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THEORETICAL ASPECTS OF THE SIMPLIFIED P_n EQUATIONS

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In celebration of the 50th anniversary of the simplified P_n *equations (*SP_n*), this work reviews the theory underpinning the* SP_n *equations for neutral particle transport. We recount the derivation of these equations by Gelbard's formal procedure and by more recent asymptotic and variational analyses. The relation between the* SP_n *equations and several other low order approximations is discussed. Also, the conditions under which the* SP_n *equations are equivalent to the full* P_n *equations of the same order are discussed as well as the accuracy of the* SP_n *equations. Several open problems in the theory of the* SP_n *equations are posed.*

Keywords: Simplified P_n method, Transport theory

1. Introduction

The solution of linear transport problems is difficult because of the rich phase space; in general there are seven independent variables: three for space, two describing a direction on the unit sphere, one for speed or energy, and one for time. Obtaining energy and time dependent solutions to 3-D transport problems is still challenging, even on petascale computers. Imagine the situation 50 years ago when the simplified P_n (SP_n) method was developed by Ely Gelbard: computer resources were strained to solve 3-D *diffusion* problems. In such a situation the notion of solving transport problems in higher dimensions could quite rightly be considered an academic curiosity to those who needed to design and analyze real systems. To solve transport problems in three

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spatial dimensions would be several orders of magnitude larger than the resource-straining diffusion calculations.

It is into this fray that Gelbard introduced the simplified P_n method (Gelbard, 1960, 1961, 1962). It was a middle ground between diffusion and transport that could be solved using the computational resources of the time. The simplified P_n method was in some sense the product of a day dream that imagined what would happen if the spherical harmonics (P_n) method in general geometry was as nice as it is in slab geometry (although it is not clear if this was the genesis of Gelbard's original derivation). In slab geometry the P_n equations can be written as a system of 1-D diffusion equations—in general geometry this is not possible. It was by the process of writing these 1-D equations in a 3-D form that led to Gelbard's formal derivation of the simplified P_n or SP_n equations. These equations were equivalent to the P_n equations in slab geometry and in other narrow circumstances. In general geometry initial numerical results suggested that SP_n was superior to diffusion.

For some time the SP_n equations existed in theoretical limbo. The only theoretical justification was, to paraphrase Anselm of Canterbury's dictum[1]—"Gelbard could do it, it was appropriate, therefore he did it." In the end, it was the success of the numerical results that were the ultimate justification. It should be noted, however, that SP_n was not widely accepted as an approximate transport method because of the lack of a true theoretical foundation. It was not until the 1990s that this foundation was poured. Pomraning (1993) and Larsen, Morel, and McGhee (1993) independently presented analyses that showed that the SP_n equations were an asymptotic correction to standard diffusion theory (in the case of Larsen et al.) and asymptotically related to the slab geometry P_n equations (in the case of Pomraning). It should be noted that asymptotic derivations also provide a justification for Gelbard's formal derivation. The asymptotic derivations could have landed at many systems of equations that would ultimately be equivalent to the SP_n equations as written by Gelbard but would not have their elegant structure. In other words, Gelbard's derivation guided the asymptotic derivations.

[1]The original Latin phrase is "*potuit, decuit, ergo fecit.*"

The SP_n equations can also be derived using a variational analysis. The first of these analyses appeared in Pomraning's paper where the asymptotic derivation was presented. This derivation was restricted to a uniform, infinite medium with anisotropic scattering. Pomraning's variational analysis was able to produce an arbitrary order SP_n approximation. Later, a finite medium with material interfaces and boundary conditions, along with multigroup treatments, were treated to derive the SP_2 equations by Tomasevic and Larsen (1996) and for the SP_3 equations by Brantley and Larsen (2000). These later variational analyses were by necessity algebraically messy but were able to derive "Marshak-like" boundary conditions as well as interface conditions for the SP_n equations.

The asymptotic and variational derivations and subsequent work (Larsen, Morel, and McGhee, 1996; Frank et al., 2007) led to a groundswell of support for the SP_n method. In the past decade the SP_n method has been applied to the radiative cooling of industrially produced glass (see Frank et al.(this issue) for a review), infrared transfer in combustion and reactive flows (Schneider et al., 2008; Seaïd et al., 2004; Teleaga and Seaïd, 2008; Pinnau and Seaïd, 2008; Banda, Seaïd, and Teleaga, 2008), crystal growth (Backofen et al., 2004), radiative transfer in biological tissues (Klose and Larsen, 2006; Chu, Klose, and Dehghani, 2008; Domínguez and Bérubé-Lauzière, 2010), electron transport (Josef and Morel, 1998), and plasma spectroscopy (Ségur et al., 2006; Capeillere et al., 2008). All of these applications are in addition to the use of SP_n methods in nuclear engineering (Beckert and Grundmann, 2008; Kotiluoto, Pyyry, and Helminen, 2007; Hébert, 2010), as was the original application intended for the SP_n method.

Although there is a theoretical foundation for the SP_n equations, these equations are not effective for solving *all* types of transport problems. As the derivations below will detail in a more precise fashion, if the problem is not (1) "close" to diffusive or (2) locally 1-D, SP_n can give answers worse than diffusion. This is due to the fact that the SP_n equations are an asymptotic approximation to the transport equation. Away from the appropriate asymptotic limit, there is no guarantee that the SP_n equations are accurate. Of course, not all hope is lost: in certain cases the SP_n equations can be shown to be equivalent to the P_n equations,

which are known to be convergent. In these cases the answer will be as accurate as the P_n solution.

In this study we will review the underlying theory of the SP_n equations. First we will present four ways to derive the SP_n equations: Gelbard's original "derivation," two asymptotic derivations, and a variational derivation. After detailing these derivations we discuss, in Section 5, the important theoretical aspect of the SP_n equations that under certain circumstances they are equivalent to the full P_n equations. Alternate forms of the SP_n equations are presented and discussed in Section 6. Before concluding the review we highlight several open questions in the theory of the SP_n equations.

The lion's share of the exposition will deal with odd-order SP_n equations for mono-energetic, steady-state transport problems. The choice of mono-energetic and steady problems was made to make the derivations and discussions as uncluttered as possible with complicated details that do not provide further insight into the theory. In several places we mention how things change in the time dependent case and point the reader to the primary sources for the full details. Focusing on mono-energetic problems is only a minor restriction: if the multigroup method is used for energy dependent problems, the equation for each group looks like a mono-energetic transport equation with a source that couples the other groups. Also, we will almost exclusively deal with odd-order SP_n equations. While we do not focus on SP_2 equations or other even-order SP_n equations, these equations are important waypoints in the development of SP_n in both theoretical and computational aspects. For example the work of Tomasevic and Larsen (1996) on a variational derivation of the SP_2 equations motivated Noh and Miller (1996) to study the use of SP_2 synthetic acceleration of the discrete ordinates equations.

2. Formal Derivation of the Simplified P_n Equations

The energy independent, steady transport equation for the angular flux of neutral particles is

$$\hat{\Omega} \cdot \nabla \psi + \sigma_t \psi = \frac{1}{4\pi} \int_{4\pi} \sigma_s (\hat{\Omega}' \cdot \hat{\Omega}) \psi (\vec{r}, \hat{\Omega}') \, d\hat{\Omega}' + \frac{Q}{4\pi}. \qquad (1)$$

Here $\psi(\vec{r}, \hat{\Omega})$ $(\mathrm{cm}^{-2}\,\mathrm{s}^{-1})$ is the angular flux of particles, $\hat{\Omega} = (\mu, \gamma) \in \mathbb{S}_2$ is a point on the unit sphere where $\mu \in [-1, 1]$ is the cosine of the polar angle and $\gamma \in [0, 2\pi]$ is the azimuthal angle, σ_t (cm^{-1}) is the total interaction macroscopic cross-section, $\sigma_s(\hat{\Omega}' \cdot \hat{\Omega})$ (cm^{-1}) is the differential scattering macroscopic cross-section, and Q is a prescribed, isotropic source. The boundary conditions for the transport equation prescribe the angular flux coming into the system,

$$\psi(\vec{r}, \hat{\Omega}) = \Psi^-(\hat{\Omega}), \quad \text{for } \hat{\Omega} \cdot \hat{n} < 0,\ \vec{r} \in \partial\Gamma \tag{2}$$

with $\hat{n}$ the outward normal of the boundary of the domain of interest Γ. From this equation we can proceed in several different ways to derive the SP_n equations. The original derivation of the SP_n equations by Gelbard (1960, 1961, 1962, 1968) involved an ad hoc substitution of multivariable differential operators. To begin we restrict Eq. (1) to 1-D slab geometry (Bell and Glasstone, 1970; Case and Zweifel, 1967):

$$\mu \frac{\partial \psi}{\partial x} + \sigma_t \psi = \frac{1}{2} \int_{-1}^{1} \sigma_s(\mu_0)\psi(x, \mu')\, d\mu' + \frac{Q}{2}, \tag{3}$$

where $\mu_0 = \hat{\Omega}' \cdot \hat{\Omega}$. We then take Legendre polynomial moments in μ of the 1-D equation and use recursion relations for these polynomials to get the slab geometry P_n equations:

$$\frac{d\phi_1}{dx} + \sigma_0 \phi_0 = Q, \tag{4a}$$

$$\frac{n}{2n+1}\frac{d}{dx}\phi_{n-1} + \frac{n+1}{2n+1}\frac{d}{dx}\phi_{n+1} + \sigma_n \phi_n = 0 \quad \text{for } n > 0. \tag{4b}$$

