of generalized Lagrangian basis sets can be constructed. We refer to these sets as generalized Lagrangian basis sets because the sets corresponding to global polynomial interpolation are classically known as Lagrange interpolatory polynomials.

3.3 Collocation Operator Construction

Generalized Lagrangian basis sets can easily be used to define a collocation operator, P , which projects from a general space G onto the interpolatory space. In particular, given any $g(x) \in G$, we define P such that

$$Pg(x) = \sum_{i=1}^N g_i B_i(x) \quad (3.3.1)$$

where

$$g_i = g(x_i), i = 1, N .$$

It is clear from expression 3.2.3 that

$$Pg(x_i) = g(x_i), i = 1, N \quad (3.3.2)$$

and further that $P^2 = P$. Thus the operator so defined is a valid collocation operator. As demonstrated in Chapter 6, the operators used in our collocation technique for the solution of the transport equation are defined in terms of generalized Lagrangian basis sets.

3.4 Examples

Suppose that we wish to construct a collocation operator with collocation points at $x_1 = -1.0$ and $x_2 = 1.0$ which projects onto the space of linear functions defined over $[-1.0, 1.0]$. Let H denote the global linear interpolation operator. Then from definition 3.2.2 it follows that

$$\begin{aligned} B_1(x) &= H(\vec{e}_1) \quad , \quad (3.4.1) \\ &= 0.5 (1.0 + x) \quad , \end{aligned}$$

and that

$$\begin{aligned} B_2(x) &= H(\vec{e}_2) \quad , \quad (3.4.2) \\ &= 0.5 (1.0 - x) \quad . \end{aligned}$$

It is easily seen that given the ordinate values y_1 and y_2 corresponding to $x_1 = -1.0$ and $x_2 = 1.0$, the line which interpolates these points is

$$Y(x) = y_1 0.5(1.0 - x) + y_2 0.5(1.0 + x) \quad (3.4.3)$$

Thus following expression 3.3.1,

$$Pg(x) = g(x_1) 0.5(1.0 - x) + g(x_2) 0.5(1.0 + x) \quad (3.4.4)$$

If global polynomial interpolation is applied on an arbitrary interval containing the interpolation points, $\{x_i\}_{i=1}^N$, the corresponding generalized Lagrangian basis functions can be expressed as

$$B_i(x) = \frac{(x - x_1) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_N)}{(x_i - x_1) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_N)}, \quad i=1, N \quad (3.4.5)$$

As previously noted, these functions are also known as the Lagrange interpolatory polynomials.

CHAPTER 4

THE NEUTRON TRANSPORT AND STANDARD DIFFUSION EQUATIONS

4.1 The Transport Equation

Our collocation method is developed for the solution of the one-speed integro-differential neutron transport equation in slab geometry with either symmetric or asymmetric scattering. This equation is said to be a one-speed equation because it is based upon the assumption that the particles have a single speed or energy which does not change during the transport process. This assumption is almost never valid, so it would seem that a method for solving the one-speed equation would be of little practical use. However, the energy-dependent transport equation can be reduced to a coupled system of one-speed equations by means of an approximation technique known as the multi-group method (Bell and Glasstone, 1970). Under this approach, each one-speed equation yields the transport solution for particles having energies within a particular range or energy group. Any method for solving the one-speed equation can be directly applied to the solution of the multi-group equations. Thus energy-dependent transport calculations can be performed using our

collocation method even though it is explicitly developed only for the solution of the one-speed equation.

The traditional neutron transport equation treats only symmetric scattering. When the scattering is asymmetric, the equation which we solve is more accurately referred to as the linearized Boltzmann transport equation rather than the neutron transport equation. However, for simplicity we henceforth refer to it as the neutron transport equation in all cases.

The neutron transport equation can be expressed as follows:

$$\begin{aligned} \mu \frac{\partial}{\partial z} \psi(z, \mu) + \{\sigma_a + \sigma_s(\mu)\} \psi(z, \mu) & \quad (4.1.1) \\ & = 2\pi \int_{-1}^{+1} \sigma_s(\mu_1 \rightarrow \mu) \psi(z, \mu_1) d\mu_1 + Q(z, \mu) . \end{aligned}$$

where,

z = a direction variable defined in Figure 1,

$\psi(z, \mu)$ = The flux of particles at position z traveling within the differential solid angle defined by μ per steradian of that solid angle. This quantity is generally known as the angular flux and has units of particles/(area-time-steradian),

Figure 1. Geometry for Transport Equation.

$\sigma_s(\mu_1 \rightarrow \mu_2)$ = the probability per unit pathlength that a particle traveling within the differential solid angle defined by μ_1 will scatter into the differential solid angle defined by μ_2 per steradian of that solid angle. This function is generally referred to as the scattering kernel and has units of (pathlength-steradian)⁻¹,

σ_a = the probability per unit pathlength that a particle will undergo an absorptive interaction. This quantity is known as the macroscopic absorption cross section and has units of (pathlength)⁻¹,

$\sigma_s(\mu)$ = the probability per unit pathlength that a particle traveling within the differential solid angle defined by a μ will undergo a scattering interaction. This quantity is known as the total macroscopic scattering cross section and has units of (pathlength)⁻¹,

$Q(z, \mu)$ = the source of particles at position z traveling within the differential solid angle defined by μ per steradian of that solid angle. This quantity has units of particles/(volume-time-steradian).

The transport equation is a mathematical expression of the physical principle of particle conservation. It directly reflects the fact that in steady-state, the

rate at which particles enter any region of phase space must be equal to the rate at which particles leave it. This can be clearly seen through the physical interpretation of each term.

Let $d\chi = 2\pi d\mu \, dx dy dz$, then

$\mu \frac{\partial}{\partial z} \psi(z, \mu) d\chi$ = the net particle leakage rate due to streaming for the differential phase space volume defined by $d\chi$.

$\sigma_a \psi(z, \mu) d\chi$ = the rate at which particles are absorbed within the differential phase space volume defined by $d\chi$.

$\sigma_s(\mu) \psi(z, \mu) d\chi$ = the rate at which particles scatter out of the differential phase space volume defined by $d\chi$.

$2\pi \int_{-1}^{+1} \sigma(\mu_1 \rightarrow \mu_2) \psi(z, \mu_1) d\mu_1 d\chi$ = the rate at which particles scatter into the differential phase space volume $d\chi$.

$Q(z, \mu) d\chi$ = the rate at which particles are created within the differential phase space volume defined by $d\chi$.

Thus we see that the equation mathematically states that within each differential phase space element,

Leakage + Absorption + Outscatter = Inscatter + Source.

4.2 The Scalar Balance Equation

Scattering is a conservative process because particles are neither created nor destroyed. Every particle which scatters out of one direction must scatter into another. Thus from the definitions of the scattering cross section and scattering kernel, it follows that

$$\sigma_s(\mu) = 2\pi \int_{-1}^{+1} \sigma_s(\mu \rightarrow \mu_2) d\mu_2 \quad . \quad (4.2.1)$$

Furthermore, if equation 4.2.1 is multiplied by $\psi(z, \mu)$ and integrated over all directions, we obtain

$$2\pi \int_{-1}^{+1} \sigma_s(\mu) \psi(z, \mu) d\mu = 2\pi \int_{-1}^{+1} 2\pi \int_{-1}^{+1} \sigma_s(\mu \rightarrow \mu_2) \psi(z, \mu) d\mu d\mu_2 \quad . \quad (4.2.2)$$

Equation 4.2.2 simply expresses that fact that the rate at which particles scatter out of all directions must be equal to the rate at which particles scatter into all directions.

Hence if equation 4.1.1 is integrated over all directions, the following equation results:

$$\frac{d}{dz} J(z) + \sigma_a \phi(z) = q(z) \quad , \quad (4.2.3)$$

where the net current, $J(z)$, is defined by

$$J(z) = 2\pi \int_{-1}^{+1} \mu \psi(z, \mu) d\mu ,$$

the scalar flux, $\phi(z)$, by

$$\phi(z) = 2\pi \int_{-1}^{+1} \psi(z, \mu) d\mu ,$$

and the scalar source, $q(z)$, by

$$q(z) = 2\pi \int_{-1}^{+1} Q(z, \mu) d\mu .$$

This equation is called the scalar balance equation. It expresses the physical fact that if one averages over all directional components of phase space,

$$\text{Leakage} + \text{Absorption} = \text{Source}.$$

The outscatter and inscatter terms appearing in equation 4.1.1 do not appear in equation 4.2.3 because, as shown by equation 4.2.2, the scalar inscatter and outscatter terms are equal and, hence, cancel each other.

When one applies an approximation method such as our collocation method or the S_n method to the transport equation, an approximate transport equation is obtained. An approximate transport equation is said to be conservative if the scalar inscatter and outscatter rates consistent with that equation are equal. Many types of approximate equations (including our collocation equations and the S_n equations) can be efficiently solved using iterative methods in conjunction with convergence acceleration techniques. The most effective convergence acceleration methods can only be applied to conservative equations. Thus it is important to retain the conservative property whenever possible in deriving approximations to the transport equation.

4.3 The Standard Diffusion Equation

The standard diffusion equation treats only symmetric scattering. For this case the differential scattering cross section depends only upon $\mu_0 = \hat{\Omega}_1 \cdot \hat{\Omega}_2$. This equation can be obtained from the transport equation by the application of a Galerkin projection technique known as the P_1 spherical-harmonics approximation and takes the following form in one-dimensional slab geometry (Bell and Glasstone, 1970):

$$-D \frac{d^2}{dz^2} \phi(z) + \sigma_a \phi(z) = q(z) , \quad (4.3.1)$$

where

$$D = \left[3(\sigma_a + \sigma_o - \sigma_1) \right]^{-1} ,$$

$$\sigma_o = 2\pi \int_{-1}^{+1} \left(\frac{d\sigma_s}{d\mu_o} \right) d\mu_o ,$$

$$\sigma_1 = 2\pi \int_{-1}^{+1} \left(\frac{d\sigma_s}{d\mu_o} \right) \mu_o d\mu_o ,$$

and

$$\frac{d\sigma_s}{d\mu_o}(\mu_o) = \text{the differential scattering cross section.}$$

Note that this equation follows directly from the scalar balance equation, equation 4.2.3, under the assumption that

$$J = -D \frac{d}{dz} \phi(z) . \quad (4.3.2)$$

Expression 4.3.2 is known as Fick's Law. It can be shown from the P_1 approximation that Fick's Law is valid whenever the behavior of the angular flux is approximately linear in μ (Bell and Glasstone, 1970). Thus the diffusion equation is most accurate for problems with spatially distributed isotropic sources.

One of the most important uses of the diffusion equation arises in the numerical solution of the transport equation. It can be used in an algorithm to evaluate the iterative convergence of the transport solution. This algorithm is known as diffusion-synthetic acceleration and is fully discussed in Chapter 5.

CHAPTER 5

THE STANDARD S_n TECHNIQUE

5.1 Introduction

The primary purpose of this chapter is to discuss the standard S_n or discrete-ordinates technique for the numerical solution of the one-dimensional neutron transport equation in slab geometry. Due to the difficulties associated with direct solution techniques, essentially all production transport codes available to the scientific community employ the S_n treatment in the angular variables. Thus a discussion of this technique is presented in order to provide the reader with a standard with which our collocation technique can be compared.

5.2 Derivation of the Equations

Only symmetric scattering is treated in the S_n method. In this case, the scattering kernel which appears in equation 4.1.1 can be expressed as

$$\sigma_s(\mu' \rightarrow \mu) = \frac{1}{2\pi} \int_0^{2\pi} \left(\frac{d\sigma_s}{d\mu_0} \right) d\phi, \quad (5.2.1)$$

where

$$\mu_0 = \vec{\Omega}' \cdot \vec{\Omega} = \mu' \mu + \sqrt{(1 - \mu'^2)(1 - \mu^2)} \cos \phi ,$$

and

$$\frac{d\sigma_s}{d\mu_0} = \text{the macroscopic differential scattering cross section.}$$

The derivation of the S_n equations is begun by approximating the scattering kernel with a finite Legendre polynomial expansion:

$$\sigma_s(\mu' \rightarrow \mu) = \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_\ell P_\ell(\mu') P_\ell(\mu) , \quad (5.2.2)$$

where

$$\sigma_\ell = 2\pi \int_{-1}^{+1} \left(\frac{d\sigma_s}{d\mu_0} \right) P_\ell(\mu_0) d\mu_0$$

and

$L = \text{some finite integer.}$

The following properties of the Legendre polynomials are used extensively:

$$\int_{-1}^{+1} P_i(\mu) P_j(\mu) d\mu = \left(\frac{2}{2i+1} \right) \delta_{ij} \quad (5.2.3a)$$

and

$$P_0(\mu) = 1.0 \quad (5.2.3b)$$

From expressions 4.2.1, 5.2.2, and 5.2.3, it follows that

$$\sigma_s(\mu) = \sigma_0 \quad (5.2.4)$$

Substituting expressions 5.2.2 and 5.2.4 into equation 4.1.1, we obtain

$$(5.2.5)$$

$$\mu \frac{\partial}{\partial z} \psi(z, \mu) + (\sigma_a + \sigma_0) \psi(z, \mu) = 2\pi \int_{-1}^{+1} \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_\ell P_\ell(\mu') P_\ell(\mu) \psi(z, \mu') d\mu' + Q(z, \mu) \quad .$$

Next the inscatter integral is approximated with some standard quadrature formula. Such formulas are defined in terms of a set of quadrature directions, $\{\mu_j\}_{j=1}^N$, and associated weights, $\{w_j\}_{j=1}^N$, such that

$$\sum_{j=1}^N f(\mu_j) w_j \approx \int_{-1}^{+1} f(\mu) d\mu \quad (5.2.6)$$

Applying this formula to equation 5.2.5 gives the approximating equation

$$\mu \frac{\partial}{\partial z} \psi(z, \mu) + (\sigma_a + \sigma_o) \psi(z, \mu) = \quad (5.2.7)$$

$$2\pi \sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu_j) P_{\ell}(\mu) \psi(z, \mu_j) w_j + Q(z, \mu) \quad .$$

Finally, equation 5.2.7 is discretized at the quadrature directions resulting in an NxN system of coupled differential equations for the discrete angular flux values:

$$\mu_i \frac{\partial}{\partial z} \psi(z, \mu_i) + (\sigma_a + \sigma_o) \psi(z, \mu_i) = \quad (5.2.8)$$

$$2\pi \sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu_j) P_{\ell}(\mu_i) \psi(z, \mu_j) w_j + Q(z, \mu_i), \quad i=1, N \quad .$$

In order to obtain a computer solution, the spatial variable must also be discretized. Because identical spatial variable treatments can be used for both the S_n and collocation equations, there is no need to consider the spatial variable treatment at this point. However, because it plays an important role in the diffusion-synthetic algorithm, the standard discrete-ordinates spatial treatment is described in Section 5.4.

In order to ensure that equation 5.2.8 be conservative, a restriction must be placed upon the order of

the kernel expansion. In particular, the order must be less than or equal to the maximum degree of polynomial for which the quadrature is exact (Bell and Glasstone, 1970).

Gauss quadrature formulas are generally used in transport calculations. One reason is that an N-point Gauss quadrature set integrates all polynomials of degree $2N-1$ or less exactly. The other reason is that the S_n equations in one-dimensional slab geometry with an N-point Gauss quadrature set are equivalent to the spherical-harmonics (P_n) equations of order $N-1$ (Bell and Glasstone, 1970). This is obviously a highly desirable property.

5.3 An Extension to Include Asymmetric Scattering

A straightforward way to extend the S_n technique to include asymmetric scattering is simply to approximate the scattering kernel with a tensor-product Legendre expansion

$$\sigma_s(\mu' \rightarrow \mu) = \sum_{\ell=0}^L \sum_{m=0}^L \frac{(2\ell+1)(2m+1)}{8\pi} \sigma_{\ell,m} P_\ell(\mu') P_m(\mu), \quad (5.3.1)$$

where

$$\sigma_{\ell,m} = \int_{-1}^{+1} 2\pi \int_{-1}^{+1} \sigma_s(\mu_1 \rightarrow \mu_2) P_\ell(\mu_1) P_m(\mu_2) d\mu_1 d\mu_2.$$

From expressions 4.2.1 and 5.2.3, it is easily seen that

$$\sigma_s(\mu) = \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{\ell,0} P_{\ell}(\mu) \quad . \quad (5.3.2)$$

Making the appropriate substitutions, equation 5.2.8 becomes

$$\mu_i \frac{\partial}{\partial z} \psi(z, \mu_i) + \left(\sigma_a + \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{\ell,0} P_{\ell}(\mu_i) \right) \psi(z, \mu_i) = \quad (5.3.3)$$

$$2\pi \sum_{j=1}^N \sum_{\ell=0}^L \sum_{m=0}^L \frac{(2\ell+1)(2m+1)}{8\pi} \sigma_{\ell,m} P_{\ell}(\mu_j) P_m(\mu_i) \psi(z, \mu_j) w_j$$

$$+ Q(z, \mu_i), \quad i=1, N \quad .$$

If equation 5.3.3 is to be conservative, the expression

$$\sum_{i=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{\ell,0} P_{\ell}(\mu_i) \psi(z, \mu_i) w_i = \quad (5.3.4)$$

$$2\pi \sum_{i=1}^N \sum_{j=1}^N \sum_{\ell=0}^L \sum_{m=0}^L \frac{(2\ell+1)(2m+1)}{8\pi} \sigma_{\ell,m} P_{\ell}(\mu_j) P_m(\mu_i) \psi(z, \mu_j) w_i w_j$$

must hold for arbitrary values of the angular flux.

