

ASYMPTOTIC P_N -EQUIVALENT S_{N+1} EQUATIONS

J.E. Morel^a, J.C. Ragusa^a, M.L. Adams^a, G. Kanschat^b

^aDepartment of Nuclear Engineering

^bDepartment of Mathematics

Texas A&M University
College Station, TX 77843

Abstract

The 1-D one-speed slab-geometry P_N equations with isotropic scattering can be modified via an alternative moment closure to preserve the two asymptotic eigenmodes associated with the transport equation. Pomraning referred to these equations as the asymptotic P_N equations. It is well-known that the 1-D slab-geometry S_{N+1} equations with Gauss quadrature are equivalent to the standard P_N equations. In this paper, we first show that if any quadrature set meets a certain criterion, the corresponding S_{N+1} equations will be equivalent to a set of P_N equations with a quadrature-dependent closure. We then derive a particular family of quadrature sets that make the S_{N+1} equations equivalent to the asymptotic P_N equations. Next we theoretically demonstrate several of the properties of these sets, relate them to an existing family of quadratures, numerically generate several example quadrature sets, and give numerical results that confirm several of their theoretically predicted properties.

Keywords

P_N equations, S_N equations, asymptotic decay lengths.

Running Head

Asymptotic S_{N+1} Equations

Corresponding Author

Jim E. Morel, Phone: (979)845-6072, FAX: (979)845-6075, E-mail: morel@tamu.edu.

1 Introduction

Pomraning developed a generalized P_N method based upon alternatives to the usual closure that assumes the angular flux moment corresponding to P_{N+1} is zero [1]. This generalized approach takes two forms. One preserves forward-peaked and backward-peaked delta-function solutions, and the other preserves the two asymptotic eigenmodes associated with the exact transport solution. We refer to the latter approximation as the asymptotic P_N equations. Both of the asymptotic modes have a decay length that is larger than those of all other eigenmodes, so the asymptotic modes dominate at deep penetration in a homogeneous medium.

It is well known that in 1-D slab geometry the S_{N+1} equations with Gauss quadrature are equivalent to the standard P_N equations. The purpose of this paper is to demonstrate that an analogous equivalence exists between the S_{N+1} equations with appropriate quadrature and the asymptotic P_N equations. Several families of S_N quadrature sets that preserve the transport asymptotic decay length were derived by Ganguley, et al. [2]. Although these sets were derived without consideration of P_N equations, we have found that our family of asymptotic quadratures is identical to one of those families. We have no proof of this property, but rather have simply observed it by comparing quadrature sets that we generated with those published by Ganguley, et. al.

The remainder of this paper is organized as follows. First we derive Pomraning's asymptotic P_N equations. Next we show that under the assumption of a certain property of the quadrature set, the S_{N+1} equations are equivalent to the P_N equations with a truncation determined by the quadrature set. This is a general property independent of Pomraning's closure. The particular quadrature sets that produce Pomraning's asymptotic closure are next derived. Various properties of these sets are then demonstrated including certain properties that Ganguly, et al., did not make reference to. Boundary conditions and interface

conditions are next given for the S_{N+1} equations corresponding to our asymptotic quadrature sets. We then discuss the equations that Ganguley, et al., used to generate the quadrature sets that are identical to ours. Finally, we numerically generate several of our sets and numerical demonstrate several of their properties.

2 The Asymptotic P_N Equations

The purpose of this section is to derive Pomraning's asymptotic P_N equations. We begin with the transport equation:

$$\mu \frac{\partial \psi}{\partial z} + \sigma_t \psi = \frac{\sigma_s}{2} \phi + \frac{q}{2}, \quad (1)$$

where $\psi(z, \mu)$ ($p/cm^2 - sec - steradian$) is the angular flux, μ is the cosine of the polar angle associated with the particle direction, σ_t (cm^{-1}) is the macroscopic total cross section, σ_s (cm^{-1}) is the macroscopic scattering cross section, $q(z)/2$ ($p/cm^3 - sec - steradian$) is the inhomogeneous source, and $\phi(z)$ ($p/cm^2 - sec$) is the scalar flux:

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

It is convenient for our purposes to re-express the spatial variable in Eq. (1) in mean-free-paths. Let x denote this variable, then

$$x = \sigma_t z, \quad (3)$$

and Eq. (1) becomes

$$\mu \frac{\partial \psi}{\partial x} + \psi = \frac{c}{2} \phi + \frac{\rho}{2}, \quad (4)$$

where $c = \sigma_s/\sigma_t$ is the scattering ratio and $\varrho = q/\sigma_t$. We next take the k 'th Legendre moment of the transport equation by first multiplying Eq. (1) by the k 'th Legendre polynomial, $P_k(\mu)$, and integrating over all directions. Using the identity

$$\mu P_k(\mu) = \frac{k+1}{2k+1} P_{k+1}(\mu) + \frac{k}{2k+1} P_{k-1}(\mu) , \quad (5)$$

and taking the moments for $k = 0, N$, with N restricted to odd values, we obtain the following system of exact moment equations:

