THEORETICAL ASPECTS OF THE SIMPLIFIED \(P_n\) EQUATIONS

RYAN G. McCLARREN

Department of Nuclear Engineering, Texas A&M University,
College Station, TX

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
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; Dominguez 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, Pyry, 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

$$\hat{\Omega} \cdot \nabla \psi + \sigma_t \psi = \frac{1}{4\pi} \int_{4\pi} \sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}') d\hat{\Omega}' + \frac{Q}{4\pi}. \quad (1)$$
Here $\psi(\vec{r}, \hat{\Omega})$ (cm$^{-2}$ s$^{-1}$) is the angular flux of particles, $\hat{\Omega} = (\mu, \gamma) \in S_2$ 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, $\sigma_t$ (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,

$$\psi(\vec{r}, \hat{\Omega}) = \Psi^-(\hat{\Omega}), \quad \text{for } \hat{\Omega} \cdot \hat{n} < 0, \quad \vec{r} \in \partial \Gamma$$  \hspace{1cm} (2)

with $\hat{n}$ the outward normal of the boundary of the domain of interest $\Gamma$. 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):

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

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

$$\frac{d\phi_1}{dx} + \sigma_0 \phi_0 = Q,$$ \hspace{1cm} (4a)

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

In these equations we have used the definitions

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

and

$$\sigma_n = \sigma_t - \sigma_{sn},$$ \hspace{1cm} (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 \( n \)th 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 \( \psi \) and the incoming angular flux at the boundary, \( \Psi^- \). For an \( N \)th order expansion where \( N \) is odd there are \( (N+1)/2 \) boundary conditions:

\[
2\pi \int_{0}^{\pm 1} P_{2m-1}(\mu) \psi \, d\mu = \sum_{n=0}^{N} \frac{2n+1}{2} \phi_n(x) \int_{0}^{\pm 1} P_{2m-1}(\mu) P_n(\mu) \, d\mu
= 2\pi \int_{0}^{\pm 1} P_{2m-1}(\mu) \Psi^- (x, \mu) \, d\mu,
\]

for \( x = 0, X, \) and \( m = 1, 2, \ldots, (N+1)/2 \).

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
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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 $\mu_m$ 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

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

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 $n$, $\phi_n$ was replaced by a vector,

$$\phi_n \rightarrow \vec{\phi}_n = (\phi_n^x, \phi_n^y, \phi_n^z)^T.$$
then in the even \( n \) equations the derivative in \( x \) is replaced by a divergence,

\[
\frac{d}{dx} \rightarrow \nabla \cdot ,
\]

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

\[
\frac{d}{dx} \rightarrow \nabla .
\]

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

\[
\nabla \cdot \phi_1 + \sigma_0 \phi_0 = Q, \quad (7a)
\]

\[
\frac{n}{2n+1} \nabla \phi_{n-1} + \frac{n+1}{2n+1} \nabla \phi_{n+1} + \sigma_n \phi_n = 0 \quad \text{for odd } n. \quad (7b)
\]

\[
\frac{n}{2n+1} \nabla \cdot \phi_{n-1} + \frac{n+1}{2n+1} \nabla \cdot \phi_{n+1} + \sigma_n \phi_n = 0 \quad \text{for even } n > 0. \quad (7c)
\]

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 \( \phi_n \) with the \( SP_n \) unknowns and \( \mu \) with \( \hat{n} \cdot \hat{\Omega} \) where \( \hat{n} \) is the unit inward normal to the boundary to get

\[
\sum_{n \text{ even}}^{N} \frac{2n+1}{4\pi} \phi_n(\vec{r}) \int_{\hat{n} \cdot \hat{\Omega} > 0} P_{2m-1}(\hat{n} \cdot \hat{\Omega}) P_n(\hat{n} \cdot \hat{\Omega}) \, d^2 \hat{\Omega}
\]

\[+ \sum_{n \text{ odd}}^{N} \frac{2n+1}{4\pi} \hat{n} \cdot \frac{\phi_n(\vec{r})}{\int_{\hat{n} \cdot \hat{\Omega} > 0} P_{2m-1}(\hat{n} \cdot \hat{\Omega}) P_n(\hat{n} \cdot \hat{\Omega}) \, d^2 \hat{\Omega}} \]

\[= \int_{\hat{n} \cdot \hat{\Omega} > 0} P_{2m-1}(\hat{n} \cdot \hat{\Omega}) \Psi^{-}(\vec{r}, \hat{\Omega}) \, d^2 \hat{\Omega}, \]

for \( \vec{r} \in \partial \Gamma \) and \( m = 1, 2, \ldots, (N + 1)/2. \) \( (8) \)
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

$$\hat{n} \cdot \phi_1,$$

$$n\phi_{n-1} + (n + 1)\phi_{n+1} \quad \text{for } n \quad \text{odd},$$

$$n(\hat{n} \cdot \vec{\phi}_{n-1}) + (n + 1)(\hat{n} \cdot \vec{\phi}_{n+1}) \quad \text{for } n \text{ even},$$