This is simply the numerical equivalent of expression 4.2.2. It is convenient to re-state expression 5.3.4 as follows:

$$\sum_{i=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{\ell,0} P_{\ell}(\mu_i) \psi(z, \mu_i) w_i = \quad (5.3.5)$$

$$\sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{2} P_{\ell}(\mu_j) \psi(z, \mu_j) w_j \sum_{m=0}^L \sum_{i=1}^N \frac{2m+1}{2} \sigma_{\ell,m} P_m(\mu_i) w_i \quad .$$

If we assume that the quadrature formula exactly integrates all polynomials of order L or less, the right side of expression 5.3.5 becomes

$$\sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{2} \sigma_{\ell,0} P_{\ell}(\mu_j) \psi(z, \mu_j) w_j \quad (5.3.6)$$

which is clearly equivalent to the left side of the expression.

Thus in both the symmetric and asymmetric cases, the expansion order must be less than or equal to the maximum degree of polynomial for which the quadrature formula is exact if particle conservation is to be assured.

5.4 Discrete-Ordinates Spatial Variable Treatment

Although explicit low-order finite-element methods have been used (Hill, 1975), finite-difference treatments are standard in discrete-ordinates codes. In this section, we apply the most common finite-difference treatment to the S_n equations (equation 5.2.8).

Let $[z_{k-1/2}, z_{k+1/2}]$ denote a spatial mesh cell with $z_{k-1/2} < z_{k+1/2}$. From the mean value theorem, it follows that there exists a $z_1 \in (z_{k-1/2}, z_{k+1/2})$ such that the following equation, obtained upon integrating equation 5.2.8 over the mesh cell, is exact:

(5.4.1)

$$\mu_i (\psi_{k+1/2,i} - \psi_{k-1/2,i}) + (\sigma_a + \sigma_o) \psi_{k,i} \Delta_k = (S_{k,i} + Q_{k,i}) \Delta_k, \quad i=1, N, \quad ,$$

where

$$\psi_{k,i} = \psi(z_k, \mu_i) \quad ,$$

$$\Delta_k = z_{k+1/2} - z_{k-1/2} \quad ,$$

and

$$S_{k,i} = 2\pi \sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell + 1}{4\pi} \sigma_\ell P_\ell(\mu_i) P_\ell(\mu_j) \psi_{k,j} w_j \quad .$$

Equation 5.4.1 consists of N equations with $3N$ unknowns. In general, N flux values can be assumed to be known at the end points of the cell. In order to solve for the remaining fluxes, N additional equations must be specified by assuming some relationships between the endpoint and midpoint fluxes. The most common one is the so-called diamond difference relationship (Bell and Glasstone, 1970):

$$\psi_{k,i} = 0.5(\psi_{k+\frac{1}{2},i} + \psi_{k-\frac{1}{2},i}), i=1,N \quad . \quad (5.4.2)$$

The discrete-ordinates equations are usually solved by iteration. In order to assure stability, the iteration must proceed in the direction of particle motion. For instance, consider a problem with particles incident upon the left face of a slab with vacuum boundary conditions as shown in Figure 2. For simplicity, we assume an even number of directions with $\mu_i > 0$ for $i = 1, N/2$, and $\mu_i < 0$ for $i = N/2 + 1, N$. The iteration begins at the left face because the forward-directed fluxes are prescribed there by the boundary conditions. In a left-to-right sweep of the mesh, the forward-directed midpoint and endpoint fluxes are successively found using the following equations which are obtained from equations 5.4.1 and 5.4.2:

$$\psi_{k,i}^{\ell} = \frac{\mu_i^2 \psi_{k-\frac{1}{2},i}^{\ell} + (S_{k,i}^{\ell-1} + Q_{k,i}) \Delta_k}{2\mu_i + (\sigma_a + \sigma_o) \Delta_k} \quad , \quad (5.4.3a)$$

and

$$\psi_{k+\frac{1}{2},i}^{\ell} = 2\psi_{k,i}^{\ell} - \psi_{k-\frac{1}{2},i}^{\ell} \quad i=1,N/2 \quad . \quad (5.4.3b)$$

The superscript ℓ denotes the iteration index. Note

Figure 2. Discrete-Ordinates Problem Geometry.

that the scattering sources are calculated with the midpoint fluxes from the previous iteration. Lacking any a priori knowledge of the solution, the scattering sources are generally set to zero on the first iteration. The forward sweep is continued until the forward-directed fluxes are obtained at the right face of the slab.

The backward-directed fluxes are known to be zero at the right face from the vacuum boundary condition. A right-to-left sweep of the mesh is next begun similarly solving for the midpoint and endpoint backward-directed fluxes. The following equations are used:

$$\psi_{k,i}^{\ell} = \frac{-\mu_i 2\psi_{k+\frac{1}{2},i}^{\ell} + (S_{k,i}^{\ell-1} + Q_{k,i})\Delta_k}{-2\mu_i + (\sigma_a + \sigma_o)\Delta_k}, \quad (5.4.4a)$$

and

$$\psi_{k-\frac{1}{2},i}^{\ell} = 2\psi_{k,i}^{\ell} - \psi_{k+\frac{1}{2},i}^{\ell} \quad i = N/2 + 1, N. \quad (5.4.4b)$$

The first iteration is completed when the backward-directed fluxes are found at the left face. The iterations are continued until the fluxes converge to within a prescribed tolerance, TOL. A popular criterion is

$$\max_k \left[1.0 - \sum_i \psi_{k,i}^{l-1} w_i / \sum_i \psi_{k,i}^l w_i \right] < \text{TOL} \quad . \quad (5.4.5)$$

It can be seen from equations 5.4.3 and 5.4.4 that negative endpoint flux values can be obtained if the quantity $(\sigma_o + \sigma_a)\Delta_k$ is too large. Negative fluxes can be avoided by using step-differencing rather than diamond-differencing:

$$\psi_{k,i} = \psi_{k+1/2,i} , \mu_i > 0 , \quad (5.4.6a)$$

and

$$\psi_{k,i} = \psi_{k-1/2,i} , \mu_i < 0 . \quad (5.4.6b)$$

In this case, equations 5.4.3a and 5.4.3b take the following form

$$\psi_{k,i}^l = \frac{\mu_i \psi_{k-1/2,i}^l + (S_{k,i}^{l-1} + Q_{k,i})\Delta_k}{\mu_i + (\sigma_a + \sigma_o)\Delta_k} , \mu_i > 0 \quad , \quad (5.4.7a)$$

and

$$\psi_{k,i}^l = \frac{-\mu_i \psi_{k+1/2,i}^l + (S_{k,i}^{l-1} + Q_{k,i})\Delta_k}{-\mu_i + (\sigma_a + \sigma_o)\Delta_k} , \mu_i < 0 \quad . \quad (5.4.7b)$$

Because step-differencing is not as accurate as diamond-differencing, step-differencing is generally used in a

calculation only after diamond-differencing has been used and a negative flux value has been detected.

5.5 Convergence Acceleration

The discrete-ordinates equations are generally solved iteratively. In operator notation, the transport equation can be expressed as

$$(L - S)\psi = Q \quad , \quad (5.5.1)$$

where

$$L = \mu \frac{\partial}{\partial z} + \sigma_a + \sigma_s \quad ,$$

and

$$S = 2\pi \int_{-1}^{+1} d\mu' \sigma_s(\mu' \rightarrow \mu) \quad .$$

The iterative form of the equation which is used is

$$\psi^{\ell+1} = L^{-1} S \psi^{\ell} + L^{-1} Q \quad , \quad (5.5.2)$$

where ℓ denotes the iteration index. This physically corresponds to an order-of-scatter approach, i.e.,

$$\begin{aligned} \psi^0 &= L^{-1} Q = \text{the unscattered flux,} \\ \psi^1 &= L^{-1} (\psi^0 + S\psi^0) = \text{the unscattered plus once-} \\ &\quad \text{scattered flux,} \\ &\cdot \\ &\cdot \\ &\cdot \\ &\text{etc.} \end{aligned}$$

The convergence rate of this sequence becomes increasingly poor as the dominance ratio, $c = \sigma_s / (\sigma_s + \sigma_a)$, approaches unity. In fact, the convergence rate is so poor when $c = 1$ that convergence effectively cannot be obtained. Thus convergence acceleration is essential for these types of problems. Although many acceleration techniques such as the Chebychev and rebalance methods (Hill, 1975) are commonly employed in production transport codes, only the diffusion-synthetic method is effective when $c = 1$. Furthermore, this technique has been shown to be the most effective for any type of problem (Miller, 1978). Hence we discuss only this method.

We begin by considering an equation of the general form

$$(A - B)\psi = Q \quad (5.5.3)$$

with the associated iterative equation,

$$\psi^{l+1} = M \psi^l + A^{-1}Q \quad (5.5.4)$$

where

$$M = A^{-1}B .$$

The transport equation is clearly of this form. The operator M is called the iteration operator. A necessary and sufficient condition for the convergence of the

sequence given by equation 5.5.4 is that the spectral radius (the magnitude of the largest eigenvalue) of M be less than unity. Furthermore, as the spectral radius gets smaller, the convergence rate increases. Defining the residual, r^ℓ , as

$$r^\ell = \psi^\ell - \psi^{\ell-1} \quad , \quad (5.5.5)$$

it follows from equation 5.5.4 that

$$r^\ell = Mr^{\ell-1} \quad . \quad (5.5.6)$$

Clearly,

$$\begin{aligned} \psi &= \psi^\ell + \sum_{k=1}^{\infty} r^{\ell+k} \quad , \quad (5.5.7) \\ &= \psi^\ell + (M + M^2 + M^3 + \dots)r^\ell \quad , \\ &= \psi^\ell(1 + M + M^2 + \dots)Mr^{\ell-1} \quad . \end{aligned}$$

Because the spectral radius of M is less than unity, the operator series appearing in the above equation converges to $(I-M)^{-1}$ (Isaacson and Keller, 1966). Thus

$$\begin{aligned} \psi &= \psi^\ell + (I - M)^{-1}Mr^{\ell-1} \quad , \quad (5.5.8) \\ &= \psi^\ell + (A - B)Br^{\ell-1} \quad . \end{aligned}$$

As it stands, this equation is no more useful

than equation 5.5.1 because $(A-B)$ must be directly inverted to solve it and if $A-B$ were easily invertible, we would not be iterating in the first place. However, suppose that an easily invertible operator, T , can be found which "closely" approximates $A-B$. Then equation 5.5.8 suggests that if T^{-1} were substituted for $(A-B)^{-1}$ in that equation, the resulting solution might be quite "close" to the exact solution. This is the basic idea of all synthetic acceleration methods. The operator T is usually referred to as the low-order operator. The accelerated iterative algorithm can be expressed as

$$\psi^{\ell+1} = \tilde{\psi}^{\ell} + T^{-1}B\tilde{r}^{\ell} \quad , \quad (5.5.9)$$

where

$$\tilde{\psi}^{\ell} = M \psi^{\ell} + A^{-1}Q$$

$$\tilde{r}^{\ell} = \tilde{\psi}^{\ell} - \psi^{\ell} \quad .$$

With considerable manipulation, it can be shown that this algorithm is equivalent to the following iterative equation (Reed, 1971),

$$\psi^{\ell+1} = [I - T^{-1}(A - B)] M \psi^{\ell} + (I + T^{-1}B)A^{-1}Q \quad . \quad (5.5.10)$$

This form of the equation clearly reflects the fact that the spectral radius of the accelerated iteration operator goes to zero as T more closely approximates $(A-B)$.

In diffusion-synthetic acceleration, the low-order operator is the diffusion operator. There are actually three different variations of diffusion-synthetic acceleration: the source correction, diffusion coefficient correction, and removal correction schemes (Alcouffe, 1977). The last two schemes are actually non-linear and do not correspond to the general development which has been presented. The source correction scheme does correspond, however, and it is the only scheme which we apply to the collocation equations.

The accelerated iterative algorithm for the source correction scheme can be expressed as

$$\tilde{\psi}^{\ell} = L^{-1}S \psi^{\ell} + L^{-1}Q, \quad (5.5.11a)$$

$$\phi^{\ell+1} = T^{-1}(Q - \tilde{C}^{\ell}), \quad (5.5.11b)$$

$$\psi^{\ell+1} = \psi^{\ell} (\phi^{\ell+1}/\phi^{\ell}) \quad (5.5.11c)$$

where

$$T = -D \frac{d^2}{dz^2} + \sigma_a, \quad (5.5.11d)$$

$$\tilde{C}^{\ell} = \frac{d}{dz} \tilde{J}^{\ell} + D \frac{d^2}{dz^2} \tilde{\phi}^{\ell}. \quad (5.5.11e)$$

Note that information from the latest transport iteration is used to construct a source correction term, $\tilde{C}^{\ell}$,

which in some measure corrects for the inaccuracy of Fick's Law. The improved scalar flux solution which results is then used to renormalize the scattering source. It is effectively the scalar component (magnitude) of the scattering source which is being accelerated.

It is instructive to write out equation 5.4.11 in full:

$$-D \frac{d^2}{dz^2} \phi^{l+1} + \sigma_a \phi^{l+1} = q - \frac{d}{dz} \tilde{J}^l - D \frac{d^2}{dz^2} \tilde{\phi}^l \quad . \quad (5.5.12)$$

Note that upon convergence, this equation simply becomes the scalar balance equation (equation 4.2.3),

$$\frac{d}{dz} \tilde{J} + \sigma_a \tilde{\phi} = \tilde{q} \quad . \quad (5.5.13)$$

This demonstrates that if the accelerated algorithm converges, it converges to the transport solution. An algorithm with this property is said to be consistent.

We have thus far discussed only the continuous case. Additional considerations come into play in the discretized case. Care must be taken to difference the diffusion equation in a manner which is consistent with the differencing of the transport equation. Early investigators simply diamond-differenced the diffusion

equation for use with the diamond-differenced transport equation. This procedure leads to algorithm which is consistent, but unstable (not always convergent). Although Reed (1971) made considerable progress, it was Alcouffe (1977) who solved the instability problem. As previously mentioned, the diffusion equation can be derived from the P_1 equations. Alcouffe discovered that diamond-differencing the P_1 equations and then deriving the corresponding discretized diffusion equation is not equivalent to simply diamond-differencing the diffusion equation. The former procedure leads to an algorithm which is both consistent with the diamond-differenced transport equation and stable when appropriate boundary conditions are used. Because step-differencing is often used for negative flux fixup, additional steps must be taken to ensure an algorithm which is both consistent and stable in general. Alcouffe gives the following general diffusion equation for the interior mesh cells for use in the diffusion synthetic acceleration algorithm:

$$\begin{aligned} \frac{-D}{\Delta_{k+1}} \left(\phi_{k+3/2}^{\ell+1} - \phi_{k-1/2}^{\ell+1} \right) + \frac{D}{\Delta_k} \left(\phi_{k+1/2}^{\ell+1} - \phi_{k-1/2}^{\ell+1} \right) + (\tilde{\sigma}_a \Delta)^{\ell} \phi_{k+1/2}^{\ell+1} \\ = 0.5 (q_{k+1} \Delta_{k+1} + q_k \Delta_k) - \tilde{C}_k^{\ell} \end{aligned} \quad , \quad (5.5.14a)$$

where,

$$(\tilde{\sigma}_a \Delta)^l = 0.5 \left(\sigma_a \tilde{\phi}_{k+1}^l \Delta_{k+1} + \sigma_a \tilde{\phi}_k^l \Delta_k \right) , \quad (5.5.14b)$$

and

(5.5.14c)

$$\tilde{C}_k^l = \left(\tilde{j}_{k+1}^l - \tilde{j}_k^l \right) - \left[-\frac{D}{\Delta_{k+1}} \left(\tilde{\phi}_{k+3/2}^l - \tilde{\phi}_{k+1/2}^l \right) + \frac{D}{\Delta_k} \left(\tilde{\phi}_{k+1/2}^l - \tilde{\phi}_{k-1/2}^l \right) \right] .$$

As in the continuous case, the source correction factor, $\tilde{C}_k^l$, compensates for the inaccuracy of Fick's Law.

Alcouffe introduces the non-linear correction factor, $(\sigma_a \Delta)^l$, in order to achieve consistency with both diamond and step-differencing. Although it is not explicitly mentioned by Alcouffe, it is important to note that whenever step-differencing is used, the midpoint currents appearing in expression 5.5.14c must be evaluated by linearly averaging the adjacent endpoint currents. The currents so obtained correspond to the actual midpoint currents only when diamond-differencing is used.

