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SIMPLIFIED P_N EQUATIONS WITH ANISOTROPIC SCATTERING

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ASYMPTOTIC DERIVATION OF THE MULTIGROUP P_1 AND SIMPLIFIED P_N EQUATIONS WITH ANISOTROPIC SCATTERING

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ABSTRACT

The multigroup P_1 and Simplified P_N equations are shown to be a family of asymptotic approximation to the multigroup transport equation with anisotropic scattering. The physical assumptions are that the material system is optically thick, the probability of absorption is small, and the mean scattering angle $\bar{\mu}_0$ is not close to unity.

I. INTRODUCTION

The Simplified P_N (SP_N) equations were originally proposed by Gelbard in the early 1960's as a relatively easy way to include additional transport physics into the P_1 model without resorting to the more complicated P_N equations.¹⁻³ During the succeeding 30 years, other researchers⁴⁻¹³ have experimented computationally with the SP_N equations and have usually concluded that SP_N solutions are significantly more transport-like than diffusion solutions. For example, Gamino^{12,13} has reported that low-order SP_N solutions often capture "greater than 80%" of the transport corrections to diffusion theory.

One of the reasons for this success is that in planar geometry, the SP_N equations exactly reduce to the P_N (and hence S_{N+1}) equations. However, recent theoretical work¹⁴⁻²¹ has explained other reasons for these successful computational results: SP_N theory is an asymptotic correction to P_1 theory for problems in which P_1 theory is an asymptotic approximation to transport theory. Also, the SP_N equations have been derived variationally in certain cases. These asymptotic and variational derivations have mostly been limited to one-group transport problems with isotropic scattering. However, Larsen has recently sketched a derivation of the SP_N equations for multigroup transport problems with isotropic scattering.¹⁹

In this paper, we extend the analysis in Ref. 19 and derive the SP_N equations as an asymptotic limit of the fully general 3-D multigroup transport equation with arbitrary anisotropic scattering. Our physical assumptions are that the system is optically thick, that scattering dominates absorption, and that the mean scattering angle $\bar{\mu}_0$ is not close to unity. In such circumstances, we show that multigroup P_1 theory is the leading-order asymptotic expansion of the transport equation, that multigroup SP_2 theory is the first asymptotic correction to P_1 theory, and that multigroup SP_3 theory is the second asymptotic correction to P_1 theory. Our analysis can be continued for $N > 3$, but we will not do so here.

The remainder of this paper is organized as follows. In Sec. II we establish notation and derive, by the conventional method, the multigroup SP_2 and SP_3 equations. In Sec. III we asymptotically derive the multigroup P_1 , SP_2 , and SP_3 equations. We conclude with numerical results in Sec. IV and a brief discussion in Sec. V.

II. CONVENTIONAL DERIVATION OF THE SP_N EQUATIONS

We shall consider the multigroup transport equation

$$\Omega_i \frac{\partial}{\partial x_i} \psi(\mathbf{x}, \Omega) + \Sigma_t(\mathbf{x}) \psi(\mathbf{x}, \Omega) = \int_{4\pi} \Sigma_s(\mathbf{x}, \Omega \cdot \Omega') \psi(\mathbf{x}, \Omega') d^2\Omega' + \frac{Q(\mathbf{x})}{4\pi} , \quad \mathbf{x} \in V , \quad |\Omega| = 1 , \quad (1)$$

defined in a physical region V . The notation in Eq. (1) is standard: $\underline{x} = (x_1, x_2, x_3)$ is the spatial variable; $\underline{\Omega} = (\Omega_1, \Omega_2, \Omega_3)$ with $|\underline{\Omega}| = 1$ is the angular variable; $\psi(\underline{x}, \underline{\Omega})$ is a $G \times 1$ vector whose g -th component is the angular flux of neutrons in group g at the point \underline{x} travelling in the direction $\underline{\Omega}$; $\Sigma_t(\underline{x})$ is the total cross section (a $G \times G$ diagonal matrix), $\Sigma_s(\underline{x}, \mu_0)$ is the differential scattering cross section (a $G \times G$ matrix); $Q(\underline{x})$ is the interior source (a $G \times 1$ vector); and we use the summation convention: repeated subscripts are summed from 1 to 3. The boundary condition is

$$\psi(\underline{x}, \underline{\Omega}) = \psi^b(\underline{x}, \underline{\Omega}) , \quad \underline{x} \in \partial V , \quad \underline{\Omega} \cdot \underline{n} < 0 , \quad (2)$$

where ψ^b is the prescribed incident angular flux and \underline{n} is the unit outer normal. The differential scattering cross section has the expansion

$$\Sigma_s(\underline{x}, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \Sigma_{sn}(\underline{x}) P_n(\mu_0) , \quad (3)$$

where $P_n(\mu)$ is the Legendre polynomial of order n .