In these equations we have used the definitions

$$\phi_n(x) = \int_{-1}^{1} P_n(\mu)\psi(x, \mu)\, d\mu, \tag{5a}$$

and

$$\sigma_n = \sigma_t - \sigma_{sn}, \tag{5b}$$

where the moments of the differential scattering cross section are defined by

$$\sigma_{sn} = \int_{-1}^{1} P_n(\mu_0)\sigma_s(\mu_0')\, d\mu_0,$$

where P_n is the nth degree Legendre polynomial. The angular flux is reconstructed as

$$\psi = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} P_n(\mu)\phi_n,$$

and the differential scattering cross-section is

$$\sigma_s(\mu', \mu) = \sum_{n=0}^{\infty} \frac{2n+1}{2} P_n(\mu)P_n(\mu')\sigma_{sn}.$$

Note that $\sigma_0 = \sigma_t - \sigma_s \equiv \sigma_a$, the absorption cross-section, and that $\sigma_1 \equiv \sigma_{tr}$, the so-called transport cross-section. In practice the P_n equations are solved by truncating the expansion at some order N. To close the equations we assume here that $\phi_{N+1} = 0$, although many other closures are possible (see, for example, Brunner, 2001; Hauck and McClarren, 2010; Oh and Holloway, 2008; Buet and Despres, 2006; Frank et al. 2007; Pomraning, 1964).

The Marshak boundary conditions for the P_n equations are obtained by equating half-range moments of ψ and the incoming angular flux at the boundary, Ψ^-. For an Nth order expansion where N is odd there are $(N+1)/2$ boundary conditions:

$$2\pi \int_0^{\pm 1} P_{2m-1}(\mu)\psi\, d\mu = \sum_{n=0}^{N} \frac{2n+1}{2}\phi_n(x) \int_0^{\pm 1} P_{2m-1}(\mu)P_n(\mu)\, d\mu$$
$$= 2\pi \int_0^{\pm 1} P_{2m-1}(\mu)\Psi^-(x, \mu)\, d\mu,$$
$$\text{for } x = 0, X, \text{ and } m = 1, 2, \ldots, (N+1)/2. \quad (6)$$

In Eq. (6) the positive sign in the integration limits is chosen if $x = 0$ (the left edge of the system), and at $x = X$ the integrals

go from -1 to 0. Mark boundary conditions can be derived in a similar manner by replacing the P_{2m-1} functions by a Dirac delta functions, $\delta(\mu - \mu_m)$ where the μ_m are the roots of $P_{N+1}(\mu)$. For even-order expansions the subject of boundary conditions is more subtle (Lewis and Miller, 1984). Rulko and Larsen (1993) derived boundary conditions for P_2 using a variational analysis, and more recently Schaefer, Frank, and Levermore (2009) showed that a diffusive closure for the equations can resolve the issue.

The P_n equations also have conditions at a material interface. These can be found by integrating the equations in a vanishing neighborhood of the material interface to get that

$$\phi_1,$$
$$n\phi_{n-1} + (n+1)\phi_{n+1}, \quad \text{for } 1 < n < N-1,$$

and

$$\phi_{N-1},$$

must be continuous at a material interface.

The P_n equations are quite accurate for slab geometry problems and they can provide spectral convergence to the transport solution (Davison, 1960; Kofink, 1958; Guo, 1995; Yaun, 2000; Boyd, 2001). Extending these equations to multi-dimensional or curvilinear geometries is exceedingly complicated. In these cases (except for 1-D spherical geometry) the angular variable must be expanded in spherical harmonics. This complication arises because the other component in the angular variable needs to be included in the expansion. These extra degrees of freedom make the number of equations that need to be solved increase as N^2 rather than linearly in N as in the slab case. Not only do the number of equations increase, but the coupling of moments through the streaming operator loses its simple structure.

The desire to have a system of moment equations in multi-dimensional geometries with the simplicity of the slab geometry P_n equations led Gelbard (1961) to formally carry out an ad hoc replacement of terms in the P_n equations. First, for odd values of n, ϕ_n was replaced by a vector,

$$\phi_n \to \vec{\phi}_n = \left(\phi_n^x, \phi_n^y, \phi_n^z\right)^{\mathrm{t}},$$

then in the even n equations the derivative in x is replaced by a divergence,

$$\frac{d}{dx} \to \nabla\cdot,$$

and in the odd n equations the x derivative is changed to a gradient,

$$\frac{d}{dx} \to \nabla.$$

This allows us to write the first-order form of the SP_n equations as

$$\nabla \cdot \vec{\phi}_1 + \sigma_0\phi_0 = Q, \tag{7a}$$

$$\frac{n}{2n+1}\nabla\phi_{n-1} + \frac{n+1}{2n+1}\nabla\phi_{n+1} + \sigma_n\vec{\phi}_n = 0 \text{ for odd } n. \tag{7b}$$

$$\frac{n}{2n+1}\nabla\cdot\vec{\phi}_{n-1} + \frac{n+1}{2n+1}\nabla\cdot\vec{\phi}_{n+1} + \sigma_n\phi_n = 0 \text{ for even } n > 0. \tag{7c}$$

The boundary conditions for the SP_n equations can be obtained by making simple replacements in the Marshak boundary conditions given in Eq. (6). Namely we replace the ϕ_n with the SP_n unknowns and μ with $\hat{n}\cdot\hat{\Omega}$ where $\hat{n}$ is the unit inward normal to the boundary to get

$$\begin{aligned}
&\sum_{n\,\text{even}}^{N} \frac{2n+1}{4\pi}\phi_n(\vec{r}) \int_{\hat{n}\cdot\hat{\Omega}>0} P_{2m-1}(\hat{n}\cdot\hat{\Omega})P_n(\hat{n}\cdot\hat{\Omega})\, d^2\hat{\Omega} \\
&\quad + \sum_{n\,\text{odd}}^{N} \frac{2n+1}{4\pi}\hat{n}\cdot\vec{\phi}_n(\vec{r}) \int_{\hat{n}\cdot\hat{\Omega}>0} P_{2m-1}(\hat{n}\cdot\hat{\Omega})P_n(\hat{n}\cdot\hat{\Omega})\, d^2\hat{\Omega} \\
&\quad = \int_{\hat{n}\cdot\hat{\Omega}>0} P_{2m-1}(\hat{n}\cdot\hat{\Omega})\Psi^-(\vec{r},\hat{\Omega})\, d^2\hat{\Omega}, \\
&\qquad\qquad \text{for } \vec{r}\in\partial\Gamma \text{ and } m = 1, 2, \ldots, (N+1)/2.
\end{aligned} \tag{8}$$

These boundary conditions are a collection of 1-D Marshak boundary conditions where the SP_n unknowns are interpreted as components of a Legendre polynomial expansion.
The interface conditions for the SP_n equations are found from the slab geometry interface conditions to be for a N odd

$$\begin{aligned}
&\hat{n}\cdot\phi_1,\\
&n\phi_{n-1}+(n+1)\phi_{n+1} \quad \text{for } n \quad \text{odd},\\
&n(\hat{n}\cdot\vec{\phi}_{n-1})+(n+1)(\hat{n}\cdot\vec{\phi}_{n+1}) \quad \text{for } n \text{ even},
\end{aligned}$$

and

$$\phi_{N-1}$$

are continuous at a material interface with outward normal $\hat{n}$.