Equations for the boundary mesh cells can be obtained from the standard equation corresponding to

a vacuum boundary condition (Alcouffe, 1978). That equation takes the following form for the first mesh cell:

$$\frac{-D}{\Delta_1} (\phi_{3/2} - \phi_{1/2}) + 0.5\phi_{1/2} + 0.5\sigma_a\phi_1\Delta_1 = 0.5q_1\Delta_1. \quad (5.5.15)$$

Alcouffe obtains a consistent and stable equation from the above equation by applying correction factors in the following manner:

$$\frac{-D}{\Delta_1} (\phi_{3/2}^{\ell+1} - \phi_{1/2}^{\ell+1}) + 0.5\phi_{1/2}^{\ell+1} + 0.5(\tilde{\sigma}_a\Delta)^{\ell}\phi_{1/2}^{\ell+1} = 0.5q_1\Delta_1 - \tilde{C}_1^{\ell}. \quad (5.5.16a)$$

where,

$$(\tilde{\sigma}_a\Delta)^{\ell} = \sigma_a\tilde{\phi}_1^{\ell}\Delta_1 / \tilde{\phi}_{1/2}^{\ell}, \quad (5.5.16b)$$

and

$$\tilde{C}_1^{\ell} = 0.5(\tilde{J}_{3/2} - \tilde{J}_{1/2}) - \left[-\frac{D}{\Delta_1} (\tilde{\phi}_{3/2}^{\ell} - \tilde{\phi}_{1/2}^{\ell}) + 0.5\tilde{\phi}_{1/2}^{\ell} \right]. \quad (5.5.16c)$$

Note that upon convergence, the above equation goes over to the scalar balance equation for the first mesh cell,

$$\tilde{J}_{3/2} - \tilde{J}_{1/2} + \sigma_a\tilde{\phi}_1\Delta_1 = q_1\Delta_1. \quad (5.5.17)$$

Thus it is consistent. Although equation 5.4.16 is obtained through the application of a vacuum boundary condition, it is used regardless of the actual boundary condition imposed upon the transport solution. The correction factors effectively compensate for the inaccuracy of the vacuum boundary condition.

Alcouffe (1977) has rigorously proven that his algorithm is unconditionally stable for infinite-medium problems. For finite-medium problems, where boundary conditions come into play, his method has been computationally found to be unconditionally stable, however, no rigorous proof of this property has been given.

CHAPTER 6

THE COLLOCATION METHOD

6.1 Introduction

The theory of our collocation method is presented in this chapter. It is first developed for symmetric scattering and then extended to treat asymmetric scattering.

6.2 Derivation of Symmetric Scattering Equations

The collocation equation for symmetric scattering is derived in a manner analogous to that described in Chapter 2. After briefly discussing the equation to be solved, we define a trial space and a collocation operator which projects onto it. The approximate solution is assumed to be an element of the trial space and the collocation equation is then obtained by requiring the projection of the associated residual to be zero.

Under the assumption of symmetric scattering, the transport equation (equation 4.1.1) can be expressed as

$$\mu \frac{\partial}{\partial z} \psi(z, \mu) + (\sigma_a + \sigma_s) \psi(z, \mu) = 2\pi \int_{-1}^{+1} \sigma_s(\mu' + \mu) \psi(z, \mu') d\mu' + Q(z, \mu), \quad (6.2.1)$$

where

$$\sigma_s(\mu' \rightarrow \mu) = \frac{1}{2\pi} \int_0^{2\pi} \frac{d\sigma_s}{d\mu_0} d\phi ,$$

$\frac{d\sigma_s}{d\mu_0}$ = the differential scattering cross section,

$$\mu_0 = \vec{\Omega}' \cdot \vec{\Omega} = \mu'\mu + \sqrt{(1 - \mu'^2)(1 - \mu^2)} \cos \phi ,$$

$$\sigma_s = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu) d\mu , \quad \text{(Note that the total scattering cross section is independent of the incident particle direction with symmetric scattering.)}$$

Let P be a collocation operator defined with respect to the generalized Lagrangian basis set, $\{B_i(\mu)\}_{i=1}^N$, having collocation points, $\{\mu_i\}_{i=1}^N$. Then for any function, $f(z, \mu)$, defined for arbitrary z and $\mu \in [-1, +1]$,

$$P[f(z, \mu)] = \sum_{i=1}^N f(z, \mu_i) B_i(\mu) . \quad (6.2.2)$$

The collocation solution is assumed to be an element of the trial space spanned by the Lagrangian basis set,

$$\psi(z, \mu) = \sum_{i=1}^N \psi_i(z) B_i(\mu) , \quad (6.2.3)$$

where

$$\psi_i(z) = \psi(z, \mu_i) , \quad i = 1, N.$$

The collocation equation is obtained by substituting expression 6.2.3 into equation 6.2.1 and operating on that equation from the left with P. The result is

$$\begin{aligned} & \sum_{i=1}^N \mu_i \frac{d}{dz} \psi_i(z) B_i(\mu) + (\sigma_a + \sigma_s) \sum_{i=1}^N \psi_i(z) B_i(\mu) \\ &= \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \psi_j(z) \right] B_i(\mu) + \sum_{i=1}^N Q_i(z) B_i(\mu) , \end{aligned} \quad (6.2.4a)$$

where

$$k_{ij} = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu_i) B_j(\mu') d\mu' . \quad (6.2.4b)$$

Note that the solution itself as well as each term in the transport equation has a continuous representation in μ . In particular, the discrete values of the angular flux are chosen such that

$$\frac{d}{dz} J(z, \mu) + (\sigma_a + \sigma_s) \psi(z, \mu) = S(z, \mu) + Q(z, \mu) \quad (6.2.1)$$

at each value of z and for all $\mu \in [-1, +1]$, where

$$J(z, \mu) = \sum_{i=1}^N \mu_i \psi_i(z) B_i(\mu) , \quad (6.2.2)$$

$$\psi(z, \mu) = \sum_{i=1}^N \psi_i(z) B_i(\mu) , \quad (6.2.3)$$

$$S(z, \mu) = \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \psi_j(z) \right] B_i(\mu) , \quad (6.2.4)$$

and

$$Q(z, \mu) = \sum_{i=1}^N Q_i(z) B_i(\mu) . \quad (6.2.5)$$

It follows from expression 3.2.3 that if equation 6.2.4a is successively evaluated at each of the collocation points, the following system of equations for the discrete angular flux values is obtained:

$$\mu_i \frac{d}{dz} \psi_i(z) + (\sigma_a + \sigma_s) \psi_i(z) = \sum_{j=1}^N k_{ij} \psi_j(z) + Q(z) , \quad (6.2.6)$$

Equation 6.2.4a demonstrates the continuous nature of the collocation solution while equation 6.2.6 demonstrates its discrete nature. We shall refer to equations 6.2.4 and 6.2.6 as the continuous and discrete collocation equations, respectively. It is important to remember, however, that the two equations are fully equivalent as solving either of them is equivalent to solving the other.

It is easily seen that the collocation equations will be conservative if the equation

$$\begin{aligned} \sigma_s 2\pi \int_{-1}^{+1} \sum_{i=1}^N \psi_i(z) B_i(\mu) d\mu \\ = 2\pi \int_{-1}^{+1} \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \psi_j(z) \right] B_i(\mu) d\mu \end{aligned} \quad (6.2.7)$$

holds for every element of the trial space. Due to the linear nature of the trial space, the above expression holds for each element of the trial space if it holds for each basis function. Thus, we can decompose expression 6.2.7 into N distinct requirements,

$$\sigma_s 2\pi \int_{-1}^{+1} B_j(\mu) d\mu = 2\pi \int_{-1}^{+1} \sum_{i=1}^N k_{ij} B_i(\mu) d\mu, \quad j=1, N. \quad (6.2.8)$$

The conditions under which the above requirements will be met become clear when the matrix elements, k_{ij} , are

properly interpreted. The exact scattering source corresponding to the j 'th basis function can be expressed as

$$S_j^*(\mu) = 2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu) B_j(\mu') d\mu' . \quad (6.2.9)$$

From expression 6.2.4b, it is clear that the scattering matrix elements are simply the N discrete values of the j 'th exact scattering source,

$$k_{ij} = S_{j_i}^*(\mu_i), \quad i=1,N, \quad j=1,N . \quad (6.2.10)$$

The j 'th scattering source which is consistent with the collocation equations and appears in expression 6.2.8 is the projection of the exact source,

$$S_j(\mu) = P[S_j^*(\mu)] = \sum_{i=1}^N k_{ij} B_i(\mu) . \quad (6.2.11a)$$

Due to the conservative property of the scattering kernel (expression 4.2.2), we know that

$$\sigma_s 2\pi \int_{-1}^{+1} B_j(\mu) d\mu = 2\pi \int_{-1}^{+1} S_j^*(\mu) d\mu, \quad j=1,N. \quad (6.2.11b)$$

If the scattering operator maps the trial space to itself, the exact scattering sources and their projections will be identical. Thus, particle conservation is assured in this case.

There are two notable instances in which this occurs. If the scattering is isotropic, all of the exact scattering sources are constant functions of μ . Since any reasonable trial space contains the constant function, it follows that the collocation equation is always conservative with isotropic scattering. It is well known that the Legendre polynomials are eigenfunctions of every symmetric scattering operator. In particular

(6.2.12a)

$$2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu) P_\ell(\mu') d\mu' = \sigma_\ell P_\ell(\mu), \quad \ell=0, \infty,$$

where

$$\sigma_\ell = 2\pi \int_{-1}^{+1} \frac{d\sigma_s}{d\mu_0} P_\ell(\mu_0) d\mu_0. \quad (6.2.12b)$$

Since the Legendre polynomials form a basis for any global polynomial trial space, it follows that the collocation equation is always conservative

with a global polynomial trial space regardless of the anisotropy of the scattering.

There are many types of trial spaces which are of interest, such as piecewise polynomial trial spaces, for which conservation is not guaranteed. This difficulty can be easily overcome by employing an ad hoc procedure to enforce particle conservation in the collocation equations. Since lack of conservation is entirely due to incorrect magnitudes of the consistent basis function scattering sources, one need only normalize these sources to enforce conservation. We choose normalization factors, $\{\gamma_j\}_{j=1}^N$ such that

(6.2.13)

$$2\pi \int_{-1}^{+1} \gamma_j S_j(\mu) d\mu = \sigma_s 2\pi \int_{-1}^{+1} B_j(\mu) d\mu, \quad j=1, N.$$

The result is

$$\gamma_j = \sigma_s w_j / \sum_{i=1}^N k_{ij} w_i, \quad (6.2.14a)$$

where

$$w_j = 2\pi \int_{-1}^{+1} B_j(\mu) d\mu . \quad (6.2.14b)$$

Strictly conservative equations are obtained by substituting $k_{ij}\gamma_j$ for k_{ij} in equations 6.2.4a and 6.2.6 respectively,

$$\begin{aligned} & \sum_{i=1}^N \mu_i \frac{d}{dz} \psi_i(z) B_i(\mu) + (\sigma_a + \sigma_s) \sum_{i=1}^N \psi_i(z) B_i(\mu) \\ &= \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \gamma_j \psi_j(z) \right] B_i(\mu) + \sum_{i=1}^N Q_i(z) B_i(\mu) , \end{aligned} \quad (6.2.15)$$

and

$$\mu_i \frac{d}{dz} \psi(z) + (\sigma_a + \sigma_s) \psi_i(z) = \sum_{j=1}^N k_{ij} \gamma_j \psi_j(z) + Q_i(z), \quad i=1, N . \quad (6.2.16)$$

The consistent scalar balance equation is obtained by integrating equation 6.2.15 over all directions. The result is

$$\frac{d}{dz} J(z) + \sigma_a \phi(z) = q(z) , \quad (6.2.17)$$

where

$$J(z) = \sum_{i=1}^N \mu_i \psi_i(z) w_i ,$$

$$\phi(z) = \sum_{i=1}^N \psi_i(z) w_i ,$$

$$q(z) = \sum_{i=1}^N Q_i(z) w_i .$$

If the normalization factors are not within a few percent of unity, the accuracy of the collocation solution is questionable. A substantial lack of particle conservation clearly indicates that the exact and consistent basis function scattering sources are quite different from one another. This difference directly affects the accuracy of the solution by contributing to its associated residual (see theorem 2.3.1). This residual can be expressed as

$$R(z, \mu) = R_1(z, \mu) - R_2(z, \mu) - R_3(z, \mu) , \quad (6.2.18a)$$

where

$$R_1(z, \mu) = \mu \sum_{i=1}^N \frac{d}{dz} \psi_i(z) B_i(\mu) - \sum_{i=1}^N \mu_i \frac{d}{dz} \psi_i(z) B_i(\mu) , \quad (6.2.18b)$$

(6.2.18c)

$$R_2(z, \mu) = \sum_{i=1}^N \psi_i(z) S_i^*(\mu) - \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \gamma_j \psi_j(z) \right] B_i(\mu) ,$$

$$R_3(z, \mu) = Q(z, \mu) - \sum_{i=1}^N Q_i(z) B_i(\mu) . \quad (6.2.18d)$$

By normalizing we ensure that

$$2\pi \int_{-1}^{+1} R_2(z, \mu) d\mu = 0 . \quad (6.2.19)$$

However, it can be shown that

$$R_2(z, \mu_j) = \sum_{i=1}^N \psi_i(z) S_i^*(\mu_j) (1 - \gamma_i) , \quad j=1, N . \quad (6.2.20)$$

Thus the departure of the normalization factors from unity directly contributes to non-zero values of the residual at the collocation points.

It is important to note that if the scattering kernel is expressible in terms of the basis functions, i.e.,

$$\sigma_s(\mu' \rightarrow \mu) = \sum_{i=1}^N \sum_{j=1}^N \sigma(\mu_i \rightarrow \mu_j) B_i(\mu') B_j(\mu) , \quad (6.2.21)$$

the exact basis function scattering sources are contained within the trial space. Thus if the trial space is chosen such that the above expression is approximately correct, normalization factors correspondingly close to unity are obtained. Restricting consideration to physically reasonable scattering kernels and standard interpolation schemes, it can be expected that as the number of collocation points is "correctly" increased (in such a way that the maximum distance between adjacent collocation points approaches zero), the basis function expansion for the kernel will become increasingly accurate. Thus one can simply increase the number of collocation points until the normalization factors are sufficiently close to unity.

It is important to note that the discrete collocation equation given in equation (6.2.16) has the same algebraic structure as the standard S_n equation (equation 5.2.3). Thus the iterative methods used to solve the S_n equation can similarly be applied to the collocation equation. In addition, because the collocation equation is strictly conservative, convergence

acceleration techniques generally applied to the S_n equation can also be expected to be applicable. Thus the collocation approach, like the finite-element approach, gives a consistent continuous angular flux representation, but unlike the finite-element approach, the resulting equations can be solved with standard S_n techniques. We feel that this is the most significant advantage of the collocation approach.

Our collocation method is more flexible with respect to cross-section representation because Legendre expansions are not required. However, if the use of such expansions is desirable, an alternate method for normalizing the collocation scattering source can be employed which is more efficient in certain instances. We begin the development of this method by assuming the use of a Legendre expansion of degree L . In this case, the unnormalized collocation scattering source can be expressed as

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_\ell P_\ell(\mu') P_\ell(\mu_i) \psi_j(z) B_j(\mu') d\mu' , \quad (6.2.22)$$

$$i=1, N .$$

By interchanging the order of summation, we obtain

$$S(z, \mu_i) = \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_{\ell} \phi_{\ell}(z) P_{\ell}(\mu), \quad i=1, N, \quad (6.2.23a)$$

where

$$\phi_{\ell}(z) = \sum_{j=1}^N \psi_j(z) B_{j\ell}, \quad \ell=0, L, \quad (6.2.23b)$$

and

$$B_{j\ell} = 2\pi \int_{-1}^{+1} B_j(\mu) P_{\ell}(\mu) d\mu, \quad \ell=0, L. \quad (6.2.23c)$$

The coefficients, $\{\phi_{\ell}(z)\}_{\ell=0}^L$, are the first $L+1$ Legendre moments of the angular flux. In many instances, the scalar flux $(\phi_0(z))$ is the only quantity of interest. If scattering source normalization is not necessary and $L+1 < N$, a significant reduction in computer storage requirements can be achieved in such calculations by storing only the $L+1$ flux moments needed to calculate the scattering source rather than the complete angular flux. However, if normalization is necessary and the standard procedure is employed, expression 6.2.23a remains valid but expression 6.2.23b becomes

$$\phi_{\ell}(z) = \sum_{j=1}^N \psi_j(z) B_{j\ell} \gamma_j, \quad \ell=1, N. \quad (6.2.24)$$

Unfortunately, these modified coefficients no longer represent the Legendre moments of the flux. Under these circumstances, the flux moments of interest would have to be stored in addition to these coefficients.