The standard derivation of the SP_N equations is partly motivated by the following observation. If we write the planar-geometry P_1 equations that correspond to Eq. (1),

$$\frac{d}{dx} \phi_1(x) + [\Sigma_t(x) - \Sigma_{s0}(x)] \phi_0(x) = Q(x) , \quad (4)$$

$$\frac{1}{3} \frac{d}{dx} \phi_1(x) + [\Sigma_t(x) - \Sigma_{s1}(x)] \phi_1(x) = 0 , \quad (5)$$

and we formally

1. replace the scalar derivative $\frac{d}{dx}$ by the gradient operator $\frac{\partial}{\partial x_i}$,
2. replace all odd-order moments $\phi_n(x)$ by $\phi_{n,i}(\underline{x})$,
3. replace all even-order moments $\phi_n(x)$ by $\phi_n(\underline{x})$,

then we obtain

$$\frac{\partial}{\partial x_i} \phi_{1,i}(\underline{x}) + [\Sigma_t(\underline{x}) - \Sigma_{s0}(\underline{x})] \phi_0(\underline{x}) = Q(\underline{x}) , \quad (6)$$

$$\frac{1}{3} \frac{\partial}{\partial x_i} \phi_0(\underline{x}) + [\Sigma_t(\underline{x}) - \Sigma_{s1}(\underline{x})] \phi_{1,i}(\underline{x}) = 0 , \quad i = 1, 2, 3 . \quad (7)$$

These are the familiar 3-D multigroup P_1 equations. By using Eq. (7) to eliminate $\phi_{1,i}$ from Eq. (6), we obtain the following system of G coupled diffusion equations in the G unknowns $\phi_0(\underline{x})$:

$$-\frac{\partial}{\partial x_i} \left(\frac{1}{3} \Sigma_{a1}^{-1} \right) \frac{\partial}{\partial x_i} \phi_0 + \Sigma_{a0} \phi_0 = Q . \quad (8)$$

(Here we have defined the $G \times G$ matrices

$$\Sigma_{an} \equiv \Sigma_t - \Sigma_{sn} , \quad n \geq 0 . \quad (9)$$

Also, boundary conditions for Eqs. (6) and (7) [or (8)] can be obtained formally from planar-geometry boundary conditions for Eqs. (4) and (5) by simply replacing ϕ_1 by $n_i \phi_{1,i}$ (where, again, $\underline{n} = (n_1, n_2, n_3)$ is the unit outer normal).

Applying this same formal procedure to the planar-geometry P_2 equations, one obtains the following SP₂ equations:

$$\frac{\partial}{\partial x_i} \phi_{1,i}(\underline{x}) + \Sigma_{a0}(\underline{x}) \phi_0(\underline{x}) = Q(\underline{x}) , \quad (10)$$

$$\frac{\partial}{\partial x_i} \left[\frac{1}{3} \phi_0(\underline{x}) + \frac{2}{3} \phi_2(\underline{x}) \right] + \Sigma_{a1}(\underline{x}) \phi_{1,i}(\underline{x}) = 0 , \quad i = 1, 2, 3 , \quad (11)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[\frac{2}{5} \phi_{1,i}(\underline{x}) \right] + \Sigma_{a2}(\underline{x}) \phi_2(\underline{x}) = 0 . \quad (12)$$

By using Eqs. (11) and (12) to eliminate $\phi_{1,i}$ and ϕ_2 from Eqs. (10), one reduces these equations to the following G coupled diffusion equations in the G unknowns $\phi_i(\underline{x})$:

$$-\frac{\partial}{\partial \mathbf{x}_i} \left(\frac{1}{3} \Sigma_{a1}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} \left[\phi_0 + \frac{4}{5} \Sigma_{a2}^{-1} (\Sigma_{a0} \phi_0 - Q) \right] + \Sigma_{a0} \phi_0 = Q . \quad (13)$$

In contrast, the full P_2 equations have 9G equations and unknowns. Boundary conditions for Eqs. (10)-(12) [or (13)] can be obtained from planar-geometry conditions using the same formal procedure as with the P_1 equations.