$$\frac{d\Phi_1}{dx} + (1-c)\Phi_0 = \varrho , \quad (6)$$

$$\frac{k+1}{2k+1} \frac{d\Phi_{k+1}}{dx} + \frac{k}{2k+1} \frac{d\Phi_{k-1}}{dx} + \Phi_k = 0 , \quad k = 1, N-1, \quad (7)$$

$$\frac{N+1}{2N+1} \frac{d\Phi_{N+1}}{dx} + \frac{N}{2N+1} \frac{d\Phi_{N-1}}{dx} + \Phi_N = 0 , \quad (8)$$

where the k 'th Legendre moment of the angular flux is given by

$$\Phi_k(x) = \int_{-1}^{+1} P_k(x, \mu) \psi(x, \mu) d\mu , \quad (9)$$

and $\sigma_a = \sigma_t - \sigma_s$ (cm^{-1}) is the macroscopic absorption cross section. These moment equations are exact, but the system is open because there are $N+1$ unknowns and N equations. The standard P_N approximation is simply to set $\Phi_{N+1} = 0$. Pomraning obtains the asymptotic closure by assuming that the solution is given by a linear combination of the Legendre polynomials of degree $N-2$ or less and the two asymptotic transport modes. These modes have the following form:

$$\psi_\nu^+(x, \mu) = \frac{a^+}{1 + \nu\mu} \exp(\nu x) , \quad (10)$$

and

$$\psi_{\nu}^{-}(x, \mu) = \frac{a^{-}}{1 - \nu\mu} \exp(-\nu x) , \quad (11)$$

where each a^{\pm} is an arbitrary constant, and ν is the decay constant or the reciprocal of the asymptotic decay length that satisfies the following dispersion relation,

$$\frac{2\nu}{c} = \ln \frac{1 + \nu}{1 - \nu} , \quad (12)$$

Because $0 \leq c \leq 1$, ν is real and continuously varies from zero to one as c varies from one to zero. Equation (12) admits negative μ values as well, but we have accounted for these values by defining ψ^{\pm} . The generalized closure is mechanically expressed in terms of a constant, α_N , where

$$\Phi_{N+1} = \alpha_N \Phi_{N-1} . \quad (13)$$

Thus Eq. (8) becomes

$$\left[\alpha_N \frac{N+1}{2N+1} + \frac{N}{2N+1} \right] \frac{d\Phi_{N-1}}{dx} + \Phi_N = 0 . \quad (14)$$

Due to the orthogonality of the Legendre polynomials and the assumption that the solution is given by a linear combination of the Legendre polynomials of degree $N-2$ or less and the two asymptotic transport modes, only the asymptotic modes contribute to Φ_{N-1} and Φ_{N+1} . Thus

$$\alpha_N = \frac{\int_{-1}^{+1} P_{N-1}(\mu) [a^{+} \exp(\nu x)(1 + \nu\mu)^{-1} + a^{-}(x) \exp(-\nu x)(1 + \nu\mu)^{-1}] d\mu}{\int_{-1}^{+1} P_{N+1}(\mu) [a^{+} \exp(\nu x)(1 + \nu\mu)^{-1} + a^{-} \exp(-\nu x)(1 + \nu\mu)^{-1}] d\mu} \quad (15)$$

Since both $P_{N-1}(\mu)$ and $P_{N+1}(\mu)$ are even functions of μ , and $\psi_\nu^+(\mu) = \psi_\nu^-(-\mu)$, Eq. (15) reduces to

$$\alpha_N = \frac{\int_{-1}^{+1} P_{N-1}(\mu)(1 + \nu\mu)^{-1} d\mu}{\int_{-1}^{+1} P_{N+1}(\mu)(1 + \nu\mu)^{-1} d\mu} . \quad (16)$$

For a given value of N , the constant α_N is purely a function of c and continuously varies from zero to one as c varies from one to zero. This constant can be directly evaluated numerically using adaptive quadrature integration for any values of c other than zero and one. However, as previously noted, $c = 1$ yields $\alpha_N = 0$ and $c = 0$ yields $\alpha_N = 1$. As $c \rightarrow 1$, the modal functions become isotropic and as $c \rightarrow 0$, (with proper normalization) they become delta-functions at $\mu = \pm 1$.

3 General Equivalence of S_{N+1} and P_N Equations

In this section we first show that if any quadrature set meets a certain general criterion, the S_{N+1} equations formed with that set will be equivalent to a set of P_N equations with a closure determined by the quadrature. We begin our consideration of the general S_{N+1} equations by assuming a standard $(N + 1)$ -point quadrature set for discrete-ordinates calculations: $\{\mu_m, w_m\}_{m=1}^{N+1}$, where the weights sum to 2, the quadrature points are symmetric about $\mu = 0$, and the set exactly integrates at least 1, μ , and μ^2 . The corresponding S_{N+1} equations can be written as follows:

$$\mu_m \frac{d\psi_m}{dx} + \psi_m = \frac{c}{2}\phi + \frac{\varsigma}{2} , \quad m = 1, N + 1, \quad (17)$$

where $\psi_m(x) = \psi(x, \mu_m)$ and

$$\phi(x) = \sum_{m=1}^{N+1} \psi_m(x) w_m . \quad (18)$$

We next take the k 'th Legendre moment of Eq. (17) using the quadrature formula:

$$\sum_{m=1}^{N+1} P_k(\mu_m) \left[\mu_m \frac{d\psi_m}{dx} + \psi_m - \frac{c}{2}\phi + \frac{\varsigma}{2} \right] w_m = 0 . \quad (19)$$