This difficulty can be circumvented by applying a single normalization factor to the complete source. In particular, the normalized source can be expressed as

$$S(z, \mu_i) = \gamma(z) \left[\sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_{\ell} \phi_{\ell}(z) P_{\ell}(\mu_i) \right], \quad i=1, N, \quad (6.2.25a)$$

where

$$\gamma(z) = \sigma_0 \phi_0 / \sum_{\ell=0}^L \frac{2\ell+1}{4\pi} \sigma_{\ell} \phi_{\ell}(z) W_{\ell}, \quad (6.2.25b)$$

and

$$W_{\ell} = \sum_{i=1}^N P_{\ell}(\mu_i) w_i. \quad (6.2.25c)$$

The only disadvantage of this approach is that the normalization factor depends explicitly upon the angular flux rather than on the basis functions. This means that the normalization factor must be calculated each time that the source is calculated. Under the standard approach, the rebalance factors depend only upon the basis functions and need only be calculated once. Thus the alternate method is less efficient in terms of computing time. However, it can be seen from equation 6.3.5 that if the coefficients, $\{W_\ell\}_{\ell=0}^L$, are precalculated, the calculation of the normalization factor and the normalized source is equivalent to the calculation of the normalized source under the standard approach with a single extra direction. Thus, the relative increase in computing time incurred under the alternate approach can be expected to be quite small.

In concluding this section, we wish to make the important point that our method can always be made comparable to the S_n method in terms of total computational cost (time and storage). However, in order to do so in multigroup (energy-dependent) calculations, it is necessary to employ the alternate scattering source normalization technique. The reasons for this lie in the structure of the multigroup equations (Bell and Glasstone, 1970) and the construction of modern S_n codes (Hill, 1975).

6.3 Characteristics of Particular Basis Sets (Symmetric Case)

In this section we discuss the characteristics of some specific basis sets. Since generalized Lagrangian basis sets can be uniquely defined in terms of a set of N discrete directions or collocation points, $\{\mu_i\}_{i=1}^N$, and an appropriate interpolation scheme (see Section 3.2), we shall refer to specific basis sets in terms of these quantities. Although the choice of collocation points is arbitrary, only even-numbered sets with point arrangements symmetric about $\mu = 0$ will be considered. In doing so, we ensure that the principle of optical reciprocity is maintained in calculations. This principle simply states that the directed flux at $\vec{r}$ in direction $\vec{\Omega}_1$ due to a unit source at $\vec{r}_0$ radiating in direction $\vec{\Omega}_2$ is the same as the directed flux at $\vec{r}_0$ in direction $-\vec{\Omega}_2$ due to a unit source at $\vec{r}$ radiating in direction $-\vec{\Omega}_1$.

Some of the most interesting basis sets are those based upon global polynomial interpolation with collocation points corresponding to Gauss quadrature points. We refer such basis sets as Gauss collocation sets. The Gauss quadrature points corresponding to a N -point set are the roots of the Legendre polynomial of degree N . We refer to the S_n equations obtained

with Gauss quadrature sets as Gauss S_n equations. The Gauss collocation and Gauss S_n equations are equivalent (i.e., they yield identical solutions for the same problem when similar boundary conditions are applied). It is not difficult to show this. Since the collocation and quadrature points are identical, it is clear that the leakage, removal, and inhomogeneous source terms appearing in the S_n and collocation equations (equations 5.2.8 and 6.2.16) are identical. Thus, to demonstrate equivalence, we need only show that the inscatter terms are identical.

With a global polynomial trial space, normalization is not necessary and the collocation inscatter term for the i 'th direction is

$$S(z, \mu_i) = \sum_{j=1}^N k_{ij} \psi_j(z) . \quad (6.3.1)$$

Following expression 6.2.4b, we find that

$$S(z, \mu_i) = \sum_{j=1}^N 2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu_i) \psi_j(z) B_j(\mu') d\mu' . \quad (6.3.2)$$

Expanding the scattering kernel in Legendre polynomials gives

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^{\infty} \int_{-1}^{+1} \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu') P_{\ell}(\mu_i) \psi_j(z) B_j(\mu') d\mu' . \quad (6.3.3)$$

Since each basis function is a polynomial of degree $N-1$, each one can be expanded in a Legendre polynomial expansion of similar degree. Thus, due to the orthogonality of the Legendre polynomials, the summation can be truncated at $\ell = N - 1$,

(6.3.4)

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^{N-1} \int_{-1}^{+1} \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu') P_{\ell}(\mu_i) \psi_j(z) B_j(\mu') d\mu'.$$

It is well known that the Gauss quadrature formula of order N exactly integrates all polynomials of degree $2N - 1$ or less. Therefore the integrals appearing in expression 6.3.4 can be replaced by the Gauss quadrature formula,

(6.3.5a)

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^{N-1} \sum_{k=1}^N \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu_k) P_{\ell}(\mu_i) \psi_j(z) B_j(\mu_k) w_k^*.$$

Using expression 3.2.3, the above expression reduces to

(6.3.5b)

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^{N-1} \frac{2\ell+1}{4\pi} \sigma_{\ell} P_{\ell}(\mu_j) P_{\ell}(\mu_i) \psi_j(z) w_j^*.$$

This expression is equivalent to the Gauss S_n inscatter term with a Legendre cross-section expansion of degree $N - 1$. Thus the Gauss S_n and Gauss collocation equations of order N are equivalent whenever a cross-section expansion of degree $N - 1$ is used in the Gauss S_n equations of order N . The equations are also equivalent if an expansion of lower order is used and the scattering kernel is exactly expressible in terms of that expansion. The equations will not be equivalent if cross-section expansions of degree greater than N are used because the quadrature integration will not be exact. It should be noted that although the Gauss quadrature correctly integrates an N 'th degree expansion, there is no point in employing one. The contribution of the N 'th term is identically zero due to the orthogonality of the Legendre polynomials.

Perhaps the most important property of the Gauss collocation equations is that they can be Galerkin-equivalent (see Chapter 2). To demonstrate this equivalence, it is sufficient to show that the collocation residual, given by equation 6.2.19, is orthogonal to the trial space. Throughout the following analysis, the class of polynomials of degree N is intended to include all polynomials of degree N or less.

Due to the nature of the collocation projection, the residual is always zero at the collocation points,

$$R(z, \mu_i) = 0, \quad i=1, N. \quad (6.3.6)$$

Thus clearly,

$$R(z, \mu_i) B_j(\mu_i) w_i^* = 0, \quad i=1, N, \quad j=1, N, \quad (6.3.7)$$

where $\{w_i^*\}_{i=1}^N$ denotes the N-point Gauss quadrature weights. Summing over all i gives

$$\sum_{i=1}^N R(z, \mu_i) B_j(\mu_i) w_i^* = 0, \quad j=1, N. \quad (6.3.8)$$

Because the trial space is composed of global polynomials, the inscatter component of the residual, $R_2(z, u)$ (see equation 6.2.19), is identically zero. If we assume that the inhomogeneous source is expressible as a polynomial in u of degree N , i.e.,

$$Q(z, u) = \sum_{\ell=0}^N Q_\ell(z) u^\ell, \quad (6.3.9)$$

the residual is a polynomial in u of degree N and the products

$$R(z, \mu) B_j(\mu) \quad , \quad i=1, N, \quad (6.3.10)$$

will be polynomials in μ of degree $2N-1$. Since the Gauss quadrature formula exactly integrates such polynomials, the summation in equation 6.2.8 can be replaced by an integral,

$$\int_{-1}^{+1} R(z, \mu) B_j(\mu) d\mu = 0 \quad , \quad j=1, N, \quad (6.3.11)$$

which shows that the residual is orthogonal to the trial space. Thus we see that the Gauss collocation solution of order N is Galerkin-equivalent whenever the inhomogeneous source is expressible as a polynomial in μ of degree N .

The spherical harmonics solution of order N (the P_{N-1} solution) is a Galerkin solution corresponding to the trial space of global polynomials in μ of degree $N-1$. Since the Galerkin solution is unique for any trial space, it follows that the Gauss collocation equations of order N and the P_{N-1} equations are equivalent whenever the collocation equations are Galerkin equivalent. As noted in Chapter 5, it is

well known that equivalence exists under certain conditions between the Gauss S_n and spherical harmonics equations. Thus the equivalence between the Gauss collocation and spherical-harmonics equations is expected because of the Gauss collocation-Gauss S_n equivalence.

Another interesting group of generalized Lagrangian basis sets are the double-Gauss sets. These sets are generated with independent polynomial interpolations on the intervals $[-1,0]$ and $[0,+1]$ respectively and have collocation points corresponding to the double-Gauss quadrature points. As might be expected, the double-Gauss collocation equations can be equivalent to both the double-Gauss S_n and the double- P_n equations (Galerkin equivalent). The analysis demonstrating this equivalence is analogous to that for the Gauss collocation equations. Therefore, we shall omit it and simply state the results. The double-Gauss collocation equations of order N are equivalent to the double Gauss S_n equations of order N only when the scattering kernel is exactly expressible in terms of a Legendre polynomial expansion of degree $N/2$ or less and the exact expansion is used in the S_n equations. The double-Gauss collocation equations of order N are equivalent to the double $P_{N/2-1}$ equations only if the scattering kernel is exactly expressible in terms of a Legendre

polynomial expansion of degree $N/2$ or less and the inhomogeneous source is exactly expressible as a double polynomial in μ of degree $N/2$ or less, i.e.,

$$Q(z, \mu) = \sum_{\ell=0}^{N/2} Q_{\ell}^{+}(z) \mu^{\ell} , \quad \mu \geq 0 , \quad (6.3.12a)$$

$$= \sum_{\ell=0}^{N/2} Q_{\ell}^{-}(z) \mu^{\ell} , \quad \mu < 0 . \quad (6.3.12b)$$

Negative angular fluxes are sometimes obtained in discrete ordinates calculations. There are only two reasons for these occurrences. Either the spatial mesh is too large or the scattering source is negative due to negative oscillations in the scattering kernel expansion. The former problem can be remedied using standard negative-flux-fixup techniques. The latter problem can sometimes be dealt with simply by increasing the degree of the cross-section expansion. However, this is not always practical because in most cases the scalar flux solutions are quite good and the negative angular flux values occur only at those directions for which the angular flux is nearly zero. This type of problem can be completely avoided using the collocation method in conjunction with a generalized Lagrangian basis set which is positive. By this we mean a set which satisfies

$$B_j(\mu) \geq 0, \mu \in [-1, +1], \quad j=1, N. \quad (6.3.13)$$

Since any physically meaningful scattering kernel satisfies

$$\sigma_s(\mu' \rightarrow \mu) \geq 0, \quad \mu', \mu \in [-1, +1], \quad (6.3.14)$$

it follows that all of the scattering matrix elements, k_{ij} given by equation 6.2.4b are positive if the basis set is positive. This in turn ensures positive angular flux solutions (neglecting spatial mesh considerations). A more precise way of stating this result is that the positivity of the transport operator is preserved by the collocation projection.

Any generalized Lagrangian basis set generated with piecewise-linear interpolation and having collocation points at the endpoints of the interval of interpolation is positive. Such sets are computationally investigated in Chapter 8.

Due to the close parallel between the collocation and S_n equations, it is natural to ask if the collocation method can be viewed as simply being a mathematically formal means of deriving S_n equations. For reasons which we now discuss, this viewpoint is generally valid only for the case of isotropic scattering.

Assuming that the collocation trial space contains the constant function, $f(\mu) = 1.0$, it follows that

$$\sum_{i=1}^N B_i(\mu) = 1.0. \quad (6.3.15)$$

Integrating over all μ gives

$$\sum_{i=1}^N w_i^+ = 2.0, \quad (6.3.16a)$$

where

$$w_i^+ = \int_{-1}^{+1} B_i(\mu) d\mu.$$

These weights together with the collocation points, $\{\mu_i\}_{i=1}^N$, constitute a valid quadrature set because the weights sum to 2.0. In addition, this quadrature set integrates all elements of the trial space exactly (note that these weights differ from those given in expression 6.2.4b only by a factor of 2π). When this quadrature set is used in the S_N equations, we obtain what we refer to as the companion S_N equations. When the scattering is isotropic, the companion S_N equations will be identical to the discrete collocation

equations. Although the S_n approach does not explicitly include the continuous representation inherent in the collocation approach, it is clear that the two approaches always yield the same discrete angular flux and scalar transport quantities (scalar flux, net current, etc.) and thus are really equivalent in this instance.

However, for the case of anisotropic scattering, the collocation and S_n equations are equivalent only if the companion quadrature set exactly performs the inscatter integral. In particular, it is necessary that

$$2\pi \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu_i) B_j(\mu') d\mu' = 2\pi \sigma_s(\mu_j \rightarrow \mu_i) w_j^+, \quad i=1,N, \quad j=1,N. \quad (6.3.16)$$

In arbitrarily choosing basis sets (interpolation schemes and collocation points), this condition is rarely met. Thus for the case of anisotropic scattering, the collocation and S_n methods are indeed fundamentally different. Unfortunately, it is essentially impossible to determine a priori whether the collocation or companion S_n solution is more accurate for a particular problem. Nonetheless, there are two instances in which the collocation approach is preferred. If the companion quadrature set is not sufficiently accurate to ensure particle conservation, the S_n approach is clearly undesirable. This is often

the case when piecewise polynomial trial spaces of low degree (relative to the dimensionality of the space) are employed in problems with substantially anisotropic scattering. As noted previously, the collocation scattering source is exact whenever a global polynomial trial space is employed. If the companion S_n quadrature set cannot exactly evaluate the inscatter integral, the S_n scattering source is not exact. This does not mean that the S_n solution is always less accurate than the collocation solution. However, the collocation solution can be expected to be more accurate for most problems. Thus, the collocation method is preferred whenever global polynomial trial spaces are employed. It should be noted that the companion quadrature set is never exact in problems with full anisotropy (a P_{N-1} expansion with N collocation points) and other than Gauss collocation points.

Overall, we feel that the primary advantage of the collocation approach relative to the S_n approach is its versatility. Because the inscatter integral is performed exactly rather than with quadrature formulas, there is a great deal more freedom in choosing an angular flux representation. Computational examples demonstrating this versatility are given in Chapter 8.

5.4 Derivation of Asymmetric Scattering Equations

The derivation of the asymmetric scattering equations is identical to the derivation of the symmetric scattering equations with the exception that the full asymmetric form of the transport equation given by equation 4.1.1 is used. The continuous and discrete collocation equations obtained are respectively

$$\begin{aligned} \sum_{i=1}^N \mu_i \frac{d}{dz} \psi_i(z) B_i(\mu) + \sum_{i=1}^N (\sigma_a + \sigma_{si}) \psi_i(z) B_i(\mu) \\ = \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \psi_j(z) \right] B_i(\mu) + \sum_{i=1}^N Q_i(z) B_i(\mu) , \end{aligned} \quad (6.4.1a)$$

and

$$\mu_i \frac{d}{dz} \psi_i(z) + (\sigma_a + \sigma_{si}) \psi_i(z) = \sum_{j=1}^N k_{ij} \psi_j(z) + Q_i(z) , \quad i=1, N, \quad (6.4.1b)$$

where

$$\sigma_{si} = \sigma_s(\mu_i) , \quad i=1, N,$$

and the scattering matrix elements, k_{ij} , are defined as in equation 6.2.4b. The only obvious difference

between these and the symmetric equations is the dependence of the scattering cross section upon μ . However, the scattering source is also significantly different, but the generalized definition of the scattering matrix elements masks this difference.

One general effect of the asymmetry is to make the transport equation more difficult to solve from the viewpoint of approximation theory. This is most readily seen by noting that the residual corresponding to equation 6.4.1 contains an extra term,

$$R_4(z, \mu) = \sigma_s(\mu) \sum_{i=1}^N \psi_i(z) B_i(\mu) - \sum_{i=1}^N \sigma_{si} \psi_i(z) B_i(\mu), \quad (6.4.2)$$

which does not occur in the symmetric residual given by equation 6.2.18a. An additional residual term is really just an additional source of error. Thus, asymmetric scattering can give rise to more sources of error than anisotropic scattering.

Particle conservation is more difficult to obtain with asymmetric scattering. In the symmetric case, conservation is guaranteed if the inscatter operator maps the trial space to itself. In the asymmetric case, both the inscatter and outscatter operators must map

the trial space to itself to ensure conservation. However, it can be seen that the outscatter operator can never map the trial space to itself unless the total scattering cross section is a constant. Although it is possible to have asymmetric scattering with a constant scattering cross section, such scattering would almost never occur in physically realistic systems. Thus particle conservation can rarely be ensured in the asymmetric case.

Additional care must be exercised in developing an ad hoc procedure for enforcing particle conservation. As in the symmetric case, it is always possible to normalize the consistent basis function scattering sources so that conservation is achieved. The equation which the normalization factors must satisfy is

$$2\pi \int_{-1}^{+1} \gamma_j S_j(\mu) d\mu = 2\pi \int_{-1}^{+1} \sigma_{sj} B_j(\mu) d\mu, \quad j=1,N, \quad (6.4.3)$$

which directly corresponds to equation 6.2.13.