Also, applying the same formal procedure to the planar geometry P_3 equations, one obtains the following SP_3 equations:

$$\frac{\partial}{\partial \mathbf{x}_i} \phi_{1,i}(\underline{x}) + \Sigma_{a0}(\underline{x}) \phi_0(\underline{x}) = Q(\underline{x}) , \quad (14)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[\frac{1}{3} \psi_0(\underline{x}) + \frac{2}{3} \phi_2(\underline{x}) \right] + \Sigma_{a1}(\underline{x}) \phi_{1,i}(\underline{x}) = 0 , \quad i = 1, 2, 3 , \quad (15)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[\frac{2}{5} \phi_{1,i}(\underline{x}) + \frac{3}{5} \phi_{3,i}(\underline{x}) \right] + \Sigma_{a2}(\underline{x}) \phi_2(\underline{x}) = 0 , \quad (16)$$

$$\frac{\partial}{\partial \mathbf{x}_i} \left[\frac{3}{7} \phi_2(\underline{x}) \right] + \Sigma_{a3}(\underline{x}) \phi_{3,i}(\underline{x}) = 0 , \quad i = 1, 2, 3 . \quad (17)$$

By using Eqs. (15) and (17) to eliminate $\phi_{1,i}$ and $\phi_{3,i}$ from Eqs. (14) and (16), and slightly rearranging, one obtains the following 2G coupled diffusion equations in the 2G unknowns $\phi_0(\underline{x})$ and $\phi_2(\underline{x})$:

$$-\frac{\partial}{\partial \mathbf{x}_i} \left(\frac{1}{3} \Sigma_{a1}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} (\phi_0 + 2\phi_2) + \Sigma_{a0} \phi_0 = Q , \quad (18)$$

$$-\frac{\partial}{\partial \mathbf{x}_i} \left(\frac{9}{35} \Sigma_{a3}^{-1} \right) \frac{\partial}{\partial \mathbf{x}_i} \phi_2 + \Sigma_{a2} \phi_2 = \frac{2}{5} (\Sigma_{a0} \phi_0 - Q) . \quad (19)$$

In contrast, the full P_3 equations have 16G equations and unknowns. Boundary conditions for Eqs. (14)-(17) can be obtained from planar-geometry conditions using the same formal procedure as with the P_1 equations.

Of course, the above derivations of the SP_2 and SP_3 equations are ad-hoc. This apparent lack of a solid theoretical basis has likely contributed to the historical neglect of the SP_N equations, even though the computational experience with these equations has been quite favorable.

III. ASYMPTOTIC DERIVATION OF THE P_1 AND SP_N EQUATIONS

We consider Eq. (1) for optically thick systems that are dominated by scattering, for which scattering is not extremely forward-peaked, and for which the solution ψ is $O(1)$. Such a situation occurs if Σ_t , Σ_s , and Q satisfy:

$$\Sigma_t(\underline{x}) = \frac{1}{\varepsilon} \sigma_t(\underline{x}) , \quad (20)$$

$$\Sigma_{sn}(\underline{x}) = \frac{1}{\varepsilon} \sigma_{sn}(\underline{x}) , \quad n \geq 0 , \quad (21)$$

$$Q(\underline{x}) = \varepsilon q(\underline{x}) , \quad (22)$$

$$\sup_{\|u\|=1} \|(\sigma_t - \sigma_{sn})^{-1} u\| = \begin{cases} O(\varepsilon^{-2}) & , n=0 \\ O(1) & , n \geq 1 \end{cases} , \quad (23)$$

where σ_t , σ_s , and q are $O(1)$ and ε is a small, positive dimensionless parameter. Eq. (20) implies that the mean free path is small, of $O(\varepsilon)$, so the system V is $O(\varepsilon^{-1})$ mean free paths thick. It can be shown that Eq. (23) for $n = 0$

holds if the probability of absorption is small, of $O(\varepsilon^2)$, and for $n \geq 1$ holds if scattering is not highly forward-peaked. (These results are independent of the kind of group-to-group coupling that exists due to scattering; these coupling terms can be $O(1)$, or they can be small.) Eqs. (20)-(23) imply that the infinite-medium solution

$$\psi = \frac{1}{4\pi} (\Sigma_t - \Sigma_{s0})^{-1} Q = \frac{1}{4\pi} \left[\frac{1}{\varepsilon} (\sigma_t - \sigma_{s0}) \right]^{-1} \varepsilon q = \frac{1}{4\pi} (\sigma_t - \sigma_{s0})^{-1} \varepsilon^2 q \quad (24)$$

is $O(1)$. If we define

$$\sigma_s(\underline{x}, \mu_0) = \varepsilon \Sigma_s(\underline{x}, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} \sigma_{sn}(\underline{x}) P_n(\mu_0) \quad , \quad (25)$$

then Eq. (1) may be written as

$$\Omega_i \frac{\partial}{\partial x_i} \psi(\underline{x}, \underline{\Omega}) + \frac{1}{\varepsilon} \sigma_t(\underline{x}) \psi(\underline{x}, \underline{\Omega}) = \frac{1}{\varepsilon} \int_{4\pi} \sigma_s(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' + \varepsilon \frac{q(\underline{x})}{4\pi} \quad . \quad (26)$$