The simple structure of the SP_n equations can be exploited to eliminate the vector unknowns. From each odd n equation we get

$$\vec{\phi}_n=-\frac{1}{\sigma_n}\left(\frac{n}{2n+1}\nabla\phi_{n-1}+\frac{n+1}{2n+1}\nabla\phi_{n+1}\right), \tag{9}$$

assuming $\sigma_n\neq 0$. Then using this relation in the even equations we get the second-order form of the SP_n equations

$$-\nabla\cdot\frac{1}{3\sigma_1}\nabla\phi_0-\nabla\cdot\frac{2}{3\sigma_1}\nabla\phi_2+\sigma_0\phi_0=Q, \tag{10a}$$

$$\begin{aligned}
&-\nabla\cdot\left(\frac{n(n-1)}{(2n+1)(2n-1)\sigma_{n-1}}\right)\nabla\phi_{n-2}\\
&-\nabla\cdot\left(\frac{(n+1)(n+2)}{(2n+1)(2n+3)\sigma_{n+1}}\right)\nabla\phi_{n+2}\\
&-\nabla\cdot\left(\frac{n^2}{(2n+1)(2n-1)\sigma_{n-1}}+\frac{(n+1)^2}{(2n+1)(2n+3)\sigma_{n+1}}\right)\nabla\phi_n\\
&\qquad+\sigma_n\phi_n=0, \quad \text{for } n=2,4,\ldots,N-1.
\end{aligned} \tag{10b}$$

The second-order form is useful because it makes the SP_n equations look like a set of coupled diffusion equations.

It is obvious that the SP_n equations, in either form, are equivalent to the P_n equations in slab geometry. The SP_n equations are also equivalent to the P_n equations in general geometry; however, this is true only under certain special conditions that we shall describe later. The perhaps surprising upshot of this formal derivation is that this simplified form of the P_n equations is equivalent to the full P_n equations in certain cases. On the downside this derivation does not lead to an expression for the angular flux in terms of moments. Later, in the variational derivation of the SP_n equations, we will be able to reconstruct the angular flux from the unknowns.

2.1. SP_1 and SP_3 Equations

To demonstrate what the SP_n equations look like in a concrete sense here we write out the equations for expansions in two and four unknowns. In first order form the SP_1 equations are

$$\nabla \cdot \vec{\phi}_1 + \sigma_a \phi_0 = Q, \tag{11a}$$

$$\frac{1}{3}\nabla \phi_0 + \sigma_{tr}\vec{\phi}_1 = 0. \tag{11b}$$

The boundary conditions for the SP_1 equations are, using Eq. (6),

$$\frac{1}{2}\phi_0(\vec{r}) + \hat{n}\cdot\vec{\phi}_1(\vec{r}) = 2\int_{\hat{n}\cdot\hat{\Omega}>0} P_1(\hat{n}\cdot\hat{\Omega})\Psi^-(\vec{r},\hat{\Omega})\, d^2\hat{\Omega}, \quad \text{for } \vec{r}\in\partial\Gamma. \tag{12}$$

In second-order form the SP_1 equations are

$$-\nabla\cdot\frac{1}{3\sigma_{tr}}\nabla\phi_0 + \sigma_a\phi_0 = Q. \tag{13}$$

This is equivalent to the diffusion approximation to transport in general geometry. This implies that the SP_1 and P_1 equations are the same in general geometry. The boundary condition for the

second-order form equation is

$$\frac{1}{2}\phi_0(\vec{r}) - \frac{1}{3\sigma_{tr}}\hat{n}\cdot\nabla\phi_0(\vec{r}) = 2\int_{\hat{n}\cdot\hat{\Omega}>0} P_1(\hat{n}\cdot\hat{\Omega})\Psi^-(\vec{r},\hat{\Omega})\,d^2\hat{\Omega}, \quad \text{for } \vec{r}\in\partial\Gamma. \tag{14}$$

Next we'll look at the SP_3 equations. The SP_3 equations are in first-order form

$$\nabla\cdot\vec{\phi}_1 + \sigma_a\phi_0 = Q, \tag{15a}$$

$$\frac{1}{3}\nabla\phi_0 + \frac{2}{3}\nabla\phi_2 + \sigma_{tr}\vec{\phi}_1 = 0, \tag{15b}$$

$$\frac{2}{5}\nabla\cdot\vec{\phi}_1 + \frac{3}{5}\nabla\cdot\vec{\phi}_3 + \sigma_2\phi_2 = 0, \tag{15c}$$

$$\frac{3}{7}\nabla\phi_2 + \sigma_3\vec{\phi}_3 = 0. \tag{15d}$$

The boundary conditions for the first-order form of the SP_3 equations can be obtained from Eq. (8).

There are two equations in the second-order form of the SP_3 equations:

$$-\nabla\cdot\frac{1}{3\sigma_{tr}}\nabla\phi_0 - \nabla\cdot\frac{2}{3\sigma_{tr}}\nabla\phi_2 + \sigma_a\phi_0 = Q, \tag{16a}$$

$$-\nabla\cdot\frac{2}{15\sigma_{tr}}\nabla\phi_0 - \nabla\cdot\left(\frac{4}{15\sigma_{tr}} + \frac{9}{35\sigma_3}\right)\nabla\phi_2 + \sigma_2\phi_2 = 0. \tag{16b}$$

The first of these equations is the diffusion equation with a correction term involving ϕ_2.

The SP_3 equations can be manipulated into a form that resembles a two group diffusion equation by defining $\hat{\phi}_0 = \phi_0 + 2\phi_2$. Using this new variable, Eq. (16a) becomes

$$-\nabla\cdot\frac{1}{3\sigma_t}\nabla\hat{\phi}_0 + \sigma_a\hat{\phi}_0 = 2\sigma_a\phi_2 + Q. \tag{17a}$$

this is a diffusion equation for $\hat{\phi}_0$ coupled to ϕ_2 through an interaction term. We can also get such an equation for ϕ_2 using the definition of $\hat{\phi}_0$:

$$-\nabla \cdot \frac{9}{35\sigma_t}\nabla\phi_2 + \left(\sigma_2 + \frac{4}{5}\sigma_a\right)\phi_2 = \frac{2}{5}(\sigma_a\hat{\phi}_0 - Q). \quad (17b)$$

These equations can be solved with a two-group diffusion code by properly setting the diffusion coefficients and cross-sections or with a one-group diffusion code utilizing an iteration strategy for the coupling terms. This iterative strategy is known as the FLIP iteration strategy (Gelbard, 1968).

2.2. *Time-dependent SP_n equations*

The SP_n equations for time dependent problems can be derived in a similar formal manner as the steady-state SP_n equations. The time dependent P_n equations in 1-D slab geometry have a term that is the partial derivative with respect to time of ϕ_n divided by the particle speed in each equation. Therefore to get the SP_n equations in time-dependent form we simply add such a term to each of the SP_n equations in first-order form:

$$\frac{1}{v}\frac{\partial\phi_0}{\partial t} + \nabla\cdot\vec{\phi}_1 + \sigma_0\phi_0 = Q, \quad (18a)$$

$$\frac{1}{v}\frac{\partial\vec{\phi}_n}{\partial t} + \frac{n}{2n+1}\nabla\phi_{n-1} + \frac{n+1}{2n+1}\nabla\phi_{n+1} + \sigma_n\vec{\phi}_n = 0 \quad \text{for odd } n, \quad (18b)$$

$$\frac{1}{v}\frac{\partial\phi_n}{\partial t} + \frac{n}{2n+1}\nabla\cdot\vec{\phi}_{n-1} + \frac{n+1}{2n+1}\nabla\cdot\vec{\phi}_{n+1} + \sigma_n\phi_n = 0 \quad \text{for even } n > 0. \quad (18c)$$

The reader's attention is drawn to the fact that the time dependent SP_n equations will not have a simple second-order form because we cannot write the odd order unknowns in terms of spatial derivatives of even unknowns due to the addition of the time derivative.

The initial conditions for these equations are not obvious due to the fact that beyond $\vec{\phi}_1$ we cannot interpret the SP_n unknowns as moments of the initial angular flux. The most obvious initial condition is to set

$$\phi_0(\vec{r}, 0) = \int_{4\pi} I(\vec{r}, \hat{\Omega})\, d^2\hat{\Omega}, \quad \text{and}$$
$$\vec{\phi}_1(\vec{r}, 0) = \int_{4\pi} I(\vec{r}, \hat{\Omega})\hat{\Omega}\, d^2\hat{\Omega}, \tag{19}$$

where $I(\vec{r}, \hat{\Omega})$ is the initial angular flux. The other unknowns can initially be set to zero. We will return to the point of initial conditions below in the discussion of an asymptotic derivation of the time dependent SP_n equations.