Although it is simple and effective, we do not recommend this procedure. It is always appropriate to normalize the scattering sources in the symmetric case because the lack of conservation is always due to disparity between the consistent and exact scattering

sources. However, in the asymmetric case, lack of conservation can be caused both by disparity between the consistent and exact scattering sources and by disparity between the consistent and exact outscatter terms. Thus it is appropriate to do two separate normalizations on each term. Normalizing the outscatter term is equivalent to normalizing the discrete scattering cross-section values. The cross-section normalization factors, $\{\alpha_i\}_{i=1}^N$, are chosen so that

$$2\pi \int_{-1}^{+1} \alpha_i \sigma_{si} B_i(\mu) d\mu = 2\pi \int_{-1}^{+1} \sigma_s(\mu) B_i(\mu) d\mu , \quad i=1, N. \quad (6.4.4)$$

The result is

$$\alpha_i = \bar{\sigma}_{si} / \sigma_{si} , \quad i=1, N, \quad (6.4.5a)$$

where

$$\bar{\sigma}_{si} = \frac{2\pi \int_{-1}^{+1} \sigma_s(\mu) B_i(\mu) d\mu}{2\pi \int_{-1}^{+1} B_i(\mu) d\mu} , \quad i=1, N . \quad (6.4.5b)$$

Note that these normalization factors have the effect of replacing the cross-section values evaluated at the collocation points with average cross-section values where the respective basis functions serve as the weighting function. By using the average cross-section values, the consistent and exact integral scattering densities are the same, i.e.

$$2\pi \int_{-1}^{+1} \sum_{i=1}^N \sigma_{si} \alpha_i \psi_i(z) B_i(\mu) d\mu = 2\pi \int_{-1}^{+1} \sigma_s(\mu) \sum_{i=1}^N \psi_i(z) B_i(\mu) d\mu . \quad (6.4.6)$$

This is clearly a highly desirable property. If the normalized cross-section values are substituted into equation 6.4.3, the right side of that equation becomes exact and the equation which the scattering source normalization factors must satisfy is obtained,

$$2\pi \int_{-1}^{+1} \gamma_j S_j(\mu) d\mu = 2\pi \int_{-1}^{+1} \sigma_{sj} \alpha_j B_j(\mu) d\mu , \quad j=1, N. \quad (6.4.7)$$

The result is

$$\gamma_j = \sigma_{sj} \alpha_j w_j / \sum_{i=1}^N k_{ij} w_i , \quad (6.4.8)$$

where the weights are the standard collocation weights defined in equation 6.2.14b.

The final conservative forms of the collocation equations are

$$\begin{aligned} & \sum_{i=1}^N \mu_i \frac{d}{dz} \psi_i(z) B_i(\mu) + \sum_{i=1}^N (\sigma_a + \sigma_{si} \alpha_i) \psi_i(z) B_i(\mu) \\ &= \sum_{i=1}^N \left[\sum_{j=1}^N k_{ij} \gamma_j \psi_j(z) \right] B_i(\mu) + \sum_{i=1}^N Q_i(z) B_i(\mu) , \end{aligned} \quad (6.4.9a)$$

and

$$\begin{aligned} & \mu_i \frac{d}{dz} \psi_i(z) + (\sigma_a + \sigma_{si} \alpha_i) \psi_i(z) = \sum_{j=1}^N k_{ij} \gamma_j \psi_j(z) + Q_i(z) , \\ & i=1, N, \end{aligned} \quad (6.4.9b)$$

respectively. If equation 6.4.9a is integrated over all directions, the scalar balance equation (equation 6.2.17) is obtained.

6.5 Characteristics of Particular Basis Sets

(Asymmetric Case)

As in the symmetric case, Gauss collocation sets are particularly interesting. We first wish to demonstrate that the Gauss collocation and Gauss S_n equations of order N are equivalent whenever the scattering kernel is exactly expressible as a tensor-product polynomial expansion of degree N or less and that expansion is employed in the S_n equations. It is apparent in comparing equations 6.4.9b and 5.3.3 respectively, that it is only necessary to show that the respective outscatter and inscatter terms are identical.

From equations 6.4.5a and 6.4.5b it follows that the average cross section values can be expressed as

$$\bar{\sigma}_{si} = \frac{2\pi \int_{-1}^{+1} \sigma_s(\mu) B_i(\mu) d\mu}{w_i}, \quad i=1, N, \quad (6.5.1)$$

where the weights are the standard collocation weights defined in equation 6.2.14b. We shall demonstrate that these weights differ from the Gauss quadrature weights only by a factor of 2π .

Clearly,

$$\sum_{i=1}^N f(\mu_i) w_i = 2\pi \int_{-1}^{+1} f(\mu) d\mu, \quad (6.5.2)$$

whenever $f(\mu)$ is a polynomial of degree $N-1$ or less (i.e., an element of the trial space). Thus these weights must satisfy

$$V \vec{w} = 2\pi \vec{m}, \quad (6.5.3)$$

where

$$V = \begin{bmatrix} 1 & 1 & \dots & 1 \\ \mu_1 & \mu_2 & \dots & \mu_N \\ \vdots & \vdots & \ddots & \vdots \\ \mu_1^{N-1} & \mu_2^{N-1} & \dots & \mu_N^{N-1} \end{bmatrix},$$

$$\vec{w} = (w_1, w_2, \dots, w_N),$$

$$\vec{m} = (m_1, m_2, \dots, m_N),$$

and

$$m_i = \int_{-1}^{+1} \mu^{i-1} d\mu, \quad i=1, N.$$

Because the Gauss quadrature formula exactly integrates all polynomials of degree $N-1$ or less, the Gauss weights, $\{w_i^*\}_{i=1}^N$, satisfy

$$V \vec{w}^* = \vec{m} \quad (6.5.4)$$

Since the matrix V is nonsingular, it follows from equations 6.5.3 and 6.5.4 that the collocation weights can differ from the Gauss weights only by a factor of 2π .

If the scattering kernel is exactly expressible as a polynomial of degree $N-1$, the integrand appearing in the numerator of expression 6.5.1 is a polynomial of degree $2N-2$ or less. Because of the equivalence between the Gauss and collocation weights, the integral can be exactly evaluated with the collocation weights,

$$\bar{\sigma}_{si} = \frac{\sum_{k=1}^N \sigma_{sk} B_i(\mu_k) w_k}{w_i}, \quad i=1, N. \quad (6.5.5)$$

Using expression 3.2.3, the above expression reduces to

$$\bar{\sigma}_{si} = \frac{\sigma_{si} w_i}{w_i} = \sigma_{si}, \quad i=1, N. \quad (6.5.6)$$

Thus, the outscatter terms are indeed identical.

The collocation scattering source can be expressed as

$$S(z, \mu_i) = 2\pi \sum_{j=1}^N \sum_{\ell=0}^{N-1} \sum_{m=0}^{N-1} \int_{-1}^{+1} \left[\frac{(2\ell + 1)(2m + 1)}{8\pi} \right. \\ \left. \sigma_{\ell, m} P_{\ell}(\mu') P_m(\mu_i) \psi_j(z) B_j(\mu') \right] d\mu' , \quad i=1, N . \quad (6.5.7)$$

Because the integrand is a polynomial of degree $2N-2$ or less, the Gauss quadrature formula can be used to evaluate the integral. When this is done, the above expression reduces to the Gauss S_N scattering source. It is clear that the scattering operator maps the trial space to itself. Thus the scattering source normalization factors are unity and the collocation and S_N scattering terms are identical. With expansion orders greater than N , the quadrature integrations would not be exact and equivalence would be lost.

As in the symmetric scattering case, the Gauss collocation solution is Galerkin-equivalent only if the collocation residual is a polynomial of degree N . This happens only if the scattering cross section, scattering kernel, and inhomogeneous source, are exactly expressible as polynomials of degree 1, N , and N

respectively. These conditions can be expected to be met much less often than the corresponding conditions for the symmetric case.

Similar results are obtained for the double-Gauss collocation equations. In particular, the double-Gauss collocation and S_n equations of order N are equivalent only if the scattering kernel is exactly expressible as a polynomial of order $N/2$ or less and that expansion is employed in the S_n equations. The double-Gauss collocation equations of order N will be Galerkin-equivalent only if the scattering cross section, scattering kernel, and inhomogeneous source are exactly expressible as polynomials of degree, 1, $N/2$, and $N/2$, respectively.

The remarks made for the symmetric scattering case regarding positive basis sets also apply to the asymmetric scattering case. The positivity of the collocation equation is one of the few properties which is not affected by scattering asymmetry.

The final point that we wish to make concerns the relative computational effort required to generate scattering sources for the asymmetric collocation and S_n methods. It can be seen from expression 6.2.4b that the evaluation of each element of the collocation scattering matrix requires a one-dimensional integral. Thus N^2 total integrals must be performed for an N 'th order equation. On the

other hand, each tensor-product Legendre expansion coefficient appearing in the S_n equation requires a two-dimensional integral (see expression 5.3.1). In a problem with strong asymmetry (i.e., an $N-1$ degree expansion with a quadrature set of order N), N^2 two-dimensional integrals are required. If each one-dimensional collocation integral requires X units of computational effort to evaluate, each two-dimensional S_n integral can be expected to require approximately X^2 units. Thus, the total computational effort required for the collocation integrals is $(NX)^2 = N^2X^2$, while the corresponding effort required for the S_n integrals is $(NX^2)^2 = N^2X^4$. In problems with strong asymmetry, it is clear that the collocation method is significantly more efficient than the S_n method in terms of cross-section processing requirements. In problems with weak asymmetry (i.e., an L degree expansion with a quadrature set of order N where $L \ll N$), the use of Legendre expansions is desirable. It should be noted that for such problems a modified asymmetric collocation method can be employed which is analogous to the modified symmetric collocation method discussed in Section 2.6. Under this approach, the computational efficiency of the collocation method becomes comparable to that of the S_n method for problems with weak asymmetry.

CHAPTER 7

THE ASYMMETRIC DIFFUSION EQUATION

7.1 Introduction

In this chapter, we derive a diffusion equation which treats scattering with polar asymmetries. After an analysis of the effects of scattering asymmetries on the diffusion solution, we present the analytic solution to a particularly interesting problem. Finally, we discuss our utilization of the asymmetric diffusion equation in an algorithm to accelerate the iterative convergence of collocation solutions.

7.2 Derivation of the Asymmetric Diffusion Equation

Our asymmetric diffusion equation is obtained from the asymmetric transport equation by the application of a Galerkin projection technique corresponding to a trial space which is linear in μ . We choose to represent each element of the trial space in the form

$$t(z, \mu) = \frac{1}{4\pi} t_0(z) + \frac{3}{4\pi} t_1(z) \mu . \quad (7.2.1)$$

Under this representation, the expansion coefficients

$t_0(z)$ and $t_1(z)$ represent, respectively, the scalar flux and net current corresponding to $t(z, \mu)$. The Galerkin operator projecting onto this trial space operates on a general function as follows:

$$P [g(z, \mu)] = \frac{1}{4\pi} g_0(z) + \frac{3}{4\pi} g_1(z) \mu , \quad (7.2.2)$$

where

$$g_0(z) = 2\pi \int_{-1}^{+1} g(z, \mu) d\mu ,$$

and

$$g_1(z) = 2\pi \int_{-1}^{+1} g(z, \mu) \mu d\mu .$$

We begin the derivation of the diffusion equation by assuming that the transport solution is an element of the trial space.

$$\phi(z, \mu) = \frac{1}{4\pi} \phi_0(z) + \frac{3}{4\pi} \phi_1(z) \mu . \quad (7.2.3)$$

This expression is substituted into equation 4.1.1 and that equation is then operated on by P. Under the additional assumption of an isotropic inhomogenous source (standard in diffusion theory), the following equations result,

$$\frac{d}{dz} \phi_1(z) + \sigma_a \phi_0(z) = q_0(z) , \quad (7.2.4a)$$

and

$$\begin{aligned} \frac{1}{3} \frac{d}{dz} \phi_0(z) + \sigma_a \phi_1(z) + \frac{1}{2} \sigma_{10} \phi_0(z) + \frac{3}{2} \sigma_{20} \phi_1(z) \\ = \frac{1}{2} \sigma_{10} \phi_0(z) + \frac{3}{2} \sigma_{11} \phi_1(z) , \end{aligned} \quad (7.2.4b)$$

where

$$\sigma_{n,m} = 2\pi \int_{-1}^{+1} \int_{-1}^{+1} \sigma_s(\mu' \rightarrow \mu) \mu^n \mu'^m d\mu' d\mu .$$

Equation 7.2.4a is simply the scalar balance equation. With some rearrangement, equation 7.2.4b is seen to yield a modified form of Fick's law,

$$\phi_1(z) = -D \left[\frac{d}{dz} \phi_0(z) + \frac{3}{2} (\phi_{10} - \phi_{01}) \phi_0(z) \right] \quad (7.2.5a)$$

where

$$D = \frac{1}{3(\sigma_a + \frac{3}{2}\sigma_{20} - \frac{3}{2}\sigma_{11})} \quad (7.2.5b)$$

By substituting from equation 7.2.5a into equation 7.2.4a, we obtain the desired diffusion equation,

$$-D \left[\frac{d^2}{dz^2} \phi(z) + \frac{3}{2} (\sigma_{10} - \sigma_{01}) \frac{d}{dz} \phi(z) \right] + \sigma_a \phi(z) = q(z) \quad (7.2.6)$$

Equation 7.2.6 reduces to the standard diffusion equation (equation 4.3.1) under the assumption of symmetric scattering. Upon comparing the two equations, it is seen that asymmetric scattering can give rise to a first-order derivative term which does not appear with symmetric scattering. A term of this form is known as a drift term. We later give a specific example which shows that its presence can radically alter the asymptotic nature of the diffusion solution.

7.3 Qualitative Effects of Asymmetric Scattering

In order to demonstrate some of the qualitative effects of asymmetric scattering, we consider four particularly simple types of scattering kernels,

$$\sigma_1(\mu' \rightarrow \mu) = \frac{1}{4\pi} \sigma_s , \quad (7.3.1a)$$

$$\sigma_2(\mu' \rightarrow \mu) = \frac{1}{4\pi} \sigma_s (1 + 3\beta\mu'\mu) , \quad (7.3.1b)$$

$$\sigma_3(\mu' \rightarrow \mu) = \frac{1}{4\pi} \sigma_s (1 + 3\beta\mu'^2) , \quad (7.3.1c)$$

$$\sigma_4(\mu' \rightarrow \mu) = \frac{1}{4\pi} \frac{\sigma_s}{1+\beta} (1 + 3\beta\mu'^2) . \quad (7.3.1d)$$

The first kernel corresponds to symmetric isotropic scattering, the second to symmetric linearly-anisotropic scattering, and the third and fourth to asymmetric isotropic scattering with respective linear and quadratic dependences of the total scattering cross section upon the incident particle direction. It should be noted that the average value of the total scattering cross section is the same in all cases:

$$\bar{\sigma}_i = \frac{1}{2} \int_{-1}^{+1} \left[2\pi \int_{-1}^{+1} \sigma_i(\mu' \rightarrow \mu) d\mu \right] d\mu' = \sigma_s , \quad i=1,4. \quad (7.3.2)$$

Equation 7.2.5 takes the following forms for the four kernels,

$$- \frac{1}{3\sigma_s} \frac{d^2}{dz^2} \phi(z) + \sigma_a \phi(z) = q(z) , \quad (7.3.3a)$$

$$\frac{-1}{3\sigma_s(1-\beta)} \frac{d^2}{dz^2} \phi(z) + \sigma_a \phi(z) = q(z) , \quad (7.3.3b)$$

$$- \frac{1}{3\sigma_s} \frac{d^2}{dz^2} \phi(z) - \beta \frac{d}{dz} \phi(z) + \sigma_a \phi(z) = q(z) , \quad (7.3.3c)$$

$$\frac{-5(1+\beta)}{3\sigma_s(5+9\beta)} \frac{d^2}{dz^2} \phi(z) + \sigma_a \phi(z) = q(z) . \quad (7.3.3d)$$

Equations 7.3.3a and 7.3.3b show that anisotropy does not alter the structure of the symmetric-isotropic diffusion equation, but rather simply changes the diffusion coefficient (see equation 7.2.4b). It is easily seen that a symmetric-isotropic kernel of the form,

$$\sigma(\mu' \rightarrow \mu) = \frac{1}{4\pi} \sigma_s (1 - \beta) \quad (7.3.4)$$

produces the same diffusion solution as the symmetric-anisotropic kernel (equation 7.3.1b). Similarly, equation 7.3.3d demonstrates that a symmetric-isotropic kernel of the form,

$$\sigma(\mu' \rightarrow \mu) = \frac{1}{4\pi} \sigma_s \frac{5 + 9\beta}{5(1 + \beta)} , \quad (7.3.5)$$

produces the same diffusion solution as the asymmetric-isotropic kernel (equation 7.3.1d). Thus the qualitative effect of the asymmetry corresponding to this kernel is analogous to that of the anisotropic kernel (equation 7.3.1b). We refer to this type of asymmetry as even asymmetry. Conversely, equation 7.3.3c shows that the asymmetry corresponding to the kernel given by equation 7.3.1c alters the structure of the symmetric-isotropic diffusion equation by adding a drift term. In this case, a symmetric isotropic kernel cannot be constructed which yields the same diffusion solution as does the asymmetric kernel. Thus the qualitative effect of this type of asymmetry is distinct from that of both even asymmetry and anisotropy. We refer to this type of asymmetry as odd asymmetry. Because of its distinctive nature, we henceforth discuss odd asymmetric scattering exclusively.