Now, let us define

$$\phi_0(\underline{x}) = \int_{4\pi} \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (27)$$

$$\phi_1(\underline{x}) = \int_{4\pi} \underline{\Omega}' \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (28)$$

$$P\psi(\underline{x}, \underline{\Omega}) = \frac{1}{4\pi} \int_{4\pi} \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad . \quad (29)$$

Operating on Eq. (26) by P and $(I - P)$, we obtain the balance equation

$$\frac{\partial}{\partial x_i} \phi_{1,i} + \frac{1}{\varepsilon} (\sigma_t - \sigma_{s0}) \phi_0 = \varepsilon q \quad , \quad (30)$$

and

$$(I - P) \Omega_i \frac{\partial}{\partial x_i} \psi + \frac{\sigma_t}{\varepsilon} \left(\psi - \frac{1}{4\pi} \phi_0 \right) = \frac{1}{\varepsilon} \int_{4\pi} \left(\sum_{n=1}^{\infty} \frac{2n+1}{4\pi} \sigma_{sn} P_n(\underline{\Omega} \cdot \underline{\Omega}') \right) \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad . \quad (31)$$

If we define the operator L by

$$L\psi(\underline{x}, \underline{\Omega}) \equiv \sigma_t \psi(\underline{x}, \underline{\Omega}) - \int_{4\pi} \left(\sum_{n=1}^{\infty} \frac{2n+1}{4\pi} \sigma_{sn} P_n(\underline{\Omega} \cdot \underline{\Omega}') \right) \psi(\underline{x}, \underline{\Omega}') d^2 \Omega' \quad , \quad (32)$$

then Eq. (31) may be written more compactly as

$$L\psi + \varepsilon(I - P) \Omega_i \frac{\partial}{\partial x_i} \psi = \frac{\sigma_t}{4\pi} \phi_0 \quad . \quad (33)$$

L is very similar to the collision operator [the $O(\varepsilon^{-1})$] terms in Eq. (26), but L does not contain the $n = 0$ part of the scattering operator. Thus, if scattering is isotropic, L reduces to a simple multiplicative operator. Also, from the assumptions (23), L^{-1} exists and is $O(1)$. Thus, Eq. (33) may be written

$$\left[I + \varepsilon L^{-1}(I - P) \Omega_i \frac{\partial}{\partial x_i} \right] \psi = \frac{1}{4\pi} \phi_0 \quad . \quad (34)$$

Hence,

$$\psi = \left[I + \varepsilon L^{-1}(I - P) \Omega_i \frac{\partial}{\partial x_i} \right]^{-1} \frac{\phi_0}{4\pi} \quad , \quad (35)$$

and introducing this into Eq. (28), we obtain

$$\phi_{1,i}(\underline{x}) = \frac{1}{4\pi} \int_{4\pi} \Omega_i \left[I + \varepsilon L^{-1}(I - P) \Omega_j \frac{\partial}{\partial x_j} \right]^{-1} \phi_0(\underline{x}) d^2 \Omega \quad . \quad (36)$$

Eqs. (30) and (36) are an exact system of equations for the scalar flux ϕ_0 and the current $\phi_{1,i}$. However, Eq. (36) is too complicated to be of immediate use, so we shall approximate it by expanding it for $\epsilon \ll 1$. The result is:

$$\phi_{1,i}(\underline{x}) \approx \sum_{n=0}^{\infty} \epsilon^n L_{i,n} \phi(\underline{x}) , \quad (37)$$

where the operators $L_{i,n}$ are defined by:

$$L_{i,n} \phi(\underline{x}) = \frac{(-1)^n}{4\pi} \int_{4\pi} \Omega_i [L^{-1}(I - P)\underline{\Omega} \cdot \underline{\nabla}]^n \phi_0(\underline{x}) d^2\Omega . \quad (38)$$

The first few operators $L_{i,n}$ can easily be evaluated using the following facts, which we state without proof.

1. For each i , the quantity

$$\omega_i \equiv \Omega_i \quad (39)$$

is a linear combination of spherical harmonic functions of order 1.

2. For each i and j , the quantity

$$\omega_{ij} \equiv \Omega_i \Omega_j - \frac{1}{3} \delta_{ij} \quad (40)$$

is a linear combination of spherical harmonic functions of order 2.