3. Asymptotic Derivation of the SP_n Equations

3.1. Larsen, Morel, and McGhee's Derivation

There are at least two ways that asymptotic analysis can be used to derive the SP_n equations. Neither of these derivations includes asymptotic boundary conditions. First, we will review the derivation of Larsen, Morel, and McGhee (LMM) (Larsen et al., 1993, 1996). Their analysis derived the SP_n equations for anisotropic scattering that is not highly forward peaked and included energy dependence through the multigroup method. Here we will present a derivation for isotropic scattering in the one-speed case[2]; the result for anisotropic scattering is the same as that given in the previous section. Our derivation begins by assuming an optically thick system and scaling the transport equation, Eq. (1), by a small, positive, dimensionless parameter ϵ. Specifically, we write

$$\sigma_t \to \frac{\sigma_t}{\epsilon},$$

[2]The derivation when there is anisotropic scattering requires some tensor analysis that we would rather avoid resorting to in this review.

that is that the total cross-section is large,

$$\sigma_s \to \frac{\sigma_s}{\epsilon}, \quad n \geq 0$$

that is the scattering cross-section is of the same order as the total cross-section,

$$\sigma_a \to \epsilon^2 \sigma_a,$$

that is the cross-section is small, $O(\epsilon^2)$, and finally

$$Q \to \epsilon Q,$$

that is the source is small. Making these changes the transport equation can be written as

$$\left(1 + \frac{\epsilon}{\sigma_t}\hat{\Omega}\cdot\nabla\right)\psi = \frac{1-\epsilon^2\sigma_a/\sigma_t}{4\pi}\phi + \frac{\epsilon^2 Q}{4\pi\sigma_t}, \tag{20}$$

where ϕ is the P_0 moment of ψ. If we invert the operator on the left-hand side of this equation, we get an expression for ψ in terms of ϕ and Q

$$\psi = \left(1 + \frac{\epsilon}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^{-1}\left[\frac{1-\epsilon^2\sigma_a/\sigma_t}{4\pi}\phi + \frac{\epsilon^2 Q}{4\pi\sigma_t}\right].$$

If we expand the inverse operator in a power series, assuming that ϵ is small enough to make this possible, we get

$$\begin{aligned}\psi = \Bigg(1 - \frac{\epsilon}{\sigma_t}\hat{\Omega}\cdot\nabla + \epsilon^2\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^2 - \epsilon^3\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^3 \\ + \epsilon^4\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^4) - \epsilon^5\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^5) \\ + \epsilon^6\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^6) + O(\epsilon^7)\Bigg)\left[\frac{1-\epsilon^2\sigma_a/\sigma_t}{4\pi}\phi + \frac{\epsilon^2 Q}{4\pi\sigma_t}\right].\end{aligned} \tag{21}$$

Next, we find the following identity to be useful (Frank et al., 2007)

$$\frac{1}{4\pi}\int_{4\pi}\left(\frac{1}{\sigma_t}\hat{\Omega}\cdot\nabla\right)^l d^2\hat{\Omega} = \frac{1+(-1)^l}{2}\frac{1}{n+1}\left(\frac{1}{\sigma_t}\nabla\right)^l. \quad (22)$$

Upon integrating Eq. (21) over the unit sphere and dividing by, 4π we get

$$\frac{\phi}{4\pi} = \left(1+\frac{\epsilon^2}{3}\left(\frac{1}{\sigma_t}\nabla\right)^2 + \frac{\epsilon^4}{5}\left(\frac{1}{\sigma_t}\nabla\right)^4) + O(\epsilon^6)\right) \times\left[\frac{1-\epsilon^2\sigma_a/\sigma_t}{4\pi}\phi + \frac{\epsilon^2 Q}{4\pi\sigma_t}\right],$$

which we can manipulate into

$$\begin{aligned}(1-\epsilon^2\sigma_a/\sigma_t)\phi + \frac{\epsilon^2 Q}{\sigma_t} &= \left(1+\frac{\epsilon^2}{3}\left(\frac{1}{\sigma_t}\nabla\right)^2 + \frac{\epsilon^4}{5}\left(\frac{1}{\sigma_t}\nabla\right)^4 + \frac{\epsilon^6}{7}\left(\frac{1}{\sigma_t}\nabla\right)^6 + O(\epsilon^8)\right)^{-1}\phi \\ &= \left(1-\frac{\epsilon^2}{3}\left(\frac{1}{\sigma_t}\nabla\right)^2 - \frac{4\epsilon^4}{45}\left(\frac{1}{\sigma_t}\nabla\right)^4 - \frac{44\epsilon^6}{945}\left(\frac{1}{\sigma_t}\nabla\right)^6\right)\phi + O(\epsilon^8),\end{aligned} \quad (23)$$

by once again expanding an inverse in a power series. From this equation we can derive the SP_1 through SP_3 equations by keeping terms up to a certain order in ϵ.

3.1.1. SP_1 (Diffusion) and SP_3 Equations by asymptotics

If we take terms up to $O(\epsilon^2)$ in Eq. (23) we get (after some simple manipulation)

$$-\nabla\cdot\frac{1}{3\sigma_t}\nabla\phi - \sigma_a\phi = Q, \quad (24)$$

which is the second-order form of the SP_1 equation.

If instead we keep terms up to $O(\epsilon^6)$ in Eq. (23), we get

$$\frac{\epsilon^2}{\sigma_t}(Q - \sigma_a\phi) = -\frac{\epsilon^2}{3}\left(\frac{1}{\sigma_t}\nabla\right)^2(\phi + 2\phi_2), \tag{25}$$

where ϕ_2 is given by

$$\begin{aligned}\phi_2 &= \frac{2\epsilon^2}{15}\left(1 + \frac{11\epsilon^2}{21}\left(\frac{1}{\sigma_t}\nabla\right)^2\right)\left(\frac{1}{\sigma_t}\nabla\right)^2\phi \\ &= \frac{2\epsilon^2}{15}\left(1 - \frac{11\epsilon^2}{21}\left(\frac{1}{\sigma_t}\nabla\right)^2\right)^{-1}\left(\frac{1}{\sigma_t}\nabla\right)^2\phi + O(\epsilon^5).\end{aligned} \tag{26}$$

Dropping the error term we can rearrange this equation into

$$-\epsilon^2\nabla\cdot\frac{1}{\sigma_t}\nabla\left(\frac{2}{15}\phi + \frac{11}{21}\phi_2\right) + \sigma_t\phi_2 = 0, \tag{27}$$

which is precisely the second-order form of the SP_3 equation for ϕ_2 given by Eq. (16b) with isotropic scattering. We can also rearrange Eq. (25) to get the first of the second-order form SP_3 equations:

$$-\nabla\cdot\frac{1}{3\sigma_t}\nabla(\phi + 2\phi_2) + \sigma_a\phi = Q. \tag{28}$$

This equation is the same as Eq. (16a) Therefore, from the asymptotic scaling we can also derive the SP_3 equations.

From this derivation we can see that the SP_3 equations are a correction to the diffusion (SP_1) equation that is correct through order ϵ^6. This means that SP_3 equations will have a wider domain of applicability. Of course, because this is an asymptotic limit of the transport equation, problems where ϵ is order 1 will not be well approximated by diffusion or the SP_3 equations.

3.1.2. TIME-DEPENDENT SP_n BY AN ASYMPTOTIC DERIVATION

Using the asymptotic approach similar to the LMM derivation, Frank et al. (2007) derived time-dependent SP_2 and SP_3 equations that are not exactly equivalent to those given in Eq. (18), except in the steady-state limit. These equations have been used in practical glass cooling applications (see Frank et al., this issue, for a review). In the asymptotic derivation there is an ambiguity on how to define the ϕ_2 unknown. It is this ambiguity that leads to flexibility on how the equations are formulated. A moment analysis for a 1-D time dependent problem, however, demonstrates that the asymptotically derived SP_3 equations do not capture the spatial moments of the transport solution in the same way as the P_3 moments (Densmore and McClarren, this issue).

In the asymptotic derivation of the time-dependent SP_n equations, Frank et al. (2007) noted that there are two ways to treat the initial conditions. As said previously, the value for the scalar flux, ϕ_0, is straightforward to compute given the initial angular flux. For the other unknowns, they suggest that it is possible to either set these to zero initially, solve a steady-state SP_n system, or interpret these as actual Legendre moments.