Substituting from Eq. (5) into Eq. (19), we get

$$\sum_{m=1}^{N+1} \left[\left(\frac{k+1}{2k+1} P_{k+1}(\mu_m) + \frac{k}{2k+1} P_{k-1}(\mu_m) \right) \frac{d\psi_m}{dx} + \psi_m - \frac{c}{2}\phi + \frac{\varsigma}{2} \right] w_m = 0 . \quad (20)$$

Equation (19) is trivially evaluated for $k = 0, N+1$:

$$\frac{d\Phi_1}{dx} + (1-c)\Phi_0 = \varsigma , \quad (21)$$

$$\frac{k+1}{2k+1} \frac{d\Phi_{k+1}}{dx} + \frac{k}{2k+1} \frac{d\Phi_{k-1}}{dx} + \Phi_k = 0 , \quad k = 1, N-1, \quad (22)$$

$$\frac{N+1}{2N+1} \frac{d\Phi_{N+1}}{dx} + \frac{N}{2N+1} \frac{d\Phi_{N-1}}{dx} + \Phi_N = 0 , \quad (23)$$

where the k 'th Legendre moment of the angular flux is given by

$$\Phi_k(x) = \sum_{m=1}^{N+1} P_k(\mu_m) \psi_m(x) w_m . \quad (24)$$

Note that Eqs. (21) through (23) are identical to Eqs. (6) through (8). However, it can be shown that if we assume a certain property of the quadrature formula, Eqs. (21) through (23) are closed, whereas Eqs. (6) through (8) are open unless a specific closure relating Φ_{N+1} to the lower-order flux moments is defined. The potential implicit closure of Eqs. (21) through (23) relates to the fact that all of the S_{N+1} moments are a function of $N+1$ independent angular flux values. If these angular flux values can be uniquely expressed in terms of the first $N+1$ moments, then it follows that Φ_{N+1} can be expressed in terms of these lower-order

moments, which in turn closes the system. We can begin to demonstrate a specific expression for the closure by first considering the discrete-to-moment matrix \mathbf{D} defined via Eq. (24) [3]:

$$D_{k,m} = P_k(\mu_m)w_m, \quad k = 0, N, \text{ and } m = 1, N + 1. \quad (25)$$

Note that this matrix maps $N + 1$ Legendre moments to $N + 1$ discrete angular flux values:

$$\vec{\psi} = \mathbf{D} \vec{\Phi}, \quad (26)$$

where

$$\vec{\psi} = (\psi_1, \psi_2, \dots, \psi_{N+1})^t, \quad (27)$$

and

$$\vec{\Phi} = (\Phi_0, \Phi_1, \dots, \Phi_N)^t. \quad (28)$$

If we assume that \mathbf{D} is invertible, then it follows that

$$\psi_m = \sum_{k=0}^N \mathbf{M}_{m,k} \Phi_k, \quad m = 1, N + 1. \quad (29)$$

where $\mathbf{M} = \mathbf{D}^{-1}$. Substituting from Eq. (29) into Eq. (24) for $k = N + 1$, we obtain the desired closure expression:

$$\Phi_{N+1} = \sum_{m=1}^{N+1} P_{N+1}(\mu_m) \left[\sum_{k=0}^N \mathbf{M}_{m,k} \Phi_k \right] w_m. \quad (30)$$

The matrix \mathbf{M} is called the moment-to-discrete matrix [3]. It is important to realize that if the discrete-to-moment matrix is not invertible Eqs. (21) through (23) are nonetheless

satisfied by the S_{N+1} -generated moments, but these equations cannot be solved for those moments or for the discrete angular flux values given those moments.

4 Asymptotic P_N -Equivalent S_{N+1} Equations

In this section we define a procedure for obtaining quadrature sets that yield Pomraning's closure given the value of α_N . In this regard, we want Eq. (13) to be satisfied using the quadrature definition for the moments given in Eq. (24):

$$\sum_{m=1}^{N+1} P_{N+1}(\mu_m) \psi_m w_m = \alpha \sum_{m=1}^{N+1} P_{N-1}(\mu_m) \psi_m w_m . \quad (31)$$

It is useful to rearrange Eq. (31) a bit:

$$\sum_{m=1}^{N+1} G_N(\mu_m) \psi_m w_m = 0 , \quad (32)$$

where

$$G_N(\mu) = P_{N+1}(\mu) - \alpha_N P_{N-1}(\mu) . \quad (33)$$

Note from Eq. (32) that if we choose the quadrature points to be the roots of $G_N(\mu)$, Eq. (31) is guaranteed to be satisfied independent of the values of ψ .