3. For each i, j , and k , the quantity

$$\omega_{ijk} \equiv \Omega_i \Omega_j \Omega_k - \frac{1}{5} (\Omega_i \delta_{jk} + \Omega_j \delta_{ki} + \Omega_k \delta_{ij}) \quad (41)$$

is a linear combination of spherical harmonic functions of order 3.

4. For each i, j, k , and l , the quantity

$$\begin{aligned} \omega_{ijkl} &\equiv \Omega_i \Omega_j \Omega_k \Omega_l - \frac{1}{7} (\Omega_i \Omega_j \delta_{kl} + \Omega_i \Omega_k \delta_{jl} + \Omega_i \Omega_l \delta_{jk} + \Omega_j \Omega_k \delta_{il} + \Omega_j \Omega_l \delta_{ik} + \Omega_k \Omega_l \delta_{ij}) \\ &\quad + \frac{1}{35} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \end{aligned} \quad (42)$$

is a linear combination of spherical harmonic functions of order 4.

Therefore, with L defined by Eq. (32), one has

$$L^{-1} \omega_i = (\sigma_i - \sigma_{s1})^{-1} \omega_i , \quad (43)$$

$$L^{-1} \omega_{ij} = (\sigma_i - \sigma_{s2})^{-1} \omega_{ij} , \quad (44)$$

$$L^{-1} \omega_{ijk} = (\sigma_i - \sigma_{s3})^{-1} \omega_{ijk} , \quad (45)$$

$$L^{-1} \omega_{ijkl} = (\sigma_i - \sigma_{s3})^{-1} \omega_{ijkl} . \quad (46)$$

We will now explicitly calculate $L_{i,0}$ and $L_{i,1}$. For $n = 0$,

$$L_{i,0} \phi = \frac{1}{4\pi} \int_{4\pi} \Omega_i \phi d^2\Omega = \left(\frac{1}{4\pi} \int_{4\pi} \Omega_i d^2\Omega \right) \phi = 0 , \quad (47)$$

because the integrand is an odd function of $\underline{\Omega}$. For $n = 1$,

$$L^{-1}(I - P)\underline{\Omega} \cdot \underline{\nabla} \phi = L^{-1} \omega_j \frac{\partial}{\partial x_j} \phi = (\sigma_i - \sigma_{s1})^{-1} \omega_j \frac{\partial}{\partial x_j} \phi = (\sigma_i - \sigma_{s1})^{-1} \Omega_j \frac{\partial}{\partial x_j} \phi . \quad (48)$$

Therefore, if we define

$$\sigma_{an} = \sigma_i - \sigma_{sn} = \varepsilon \Sigma_{an} , \quad n \geq 0 , \quad (49)$$

then, using Eq. (40)

$$\begin{aligned} L_{i,1}\phi &= -\frac{1}{4\pi} \int_{4\pi} \Omega_i \sigma_{a1}^{-1} \Omega_j \frac{\partial}{\partial x_j} \phi d^2\Omega = -\left(\frac{1}{4\pi} \int_{4\pi} \Omega_i \Omega_j d^2\Omega\right) \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi \\ &= -\left[\frac{1}{4\pi} \int_{4\pi} \left(\omega_{ij} + \frac{1}{3} \delta_{ij}\right) d^2\Omega\right] \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi = -\frac{1}{3} \delta_{ij} \sigma_{a1}^{-1} \frac{\partial}{\partial x_j} \phi = -\frac{1}{3} \sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \phi . \end{aligned} \quad (50)$$

Proceeding in this manner, using Eqs. (39)-(46), we obtain

$$L_{i,n}\phi = 0 \quad \text{for } n \text{ even} , \quad (51)$$

because for n even, the integral defining $L_{i,n}$ has an integrand which is an odd function of Ω . For n odd, the operators $L_{i,n}$ do not vanish and are quite complicated. However, for homogeneous-medium problems, or for heterogeneous-medium problems in which the solution behaves nearly one-dimensionally near interfaces (i.e. tangential directional derivatives at interfaces can be ignored), these operators simplify. If for $n \geq i$ we define

$$M_n \equiv \frac{\partial}{\partial x_i} \sigma_{an}^{-1} \frac{\partial}{\partial x_j} \equiv \nabla \cdot \sigma_{an}^{-1} \nabla , \quad (52)$$

then we obtain

$$L_{i,3}\phi = -\sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \sigma_{a2}^{-1} \left(\frac{4}{45} M_1\right) \phi , \quad (53)$$

and

$$L_{i,5}\phi = -\sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi . \quad (54)$$