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

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

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

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

$$-\nabla \cdot \left( \frac{n(n - 1)}{(2n + 1)(2n - 1)\sigma_{n-1}} \right) \nabla \phi_{n-2}$$

$$-\nabla \cdot \left( \frac{(n + 1)(n + 2)}{(2n + 1)(2n + 3)\sigma_{n+1}} \right) \nabla \phi_{n+2}$$

$$-\nabla \cdot \left( \frac{n^2}{(2n + 1)(2n - 1)\sigma_{n-1}} + \frac{(n + 1)^2}{(2n + 1)(2n + 3)\sigma_{n+1}} \right) \nabla \phi_n$$

$$+ \sigma_n \phi_n = 0, \quad \text{for } n = 2, 4, \ldots, N - 1. \quad (10b)$$

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

\[
\nabla \cdot \vec{\phi}_1 + \sigma_a \phi_0 = Q, \quad (11a)
\]

\[
\frac{1}{3} \nabla \phi_0 + \sigma_u \vec{\phi}_1 = 0. \quad (11b)
\]

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

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

In second-order form the $SP_1$ equations are

\[
-\nabla \cdot \frac{1}{3\sigma_{tr}} \nabla \phi_0 + \sigma_a \phi_0 = Q. \quad (13)
\]

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

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

Next we’ll look at the SP\(_3\) equations. The SP\(_3\) equations are in first-order form

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

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

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

\[
\frac{3}{7} \nabla \phi_2 + \sigma_3 \phi_3 = 0. \tag{15d}
\]

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:

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

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

The first of these equations is the diffusion equation with a correction term involving \(\phi_2\).

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

\[
-\nabla \cdot \frac{1}{3\sigma_1} \nabla \hat{\phi}_0 + \sigma_a \hat{\phi}_0 = 2\sigma_a \phi_2 + Q. \tag{17a}
\]
this is a diffusion equation for $\hat{\phi}_0$ coupled to $\phi_2$ through an interaction term. We can also get such an equation for $\phi_2$ using the definition of $\hat{\phi}_0$:

$$-\nabla \cdot \frac{9}{35 \sigma_t} \nabla \phi_2 + \left( \sigma_2 + \frac{4}{5} \sigma_a \right) \phi_2 = \frac{2}{5} (\sigma_a \hat{\phi}_0 - Q).$$  \hspace{1cm} (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 $\phi_n$ 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:

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

$$\frac{1}{v} \frac{\partial \phi_n}{\partial t} + \frac{n}{2n+1} \nabla \phi_{n-1} + \frac{n+1}{2n+1} \nabla \phi_{n+1} + \sigma_n \phi_n = 0$$  \hspace{1cm} for odd $n$, \hspace{1cm} (18b)

$$\frac{1}{v} \frac{\partial \phi_n}{\partial t} + \frac{n}{2n+1} \nabla \cdot \hat{\phi}_{n-1} + \frac{n+1}{2n+1} \nabla \cdot \phi_{n+1} + \sigma_n \phi_n = 0$$  \hspace{1cm} for even $n > 0$. \hspace{1cm} (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 \( \tilde{\phi}_1 \) we cannot interpret the \( SP_n \) unknowns as moments of the initial angular flux. The most obvious initial condition is to set

\[
\phi_0(\vec{r}, 0) = \int_{4\pi} I(\vec{r}, \hat{\Omega}) \, d^2 \hat{\Omega}, \quad \text{and}
\]

\[
\tilde{\phi}_1(\vec{r}, 0) = \int_{4\pi} I(\vec{r}, \hat{\Omega}) \hat{\Omega} \, d^2 \hat{\Omega},
\]

(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 \( \epsilon \). Specifically, we write

\[
\sigma_t \rightarrow \frac{\sigma_t}{\epsilon},
\]

\(^2\)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,

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

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

$$\sigma_a \rightarrow \epsilon^2 \sigma_a,$$

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

$$Q \rightarrow \epsilon Q,$$

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

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

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

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

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

$$\psi = \left(1 - \frac{\epsilon \hat{\Omega} \cdot \nabla}{\sigma_t} + \epsilon^2 \left(\frac{1}{\sigma_t} \hat{\Omega} \cdot \nabla\right)^2 - \epsilon^3 \left(\frac{1}{\sigma_t} \hat{\Omega} \cdot \nabla\right)^3 \right.$$  

$$+ \epsilon^4 \left(\frac{1}{\sigma_t} \hat{\Omega} \cdot \nabla\right)^4 - \epsilon^5 \left(\frac{1}{\sigma_t} \hat{\Omega} \cdot \nabla\right)^5 \right.$$  

$$+ \epsilon^6 \left(\frac{1}{\sigma_t} \hat{\Omega} \cdot \nabla\right)^6 + O(\epsilon^7) \left[1 - \frac{\epsilon^2 \sigma_a/\sigma_t}{4\pi} \phi + \frac{\epsilon^2 Q}{4\pi \sigma_t}\right]. \quad (21)$$
Next, we find the following identity to be useful (Frank et al., 2007)