We next show that the polynomial $G_N(\mu)$ has $N + 1$ real non-zero roots symmetrically located about $\mu = 0$, and if $\alpha < 1$, these roots are located within the open interval $(-1, 1)$, and if $\alpha = 1$, these roots are located within the closed interval $[-1, 1]$. Using Eq. (5), we

can rewrite $G_N(\mu)$ as follows:

$$G_N(\mu) = \frac{2N+1}{n+1} \mu P_N(\mu) - \left(\frac{N}{N+1} + \alpha \right) P_{N-1}(\mu). \quad (34)$$

We next make the following definitions:

$$G_N(\mu) = a(\mu) - b(\mu), \quad a(\mu) = \frac{2N+1}{n+1} \mu P_N(\mu), \quad b(\mu) = \left(\frac{N}{N+1} + \alpha \right) P_{N-1}(\mu). \quad (35)$$

First, nothing needs to be shown for $\alpha = 0$, since $G_N(\mu)$ is equal to $P_{N+1}(\mu)$ in this case, and $P_{N+1}(\mu)$ is known to have the desired properties.

Hence, we consider $\alpha > 0$. It is known that $P_{N-1}(\mu)$ has one real root within every interval between adjacent roots of $P_N(\mu)$. Let ξ_k and ξ_{k+1} be adjacent roots of $P_N(\mu)$. Then, we have $G_N(\xi_k) = -b(\xi_k)$ and $G_N(\xi_{k+1}) = -b(\xi_{k+1})$. Since $b(\mu)$ changes sign between these two roots, $G_N(\mu)$ must similarly change sign and thereby must have at least one root between them. Thus, $G_N(\mu)$ must have at least one root in *every* interval between roots of $P_N(\mu)$. There are $N - 1$ such intervals.

Since N is odd, $P_N(\mu)$ has $(N + 1)/2$ nonnegative roots, and $G_N(\mu)$ has $(N - 1)/2$ positive zeros on the interval $(0, \xi_N)$, where ξ_N is the largest root of P_N . Furthermore, $P_{N-1}(\xi_N)$ must be positive. This follows from the fact that $P_{N-1}(1) = 1$, so if $P_{N-1}(\xi_N)$ were negative, it would have a root on $(\xi_N, 1)$, which would not be between two roots of $P_N(\mu)$. Thus, $G_N(\xi_N) < 0$. Furthermore, since

$$P_{N-1}(1) = P_N(1) = 1 \quad \text{and} \quad \frac{2N+1}{N+1} = \frac{N}{N+1} + 1 \geq \frac{N}{N+1} + \alpha, \quad (36)$$

we find that $G_N(1) \geq 0$, so it has at least one additional root in $(\xi_N, 1]$. This root is equal

to 1 if and only if $\alpha = 1$. Thus, $G_N(\mu)$ has at least $(N + 1)/2$ positive roots. Since $G_N(\mu)$ is even, the negative of each positive root must also be a root. Thus, $G_N(\mu)$ has at least $N + 1$ roots symmetrically arranged about $\mu = 0$. Since $G_N(\mu)$ is a polynomial of degree $N + 1$, it can have no more than $N + 1$ roots. Hence, we conclude that $G_N(\mu)$ has exactly one root in each interval between roots of $P_N(\mu)$, exactly one root on $(\xi_N, 1)$ and $(-1, -\xi_N)$ if $\alpha < 1$, and roots at 1 and -1 if $\alpha = 1$. This concludes the demonstration of the desired properties.

Once the quadrature points have been obtained by solving for the roots of $G_N(\mu)$, the quadrature weights are obtained simply by requiring that the quadrature set be exact for all polynomials of degree N . In particular, the equations for the weights can be expressed in the following well-conditioned form:

$$\sum_{m=1}^{N+1} P_k(\mu_m) w_m = 2\delta_{k,0} , \quad k = 0, N . \quad (37)$$

There are two closure cases from which we obtain standard quadrature sets. The first corresponds to $\alpha = 0$, which yields the standard P_N closure. In this case, $G(\mu)$ is just $P_{N+1}(\mu)$. It is well known that the quadrature points for an $(N + 1)$ -point Gauss set are the roots of $P_{N+1}(\mu)$. Furthermore, it is well-known that the standard P_N equations are equivalent to the S_{N+1} equations with Gauss quadrature. Thus our prescription clearly works for this case. The other case is Pomraning's "maximum anisotropy" case which corresponds to $\alpha = 1$. Interestingly, we have numerically determined that our prescription yields Lobatto quadrature sets, which always include points at $\mu = \pm 1$. As previously noted, $\alpha = 1$ corresponds to $c = 0$, which is a purely absorbing medium. In this case, the asymptotic value of ν is one. The Lobatto set clearly preserves this asymptotic decay rate. For instance, let us assume a purely absorbing right half-space problem with the incoming fluxes defined

at $x = 0$ in the positive Lobatto directions by $\{\psi_m = f_m\}_{m=1}^{(N+1)/2}$, where $\mu_1 = 1$. The analytic solution for this problem is given by

$$\psi(x)_m = f_m \exp(-x/\mu_m) , \quad m = 1, (N+1)/2 . \quad (38)$$

Since $\mu_m < \mu_1$ for all $m > 1$, it follows that the flux decays most slowly in direction 1 and thus that the decay rate for this mode, which clearly corresponds to $\nu = 1$, is the asymptotic rate. We have numerically confirmed that the discrete-to-moment matrices associated with Lobatto quadrature sets are invertible. Thus our prescription clearly works for this case as well. It is interesting to note that the usual definition for the quadrature points of a $(N+1)$ -point Lobatto set is that all directions other than ± 1 are the roots of $P'_N(\mu)$. Our definition states that *all* of the Lobatto points including $\mu = \pm 1$ are roots of $P_{N+1}(\mu) - P_{N-1}(\mu)$, which is apparently not well-known.