Some insight into the nature of odd asymmetric scattering can be gained by considering the equation describing the diffusion of positive ions under the influence of an electric field (Grno and Trnovcova, 1975),

$$-D \frac{d^2 C}{dz^2} + E_z e \frac{dC}{dz} = 0 , \quad (7.3.6)$$

where

D = ion diffusion coefficient,

E_z = electric field component along z-axis
($E_x = E_y = 0$),

ϵ = ion drift mobility,

C = ion concentration.

By setting

$$\sigma_a = 0.0, \quad (7.3.7a)$$

in equation 7.3.3 and

$$D = \frac{1}{3\sigma_s}, \quad (7.3.7b)$$

$$E_z = -\beta, \quad (7.3.7c)$$

$$\epsilon = 1.0, \quad (7.3.7d)$$

in equation 7.3.6, we see that the equations are identical. Thus odd asymmetric-isotropic scattering is mathematically equivalent (within the diffusion approximation) to symmetric-isotropic scattering under the influence of an electric field. We find this result quite interesting.

Further insight into the effect of odd asymmetric scattering can be gained by considering a simple solution of equation 7.3.3c. In particular, we consider the solution corresponding to an isotropic flux of particles

incident upon a non-absorbing slab of thickness t with a vacuum boundary condition at both faces of the slab and no internal source. The problem geometry is shown in Figure 3. For this case, equation 7.3.3c takes the form,

$$-\frac{1}{3\sigma_s} \frac{d^2}{dz^2} \phi(z) - \beta \frac{d}{dz} \phi(z) = 0 , \quad (7.3.8a)$$

with

$$J(z) = \frac{-1}{3\sigma_s} \frac{d}{dz} \phi(z) - \beta \phi(z) . \quad (7.3.8b)$$

The solution to this equation has the general form,

$$\phi(z) = a + be^{-3\sigma_s \beta z} .$$

Appropriate values for the constants a and b are found by assuming a unit incident particle current and applying the standard Marshak (Bell and Glasstone, 1970) boundary conditions in conjunction with the modified form of Ficks' law (equation 7.3.8b):

Figure 3. Problem Geometry for Diffusion Calculations.

$$\hat{j}^+(0) = 2\pi \int_0^1 \left[\frac{1}{4\pi} \phi(0) + \frac{3}{4\pi} J(0)\mu \right] \mu d\mu = 1.0 , \quad (7.3.10a)$$

$$\hat{j}^-(t) = 2\pi \int_{-1}^0 \left[\frac{1}{4\pi} \phi(t) + \frac{3}{4\pi} J(t)\mu \right] \mu d\mu = 0.0 , \quad (7.3.10b)$$

The result is

$$\phi(z) = \frac{4e^{-3\sigma_s \beta t} - 4(1+2\beta)e^{-3\sigma_s \beta z}}{(1-2\beta)e^{-3\sigma_s \beta t} - (1+2\beta)} . \quad (7.3.11)$$

Since the symmetric diffusion equation is embedded within the asymmetric equation, the above expression reduces to the solution corresponding to symmetric-isotropic scattering in the limit as $\beta \rightarrow 0.0$:

$$\phi(z) = \frac{4[3\sigma_s(t-z) + 2]}{(3\sigma_s t + 4)} \quad (7.3.12)$$

In addition to the scalar flux, the fraction of particles reflected from the slab and the fraction of particles transmitted through the slab are quantities of fundamental interest. Because the incident particle

current is normalized to unity (see equation 7.3.10a), the reflected fraction is equal to the backward current at $z = 0$,

$$RF = 2\pi \int_{-1}^0 \left[\frac{1}{4\pi} \phi(0) + \frac{3}{4\pi} J(0)\mu \right] \mu d\mu . \quad (7.3.13)$$

Using equations 7.3.8b and 7.3.11 to evaluate equation 7.3.13, we find that

$$RF = \frac{(1 + 2\beta)e^{-3\sigma_s \beta t} - (1 + 2\beta)}{(1 - 2\beta)e^{-\sigma_s \beta t} - (1 + 2\beta)} . \quad (7.3.14)$$

By taking the limit of equation 7.3.14 as $\beta \rightarrow 0$, the reflected fraction corresponding to symmetric scattering is obtained,

$$RF = \frac{3\sigma_s t}{3\sigma_s t + 4.0} . \quad (7.3.15)$$

Because the slab is non-absorptive, the reflected and transmitted fractions must sum to unity. Thus,

$$TF = 1.0 - RF . \quad (7.3.16)$$

Scalar flux solutions given by expression 7.3.11 are plotted in Figure 4 as a function of z with $\sigma_s t = 100$ for $\beta = 1/3, 1/30, -1/30, \text{ and } -1/3$. Note that $1/3$ and $-1/3$ correspond to the largest and smallest values of β , respectively, for which the cross section is non-negative. Expression 7.3.12 is also plotted and is denoted by $\beta = 0$.

It is clear from these plots that even a small degree of odd asymmetric in the scattering has a drastic effect upon the behavior of the diffusion solution. For $\beta > 0$, the flux profile is depressed toward the rear of the slab and has positive curvature. As would be expected, the disparity between the symmetric and asymmetric solutions increases as the absolute value of β increases. For $\beta < 0$, the scattering cross section decreases as the particle direction approaches $\mu = -1.0$ (directly toward the front face of the slab) and increases as the particle direction approaches $\mu = 1.0$. For $\beta > 0$, this dependence is reversed. The scattering cross section decreases as the particle direction approaches $\mu = 1.0$ and increases as the particle direction approaches $\mu = -1.0$. On a statistical basis, particles tend to seek those regions of phase space where the scattering rate is lowest (i.e., a statistical analog of the "path of least resistance").

Figure 4. Diffusion Theory Flux Solutions.

Thus it follows that for $\beta > 0$, particles will preferentially seek to travel in directions close to $\mu = -1.0$, while for $\beta < 0$, particles will preferentially seek to travel in directions close to $\mu = 1.0$. The respective depression and enhancement of the flux toward the rear of the slab is clearly attributable to such a statistical process.

The electric field analogy is quite useful for predicting the behavior of the scalar flux solution. According to equation 7.3.7, the intensity of the effective field is proportional to $|\beta|$. Since equation 7.3.6 is for positive ions, the particles experience a force along the direction of the field. For $\beta < 0$, the field is directed toward the back of the slab. The observed enhancement of the flux near the rear of the slab and the increase in that enhancement as $|\beta|$ increases would be a consequence of the presence of such a field. The analysis is identical for $\beta > 0$ except that the field direction is reversed.

The most unusual effect of odd-asymmetric scattering on the diffusion solution is best recognized through an analysis of the reflected fraction (expression 7.3.14). This expression is plotted in Figure 5 as a function of slab thickness for $\beta = 1/3, 1/30, -1/30$, and $-1/3$. The reflected fraction given by expression 7.3.15 is also plotted and is denoted by $\beta = 0.0$.

Figure 5. Diffusion Theory Reflected Fraction Solutions.

The asymptotic reflected fraction is obtained in the limit as the slab thickness is increased without bound. Thus it can be thought of as the reflected fraction corresponding to a semi-infinite slab. For symmetric scattering (both isotropic and anisotropic), it is well known that the asymptotic reflected fraction predicted both by diffusion theory and exact transport theory is unity. The plots in Figure 5 clearly indicate that a value of unity is also obtained for the case of odd-asymmetric scattering when $\beta > 0$. However, when $\beta < 0$, it appears that a value less than unity is obtained. By taking the limit of expression 7.3.14 as $t \rightarrow \infty$, it is found that this is indeed the case. In particular, we obtain

$$\begin{aligned} RF_{\infty} &= 1.0 \quad , \quad \text{for } \beta > 0 \quad , & (7.3.17) \\ &= \frac{1 + 2\beta}{1 - 2\beta} \quad , \quad \text{for } \beta < 0 \quad . \end{aligned}$$

From the preferential scattering agreement and the electric field analogy, one would expect that the reflected fraction for any fixed slab thickness would decrease with decreasing β , and it is evident from Figure 5 that this is true. However, it does not seem clear that the asymptotic reflected fraction should necessarily decrease with

decreasing β whenever $\beta < 0$. Hence, we find this result quite surprising. It is of considerable interest to determine whether odd-asymmetric scattering similarly alters the asymptotic behavior of the exact transport solution. Consequently, in Chapter 8, we computationally assess the accuracy of expression 7.3.17 for predicting the exact asymptotic reflected fraction as a function of β .

7.4 Asymmetric Diffusion-Synthetic Acceleration

In this section, we discuss our method for using the asymmetric diffusion equation in a synthetic algorithm to accelerate the iterative convergence of the asymmetric collocation equation. Our method represents a straightforward extension of Alcouffe's (1977) diffusion-synthetic acceleration scheme for accelerating the convergence of the S_n equation. Alcouffe's method is directly applicable to the symmetric collocation equation and is fully discussed in Chapter 5.

Our technique is applicable to the asymmetric collocation equation under the assumption that it is spatially differenced using diamond-differencing (equation 5.4.2) with step-differencing (equation 5.4.6) for negative flux fixup. The derivation of the differenced diffusion equation for interior mesh cells is begun by diamond-differencing equations 7.2.4a and 7.2.5a, respectively:

$$J_{k+1/2} - J_{k-1/2} + \sigma_a \phi_k \Delta_k = q_k \Delta_k \quad , \quad (7.4.1a)$$

$$J_k = -D \left[(\phi_{k+1/2} - \phi_{k-1/2})/\Delta_k + 3(\sigma_{10} - \sigma_{01})/2 \right] \phi_k \quad (7.4.1b)$$

The midpoint fluxes and currents can be eliminated from these equations by using the diamond-difference relationship:

$$J_{k+1/2} - J_{k-1/2} + \sigma_a (\phi_{k+1/2} + \phi_{k-1/2}) \Delta_k/2 = q_k \Delta_k \quad , \quad (7.4.2a)$$

$$(J_{k+1/2} + J_{k-1/2})/2 = -D \left[(\phi_{k+1/2} - \phi_{k-1/2})/\Delta_k + 3(\sigma_{10} - \sigma_{01}) (\phi_{k+1/2} + \phi_{k-1/2})/4 \right] \quad (7.4.2b)$$

Adding equation 7.4.2a for two adjacent cells yields,

$$\begin{aligned} J_{k+3/2} - J_{k-1/2} + \sigma_a (\phi_{k+3/2} + \phi_{k+1/2}) \Delta_{k+1}/2 & \quad (7.4.3a) \\ + \sigma_a (\phi_{k+1/2} + \phi_{k-1/2}) \Delta_k/2 \\ = q_{k+1} \Delta_{k+1} + q_k \Delta_k \quad . \end{aligned}$$

Subtracting equation 7.4.2b for two adjacent cells gives

$$\begin{aligned}
 (J_{k+3/2} - J_{k-1/2})/2 = & -D \left[(\phi_{k+3/2} - \phi_{k+1/2}) \Delta_{k+1} \right. & (7.4.3b) \\
 & + 3(\sigma_{10} - \sigma_{01}) (\phi_{k+3/2} + \phi_{k+1/2})/4 \left. \right] \\
 & + D \left[(\phi_{k+1/2} - \phi_{k-1/2}) \Delta_k + 3(\sigma_{10} - \sigma_{01}) \right. \\
 & \left. (\phi_{k+1/2} + \phi_{k-1/2})/4 \right] .
 \end{aligned}$$

Eliminating the current from equations 7.4.3a and 7.4.3b yields the desired equation,

$$\begin{aligned}
 & -D \left[(\phi_{k+3/2} - \phi_{k+1/2})/\Delta_{k+1} + 3(\sigma_{10} - \sigma_{01}) (\phi_{k+3/2} + \phi_{k+1/2})/4 \right] \\
 & + D \left[(\phi_{k+1/2} - \phi_{k-1/2})/\Delta_k + 3(\sigma_{10} - \sigma_{01}) (\phi_{k+1/2} + \phi_{k-1/2})/4 \right] \\
 & + \left[\sigma_a (\phi_{k+3/2} + \phi_{k+1/2}) \Delta_{k+1}/2 + \sigma_a (\phi_{k+1/2} + \phi_{k-1/2}) \Delta_k/2 \right] / 2 \\
 = & (q_{k+1} \Delta_{k+1} + q_k \Delta_k) / 2 . & (7.4.4)
 \end{aligned}$$

The derivation of the boundary mesh cell equations is somewhat more complicated. We first consider the left boundary cell and begin by assuming a vacuum boundary. As shown in Figure 6, the scalar flux linearly extrapolates to zero at a distance d_e (called the linear extrapolation distance) from a vacuum boundary. The interior mesh cell equation (equation 7.4.4) represents a particle balance equation averaged over two adjacent cells. In order to utilize this equation in the derivation, we assume the existence of a "ghost" cell bounded by z_b and $z_{1/2}$ as shown in Figure 6. Equation 7.4.4 takes the following form for the ghost and boundary cells,

$$\begin{aligned}
 & (7.4.5) \\
 & -D \left[(\phi_{3/2} - \phi_{1/2}) / \Delta_1 + 3(\sigma_{10} - \sigma_{01}) (\phi_{1/2} + \phi_{3/2}) / 4 \right] \\
 & + D \left[\phi_{1/2} / d_e + 3(\sigma_{10} - \sigma_{01}) \phi_{1/2} / 4 \right] + \sigma_a (\phi_{1/2} + \phi_{3/2}) \Delta_1 / 4 \\
 & = q_1 \Delta_1 / 4 .
 \end{aligned}$$

An explicit expression for the extrapolation distance can be obtained from the standard Marshak vacuum boundary condition,

Figure 6. Left Mesh Cell Geometry.

$$2\pi \int_0^1 \left[\frac{1}{4\pi} \phi(z_{1/2}) + \frac{3}{4\pi} J(z_{1/2}) \mu \right] \mu d\mu = 0 \quad . \quad (7.4.6)$$

Substituting from equation 7.2.4a into equation 7.4.6 and integrating gives

(7.4.7)

$$\frac{1}{4} \phi(z_{1/2}) - \frac{1}{2} D \left[\frac{d}{dz} \phi(z_{1/2}) + \frac{3}{2} (\sigma_{10} - \sigma_{01}) \phi(z_{1/2}) \right] = 0.$$

With further manipulation, we obtain

$$\phi(z_{1/2}) = 2 D \frac{d}{dz} \phi(z_{1/2}) / \left[1 + 3(\sigma_{10} - \sigma_{01}) \right] \quad . \quad (7.4.8)$$

From Figure 6, it is clear that

$$d_e = \phi(z_{1/2}) / \frac{d}{dz} \phi(z_{1/2}) \quad . \quad (7.4.9)$$

Thus combining equations 7.4.8 and 7.4.9, we find that

$$d_e = 2D/[1 + 3(\sigma_{10} - \sigma_{01})]. \quad (7.4.10)$$

Finally, the desired boundary mesh cell equation is obtained by substituting from expression 7.4.10 into equation 7.4.5,

$$\begin{aligned} & -D \left[(\phi_{3/2} - \phi_{1/2})/\Delta_1 + 3(\sigma_{10} - \sigma_{01})(\phi_{1/2} + \phi_{3/2})/4 \right] \\ & + \left[1 + 3(\sigma_{10} - \sigma_{01}) \right] \phi_{1/2}/2 + 3D(\sigma_{10} - \sigma_{01})\phi_{1/2}/4 \\ & + \sigma_a(\phi_{1/2} + \phi_{3/2})\Delta_1/4 = q_1\Delta_1/4 \quad . \end{aligned} \quad (7.4.11)$$

Following an analogous procedure for the right cell bounded by $z_{K-1/2}$ and $z_{K+1/2}$ gives,

$$\begin{aligned} & \left[1 + 3(\sigma_{10} - \sigma_{01}) \right] \phi_{K+1/2}/2 - 3D(\sigma_{10} - \sigma_{01})\phi_{K+1/2}/4 \\ & + D \left[(\phi_{K+1/2} - \phi_{K-1/2})/\Delta_K + 3(\sigma_{10} - \sigma_{01})(\phi_{K+1/2} + \phi_{K-1/2})/4 \right] \\ & + \sigma_a(\phi_{K-1/2} + \phi_{K+1/2})\Delta_K/4 = q_K\Delta_K/4 \quad . \end{aligned} \quad (7.4.12)$$

Unlike Alcouffe (1977), we have chosen to employ source correction factors to compensate both for the inadequacy of Fick's law and for the use of step-differencing for negative flux fixup. Alcouffe uses non-linear correction terms to compensate for step-differencing. Because all of our correction factors are linear, our method constitutes a classical synthetic acceleration method. Thus all of the analysis presented in Chapter 5 pertaining to such methods is rigorously applicable.