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

Upon integrating Eq. (21) over the unit sphere and dividing by $4\pi$ 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

$$(1 - \epsilon^2 \sigma_a/\sigma_t) \phi + \frac{\epsilon^2 Q}{\sigma_t}$$

$$= \left( 1 + \frac{\epsilon^2}{3} \left( \frac{1}{\sigma_t} \nabla \right)^2 + \frac{\epsilon^4}{5} \left( \frac{1}{\sigma_t} \nabla \right)^4 + \frac{\epsilon^6}{7} \left( \frac{1}{\sigma_t} \nabla \right)^6 + O(\epsilon^8) \right)^{-1} \phi$$

$$= \left( 1 - \frac{\epsilon^2}{3} \left( \frac{1}{\sigma_t} \nabla \right)^2 - \frac{4 \epsilon^4}{45} \left( \frac{1}{\sigma_t} \nabla \right)^4 - \frac{44 \epsilon^6}{945} \left( \frac{1}{\sigma_t} \nabla \right)^6 \right) \phi + O(\epsilon^8),$$

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 $\epsilon$.

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

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

where $\phi_2$ is given by

$$\phi_2 = \frac{2\epsilon^2}{15} \left( 1 + \frac{11\epsilon^2}{21} \left( \frac{1}{\sigma_t} \nabla \right)^2 \right) \left( \frac{1}{\sigma_t} \nabla \right)^2 \phi$$

$$= \frac{2\epsilon^2}{15} \left( 1 - \frac{11\epsilon^2}{21} \left( \frac{1}{\sigma_t} \nabla \right)^2 \right)^{-1} \left( \frac{1}{\sigma_t} \nabla \right)^2 \phi + O(\epsilon^5). \quad (26)$$

Dropping the error term we can rearrange this equation into

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

which is precisely the second-order form of the $SP_3$ equation for $\phi_2$ 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:

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

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 $\epsilon^6$. 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 $\epsilon$ 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 \( \phi_2 \) 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, \( \phi_0 \), 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

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

(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:

\[
\frac{1}{4\pi} \int_{4\pi}^{4\pi} \sigma_s(\hat{\Omega}' \cdot \hat{\Omega}) \psi (\vec{r}, \hat{\Omega}') \, d\hat{\Omega}'
\]

\[
= \int_{0}^{2\pi} d\gamma' \int_{-1}^{1} d\mu' \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \sigma_s [ P_n(\mu)P_n(\mu')
\]

\[
+ 2 \sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} P_n^{m}(\mu)P_n^{m}(\mu') \cos m(\gamma - \gamma') ] \psi (\mu', \gamma'),
\] (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 \( \gamma \). Specifically our scaling makes the transport equation, Eq. (1),

\[
\left[ \mu \frac{\partial}{\partial z} + \epsilon \left( \sqrt{1-\mu^2}(\cos \gamma) \frac{\partial}{\partial x} + \sqrt{1-\mu^2}(\sin \gamma) \frac{\partial}{\partial y} \right) \right] \psi + \sigma_i \psi
\]

\[
= \frac{Q}{4\pi} + \int_{0}^{2\pi} d\gamma' \int_{-1}^{1} d\mu' \sum_{n=0}^{\infty} \left( \frac{2n+1}{4\pi} \right) \sigma_s [ P_n(\mu)P_n(\mu')
\]

\[
+ 2\epsilon \sum_{m=1}^{n} \frac{(n-m)!}{(n+m)!} P_n^{m}(\mu)P_n^{m}(\mu') \cos m(\gamma - \gamma') \] \psi (\mu', \gamma').
\] (31)

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

\[
\mu \frac{\partial \psi}{\partial z} + \sigma_i \psi = \frac{1}{4\pi} \int_{-1}^{1} d\mu' \sum_{n=0}^{\infty} \left( \frac{2n+1}{2} \right) \sigma_s n \psi (\mu')
\]

\[
+ \frac{Q}{4\pi} + O(\epsilon).
\] (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 \( \epsilon \) the coordinate system where the dependence on \( x, y, \) and \( \gamma \) is weak must vary slowly in space. This slow variation can be quantified by requiring
that the change in $\hat{k}$ is order $\epsilon$