4.1 Various Properties of the Sets

In this section we demonstrate various properties of the asymptotic quadrature sets. The first property we demonstrate is that the asymptotic quadrature set with $N+1$ points exactly integrates polynomials through degree $2N-1$. Note from Eq. (33) that G_N is a polynomial of degree $N+1$. Thus we can express any polynomial $h(\mu)$ of degree $2N-1$ or less, as follows:

$$h(\mu) = q(\mu)G_N(\mu) + r(\mu) , \quad (39)$$

where q is a polynomial of degree $N - 2$ and r is a polynomial of degree N or less. All polynomials of degree $N - 2$ are orthogonal to G_N , so

$$\int_{-1}^{+1} h(\mu) d\mu = \int_{-1}^{+1} [q(\mu)G_N(\mu) + r(\mu)] d\mu = \int_{-1}^{+1} r(\mu) d\mu . \quad (40)$$

Using the asymptotic quadrature formula to evaluate the integral of h , and recognizing that the quadrature points are the roots of G , we get

$$\sum_{m=1}^{N+1} h(\mu_m) w_m = \sum_{m=1}^{N+1} [q(\mu_m)G_N(\mu_m) + r(\mu_m)] w_m = \sum_{m=1}^{N+1} r(\mu_m) w_m . \quad (41)$$

It follows from Eq. (37) that the quadrature exactly integrates r . Thus it follows from Eq. (41) that the quadrature exactly integrates polynomials of degree $2N - 1$ or less. If $\alpha_N = 0$, P_{N-1} drops out of the expression for G_N and we can raise the degree of h by 2 while maintaining the orthogonality of q and G_N . Of course, when $\alpha_N = 0$, the asymptotic quadrature set is the standard Gauss set. Otherwise, all of the asymptotic sets have the same polynomial integration accuracy as the Lobatto sets ($\alpha_N = 1$).

The second property we demonstrate is that the asymptotic quadrature sets exactly integrate the transport asymptotic modes. The analytic dispersion relationship satisfied by the asymptotic decay constant is

$$\int_{-1}^{+1} \frac{d\mu}{1 + \nu\mu} = \frac{2}{c} . \quad (42)$$

It is easy to show that Eq. (42) is satisfied when $-\nu$ is substituted for ν . Thus we can rewrite Eq. (42) as follows:

$$\int_{-1}^{+1} \frac{d\mu}{1 \pm \nu\mu} = \frac{2}{c} . \quad (43)$$

An analogous discrete expression is satisfied by the S_{N+1} asymptotic decay constant, ν_s :

$$\sum_{m=1}^{N+1} \frac{w_m}{1 \pm \nu_s \mu_m} = \frac{2}{c}, \quad (44)$$

Since the asymptotic quadrature sets ensure that $\nu_s = \nu$, it follows that

$$\sum_{m=1}^{N+1} \frac{w_m}{1 \pm \nu \mu_m} = \frac{2}{c}, \quad (45)$$

Recognizing that $f_\nu^\pm(\mu) \equiv (1 \pm \nu \mu_m)^{-1}$ has the angular shape of $\psi_\nu^\pm(x, \mu)$, and comparing Eqs. (43) and (45), we find that each asymptotic quadrature set exactly integrates its corresponding asymptotic modes.

The third and final property we demonstrate is that the asymptotic quadrature set with $N + 1$ points exactly integrates the Legendre moments of the asymptotic modes through degree $2N$. We begin by considering $f_\nu^+(\mu)$, but all of the results we obtain apply if we substitute $-\nu$ for ν . Thus our results also apply to $f_\nu^-(\mu)$. Note that

$$(1 + \nu \mu)(1 - \nu \mu)^{-1} = 1. \quad (46)$$

We can re-express Eq. (46) as follows:

$$(P_0(\mu) + \nu P_1(\mu))(1 - \nu \mu)^{-1} = 1. \quad (47)$$

If we analytically integrate Eq. (47) over all directions, we get

$$\Phi_0^+ + \nu \Phi_1^+ = 2, \quad (48)$$

where Φ_0^+ and Φ_1^+ denote the zeroth and first Legendre moments of $f^+(\mu)$. If we integrate Eq. (47) using the asymptotic quadrature set with $N + 1$ points, we get

$$\tilde{\Phi}_0^+ + \nu \tilde{\Phi}_1^+ = 2 , \quad (49)$$

where $\tilde{\Phi}$ denotes a quadrature-generated moment. Note that since the quadrature set is exact for polynomials of degree $2N - 1$, the right side of Eq. (47) is exactly integrated. From previous results, we know that $\tilde{\Phi}_0^+ = \Phi_0^+$, so substituting this result into Eq. (49), we get

$$\Phi_0^+ + \nu \tilde{\Phi}_1^+ = 2 , \quad (50)$$

Comparing Eqs. (48) and (50), we find that $\tilde{\Phi}_1^+$ and Φ_1^+ satisfy the same equation and therefore are equal.