3.2. Pomraning's Asymptotic Derivation

Pomraning presented a different asymptotic derivation that highlights a different connection between the SP_n equations and the transport equation (Pomraning, 1993). Specifically, it demonstrates that if the transport solution is locally 1-D, the SP_n solution will asymptotically agree with the transport solution. We begin by writing a generic point on the unit sphere using the coordinate system

$$\hat{\Omega} = \sqrt{1-\mu^2}(\cos\gamma)\hat{i} + \sqrt{1-\mu^2}(\sin\gamma)\hat{j} + \mu\hat{k}, \qquad (29)$$

for $\mu \in [-1, 1]$, and $\gamma \in [0, 2\pi]$. We assert that this coordinate system is not necessarily fixed in space. Also, we will write the interval over the scattering kernel using the addition formula for

Legendre polynomials:

$$\frac{1}{4\pi}\int_{4\pi}\sigma_s(\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}')\,d\hat{\Omega}'$$
$$=\int_0^{2\pi}d\gamma'\int_{-1}^{1}d\mu'\sum_{n=0}^{\infty}\left(\frac{2n+1}{4\pi}\right)\sigma_{sn}\Bigg[P_n(\mu)P_n(\mu')$$
$$+2\sum_{m=1}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\mu)P_n^m(\mu')\cos m(\gamma-\gamma')\Bigg]\psi(\mu',\gamma'), \quad (30)$$

where the P_n^m are associated Legendre functions. We will use a scaling that makes the solution have weak dependence in the $\hat{i}$ and $\hat{j}$ directions and a weak dependence on the azimuthal angle γ. Specifically our scaling makes the transport equation, Eq. (1),

$$\left[\mu\frac{\partial}{\partial z}+\epsilon\left(\sqrt{1-\mu^2}(\cos\gamma)\frac{\partial}{\partial x}+\sqrt{1-\mu^2}(\sin\gamma)\frac{\partial}{\partial y}\right)\right]\psi+\sigma_t\psi$$
$$=\frac{Q}{4\pi}+\int_0^{2\pi}d\gamma'\int_{-1}^{1}d\mu'\sum_{n=0}^{\infty}\left(\frac{2n+1}{4\pi}\right)\sigma_{sn}\Bigg[P_n(\mu)P_n(\mu')$$
$$+2\epsilon\sum_{m=1}^{n}\frac{(n-m)!}{(n+m)!}P_n^m(\mu)P_n^m(\mu')\cos m(\gamma-\gamma')\Bigg]\psi(\mu',\gamma'). \quad (31)$$

In limit of $\epsilon\to 0$ Eq. (31) becomes a "1-D" transport equation:

$$\mu\frac{\partial\psi}{\partial z}+\sigma_t\psi=\frac{1}{4\pi}\int_{-1}^{1}d\mu'\sum_{n=0}^{\infty}\left(\frac{2n+1}{2}\right)\sigma_{sn}\psi(\mu')$$
$$+\frac{Q}{4\pi}+O(\epsilon). \quad (32)$$

This is not exactly a 1-D transport equation because for this to be the case we need to consider the fact that in the transport equation the spatial derivatives are evaluated with $\hat{\Omega}$ held constant. For Eq. (32) to be a 1-D transport equation to order ϵ the coordinate system where the dependence on x, y, and γ is weak must vary slowly in space. This slow variation can be quantified by requiring

that the change in $\hat{k}$ is order ϵ

$$\left(\mu\frac{\partial}{\partial z}\right)_{\hat{\Omega}}\hat{k} = O(\epsilon), \tag{33}$$

which is equivalent to requiring

$$\left(\mu\frac{\partial}{\partial z}\right)_{\hat{\Omega}}\mu = O(\epsilon). \tag{34}$$

Therefore we can say that the streaming term in Eq. (32) can be approximated by

$$\left(\mu\frac{\partial}{\partial z}\right)_{\hat{\Omega}}\psi = \left(\mu\frac{\partial}{\partial z}\right)_{\mu}\psi + O(\epsilon).$$

Now that we have quantified this error as $O(\epsilon)$, we can interpret Eq. (32) as a 1-D transport equation without increasing the order of the error.

From the 1-D transport equation we can now expand ψ in Legendre polynomials as done in Section 2 to get the P_n equations given by Eq. (4):

$$\frac{\partial\phi_1}{\partial z} + \sigma_0\phi_0 = Q,$$
$$\frac{n}{2n+1}\frac{\partial\phi_{n-1}}{\partial z} + \frac{n+1}{2n+1}\frac{\partial\phi_{n+1}}{\partial z} + \sigma_n\phi_n = 0 \quad \text{for } n > 0.$$

These are partial derivatives because we have not eliminated the dependence on x and y.

To proceed we will use the weak dependence of ψ on the x and y directions to define some quantities of equivalent asymptotic error. For any even Legendre moment we can write

$$\nabla\phi_n = \frac{\partial\phi_n}{\partial x}\hat{i} + \frac{\partial\phi_n}{\partial y}\hat{j} + \frac{\partial\phi_n}{\partial z}\hat{k} = \frac{\partial\phi_n}{\partial z}\hat{k} + O(\epsilon), \quad n\text{even}, \tag{35}$$

because the derivative of ψ in the scaled transport equation is order ϵ. Furthermore, for odd Legendre moments we define a

vector of that moment as

$$\vec{\phi}_n = \phi_n \hat{k}, \quad n \text{odd},$$

so that

$$\nabla \cdot \vec{\phi}_n = \frac{\partial \phi_n}{\partial z}, \quad n \text{odd}.$$

Using these definitions we can rewrite the P_n equations in equivalent form with the same order of asymptotic error, $O(\epsilon)$, without any reference to the z coordinate:

$$\nabla \cdot \phi_1 + \sigma_0 \phi_0 = Q, \tag{36a}$$

$$\frac{n}{2n+1}\nabla \phi_{n-1} + \frac{n+1}{2n+1}\nabla \phi_{n+1} + \sigma_n \vec{\phi}_n = 0 \quad \text{for odd } n > 0, \tag{36b}$$

$$\frac{n}{2n+1}\nabla \cdot \vec{\phi}_{n-1} + \frac{n+1}{2n+1}\nabla \cdot \vec{\phi}_{n+1} + \sigma_n \phi_n = 0 \quad \text{for even } n > 0, \tag{36c}$$

These are precisely the SP_n equations in first-order form.

Before concluding this section we note that Pomraning's derivation of the SP_n equations can, without much complication, be used to derive the time-dependent SP_n equations given by Eq. (18).

3.3. *Comparison of the Asymptotic Derivations*

The two asymptotic derivations presented above take two different approaches: the LMM derivation makes assertions about the material properties (small absorption and sources, large scattering) whereas the Pomraning derivation asserts that the solution is locally 1-D. Both approaches result in the SP_n equations to some order in the asymptotic parameter.

The main difference in the two derivations other than what is scaled is that the Pomraning derivation does not give higher order correction terms. The SP_n equations are shown to be an $O(\epsilon)$ approximation to the 1-D P_n equations regardless of the order of expansion, but there is no clear path to add a correction to make

the equations accurate to higher order in ϵ. Of course since this is an asymptotic derivation, higher order corrections may not be useful to obtain more accurate approximations.

For a given problem it is conceptually easier to recognize when the assertions of the LMM derivation are valid than those in Pomraning's derivation. Usually the problem statement will make it clear when scattering dominates absorption and sources are small. It is somewhat more difficult to infer whether the solution will be locally 1-D. Moreover, even in locally 1-D solutions the 1-D coordinate system can change rapidly making the assertions in Pomraning's derivation invalid. Consider a solution that has a shadow: in the illuminated and dark parts of the shadow the solution can be described using one spatial dimension. The coordinate system, nevertheless, changes abruptly at the edge of the shadow as the solution has strong dependence on the direction perpendicular to the shadow.

4. Variational Derivations of the SP_n Equations

It is also possible to derive the SP_n equations via a variational analysis. In this section we will present such a derivation of the SP_3 equations for the case of an infinite, uniform medium with isotropic scattering. This case will not treat boundary conditions or material interfaces or anisotropic scattering for simplicity in presentation. Most of these complications can be added in a straightforward manner, but the additional level of detail is algebraically supererogatory for this review—boundary and interface conditions are not exactly straightforward as will be discussed next. Much of the background for this type of variational derivation is well covered in the incomparable book by Bell and Glasstone (1970), and the analysis below follows closely the work of Brantley and Larsen (2000, 1997).