The source correction factors corresponding to equations 7.4.4, 7.4.11, and 7.2.12, respectively, are

(7.4.13)

$$\begin{aligned} \tilde{C}_k = & (\tilde{J}_{k+3/2} - \tilde{J}_{k-1/2})/2 - \left\{ -D \left[(\tilde{\phi}_{k+3/2} - \tilde{\phi}_{k+1/2})/\Delta_{k+1} \right. \right. \\ & + 3(\sigma_{10} - \sigma_{01})(\tilde{\phi}_{k+3/2} + \tilde{\phi}_{k+1/2})/4 \left. \right] + D \left[(\tilde{\phi}_{k+1/2} - \tilde{\phi}_{k-1/2})/\Delta_k \right. \\ & \left. \left. + 3(\sigma_{10} - \sigma_{01})(\tilde{\phi}_{k+1/2} + \tilde{\phi}_{k-1/2})/4 \right] \right\} + (\sigma_a \tilde{\phi}_{k+1} \Delta_{k+1} + \sigma_a \tilde{\phi}_k \Delta_k)/2 \\ & - \left[\sigma_a (\tilde{\phi}_{k+3/2} + \tilde{\phi}_{k+1/2}) \Delta_{k+1}/2 + \sigma_a (\tilde{\phi}_{k+1/2} + \tilde{\phi}_{k-1/2}) \Delta_k/2 \right] / 2 , \end{aligned}$$

$$\begin{aligned}
\tilde{C}_k &= (\tilde{J}_{3/2} - \tilde{J}_{1/2})/2 - \left\{ -D \left[(\tilde{\phi}_{3/2} - \tilde{\phi}_{1/2})/\Delta_1 \right. \right. \\
&\quad \left. \left. + 3(\sigma_{10} - \sigma_{01})(\tilde{\phi}_{1/2} + \tilde{\phi}_{3/2})/4 \right] \right. \\
&\quad \left. + \left[(1/2 + 3(\sigma_{10} - \sigma_{01})/2) \tilde{\phi}_{1/2} + D 3(\sigma_{10} - \sigma_{01})\tilde{\phi}_{1/2}/4 \right] \right\} \\
&\quad + \sigma_a \tilde{\phi}_1 \Delta_1/2 - \left[\sigma_a (\tilde{\phi}_{1/2} + \tilde{\phi}_{3/2}) \Delta_1/2 \right] / 2
\end{aligned} \tag{7.4.14}$$

and

$$\begin{aligned}
\tilde{C}_K &= (\tilde{J}_{K+1/2} - \tilde{J}_{K-1/2}) - \left\{ \left[(1/2 + 3(\sigma_{10} - \sigma_{01})/2) \tilde{\phi}_{K+1/2} \right. \right. \\
&\quad \left. \left. - 3D(\sigma_{10} - \sigma_{01})\tilde{\phi}_{K+1/2}/4 \right] \right. \\
&\quad \left. + D \left[(\tilde{\phi}_{K+1/2} - \tilde{\phi}_{K-1/2}) \Delta_K + 3(\sigma_{10} - \sigma_{01})(\phi_{K+1/2} + \phi_{K-1/2})/4 \right] \right\} \\
&\quad + \sigma_a \tilde{\phi}_K \Delta_K/2 - \left[\sigma_a (\tilde{\phi}_{K+1/2} + \tilde{\phi}_{K-1/2}) \Delta_K/2 \right] / 2 .
\end{aligned} \tag{7.4.15}$$

As one would expect, the correction factor for the interior mesh cell equation causes that equation to go over to the scalar balance equation averaged over the cells k and $k + 1$. Similarly, all the boundary equation correction factors cause those equations to go over to the scalar balance equation for each respective boundary cell. Thus, although the boundary cell equations were derived under the assumption of vacuum boundary conditions, they are valid regardless of the actual boundary conditions imposed upon the collocation solution.

The accelerated iterative algorithm is identical to that given by equation 5.5.11 but with L , T , and C representing the differenced asymmetric collocation equation, the differenced asymmetric diffusion equation, and the differenced asymmetric diffusion equation correction factors, respectively. Under the assumptions of symmetric scattering and pure diamond differencing, our method becomes equivalent to Alcouffe's method. As previously noted, Alcouffe's technique is directly applicable to the symmetric collocation equation. However, for the sake of consistency, we use our method to accelerate the convergence of both symmetric and asymmetric collocation solutions.

CHAPTER 8

COMPUTATIONAL RESULTS

8.1 Introduction

In this chapter, we present computational results which are primarily intended to demonstrate the validity and versatility of our collocation method. Some of the calculations also relate to a determination of the accuracy of the asymmetric diffusion equation and the effect of odd-asymmetric scattering on the asymptotic behavior of the transport solution.

All of the collocation calculations presented in this chapter were performed with a computer code written by the author. This code utilizes the standard S_n spatial treatment given by equations 5.4.3 and 5.4.4. The iterative convergence of all of the collocation solutions was accelerated using the diffusion-synthetic algorithm described in Chapter 7.

For purposes of comparison, standard discrete-ordinates and Monte Carlo calculations were also performed. The Monte Carlo calculations were performed with a code written by the author and are considered exact to within statistical error. The discrete ordinates calculations were carried out with DTF69 (Renken, 1969), a version of the DTF code

which has a first-scattered distributed source option for normal-incidence calculations.

Under this approach, no attempt is made to represent normally-incident fluxes by means of the discrete-ordinates approximation. Instead, the unscattered flux component, which is also the normal component, is analytically represented and the discrete-ordinates method is used only to solve for the scattered flux component. The use of this method is often desirable in S_n calculations because standard quadrature sets of moderate order are generally inadequate for representing normally incident fluxes.

8.2 Basis Sets

Four distinct basis sets, denoted by B1, B2, B3, and B4, respectively, are employed in the collocation calculations. The angular flux representations corresponding to each basis set are shown in Figs. 7, 8, 9, and 10, respectively. It should be noted that all of the basis sets are constructed with independent interpolations on $[-1,0]$ and $[0,+1]$. This is done so that vacuum boundary conditions can be met exactly. In addition, all of the sets satisfy the requirement set down in Chapter 6 of having an even number of collocation points symmetrically arranged about $\mu = 0$.

A rather unique feature of these sets is the use of two independent collocation points at $\mu = 0$. The use of such collocation points corresponds to the use of

Figure 7. Basis Set B1 Angular Flux Representation. Independent cubic interpolations are made on $[-1,0]$ and $[0,+1]$.

Figure 8. Basis Set B2 Angular Flux Representation. Independent piecewise-linear interpolations are made on $[-1,0]$ and $[0,+1]$.

Figure 9. Basis Set B3 Angular Flux Representation. Independent linear interpolations are made on $[-1, -0.99]$ and $[+0.99, +1]$. Independent cubic interpolations are made on $[-0.99, 0]$ and $[0, +0.99]$.

Figure 10. Basis Set B4 Angular Flux Representation. Independent piecewise-linear interpolations are made on $[-1,0]$ and $[0,+1]$.

quadrature points at $\mu = 0$ in the S_n method. The standard Gauss and double-Gauss quadrature sets never have quadrature points at $\mu = 0$. However, non-standard quadrature formulae can be constructed which do. For instance, the quadrature points of an eight-point double-Newton-Coates formula (Hildebrand, 1974) are identical to the collocation points in sets B1 and B2. Nonetheless, to our knowledge, S_n calculations with quadrature points at $\mu = 0$ have never appeared in the literature. The primary reason for this is that the S_n equations are coded in standard discrete-ordinates computer codes in such a way that they become singular if the quadrature formula has a point at $\mu = 0$. It is not clear as to why the equations are written in this way as the S_n equations can be written in non-singular form. For instance, the discretized S_n equations given in Chapter 5 (equations 5.4.3 and 5.4.4) are non-singular. This situation has never been rectified apparently because it was decided some time ago by B. G. Carlson and his co-workers at Los Alamos Scientific Laboratory that quadrature sets with points at $\mu = 0$ were undesirable because of their low accuracy, relative to that of standard sets, for integrating Legendre polynomials (Miller, 1979). In the S_n method, this is an important consideration because the degree of anisotropic scattering is limited by the quadrature accuracy. However, this is not a

consideration in the collocation method because of the manner in which the scattering sources are calculated.

Basis sets B3 and B4 have collocation points at $\mu = -0.99$ and $\mu = +0.99$ in order to allow normally incident fluxes to be represented accurately. It is important to note that set B3 is constructed with a special combination of cubic and linear interpolation. This is done in order to achieve stability as it is found that simple quartic interpolation resulted in an extremely oscillatory and unstable angular flux representation.

Sets B2 and B4 are constructed with piecewise-linear interpolation in such a way that each of their respective basis functions is positive. As pointed out in Chapter 7, such sets preserve the positivity of the transport operator.

It is important to note that the collocation points for all basis sets are indexed in ascending order. For instance, for set B1, $\mu_1 = -1$, $\mu_2 = -2/3$, . . ., etc.

8.3 Symmetric Scattering Calculations

Calculations for a total of five distinct transport problems with symmetric scattering have been performed. The following characteristics are common to all of the problems:

- (a) flux incident at left face of slab,

(b) vacuum boundaries at both faces,

(c) $\sigma_a = 0.1 \text{ cm}^{-1}$, $\sigma_s = 0.9 \text{ cm}^{-1}$,

(d) slab thickness = 10.0 cm.

The problems differ in the level of scattering anisotropy and the type of flux incidence. All calculations with anisotropic scattering employ a cross section which can be expressed as

$$\sigma_s(\mu_o) = \frac{\sigma}{2\pi} f(\mu_o) , \quad (8.3.1a)$$

where

$$f(\mu_o) = \frac{2\eta(\eta + 1)}{(1 + 2\eta - \mu_o)^2} . \quad (8.3.1b)$$

The function $f(\mu_o)$ is a normalized distribution function in μ_o which becomes increasingly forward-peaked as the parameter η is decreased. By normalized, we mean that

$$\int_{-1}^{+1} f(\mu_o) d\mu_o = 1 \quad (8.3.2)$$

for all values of η . Taking this property into account, it is easily seen that the total scattering cross section is

$$2\pi \int_{-1}^{+1} \sigma_s(\mu_0) d\mu_0 = \sigma \quad (8.3.3)$$

Thus the magnitude of the cross section is determined by σ while its anisotropy (shape) is determined by η . To illustrate the anisotropic dependence, $f(\mu_0)$ is plotted in Figs. 11, 12, and 13 for $\eta = 1.0$, $\eta = 0.1$, and $\eta = 0.001$, respectively. The scattering kernel corresponding to $\sigma_s(\mu_0)$ is given by

$$\sigma(\mu' \rightarrow \mu) = \quad (8.3.4)$$

$$\frac{\eta(\eta + 2)(1 + \eta - \mu'\mu)}{4\pi \left[(1 + \eta - \mu'\mu)^2 - (1 - \mu'^2)(1 - \mu^2) \right]^{3/2}}.$$

The remaining characteristics of each of the five problems are given in Table 1. Collocation calculations were performed for problems 1, 2, and 3 using sets B1 and B2, while sets B1, B3 and B4 were used for problems 4 and 5. Similar S_n calculations were performed using a double- S_8 Gauss quadrature set for all problems in conjunction with P_7 Legendre cross-section expansions in the problems with anisotropic scattering. It should be noted that this is the maximum permissible expansion degree for use with a double- S_8 Gauss quadrature set. Particle conservation cannot be guaranteed with expansions of higher degree. Identical spatial meshes having 50 intervals each were

Figure 11. Scattering Probability Distribution Function for $\eta = 1.0$.

Figure 12. Scattering Probability Distribution Function for $\eta = 0.1$.

Figure 13. Scattering Probability Distribution
Function for $\eta = 0.001$.

TABLE 1
Characteristics of Problems 1 Through 5

<u>Calculation</u>	<u>Flux Incidence</u>	<u>Scattering</u>
1	Isotropic	Isotropic
2	Isotropic	$\eta = 1.0$
3	Isotropic	$\eta = 0.1$
4	Normal	$\eta = 1.0$
5	Normal	$\eta = 0.001$

used in both the S_n and collocation calculations. All of the S_n and collocation solutions presented are fully converged with respect to the spatial mesh. That is to say that further refinement of the mesh changes the solution by less than a percent.

We were motivated to use a double S_8 Gauss quadrature set in the S_n calculations for several reasons. For the isotropic scattering case, the S_n calculation is equivalent to an eight-point double-Gauss collocation calculation. The basis sets for such a calculation would be constructed using independent cubic interpolations on $[-1,0]$ and $[0,+1]$ with collocation points at the double-Gauss quadrature points. Note that the trial space spanned by these basis functions is identical to that spanned by the B1 set. Furthermore, the analysis presented in Chapter 7 shows that the double-Gauss collocation solution with isotropic scattering is Galerkin-equivalent. Thus we see that in the isotropic scattering case, the S_n solution represents a standard S_n solution, a collocation solution utilizing a projection onto the B1 trial space (but having different collocation points than the B1 projection), and the Galerkin solution for the B1 trial space.

It is also significant to note that in the isotropic scattering case, the B1 and B2 calculations are equivalent to S_n calculations using double S_8 Newton-Coates and

double- S_8 composite trapezoidal rule quadrature sets, respectively. Thus, in the isotropic scattering case, the B1 and B2 collocation solutions also represent some rather unique (because of the quadrature points at $\mu = 0$) S_n solutions. Despite all the various collocation- S_n equivalences which arise in the isotropic scattering calculations, there are no equivalences in the anisotropic calculations.

Scalar flux comparisons for problem 1 are plotted in Fig. 14. The B1 and S_n solutions are in excellent agreement with the Monte Carlo solutions. However, the B2 solution is clearly the least accurate. It shows good agreement near the left face of the slab, but becomes increasingly inaccurate as the right face is approached. A maximum error of approximately 15 percent is attained. This is not too surprising as a piecewise-linear flux representation cannot be expected to be as accurate as a cubic representation.

Scalar flux comparisons for problem 2 are plotted in Fig. 15. In addition, the scattering source normalization factors for sets B1 and B2 are given in Table 2. The B1 and S_n solutions are again in excellent agreement with the Monte Carlo solution, and the B2 solution shows error similar to that of problem 1. The normalization factors are very

Figure 14. Flux Solution Comparisons for Problem 1.
 The Monte Carlo data are subject to a relative standard
 deviation of less than three percent.

Figure 15. Flux Solution Comparisons for Problem 2.
The Monte Carlo data are subject to a relative standard deviation of less than two percent.

TABLE 2

Scattering Source Normalization Factors for Problem 2

Normalization Factors

	γ_1	γ_2	γ_3	γ_4	γ_5	γ_6	γ_7	γ_8
Set B1	0.99990	1.0001	0.99997	0.99994	0.99994	0.99997	1.0001	0.99990
Set B2	0.99517	0.99914	1.0020	1.0027	1.0027	1.0020	0.99914	0.99517

near unity for both sets. This is not surprising since the scattering anisotropy in problem 2 is fairly mild.

Scalar flux comparisons for problem 3 are plotted in Fig. 16, and the normalization factors for sets B1 and B2 are given in Table 3. The S_n and B1 solutions show the same level of accuracy obtained in problems 1 and 2. However, the B2 solution is considerably more accurate. The maximum error is approximately 5 percent. The normalization factors for both the B1 and B2 sets show an increased departure from unity. This is a direct consequence of the increased scattering anisotropy. The departure of the B2 factors is clearly greater than that of the B1 factors. This is a reflection of the fact that the B1 basis gives a better scattering source representation than the B2 basis. Since the B3 scattering source is less accurate in problem 3 than in problems 1 and 2, one might be tempted to conclude that the flux solution should also be less accurate in problem 3. However, it must be remembered that there are other sources of error in the calculations. In problem 1, the scattering source is exact and only the leakage term contributes to the collocation residual. In problems 2 and 3, both the leakage and scattering source terms contribute. It is apparently the leakage term error (or equivalently, the current representation error) which dominates in all of the calculations. The

Figure 16. Flux Solution Comparisons for Problem 3.
The Monte Carlo data are subject to a relative standard deviation of less than two percent.

TABLE 3
Scattering Source Normalization Factors for Problem 3

Normalization Factors								
	γ_1	γ_2	γ_3	γ_4	γ_5	γ_6	γ_7	γ_8
Set B1	0.99141	1.0094	0.98878	1.0149	1.0149	0.98878	1.0094	0.99141
Set B2	0.93842	1.0202	1.0099	1.0063	1.0063	1.0099	1.0202	0.93842

angular flux solution is more anisotropic in problem 3 than in problems 1 and 2. The increased accuracy of the B2 solution in problem 3, therefore, indicates that the error in the current representation is less severe for the highly forward-peaked solution of problem 3 than it is for the moderately forward-peaked solutions of problems 1 and 2.