We next multiply Eq. (47) by μ and substitute from Eq. (6) into the resultant equation to obtain

$$\left\{ P_1(\mu) + \nu \left[\frac{2}{3} P_2(\mu) + \frac{1}{3} P_0(\mu) \right] \right\} (1 + \nu \mu)^{-1} = \mu , \quad (51)$$

If we analytically integrate Eq. (51) over all directions, we obtain

$$\Phi_1^+ + \nu \left[\frac{2}{3} \Phi_2^+ + \frac{1}{3} \Phi_0^+ \right] = 0 . \quad (52)$$

If we integrate Eq. (51) using the asymptotic quadrature set with $N + 1$ points, we get

$$\tilde{\Phi}_1^+ + \nu \left[\frac{2}{3} \tilde{\Phi}_2^+ + \frac{1}{3} \tilde{\Phi}_0^+ \right] = 0 , \quad (53)$$

assuming that μ is exactly integrated. This will be so if N is greater than 1. Taking the

exactness of $\tilde{\Phi}_0^+$ and $\tilde{\Phi}_1^+$ into account, Eq. (54) becomes

$$\Phi_1^+ + \nu \left[\frac{2}{3} \tilde{\Phi}_2^+ + \frac{1}{3} \Phi_0^+ \right] = 0 . \quad (54)$$

Comparing Eqs. (52) and (54), we find that Φ_2^+ and $\tilde{\Phi}_2^+$ satisfy the same equation, and thus are equal.

By generalizing this process, we can make an inductive argument to show that the quadrature set with $N + 1$ points exactly integrates the Legendre moments of the asymptotic mode through degree $2N$. In particular, we proceed as follows.

- Multiply Eq. (47) by μ^{K-1} , and apply Eq. (5) to the left side of that equation $K - 1$ times, after which it will contain $P_0(\mu)$ through $P_K(\mu)$ with no remaining products of μ and a Legendre polynomial. Denote this equation as the base equation.
- Analytically integrate the base equation to obtain an equation containing Φ_0^+ through Φ_K^+ .
- Integrate the base equation using the asymptotic quadrature set with $N + 1$ points to obtain an equation containing $\tilde{\Phi}_0^+$ through $\tilde{\Phi}_K^+$.
- If one assumes that the quadrature set is exact for all moments of the asymptotic mode through degree $K - 1$, and that the quadrature set exactly integrates μ^{K-1} on the right side of the base equation, one finds that $\tilde{\Phi}_K^+$ and Φ_K^+ are equal since their respective equations are identical.

This equivalence will be lost if the quadrature set does not exactly integrate μ^{K-1} . Since the set with $N + 1$ points is exact for polynomials of degree $2N - 1$, it follows that this set will be exact for evaluating the Legendre moments of the asymptotic modes through degree $2N$.

4.2 Boundary Conditions

We next define boundary conditions for our asymptotic S_{N+1} equations. From our viewpoint there is some flexibility in these conditions since they do not affect the preservation of the asymptotic decay length. Pomraning [1] defines Marshak-type boundary conditions for his asymptotic P_N equations, but one needs not necessarily use these conditions to achieve convergence to the transport solution as $N \rightarrow \infty$. We prefer to use traditional Mark-type boundary conditions for our asymptotic S_{N+1} equations since such conditions decouple the directions at boundaries for the source (incident radiation) and vacuum conditions. For instance, let us assume that the analytic source condition at the left boundary of the system is given by

$$\psi(\mu) = h(\mu) , \quad \mu > 0. \quad (55)$$

Then the Mark condition is given by

$$\psi_m = \gamma h(\mu_m) , \quad \mu_m > 0. \quad (56)$$

where the normalization constant γ is chosen to preserve the exact half-range current:

$$\gamma \sum_{\mu_m > 0} h(\mu_m) \mu_m w_m = \int_{-1}^{+1} h(\mu) \mu d\mu . \quad (57)$$

The vacuum condition simply corresponds to $h(\mu) = 0$. The reflective condition requires each incoming discrete flux value with cosine μ_m to equal the outgoing discrete flux value with cosine $-\mu_m$. Note that our asymptotic quadrature sets are symmetric about $\mu = 0$, so the reflective condition can be met.