For the variational analysis we will need to define an inner product of two functions of space and angle:

$$(f, g) = \int_\Gamma d^3r \int_{4\pi} d^2\hat{\Omega}\, f(\vec{r}, \hat{\Omega}) g(\vec{r}, \hat{\Omega}), \tag{37}$$

where Γ is the domain of interest. Now suppose we want to calculate the integral over all space and angle of the angular

flux, $(1, \psi)$. This integral is related to the functional (Bell and Glasstone, 1970)

$$\mathcal{J}(\Psi^*, \Psi) = (1, \Psi) - \left(\Psi^*, L\Psi - \frac{Q}{4\pi}\right), \tag{38}$$

where Ψ and Ψ^* are functions of space and angle and the operator L is the transport operator

$$L\Psi = \hat{\Omega} \cdot \nabla\Psi + \sigma_t\Psi - \frac{\sigma_s}{4\pi}\int_{4\pi} d^2\hat{\Omega}'\, \Psi(\vec{r}, \hat{\Omega}').$$

It is easy to show that if $\Psi = \psi$ where ψ is the solution to the transport equation, Eq. (1), in an isotropically scattering infinite medium, then regardless of the form of Ψ^*, $\mathcal{J}(\Psi^*, \Psi) = (1, \Psi)$. Also, if $\Psi = \psi + \delta\psi$ and $\Psi^* = \psi^* + \delta\psi^*$ where ψ^* is the solution of the adjoint transport equation with a unit source,

$$-\hat{\Omega} \cdot \psi^* + \sigma_t\psi^* = \frac{\sigma_s}{4\pi}\int_{4\pi} d^2\hat{\Omega}'\, \psi^* + 1, \tag{39}$$

and $\delta\psi$ and $\delta\psi^*$ are small, but arbitrary variations of order $O(\delta)$, then

$$\mathcal{J}(\psi + \delta\psi, \psi^* + \delta\psi^*) = (1, \psi) + O(\delta)^2.$$

That this functional is $O(\delta^2)$ can be shown using the definition of the adjoint operator and the fact that $(\delta\psi^*, \delta\psi)$ is second-order in δ.

Now to derive the SP_3 equations we need to have a form for Ψ and Ψ^*. To do this we begin with the expression for the angular flux under the slab geometry P_3 equations,

$$\begin{aligned}\psi(x, \mu) &= \frac{1}{4\pi}\left[\phi_0 + 3\mu\phi_1 + \frac{5}{2}(3\mu^2 - 1)\phi_2 + \frac{7}{2}(5\mu^3 - 3\mu)\phi_3\right] \\ &= \frac{1}{4\pi}\left[\phi_0 - \frac{\mu}{\sigma_t}\frac{d}{dx}(\phi_0 + 2\phi_2) + \frac{5}{2}(3\mu^2 - 1)\phi_2\right. \\ &\quad \left. - \frac{3}{2\sigma_t}(5\mu^3 - 3\mu)\frac{d}{dx}\phi_2\right],\end{aligned} \tag{40}$$

where the second relation is found by writing the P_n equations in second-order form. Now let us write ϕ_2 as the second derivative of a function $f(x)$,

$$\phi_2(x) = \frac{d^2}{dx^2} f(x),$$

this now makes the angular flux in Eq. (40)

$$\psi(x,\mu) = \frac{1}{4\pi}\left[\phi_0 - \frac{\mu}{\sigma_t}\frac{d}{dx}\left(\phi_0 + 2\frac{d^2}{dx^2}f\right) + \frac{5}{2}\left(3\mu^2\frac{d^2}{dx^2} - \frac{d^2}{dx^2}\right)f - \frac{3\mu}{2\sigma_t}\frac{d}{dx}\left(5\mu^2\frac{d^2}{dx^2} - 3\frac{d^2}{dx^2}\right)f\right]. \tag{41}$$

Taking Eq. (41) and making the same substitution as in the formal derivation of the SP_n equations we get a form for Ψ given by

$$\Psi(\vec{r},\hat{\Omega}) = \frac{1}{4\pi}\left[\phi_0 - \frac{\hat{\Omega}\cdot\nabla}{\sigma_t}(\phi_0 + 2\nabla^2 f) + \frac{5}{2}(3(\hat{\Omega}\cdot\nabla)^2 - \nabla^2)f - \frac{3}{2\sigma_t}(\hat{\Omega}\cdot\nabla)(5(\hat{\Omega}\cdot\nabla)^2 - 3\nabla^2)f\right], \tag{42}$$

where now ϕ_0 and f are functions of $\vec{r}$. We similarly define the adjoint test function Ψ^* by replacing $\hat{\Omega}$ by $-\hat{\Omega}$:

$$\Psi^*(\vec{r},\hat{\Omega}) = \frac{1}{4\pi}\left[\phi_0^* + \frac{\hat{\Omega}\cdot\nabla}{\sigma_t}(\phi_0^* + 2\nabla^2 f^*) + \frac{5}{2}(3(\hat{\Omega}\cdot\nabla)^2 - \nabla^2)f^* + \frac{3}{2\sigma_t}(\hat{\Omega}\cdot\nabla)(5(\hat{\Omega}\cdot\nabla)^2 - 3\nabla^2)f^*\right]. \tag{43}$$

Given these forms for Ψ and Ψ^* we are in a position to simplify $\mathcal{J}$ by performing the angular integrals. Specifically, we can use

Eq. (22) to get

$$\left(\Psi^*, L\Psi - \frac{Q}{4\pi}\right) = -\frac{1}{84\pi}\int_\Gamma d^3r \left\{7\phi_0^*\left(3Q - 3\sigma_a\phi_0 + \frac{1}{\sigma_t}\nabla^2\phi_0 + \frac{2}{\sigma_t}\nabla^4 f\right) - \nabla^2 f^*\left(105\sigma_t\nabla^2 f - \frac{14}{\sigma_t}\nabla^2\phi_0 - \frac{55}{\sigma_t}\nabla^4 f\right)\right\}. \quad (44)$$

To finish the derivation of the SP_n equations we take the first variation of the functional $\delta\mathcal{J}$ to get

$$\delta\mathcal{J} = (1, \delta\Psi) - \left(\delta\Psi^*, L\Psi - \frac{Q}{4\pi}\right) - \left(\Psi^*, L\delta\Psi - \frac{Q}{4\pi}\right).$$

We then find conditions for $\delta\mathcal{J} = 0$, that is for the functional to be stationary by setting the coefficients of $\delta\Psi$ and $\delta\Psi^*$ to be zero. This will lead to a system of equations for the forward and adjoint fluxes. Specifically we can use Eq. (44) to evaluate $(\delta\Psi^*, L\Psi - Q/4\pi)$ to get

$$\left(\delta\Psi^*, L\Psi - \frac{Q}{4\pi}\right) = -\frac{1}{84\pi}\int_\Gamma d^3r \left\{7\delta\phi_0^*\left(3Q - 3\sigma_a\phi_0 + \frac{1}{\sigma_t}\nabla^2\phi_0 + \frac{2}{\sigma_t}\nabla^4 f\right) - \delta\nabla^2 f^*\left(105\sigma_t\nabla^2 f - \frac{14}{\sigma_t}\nabla^2\phi_0 - \frac{55}{\sigma_t}\nabla^4 f\right)\right\}, \quad (45)$$

which upon setting the coefficients of $\delta\phi_0^*$ and $\delta\nabla^2 f^*$ to zero and using the definition of f gives

$$-\frac{1}{3\sigma_t}\nabla^2\phi_0 - \frac{2}{3\sigma_t}\nabla^2\phi_2 + \sigma_a\phi_0 = Q, \quad (46a)$$

$$-\frac{2}{15\sigma_t}\nabla^2\phi_0 - \frac{11}{21\sigma_t}\nabla^2\phi_2 + \sigma_t\phi_2 = 0. \quad (46b)$$

These are precisely the SP_3 equations in second-order form for a uniform medium.

Extending the analysis in this section to include material interfaces and boundary conditions greatly increases the complexity of the derivation. This involves adding terms to the functional to deal with the discontinuities at the material interfaces and problem boundaries (Bell and Glasstone, 1970), along with the additional assumption that the auxillary function f is locally 1-D at the interface or boundary. This analysis has been carried out for the SP_2 equations by Tomasevic and Larsen (1996) and for SP_3 by Brantley and Larsen (2000). The boundary conditions that result are the "Marshak-like" boundary conditions listed in Eq. (8). For material interface conditions for SP_3 the result is that at an interface the following quantities must be continuous:

$$\phi_0 + 2\phi_2,$$

$$\frac{(\hat{n} \cdot \nabla)}{3\sigma_t} (\phi_0 + 2\phi_2),$$

$$\phi_2,$$

$$9\frac{(\hat{n} \cdot \nabla)}{35\sigma_t}\phi_2,$$

where $\hat{n}$ is the outer unit normal of the material interface. These are identical to the interface conditions derived by the formal derivation. The variational analysis can also be extended to multigroup problems with anisotropic scattering for SP_2 and SP_3 in a straightforward manner (Tomasevic and Larsen, 1996; Brantley and Larsen, 2000). Pomraning did a variational derivation of the SP_n equations of arbitrary order in a uniform, infinite medium (Pomraning, 1993) with anisotropic scattering in the one-group case.