Collocation calculations were carried out for problem 4 using sets B1 and B3. The B1 calculation was performed using the first-scattered distributed source technique while the normally-incident flux was directly represented in the B3 calculation. Scalar flux comparisons for problem 4 are plotted in Fig. 17. It can be seen that the B1 and B3 calculations are in excellent agreement both with each other and with the Monte Carlo calculations. This clearly demonstrates the capability of the B3 set for representing normally-incident fluxes. Although S_n quadrature sets can be similarly designed to represent such fluxes, these sets are generally not suitable for problems such as problem 4 because they often cannot perform the anisotropic inscatter integral with sufficient accuracy. For instance, the companion quadrature set corresponding to set B3 can only be used in S_n calculations with Legendre expansions of degree 1 or less. The use of higher expansion orders will result in a lack of particle conservation.

Figure 17. Flux Solution Comparisons for Problem 4. FSDS refers to the calculation made using the first-scattered distributed source method. The Monte Carlo data are subject to a relative standard deviation of less than two percent.

Scalar flux comparisons for problem 5 are plotted in Fig. 18. The normalization factors for the B4 set are given in Table 4. The S_n calculation was performed using the first-scattered distributed source technique, but the normally incident flux was directly represented in the B4 calculation. The S_n solution fails catastrophically due to severe truncation error in the Legendre expansion for the first-scattered source. This is, of course, a direct reflection of the severe anisotropy of the scattering cross section. The severe departure from unity of two of the B4 normalization factors clearly indicates that the collocation representation for the scattering source is also inadequate. Nonetheless, the B4 representation is a positive one which yields a more accurate solution than the S_n method. Comparison with the Monte Carlo solution shows a maximum error of approximately 6 percent. It is important to realize that this problem is particularly insensitive to the substantial error which exists in the collocation scattering source. Similarly accurate flux solutions cannot always be expected when the normalization factors similarly depart from unity. However, positive basis sets can always be expected to produce physically reasonable solutions regardless of the behavior of the scattering kernel.

Figure 18. Flux Solution Comparisons for Problem 5. The Monte Carlo data are subject to a relative standard deviation of less than one percent.

TABLE 4
Scattering Source Normalization Factors for Problem 5

Normalization Factors									
γ_1	γ_2	γ_3	γ_4	γ_5	γ_6	γ_7	γ_8	γ_9	γ_{10}
0.17369	1.0625	1.0356	1.0063	1.0036	1.0036	1.0063	1.0356	1.0625	0.17369

As previously noted, the collocation calculations presented in this section were performed using the diffusion-synthetic acceleration method described in Chapter 7. The method is quite effective. For instance, the collocation calculation performed with the B1 basis set for problem 1 required 56 iterations to converge without acceleration and 6 iterations to converge with it. No attempt was made to determine the unaccelerated convergence rates for the other calculations, but the accelerated rates obtained appear to be roughly equivalent to those obtained by Alcouffe (1977) and Miller (1978) in S_n calculations. Exact comparisons with their results are impossible. However, we are confident that the diffusion-synthetic algorithm is as effective in accelerating the convergence of collocation solutions as it is in accelerating the convergence of S_n solutions.

8.4 Asymmetric Scattering Calculations

Calculations have been performed for a total of 5 problems with asymmetric scattering. In order to demonstrate the asymmetric collocation method and determine the accuracy of the asymmetric diffusion equation, collocation and Monte Carlo calculations have been made which are analogous to the diffusion calculations presented in Chapter 4. For the sake of completeness, we repeat the characteristics of the problems here. The common characteristics are:

- (a) isotropically-incident at the left face of the slab,
- (b) vacuum boundaries at both slab faces,
- (c) scattering described by the asymmetric-isotropic scattering kernel given in equation 7.3.1c,
- (d) $\sigma_a = 0.0$, $\sigma_s = 1.0 \text{ cm}^{-1}$,
- (e) slab thickness = 100.0 cm.

The problems differ only in that each corresponds to a different value of the parameter β appearing in the scattering kernel. Specifically, problems 1 through 5 correspond to the values $\beta = 1/3$, $1/30$, 0 , $-1/30$, and $\beta = -1/3$, respectively. As noted in Chapter 7, $\beta = 0$ actually corresponds to symmetric-isotropic scattering. Thus, the $\beta = 0$ solution serves as a standard against which the effects of odd-asymmetric scattering can be gauged.

All of the collocation calculations were performed using the B1 basis set and a spatial mesh having 100 intervals of uniform width. Because the scattering is isotropic, scattering source normalization factors are not necessary. However, cross-section normalization factors are necessary for all but the $\beta = 0$ case and are given in Table 5. The Monte Carlo, collocation and

TABLE 5

Cross-Section Normalization Factors for Problems 6 Through 10.

Normalization Factors

β	γ_1	γ_2	γ_3	γ_4	γ_5	γ_6	γ_7	γ_8
1/3	∞	0.61176	1.1970	0.86800	1.1320	0.90075	1.0795	0.93367
1/30	1.0148	0.98571	1.0138	0.95677	1.0133	0.98710	1.0125	0.98788
-1/30	0.98788	1.0125	0.98710	1.0133	0.98667	1.0138	0.98571	1.0148
-1/3	0.93367	1.0795	0.90075	1.1320	0.86800	1.1970	0.61176	∞

The infinite values for $\beta = 1/3$ and $\beta = -1/3$ are obtained because the corresponding point cross-section values are zero. The average cross-section values are .142 in both cases.

diffusion solutions for problems 6 through 10 are plotted in Figures 19 through 23, respectively.

The diffusion and collocation solutions are virtually indistinguishable for $\beta = 1/30$ and $\beta = 0$ and are nearly identical for $\beta = 1/3$ and $\beta = -1/30$. Both the collocation and the diffusion solutions show excellent agreement with the Monte Carlo solutions for $\beta = 1/3$, $1/30$, 0 , and $\beta = -1/30$. However, for $\beta = -1/3$, the collocation and diffusion solutions are in serious disagreement both with each other and with the Monte Carlo solution. As one would expect, the collocation solution is substantially more accurate than the diffusion solution, but the collocation solution is nonetheless inadequate. It is approximately 30 percent in error at all points.

As discussed in Chapter 7, the negative ($\beta < 0$) asymmetry in this problem tends to redistribute the particles into directions near $\mu = +1$. Thus, as particles enter the slab and begin to scatter, the angular flux starts to become forward-peaked. This process reinforces itself because the scattering particles tend to redistribute into directions which take them deeper into the slab where they continue to scatter and redistribute. Because of this reinforcement, a highly forward-peaked angular flux solution results, and this is the source of difficulty in the

Figure 19. Flux Solution Comparisons for Problem 6. The Monte Carlo data are subject to a relative standard deviation which increases from approximately one percent at $z = 0.5$ to approximately ten percent at $z = 9.5$.

Figure 20. Flux Solution Comparisons for Problem 7. The Monte Carlo data are subject to a relative standard deviation which increases from approximately one percent at $z = 0.5$ to approximately ten percent at $z = 34.5$.

Figure 21. Flux Solution Comparisons for Problem 8. The Monte Carlo data are subject to a relative standard deviation which increases from approximately one percent at $z = 0.5$ to approximately twelve percent at $z = 95.5$.

Figure 22. Flux Solution Comparisons for Problem 9. The Monte Carlo data are subject to a relative standard deviation of less than four percent.

Figure 23. Flux Solution Comparisons for Problem 10. The Monte Carlo data are subject to a relative standard deviation of less than two percent.

calculations. The diffusion and collocation trial spaces are simply inadequate for representing this forward-peaked solution.

Because the asymmetry for $\beta = 1/3$ is equal in magnitude but opposite in direction to that for $\beta = -1/3$, one might be tempted to conclude that the flux solution for $\beta = 1/3$ should be highly peaked in the backward direction. However, it is interesting to note that the redistribution process is not reinforcing in this case. As particles enter the slab and begin to scatter, the particles begin to redistribute into the backward directions but then escape before significant additional redistribution can take place. As a result, the angular flux never gets very peaked and commensurately accurate diffusion and collocation solutions are obtained.

The next matter which we wish to address concerns the effect of odd-asymmetric scattering on the asymptotic behavior of the transport solution. In particular, we are interested in its effect upon the asymptotic reflected fraction for particles isotropically incident upon a non-absorptive slab. As discussed in Chapter 7, the diffusion solution given by expression 7.3.17 indicates that the fraction is less than unity whenever $\beta < 0$. In Table 6, we compare the reflected fractions given by expression 7.3.17 for $\beta = -1/30$ and $\beta = -1/3$ with the reflected fractions

TABLE 6

Comparison of Asymptotic Reflected Fractions

Diffusion Collocation Monte Carlo

$= -1/30$	0.875	.875	$0.878 \pm 0.4\%$
$= 1/3$	0.200	.202	$0.213 \pm 1.9\%$

given by the collocation and Monte Carlo calculations for problems 9 and 10. Although these fractions for these problems are not strictly equal to asymptotic fractions, the slab is sufficiently thick that the difference between these and the true asymptotic fractions is negligible (this is suggested by the diffusion solution plots given in Figure 6 and was verified with supplementary collocation and Monte Carlo calculations). The comparison shows that the asymptotic reflected fractions are indeed less than unity when $\beta < 0$, and further that the diffusion and collocation values for $\beta = -1/3$ are very accurate even though their respective flux solutions are quite inaccurate.

The final topic of discussion concerns our asymmetric diffusion-synthetic acceleration algorithm. The algorithm was absolutely essential in all of the asymmetric scattering calculations. Convergence could not be obtained within 1000 iterations without it (we did not attempt more than 1000 iterations). This is not surprising since it is well known that S_n calculations for non-absorptive media are extremely difficult to converge. The accelerated convergence rates were similar to those obtained in the symmetric scattering calculations. For instance, the solutions for $\beta = 1/30$, 0 , and $\beta = -1/30$ converged to within a relative error criterion on the angular flux of 0.001 within 6

iterations. The solutions for $\beta = 1/3$ and $-1/3$ converged to within the same error criterion within 12 iterations. The algorithm apparently becomes less effective as the asymmetry is increased. This seems reasonable since the effectiveness of the standard synthetic acceleration method is known to decrease in S_n calculations as the anisotropy of the scattering is increased (Alcouffe, 1978).

CHAPTER 9

CONCLUSIONS AND RECOMMENDATIONS

9.1 Introduction

In this chapter we draw conclusions from our results and make recommendations for future work. We first consider the collocation method for symmetric scattering and then the collocation method for asymmetric scattering. Next, we discuss some of the implications of the equivalence under the diffusion approximation of odd-asymmetric scattering and an electric field. Finally, we give several specific applications for which the collocation methods appear to be particularly suited.

9.2 The Collocation Method for Symmetric Scattering

The collocation method for symmetric scattering has been shown to possess some of the best characteristics of both the finite-element and S_n methods. The collocation approach offers the flexibility and continuous angular flux representation of the finite-element method while having equations as amenable to efficient iterative solution as the S_n equations. For this reason, we conclude that our collocation method is a valuable alternative to these methods.

Although we have explicitly developed a method only for one-dimensional slab geometry calculations, our method easily extends to other geometries and multiple dimensions. Under this extension, the similarity in structure between the collocation and S_n equations is maintained in all but one respect. In curvilinear coordinates, the collocation method will generally give rise to an implicit representation for the streaming term rather than the explicit representation characteristic of the S_n method (Bell and Glasstone, 1970). This means that the collocation equations may require more iterations than the S_n equations. However, there is also reason to believe that the collocation representation may be more accurate. Thus we feel that the relative merits of the collocation and S_n streaming term representations should be investigated.

Because the two- and three-dimensional S_n representations for the term $\nabla \cdot \vec{\Omega}\phi$ do not preserve its rotational invariance, non-physical oscillations in the angular flux solution are observed in regions with little scattering and no sources. This is known as the ray effect and represents the most serious deficiency of the S_n method. Special quadrature sets known as directed quadrature sets can be used to reduce the severity of the effect in certain problems. Unfortunately, such sets are generally less accurate for integrating the spherical harmonics functions than

standard sets. As a result, they can usually only be employed in problems with weakly anisotropic scattering.

Multi-dimensional collocation solutions will also suffer from the ray effect. However, the versatility of the method should allow for reduction of the effect in a much larger class of problems than is possible under the standard S_n approach. This is why we strongly recommend that the collocation approach be employed in multi-dimensional calculations.

9.3 The Collocation Method for Asymmetric Scattering

We have shown that our collocation method for performing calculations with asymmetric scattering is a viable one. In the process of doing so, it has been observed that scattering asymmetry can have drastic and sometimes unexpected effects upon the transport solution. Further investigations into the effects of asymmetric scattering are clearly necessary. It would be particularly valuable to determine which types of scattering asymmetry are of most importance in practical problems.

It has been shown that the collocation and S_n approaches markedly differ with respect to cross-section processing and storage requirements. When the scattering asymmetry is strong, the collocation approach is superior. When it is weak, the two methods are comparable. In

multi-dimensional multi-group calculations, cross-section processing and storage requirements will undoubtedly be the dominant factor in choosing a method. Many calculations will simply be beyond the scope of modern computers. The seriousness of this problem is compounded by the fact that most asymmetric scattering problems of practical interest are at least two-dimensional. Thus, we feel that in developing a multi-dimensional asymmetric collocation method, primary concern should be given to the minimization of cross-section processing and storage requirements.

9.4 Odd-Asymmetric Scattering and Electric Fields

It has been shown that an equivalence exists between odd-asymmetric scattering and electric fields under the diffusion approximation. We feel certain that some type of equivalence also exists within the collocation approximation between asymmetric scattering and force fields of all types. It is strongly recommended that this matter be investigated as it may be found that methods used to treat asymmetric scattering apply equally well to the treatment of fields. This would clearly be a very exciting and useful result.

9.5 Specific Applications

In this section, we discuss a few of the applications for which our collocation methods are particularly suited.

The discussion is not intended to be comprehensive; it is simply intended to demonstrate that our methods are useful for real as well as idealized problems.

A new method for calculating the scattering sources in S_n calculations has been recently developed by Odom and Shultis (1976) for problems with highly anisotropic scattering. This method is characterized by the use of exact scattering kernel values at the quadrature points rather than Legendre expansions, and it always produces a positive angular flux solution. They have applied their technique to the problem of neutron transport in hydrogenous media (an applied problem of fundamental interest) and have obtained results clearly superior to those of the standard S_n method. Beranek and Conn (1979) have shown that this method also yields superior results in neutronics calculations for inertial confinement fusion blanket design. Our symmetric collocation method in conjunction with positive basis sets has all of the advantages of the Odom-Shultis technique in addition to several others (the most important being that our method is strictly conservative). Thus, there are definite applications for our collocation method in these same areas.

Morel (1979) has shown that standard S_n codes can be used to perform charged-particle transport calculations.

Proper treatment of the inelastic component of charged-particle scattering cross sections requires that Gauss quadrature formulae be used in one-dimensional slab and spherical geometries. Calculations cannot be performed for problems requiring a two-dimensional representation in direction (this includes all spatially multi-dimensional geometries as well as one-dimensional cylindrical geometry) because there are no two-dimensional quadrature formulae sufficiently accurate to treat the inelastic scattering cross section. These two-dimensional difficulties can be completely eliminated by using a collocation treatment for the scattering source in conjunction with spherical harmonic trial spaces. Due to both the special characteristics of such spaces and the fact that the collocation treatment need only be applied to the scattering source (a hybrid S_n -collocation technique results), the modifications required to implement this scheme in S_n codes are almost negligible. This is an important application for the collocation approach because its implementation would allow the immense computational capability developed for neutron transport problems over the last two decades to be directly applied to charged particle transport problems. The interest in charged-particle transport problems has markedly increased in recent years due to their significance in controlled fusion research.

As briefly mentioned in Chapter 1, the most obvious applications for the asymmetric collocation method relate to particle transport in anisotropic plasmas. The transport of neutral hydrogen atoms in Tokamak fusion devices is important because the interactions of these atoms with the plasma tend to cool it. The scattering cross sections for these atoms are asymmetric in the laboratory frame. Cross-section generation codes have been written (Morel and Wienke, 1977) to allow neutral hydrogen transport calculations to be performed with standard S_n codes, but scattering asymmetry has been neglected because there are currently no codes which can treat it.

The plasmas formed in laser-driven inertial-confinement fusion research are extremely anisotropic due to their rapid radial expansion. The energy deposition of energetic (suprathermal) electrons in such plasmas plays an important role in the physics of the implosion process (Moses, 1977). There appears to have been little investigation of the effects of the plasma anisotropy on the transport of these electrons. Our asymmetric collocation method would be very useful in such a study.

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