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

(33)

which is equivalent to requiring

$$
\left( \mu \frac{\partial}{\partial z} \right) \mu = O(\epsilon).
$$

(34)

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

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

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 $\psi$ 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 $\psi$ on the $x$ and $y$ directions to define some quantities of equivalent asymptotic error. For any even Legendre moment we can write

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

(35)

because the derivative of $\psi$ in the scaled transport equation is order $\epsilon$. 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:

\[
\begin{align*}
\nabla \cdot \phi_1 + \sigma_0 \phi_0 &= Q, \quad (36a) \\
\frac{n}{2n+1} \nabla \phi_{n-1} + \frac{n+1}{2n+1} \nabla \phi_{n+1} + \sigma_n \vec{\phi}_n &= 0 \quad \text{for odd } n > 0, \quad (36b) \\
\frac{n}{2n+1} \nabla \cdot \vec{\phi}_{n-1} + \frac{n+1}{2n+1} \nabla \cdot \vec{\phi}_{n+1} + \sigma_n \phi_n &= 0 \\
& \quad \text{for even } n > 0, \quad (36c)
\end{align*}
\]

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 $\epsilon$. 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:

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

where $\Gamma$ 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)

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

where \(\Psi\) and \(\Psi^*\) are functions of space and angle and the operator \(L\) is the transport operator

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

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

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

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 \(\delta\).

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

\[
\psi(x, \mu) = \frac{1}{4\pi} \left[ \phi_0 + 3\mu \phi_1 + \frac{5}{2}(3\mu^2 - 1)\phi_2 + \frac{7}{2}(5\mu^3 - 3\mu)\phi_3 \right]
\]

\[
= \frac{1}{4\pi} \left[ \phi_0 - \frac{\mu}{\sigma_t} \frac{d}{dx}(\phi_0 + 2\phi_2) + \frac{5}{2}(3\mu^2 - 1)\phi_2 - \frac{3}{2\sigma_t}(5\mu^3 - 3\mu) \frac{d}{dx} \phi_2 \right].
\]
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where the second relation is found by writing the $P_n$ equations in second-order form. Now let us write $\phi_2$ 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)

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

(41)

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

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

(42)

where now $\phi_0$ and $f$ are functions of $\vec{r}$. We similarly define the adjoint test function $\Psi^*$ by replacing $\hat{\Omega}$ by $-\hat{\Omega}$:

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

(43)

Given these forms for $\Psi$ and $\Psi^*$ we are in a position to simplify $\mathcal{J}$ by performing the angular integrals. Specifically, we can use
Eq. (22) to get

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

(44)

To finish the derivation of the \( SP_n \) equations we take the first variation of the functional \( \delta J \) to get

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

We then find conditions for \( \delta J = 0 \), 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 \( \left( \delta \Psi^*, L\Psi - \frac{Q}{4\pi} \right) \) to get

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

(45)

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

\[
\begin{align*}
-\frac{1}{3\sigma_t} \nabla^2\phi_0 - \frac{2}{3\sigma_t} \nabla^2\phi_2 + \sigma_a\phi_0 &= Q, \quad (46a) \\
-\frac{2}{15\sigma_t} \nabla^2\phi_0 - \frac{11}{21\sigma_t} \nabla^2\phi_2 + \sigma_t\phi_2 &= 0. \quad (46b)
\end{align*}
\]
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 auxiliary 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 multi-group 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 \( \sigma_t \) 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

\[
Q(x, y) = \begin{cases} 
1 & 1.75 \leq x \leq 2.25, \ 1.75 \leq y \leq 2.25 \\
1 & 2.75 \leq x \leq 3.25, \ 1.5 \leq y \leq 2.5 \\
1 & 1.75 \leq x \leq 2.25, \ 2.75 \leq y \leq 3.25 \\
1 & 3.5 \leq x \leq 4.25, \ 3.5 \leq y \leq 3.75 \\
0 & \text{otherwise} 
\end{cases} \quad (47)
\]

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, $\phi_0$, 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 $1.44 \times 10^6$ unknowns. On the other hand, $SP_7$ calculations with this many computational cells can be easily accomplished on a laptop computer.
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

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

(48)

where the $\mu_{\alpha}$ are the zeros of the Legendre polynomial of order $2n$ and the $w_{\beta}$ 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

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

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 $A$ can be easily inferred from Eq. (10b). Given this matrix form of the second-order $SP_{2n-1}$ equations, we can diagonalize the matrix $A$ 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 $A_{\infty}$ 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 $S_{PN}$ body of knowledge.

The $S_{PN}$ 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 $S_{PN}$ 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 $S_{PN}$ theory. Whether or not $S_{PN}$ 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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References