5. Equivalence of SP_n and P_n Equations

Early on in the history of the SP_n equations it was realized that there is a variety of conditions under which the SP_n and P_n equations are equivalent. This equivalence is actually quite

surprising because for a given order n the SP_n equations in second-order form has $(n+1)/2$ unknowns whereas the P_n equations have $O(n^2)$ unknowns in general geometry. A discussion of this equivalence appears in the Bettis report where the SP_n equations are first mentioned (Gelbard, 1960).

In that work Gelbard discussed the fact that for a 3-D material medium of infinite extent with a constant total cross-section and isotropic source(s) the solution to the SP_n equations and the full P_n equations are identical. This was first shown by taking both the full P_n equations and the SP_n equations and Fourier transforming each in space. It can then be shown that the resulting equation for each Fourier mode is equivalent. Other facts about the equivalence of the SP_n and P_n equations are that

- In general infinite geometry only σ_t need be constant. The absorption and scattering cross-sections do not have any restrictions on themselves independently.
- In 1-D cylindrical or spherical geometry the sources and scattering do not need to be isotropic; they are allowed to be linearly anisotropic.

The fact that only the total cross-section needs to be independent allows certain multi-material problems to be solved using SP_n. Gelbard suggested that the leakage rate from a cylinder with $\sigma_t = \omega$ that is surrounded by vacuum can be calculated using SP_n in an infinite medium where the vacuum is replaced with a material having $\sigma_a = \omega$ (Gelbard, 1961). The case of a medium surrounded by a pure absorber has been used to solve problems to high angular accuracy using SP_n equations in their A_n form (Ciolini et al., 2006).

5.1. *Numerical Demonstration of SP_n-P_n Equivalence*

To demonstrate the equivalence of the P_n and SP_n equations in a homogeneous medium we have used both methods to solve a specific problem in 2-D Cartesian geometry. This problem has $\sigma_t = 1.0$ and $\sigma_a = 0.9$ with a problem domain of $L_x = L_y = 5$.

There are prescribed sources given by

$$Q(x, y) = \begin{cases} 1 & 1.75 \le x \le 2.25,\ 1.75 \le y \le 2.25 \\ 1 & 2.75 \le x \le 3.25,\ 1.5 \le y \le 2.5 \\ 1 & 1.75 \le x \le 2.25,\ 2.75 \le y \le 3.25\,. \\ 1 & 3.5 \le x \le 4.25,\ 3.5 \le y \le 3.75 \\ 0 & \text{otherwise} \end{cases} \tag{47}$$

We used periodic boundary conditions for the test problem. Mathematically, this is equivalent to solving the PDEs on a torus.

This problem has a scattering ratio of 0.1 and is significantly outside the asymptotic limit discussed in Sec. 3. Therefore, we cannot ascribe any agreement between P_n and SP_n to asymptotic agreement between the two methods. Additionally, this test problem is not well approximated by diffusion, so we expect that a high order of n will be needed to obtain an accurate solution. Also, the test problem will have an inherently multi-dimensional solution because the problem definition is rather asymmetric. The SP_n equations were solved in even-parity form using a simple finite-difference discretization. Hence, in each computational cell there are $\frac{1}{2}(N+1)$ unknowns. The P_n equations used a linear discontinuous Galerkin discretization that is a linear, steady version of the discretization presented in McClarren et al. (2008). The P_n equations were solved in their first-order form, rather than even-parity form, because a first-order form P_n code was readily available. For a 2-D problem, the first-order P_n equations have $\frac{1}{2}(N^2+3N)+1$ unknowns per cell (in even-parity form there would be $\frac{1}{4}(N^2+2N+1)$ unknowns per cell). For our spatial grid we used $N_x = N_y = 100$.

In Fig. 1 the P_n and SP_n solutions to the test problem are compared at $N = 1$, and 5. In these figures one can see that, despite using completely different numerical methods, the P_n and SP_n solutions appear to be identical. Moreover, there is a significant difference between the $N = 1$ and $N = 5$ solutions.To more precisely demonstrate that the P_n and SP_n solutions are equivalent for this problem we look at the solution along the diagonal $x = y$ in Fig. 2. In this figure we see that the SP_n and P_n solutions lie on

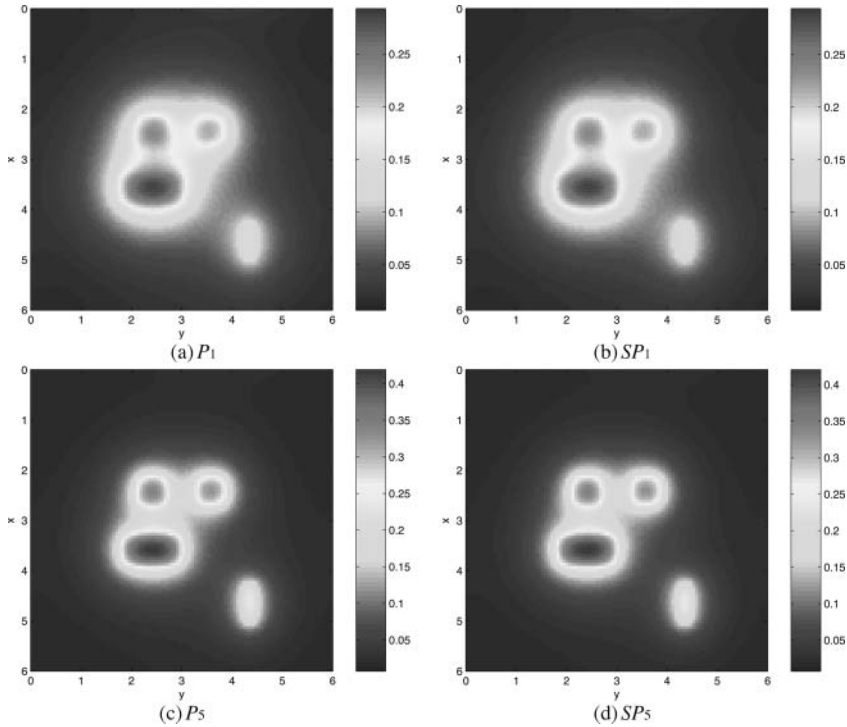

FIGURE 1 Scalar flux, ϕ_0, from several methods for the test problem. Note that the color scales are different for the $N = 5$ and $N = 1$ solutions.

top of each other. We have found that the maximum pointwise relative difference between the P_n and SP_n solution is about 0.1%. This is remarkable agreement considering the different numerical methods used and the large differences between the solutions at different N. This problem demonstrates that there exist cases where diffusion is inadequate and high-order SP_n gives accurate answers.

We did not solve the problem with P_7 or higher approximations. The principle reason for this is that the problem size becomes intractable for serial computing. For the linear discontinuous Galerkin method with $N_x = N_y = 100$, the P_7 solution requires 1.44×10^6 unknowns. On the other hand, SP_7 calculations with this many computational cells can be easily accomplished on a laptop computer.

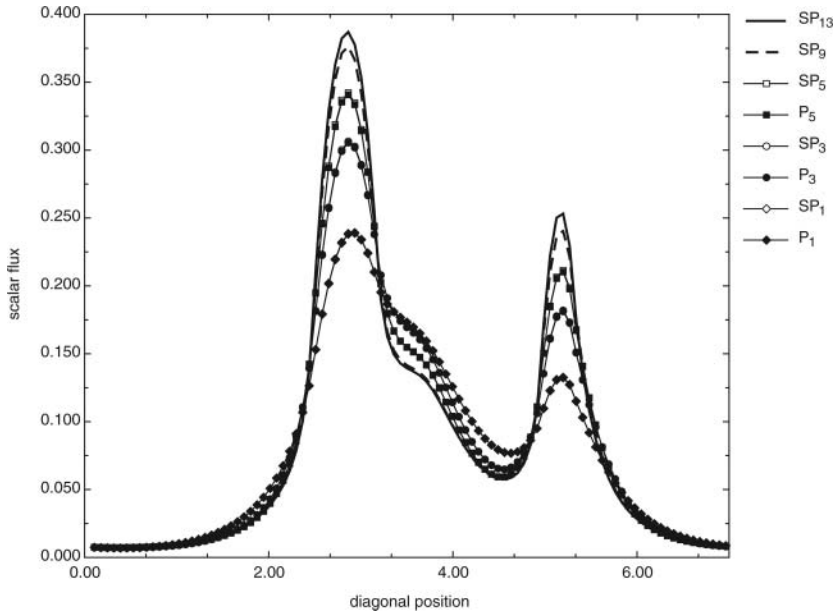

FIGURE 2 Scalar flux along the diagonal of the test problem. For most of the lines the SP_n solution is obscured by the P_n solution.