Thus, Eqs. (37) and (50)-(54) give

$$\phi_{1,i} = -\varepsilon \sigma_{a1}^{-1} \frac{\partial}{\partial x_i} \left[\frac{1}{3} \phi + \varepsilon^2 \sigma_{a2}^{-1} \left(\frac{4}{45} M_1\right) \phi + \varepsilon^4 \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi \right] + O(\varepsilon^7) . \quad (55)$$

Introducing this into the balance equation (30), we obtain

$$-\frac{\varepsilon}{3} M_1 \phi - \frac{4\varepsilon^3}{45} M_1 \sigma_{a2}^{-1} M_1 \phi - \varepsilon^5 M_1 \sigma_{a2}^{-1} \left(\frac{16}{675} M_1 + \frac{4}{175} M_3\right) \sigma_{a2}^{-1} M_1 \phi + \frac{1}{\varepsilon} (\sigma_i - \sigma_{s0}) \phi = \varepsilon q + O(\varepsilon^7) . \quad (56)$$

This is a sixth-order partial differential equation for ϕ . It is asymptotically equivalent to the transport equation (26) with $O(\varepsilon^7)$ error.

Now we shall show that the SP_N equations asymptotically agree with Eq. (56) through terms of order ε^{2N+1} . To do this, we first ignore terms in Eq. (56) of $O(\varepsilon^3)$ and obtain

$$-\frac{\partial}{\partial x_i} \left(\frac{\varepsilon}{3} \sigma_{a1}^{-1}\right) \frac{\partial}{\partial x_i} \phi_0 + \frac{1}{\varepsilon} \sigma_{a0} \phi_0 = \varepsilon q . \quad (57)$$

Using Eqs. (20)-(22) and (49), we see that this is identical to the multigroup P₁ equations (8). Thus, the multigroup P₁ equations are an asymptotic approximation to the transport equation, with an $O(\varepsilon^3)$ error.

Next, we ignore terms in Eq. (56) of $O(\varepsilon^5)$ and obtain

$$-\left(I + \frac{4\varepsilon^2}{15} M_1 \sigma_{a2}^{-1}\right) \left(\frac{\varepsilon}{3} M_1\right) \phi + \frac{1}{\varepsilon} \sigma_{a0} \phi = \varepsilon q + O(\varepsilon^5) , \quad (58)$$

or

$$-\left(I - \frac{4\varepsilon^2}{15} M_1 \sigma_{a2}^{-1}\right)^{-1} \left(\frac{\varepsilon}{3} M_1\right) \phi + \frac{1}{\varepsilon} \sigma_{a0} \phi = \varepsilon q + O(\varepsilon^5) . \quad (59)$$

Hence, dropping the error term,

$$-\frac{\varepsilon}{3}M_1\phi + \left(I - \frac{4\varepsilon^2}{15}M_1\sigma_{a2}^{-1}\right) \left(\frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q\right) = 0 , \quad (60)$$

or

$$-\frac{\varepsilon}{3}M_1 \left[\phi + \frac{4\varepsilon}{5}\sigma_{a2}^{-1} \left(\frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q \right) \right] + \frac{1}{\varepsilon}\sigma_{a0}\phi = \varepsilon q . \quad (61)$$

Using Eqs. (20)-(22) and (49), we see that this is identical to the multigroup SP₂ equations (13). Thus, the multigroup SP₂ equations are an asymptotic approximation to the transport equation with an error of O(ε^5), provided that the physical system is homogeneous or the solution has sufficiently weak tangential derivatives at material interfaces. (This proviso is not needed for the multigroup P₁ equations.)

Finally, we ignore terms in Eq. (56) of O(ε^7). The resulting equation may be written

$$-\frac{\varepsilon}{3}M_1(\phi + 2\phi_2) + \frac{1}{\varepsilon}\sigma_{a0}\phi = \varepsilon q , \quad (62)$$

where

$$\begin{aligned} \phi_2 &= \left[I + \varepsilon^2\sigma_{a2}^{-1} \left(\frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right] \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi + O(\varepsilon^6) \\ &= \left[I - \varepsilon^2\sigma_{a2}^{-1} \left(\frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right]^{-1} \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi + O(\varepsilon^6) . \end{aligned} \quad (63)$$

Dropping the error term, we may rewrite Eq. (63) as

$$\left[I - \varepsilon^2\sigma_{a2}^{-1} \left(\frac{4}{15}M_1 + \frac{9}{35}M_3 \right) \right] \phi_2 = \frac{2\varepsilon^2}{15}\sigma_{a2}^{-1}M_1\phi . \quad (64)$$