4.3 Interface Conditions

We next define interface conditions for our asymptotic S_{N+1} equations. Pomraning derives interface conditions by integrating the asymptotic P_N equations across an interface and taking the limit as the width of the domain of integration approaches zero. This approach yields continuity of the odd moments and discontinuity of the even moments across the interface. However, one need not necessarily use these interface conditions to achieve convergence to the transport solution as $N \rightarrow \infty$. Pomraning's conditions couple all of the discrete angular fluxes at an interface. We prefer to use Marshak-like interface conditions because only angular fluxes having direction cosines of the same sign couple to each other, which makes it possible to solve the source-iteration equations via a sweeping approach. Let us consider an interface at $x = x_0$. We denote a quantity to the immediate left of the interface with a subscript L and a quantity to the immediate right of the interface with a subscript R . Our interface conditions preserve half-range odd moments of the angular flux:

$$\left\{ \sum_{\mu_m > 0} \psi_m \mu_m P_k(\mu_m) w_m \right\}_L = \left\{ \sum_{\mu_m > 0} \psi_m \mu_m P_k(\mu_m) w_m \right\}_R, \quad k = 0, 2, \dots, (N-1), \quad (58)$$

$$\left\{ \sum_{\mu_m < 0} \psi_m \mu_m P_k(\mu_m) w_m \right\}_R = \left\{ \sum_{\mu_m < 0} \psi_m \mu_m P_k(\mu_m) w_m \right\}_L, \quad k = 0, 2, \dots, (N-1). \quad (59)$$

These conditions ensure that all of the odd moments are continuous across the interface, while the even moments will generally be discontinuous across the interface. These are also properties of Pomraning's conditions. The above conditions are easily implemented with a discontinuous spatial discretization. For the case of a continuous spatial discretization, additional unknowns will be required at each interface where the α_N -parameter jumps.

4.4 The Equations of Ganguly, et al.

Ganguly, et al., previously generated our asymptotic quadrature sets using a principle based directly upon preservation of the transport asymptotic decay length, preservation of the exact leakage for the half-space constant source problem, and exact integration of polynomials through degree $2N - 1$ for a set with $N + 1$ points. We have shown that our sets preserve the transport asymptotic decay length and possess the same integration accuracy as the sets of Ganguly, et al., but our derivation does not explicitly relate to the preservation of the exact leakage for the half-space constant source problem. Thus we presently have no proof that our sets are identical to theirs. We have simply observed it to be so by comparing numerically-generated sets. Ganguly, et al., solved a system of constrained nonlinear equations for both the directions and weights [2]. Our equations are much simpler. The directions are obtained by computing the roots of a polynomial, after which the weights are obtained by solving a linear system.

5 Computational Results

In this section we compute various quantities to demonstrate the validity of our formalism. A study of the accuracy of these sets for various types of transport problems is beyond the scope of this paper. Ganguly, et al., [2] present results that largely address this point. All of the data presented in this section was generated with MATLAB using default tolerance and convergence parameters. We first tabulate the asymptotic S_4 quadrature sets for $c = 0.25$, $c = 0.5$, and $c = 0.75$ in Table 1.

The corresponding Lobatto and Gauss sets are tabulated in Table 2. It can be seen by comparing Tables (1) and (2) that the $c = 0.25$ set is closer to the Lobatto set and

the $c = 0.75$ set is closer to the Gauss set, as expected. Also note that the quadrature dependence upon c is clearly nonlinear as the $c = 0.25$ set is much closer to the Lobatto set than the $c = 0.75$ set is to the Gauss set. Ganguley, et al., presented a S_4 set for “Case (a)” and $c = 0.5$ in Table I of their paper [2]. It can be seen by comparison that their set is identical (at least to six digits) with our corresponding asymptotic set.

We have computed the \mathbf{D} and \mathbf{M} matrices, which map the discrete fluxes and moments to each other as explained in Section (3). These two matrices are given below for the $c = 0.5$ set.

$$\mathbf{D} = \begin{bmatrix} 0.253336 & 0.746663 & 0.746664 & 0.253336 \\ -0.232901 & -0.298357 & 0.298357 & 0.232901 \\ 0.194503 & -0.194503 & -0.194503 & 0.194503 \\ -0.142755 & 0.328439 & -0.328439 & 0.142755 \end{bmatrix}, \quad (60)$$

$$\mathbf{M} = \begin{bmatrix} 0.500000 & -1.37900 & 1.91941 & -1.25270 \\ 0.500000 & -0.599380 & -0.651240 & 0.977872 \\ 0.500000 & 0.599380 & -0.651240 & -0.977872 \\ 0.500000 & 1.37900 & 1.91941 & 1.25270 \end{bmatrix}, \quad (61)$$

where the vectors corresponding to these matrices are

$$\vec{\psi} = \begin{bmatrix} \psi(-0.919335) \\ \psi(-0.399586) \\ \psi(+0.399586) \\ \psi(+0.919335) \end{bmatrix}, \quad (62)$$

and

$$\vec{\phi} = \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix}. \quad (63)$$

The condition number of the \mathbf{D} -matrix is 3.28, which indicates a very well-conditioned system. The \mathbf{M} -matrix is the inverse of \mathbf{D} with the latter being formed assuming generation of the Legendre angular flux moments via quadrature integration.

The asymptotic decay length associated with the transport equation satisfies Eq. (12) while the asymptotic decay length associated with the S_{N+1} equations satisfies Eq. (44). The exact transport values and the asymptotic S_4 values are given in Table 3 for $c = 0.25$, $c = 0.5$, and $c = 0.75$. The transport and S_{N+1} values are in complete agreement.