5.2. *Selengut's* P_3 *Equivalent Equations*

D.S. Selengut derived a set of P_3 equivalent SP_3 equations in 1970 in a conference paper (Selengut, 1970). In deriving these equations Selengut presented a solution to the P_3 equations in terms of the scalar flux only. Using this solution he was able to reconstruct the proper conditions that need to be satisfied at a material interface.

Despite the fact that such a method would obviously be extraordinarily useful for numerical computation (the 2 unknowns of the SP_3 equations being much smaller that the 16 unknowns for the full P_3 equations), this work was never picked up for use by other researchers. The trail may have went cold due to the nearly inscrutable structure of the paper. Also, it has been noted that the solution used to derive the interface conditions may not be the most general solution (Sanchez, 2008).

5.3. *Some Remarks on the Accuracy of* SP_n *for General Problems*

In general the SP_n solution is not equivalent to the P_n solution and therefore increasing n does not guarantee a more accurate solution (i.e., at some order n the maximum potential accuracy is obtained and going to a $n+2$ order expansion will give a worse answer). It is a common assertion based on much experience and numerical experimentation that the added work to obtain SP_n solutions beyond SP_5 or SP_7 is not wholly worthwhile. Furthermore, it has been asserted that most of the benefit of SP_n over diffusion is obtained from SP_3 (Brantley and Larsen, 2000; Smith, 1986a, 1996b). Indeed production codes exist that specifically solve the SP_3 equations (Kotiluoto, Pyyry, and Helminen, 2007).

Also, given the asymptotic derivations of the SP_n equations we do know what types of problems this approximation is well suited. The LMM derivation shows that in problems where isotropic or slightly anisotropic scattering dominates absorption and streaming the SP_n solutions are a reasonable approximation. On the other hand, Pomraning's derivation demonstrates that if the solution is locally 1-D everywhere the SP_n equations can approximate the transport solution well.

6. Alternate Forms of the SP_n Equations

The SP_n equations can be cast into several alternate but equivalent forms. As shown previously there is a form of the equations that looks like a system of multi-group diffusion equations with upscattering. This form was derived by means of a solid harmonic expansion by Ackroyd et al. (1999). This form is useful because it means that the SP_n solution can be obtained from solving a properly posed multigroup diffusion equation. Besides this form there are the A_n and canonical forms of the SP_n equations.

The A_n equations were first derived as an approximate transport method by Coppa and Ravetto (Coppa and Ravetto, 1982). The equations can be derived from the integral transport equation for a finite medium with a constant cross-section by approximating the kernel of the integral transport equation with a superposition of diffusion-like kernels. These equations take the form of a system of coupled diffusion equations, where the coupling

comes through a scattering term. The A_n equations are

$$-\nabla \cdot \left(\frac{\mu_\alpha^2}{\sigma_t} \nabla \psi_\alpha \right) + \sigma_t \psi_\alpha = \sigma_s \sum_{\beta=1}^{N} w_\beta \psi_\beta + Q, \quad \alpha = 1, 2, \ldots, n, \tag{48}$$

where the μ_α are the zeros of the Legendre polynomial of order $2n$ and the w_β are the positive weights of the Gauss-Legendre quadrature set of order $2n$. The scalar flux is also written as

$$\phi_0 = \sum_{\beta=1}^{N} w_\beta \psi_\beta.$$

It has been shown that the A_n equations are equivalent to the SP_{2n-1} equations (Ciolini et al., 2002) in the cases of isotropic and P_1 anisotropic scattering. The proof for isotropic scattering is straightforward: the second-order form of the SP_{2n-1} equations can be written as

$$-\nabla \cdot \left(\frac{1}{\sigma_t} \nabla \mathbf{A} \vec{\phi} \right) + \sigma_t \vec{\phi} = \vec{Q},$$

with $\vec{\phi} = [\phi_0, \phi_2, \ldots, \phi_{2n-1}]^t$, $\vec{Q} = [\sigma_s \phi_0 + Q, 0, \ldots, 0]^t$, and the elements of the tridiagonal $(2n-1) \times (2n-1)$ matrix $\mathbf{A}$ can be easily inferred from Eq. (10b). Given this matrix form of the second-order SP_{2n-1} equations, we can diagonalize the matrix $\mathbf{A}$ to directly derive the A_n equations.

The A_n equations with arbitrary order anisotropic scattering were called the "canonical form" of the SP_n equations by Larsen et al. (1996). The A_n or canonical form of the SP_n equations is attractive because they can be solved in a straightforward manner by a code that solves the even-parity discrete ordinates (S_n) equations or one that solves the diffusion equation. The standard source iteration technique for solving the even-parity S_n equations can converge slowly for the canonical form of SP_n equations in problems with highly anisotropic scattering unless some sort of diffusion acceleration is used.

Another form of the A_n equations (and therefore the SP_{2n-1} equations) is a boundary integral equation (Colombo, 1988; Ciolini et al., 2002). This form has been used to obtain high order A_n solutions to several problems having a constant total cross-section—a situation where the A_n solution is equivalent to the P_{2n-1} solution.

The A_n equations have a well defined limit as $n \to \infty$, and Montagnini and Ravetto (2004) used this fact to generate the Green's function for the A_∞ equations. This Green's function is a bilinear combination of the well-known Case eigenfunctions of slab geometry transport theory (Case and Zweifel, 1967).

7. The Future of SP_n and Open Problems

The development of a theoretical foundation for the SP_n equations was an important development in transport theory. There are, nevertheless, several important questions that remain unanswered regarding SP_n.

- **P_n equivalent forms of SP_n**
  As first suggested by Selengut (1970), it is in principle possible to derive SP_n equations that are equivalent to the P_n equations of the same order provided that the problem can be subdivided into subregions of constant cross-sections. That such a P_n-equivalent form of SP_n might exist is not as quixotic as it might sound. One can show that in a region of constant cross-section that SP_n and P_n solve the same equations. Therefore, the only difference between SP_n and P_n are the interface and boundary conditions that connect the solutions in these constant cross-section regions. Of course it may be possible that the extra unknowns in the P_n equations are essential in these conditions.

  Selengut claimed to have derived interface conditions for the SP_3 equations that would give solutions equivalent to those from P_3. This claim has not been independently verified, and no P_5 or higher equivalent equations have appeared in the literature. A rigorous answer to the question of whether such equivalent forms exist would be a major contribution to the theory of SP_n—especially if the answer is in the affirmative as this could revolutionize transport calculations due to small number

of unknowns in the SP_n equations relative to P_n. The solution could be to use the solid harmonics expansion of Ackroyd et al. (1999). The solid harmonics equations are both formally convergent and equivalent to the SP_n equations in a uniform medium. Therefore, it may be possible to use solid harmonics to derive P_n equivalent boundary and interface conditions.

- **Intermediate approximations**
  The SP_n equations take the form of a system of coupled diffusion equations; this compares to the full P_n equations that have complicated cross-derivative terms in second-order form. There has not been a proposed approximate form that is a middle ground between the two methods. Such a form might be derived by determining higher order corrections in Pomraning's asymptotic derivation of the SP_n equations, or through some other form. This intermediate form would be useful for treating transport problems where SP_n does not provide the required accuracy, such as problems where there are large shadows.
- **Optimal order of SP_n equations**
  Given that the SP_n equations are an asymptotic approximation to the transport equation there is an optimal finite SP_n order solution in terms of accuracy. To present there has not been an analysis of this optimal order or even a heuristic presented to determine this optimal order for a given transport problem. The knowledge of this optimal order would make SP_n solutions more valuable because it would eliminate the uncertainty in determining the balance between solution cost and accuracy. It is true that in most problems going from diffusion to SP_3 produces a large return for the extra computational effort, but in some problems going to even higher order might be beneficial.
- **SP_n closures**
  The SP_n equations are usually truncated by assuming that $\phi_{N+1} = 0$ in a similar manner to the standard P_n closure. There are of course alternate ways to close the SP_n equations and the relative benefits of these closures have not been investigated. One possibility is to take some standard P_n closures in slab geometry and make a similar replacement as in Gelbard's formal derivation. Such an approach would lead to, for example, an SP_n form of the M_3 equations (Hauck, 2011). The benefits or pitfalls of making such a closure for SP_n are by no means clear.

An analysis of these closures would be a valuable contribution to the SP_n body of knowledge.

The SP_n equations do have a strong theoretical background: specifically they are an asymptotic and variational approximation to the transport equation. They are also equivalent to the full P_n equations in several circumstances. Additionally, the SP_n equations are flexible in terms of the form one can solve them. In this review we have endeavored to highlight these points and hopefully spur new investigations into SP_n theory. Whether or not SP_n will be an important method 50 years hence remains to be seen. We can be confident, however, that there are still worthwhile research topics with this method.

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