Multiplying by σ_{a2}/ε , rearranging, and using Eq. (62), we obtain

$$-\frac{9\varepsilon}{35}M_3\phi_2 + \frac{1}{\varepsilon}\sigma_{a2}\phi_2 = \frac{2}{5} \left[\frac{\varepsilon}{3}M_1(\phi + 2\phi_2) \right] = \frac{2}{5} \left(\frac{1}{\varepsilon}\sigma_{a0}\phi - \varepsilon q \right) . \quad (65)$$

Using Eqs. (20)-(22) and (49), we see that Eqs. (62) and (65) are identical to the multigroup SP₃ equations (18) and (19). Thus, the multigroup SP₃ equations are an asymptotic approximation to the transport equation with an error of O(ε^7), provided that the physical system is homogeneous or the solution has sufficiently weak tangential derivatives at material interfaces.

IV. NUMERICAL RESULTS

In this section give a computational comparison of the multigroup P₁, SP₃, and S₄ methods with anisotropic scattering for calculating the k-eigenvalue of a small supercritical sphere of uranium. The uranium has a density of 37.4 g/cm³ and is composed of the isotopes U²³⁴, U²³⁵, and U²³⁸, with atomic fractions of 0.001054, 0.93737, and 0.05209, respectively. The sphere has a radius of 6.9355 cm. All calculations were performed with NIKE, a 3-D even-parity unstructured tetrahedral-mesh code which offers options for both the S_N and SP_N methods. The sphere was modeled with 2587 nodes and 13,120 tetrahedra. All of the calculations were performed on the massively-parallel Connection Machine-200 computer at LANL using a 12-group P₁ set of MENDEF-5 cross-sections.²³

The computational results are given in Table 1. (We also calculated a benchmark result for k_{eff} using a 1-D spherical geometry transport code with an extremely fine spatial mesh and the S₁₀₀ quadrature set; the resulting eigenvalue is k_{eff} = 1.3923, which is very close to the S₄ value given in Table 1.) It can be seen that the SP₃ eigenvalue differs from the S₄ eigenvalue by about one percent, whereas the P₁ eigenvalue differs from the S₄ eigenvalue by about five percent. Comparing CPU times, we find that the SP₃ method is about four times faster than the S₄

method. Although the P_1 method appears to be less than twice as fast as the SP_3 method, the particular solution algorithm used in NIKE is not optimal for the P_1 method and runs about twice as long as an optimal algorithm would. Thus, an optimal P_1 method would be about three times faster than the SP_3 method. Overall, our SP_N results behave as expected. For the problem considered, the SP_3 solution is much more accurate than diffusion (P_1) solution, but much less costly than the S_4 solution method.

Method	k_{eff}	CPU Time (s)
P_1	1.328	211
SP_3	1.408	300
S_4	1.390	1351

Table 1: P_1 , SP_2 , and S_4 Eigenvalues

IV. DISCUSSION

In this paper, we have shown that if the multigroup neutron transport equation with anisotropic scattering is considered for problems in which, for $\varepsilon \ll 1$,

1. the physical system is $O(\varepsilon^{-1})$ mean free paths thick,
2. the probability of absorption is $O(\varepsilon^2)$,
3. the mean scattering cosine is not close to unity,

then:

1. the P_1 equations are an asymptotic approximation to the transport equation with error $O(\varepsilon^3)$,
2. the SP_2 and SP_3 equations are an asymptotic approximation to the transport equation with respective errors $O(\varepsilon^5)$ and $O(\varepsilon^7)$, provided that either (i) the physical system is homogeneous or (ii) the system is heterogeneous, and the transport solution has weak tangential derivatives at material interfaces.

Therefore, the SP_N equations can be understood as asymptotic corrections to P_1 theory. Also, for planar geometry problems, they exactly reduce to the P_N (or, S_{N+1}) equations. In practice, the SP_N solutions are most accurate for problems that are reasonably close to ones that could be called "diffusive," or for problems that have transport regions in which the solution behaves nearly one-dimensionally. (This latter case of course includes all one-dimensional geometries.) For problems that have strong multidimensional transport effects, such as voids, with streaming regions, or geometrically complex spatial inhomogeneities, the SP_N solutions are less accurate.

In general, if a transport problem is one in which the standard diffusion or P_1 approximation is reasonably accurate (but perhaps not as accurate as desired), then the SP_N approximations should be significantly more accurate (i.e., transport-like). This is the general observation of researchers who have experimented numerically with the SP_N equations, and it is consistent with our asymptotic theory. Thus, used for the proper kinds of problems, SP_N theory can be an accurate and relatively inexpensive way of including additional transport physics in a conventional diffusion code.