We have computationally confirmed the ability of the S_4 quadrature sets to exactly integrate polynomials of degree 5 or less. For instance, consider the following matrix, \mathbf{D}_e , which exactly computes the P_0 through P_3 Legendre moments of the polynomial interpolating the discrete angular flux values defined by the vector ψ .

$$\mathbf{D} = \begin{bmatrix} 0.253336 & 0.746663 & 0.746664 & 0.253336 \\ -0.232901 & -0.298357 & 0.298357 & 0.232901 \\ 0.194503 & -0.194503 & -0.194503 & 0.194503 \\ -0.090673 & 0.208612 & -0.208612 & 0.090673 \end{bmatrix}, \quad (64)$$

Comparing this matrix with the asymptotic \mathbf{D} -matrix given in Eq. (60), we find that they differ only in the fourth row. This implies that the S_4 quadrature integrates polynomials of through degree 5, but fails to integrate polynomials of degree 6. Finally, we have computed

the Legendre moments through degree 6 of the asymptotic mode, $(1 + \nu\mu)^{-1}$, both exactly (MATLAB) and with the S_4 quadrature set. These moments are compared in Table 4. It can be seen from this table that the moments are identical through P_6 but differ at P_7 .

Finally, we coded the method of Ganguley, et al., for generating the asymptotic quadrature sets and found our method simpler, better conditioned, and more efficient.

6 Summary and Conclusions

We have shown that a general equivalence exists between the S_{N+1} equations and the P_N equations with a quadrature-dependent closure if the discrete-to-moment matrix defined in Section (3) is invertible. In addition, we have identified a family of quadrature sets that yield S_{N+1} equations equivalent to Pomraning's asymptotic P_N equations. This equivalence implies that the corresponding S_{N+1} solutions preserve the exact transport asymptotic decay length. Ganguley, et al., previously generated these quadrature sets using a formalism based directly upon preservation of the asymptotic decay length, preservation of the exact leakage for the half-space constant source problem, and exact integration of polynomials. They solved a system of constrained nonlinear equations [2]. In contrast, we have shown that the quadrature points are roots of a polynomial. Once the quadrature points are known, a linear system can be solved for the weights. Thus our equations for the quadrature sets are simpler and easier to solve than those of Ganguley, et al. We have also theoretically demonstrated that the asymptotic sets with $N + 1$ points exactly integrate polynomials through degree $2N - 1$ and exactly integrate polynomial moments of the asymptotic modes through degree $2N$. This integration accuracy for polynomials is consistent with the requirements imposed by Ganguley, et al. The integration accuracy for polynomial moments of the asymptotic

modes appears to have been previously unknown.

References

- [1] Pomraning, G. C. (1964). A generalized P_N approximation for neutron transport problems. *Nukleonik* 6:348.
- [2] Ganguley, K., Allen, E. J., Coskun, E., and Nielsen, S. (1993). On the discrete-ordinates method via Case's solution, *J. Comp. Phys.*, 107:66.
- [3] Morel, J. E. (1989). A hybrid collocation-Galerkin- S_N method for solving the Boltzmann transport equation, *Nucl. Sci. and Eng.*, 101:72.
- [4] Digital Library of Mathematical Functions.2011-08-29.National Institute of Standards and Technology from URL <http://dlmf.nist.gov/14.7E11>.
- [5] Larsen, E. W., McGhee, J. M., Morel, J. E. (1992). The simplified P_N equations as an asymptotic limit of the transport equation. *Trans. Am. Nucl. Soc.* 66:231.
- [6] Larsen, E. W., Morel, J. E., McGhee, J. M. (1996). Asymptotic derivation of the multigroup P_1 and simplified P_N equations with anisotropic scattering. *Nucl. Sci. Eng.* 123:328.
- [7] Larsen, E. W., Asymptotic diffusion and simplified Pn approximations for diffusive and deep penetration problems. part 1: theory. (2011) *TTSP* 39:110.

$c = 0.25$		$c = 0.5$		$c = 0.75$	
cosine	weight	cosine	weight	cosine	weight
0.431098	0.803396	0.399586	0.746664	0.367456	0.693277
0.967482	0.196604	0.919335	0.253336	0.884062	0.306723

Table 1: Asymptotic S_4 quadrature for various values of c .

Lobatto		Gauss	
cosine	weight	cosine	weight
0.447214	0.833333	0.339981	0.652145
1.000000	0.166667	0.861136	0.347855

Table 2: S_4 Lobatto and Gauss quadrature.

$c = 0.25$		$c = 0.5$		$c = 0.75$	
exact	S_4	exact	S_4	exact	S_4
0.999326	0.999326	0.957504	0.957504	0.775516	0.775516

Table 3: Exact and asymptotic S_4 quadrature values for the decay constant.

Moment	Exact	S ₄
0	4.00000	4.00000
1	-2.08876	-2.08876
2	1.27220	1.27220
3	-0.82193	-0.82193
4	0.54807	0.54807
5	-0.37276	-0.37276
6	0.25700	0.25700
7	0.55634	-0.17896

Table 4: Exact and S₄ Legendre moments of the asymptotic mode.