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REFERENCES

1. E.M. Gelbard, "Application of Spherical Harmonics Method to Reactor Problems," WAPD-BT-20 (September, 1960)
2. E.M. Gelbard, "Simplified Spherical Harmonics Equations and Their Use in Shielding Problems," WAPD-T-1182 (Rev. 1), (February, 1961).
3. E.M. Gelbard, "Applications of the Simplified Spherical Harmonics Equations in Spherical Geometry," WAPD-TM-294 (April, 1962).
4. C. Dawson, "Modified P_2 Approximations to the Neutron Transport Equation," DTMB-1814, David Taylor Model Basin, Dept. of Navy, Washington, D.C. (1964).
5. J.A. Davis, "Transport Error Bounds Via P_N Approximations," *Nucl. Sci. Eng.* **31**, 127 (1968).
6. D.S. Selengut, "A New Form of the P_3 Approximation," *Trans. Am. Nucl. Soc.* **13**, 625 (1970). Also published in Proc. ANS Topical Mtg., *New Developments in Reactor Mathematics and Applications*, March 29-31, 1971, Idaho Falls, CONF-710302, Vol. 2, p. 561 (1971).
7. M. Lemanska, "On the Simplified P_N Method in the 2D Diffusion Code EXTERMINATOR," *Atomkernenergie* **37**, 173 (1981).
8. K.S. Smith, "Multidimensional Nodal Transport Using the Simplified P_L Method," Proc. ANS Topical Mtg., *Reactor Physics and Safety*, Saratoga Springs, NY, p. 223, (September, 1986).
9. K.S. Smith, "Multidimensional Nodal Transport Using the Simplified P_L Method," *Trans. Am. Nucl. Soc.* **52**, 427 (1986).
10. Y.H. Liu and E.M. Gelbard, "Accuracy of Nodal Transport and Simplified P_3 Fluxes in Benchmark Tests," *Trans. Am. Nucl. Soc.* **52**, 430 (1986).
11. A.M. Mui, Y.I. Kim, and D.R. Harris, "Modified P_3 Transport Improvements for Reactor Diffusion Calculations," *Trans. Am. Nucl. Soc.* **55**, 584 (1987).
12. R.G. Gamino, "Simplified P_L Nodal Transport Applied to Two-Dimensional Deep Penetration Problems," *Trans. Am. Nucl. Soc.* **59**, 149 (1989).
13. R.G. Gamino, "Three-Dimensional Nodal Transport Using the Simplified P_L Method," Proc. ANS Topical Mtg., *Advances in Mathematics, Computations, and Reactor Physics*, April 29 - May 2, 1991, Pittsburgh, Vol. 2, Sec. 7.1, p. 3-1 (1991).
14. E.W. Larsen, J.M. McGhee, and J.E. Morel, "The Simplified P_N Equations as an Asymptotic Limit of the Transport Equation," *Trans. Am. Nucl. Soc.* **66**, 231 (1992).
15. D. Tomašević and E.W. Larsen, "The Simplified P_2 Correction to the Multidimensional Diffusion Equation," *Trans. Am. Nucl. Soc.* **66**, 232 (1992).
16. E.W. Larsen, J.E. Morel, and J.M. McGhee, "Asymptotic Derivation of the Simplified P_N Equations," Proc. ANS Topical Meeting, *Mathematical Methods and Supercomputing in Nuclear Applications, M&C + SNA '93*, April 19-23, 1993, Karlsruhe, Germany, **1**, 718 (1993).

17. G.C. Pomraning, "Asymptotic and Variational Derivations of the Simplified P_N Equations," *Ann. Nucl. Energy*, **20**, 623 (1993).
18. U. Shin, W.F. Miller, Jr., and J.E. Morel, "Asymptotic Derivation of the Time-Dependent SP_2 Equations and Numerical Calculations," *Trans. Am. Nucl. Soc.* **69**, 207 (1993).
19. E.W. Larsen, "Asymptotic Derivation of the Multigroup P_1 and SP_N Equations," *Trans. Am. Nucl. Soc.* **69**, 209 (1993).
20. D. Tomašević and E.W. Larsen, "Variational Derivation of Simplified P_2 Equations with Boundary Conditions," *Trans. Am. Nucl. Soc.* **70**, 159 (1994).
21. D. Tomašević, "Variational Derivation of the Simplified P_2 Nodal Approximation," Ph.D. Thesis, University of Michigan (September, 1994).
22. E.W. Larsen, "The Simplified P_N Equations," *Trans. ANS Winter 1994 Meeting*, to appear.
23. R.C. Little, "Replacement of Public Multigroup Libraries," Los Alamos National Laboratory Internal Memorandum X6:RCL-87-642 to Distribution (Dec. 17, 1987).