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Generalized Fokker-Planck Approximations of Particle Transport with Highly Forward-Peaked Scattering

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Abstract—*The Fokker-Planck equation is often used to approximate the description of particle transport processes with highly forward-peaked scattering. Pomraning has shown that if the physical scattering kernel is sufficiently dominated by small-angle scattering, then the Fokker-Planck equation is an asymptotic approximation to the linear Boltzmann equation. However, most physically-meaningful scattering kernels contain a sufficient amount of large-angle scattering that the asymptotic criterion is not met. Thus, in many physical problems, solutions of the Fokker-Planck equation are substantially in error. In this paper, Pomraning's asymptotic results are generalized and a new generalized Fokker-Planck (GFP) theory that robustly incorporates large-angle scattering is developed. Numerical experiments demonstrate that the resulting GFP equations are much more accurate than the standard Fokker-Planck equation.*

I. INTRODUCTION

The conventional Fokker-Planck approximation to the linear Boltzmann equation is valid if the Boltzmann scattering kernel is sufficiently peaked in the forward direction of flight.[1–4] In the classical derivation of the Fokker-Planck approximation,[1] the angular flux is Taylor-expanded in the incident directions $\underline{\Omega}'$ about the scattered direction $\underline{\Omega}$. Upon discarding higher-order terms, the integral Boltzmann scattering operator is approximated by a second-order differential Fokker-Planck operator. The resulting Fokker-Planck equation is easier to solve than the Boltzmann equation and has served as the basis of approximate analytical expressions, such as the closed-form Fermi-Eyges[5] description of narrow pencil beams of radiation. In this paper, we propose a new generalized Fokker-Planck (GFP) theory that overcomes a limitation of the classical Fokker-Planck theory: its inability to account for large-angle scattering.

To explain this more fully, we must discuss the theoretical connection between the Fokker-Planck and Boltzmann equations. Pomraning[3,4] has shown that the classical Fokker-Planck approximation is an asymptotic limit of the Boltzmann equation provided that (a) the mean-free-path is small, (b) the mean scattering cosine is nearly unity, (c) the transport cross section is $O(1)$, and (d) the differential scattering cross section contains a sufficiently small amount of large-angle scattering. Unfortunately, electron scattering kernels do not satisfy all of these conditions. The difficulty is usually with the fourth item: Physical scattering kernels contain small but sufficient amounts of large-angle scattering that Fokker-Planck theory is at best a marginal approximation to transport theory. For example, Pomraning has shown that the often-used Henyey-Greenstein kernel (for photon transport through cosmic dust or atmospheres) contains so much large-angle scattering that it does not have a Fokker-Planck limit at all, and the screened Rutherford scattering kernel (for electron transport) has a valid Fokker-Planck limit only when the screening parameter is unphysically small.[3,6]

Thus, because of large-angle scattering in physical problems, solutions of the classical Fokker-Planck equation have limited accuracy for electron transport.[7] To improve this accuracy, the Boltzmann-Fokker-Planck (BFP) equation[8–11] was formulated. This equation contains Fokker-Planck (differential) terms to describe small-angle scattering and Boltzmann (integral) terms to describe large-angle scattering. Numerical solutions of the BFP equation usually agree with experiments much

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better than solutions of the classical Fokker-Planck equation. Thus, the Boltzmann scattering terms included in the BFP equation are a successful way to incorporate large-angle scattering into the classical Fokker-Planck approximation.

In this paper, we propose an alternative GFP approximation, which has much in common with both the classical Fokker-Planck and the BFP approximations. The new GFP equations can be written either as a system of coupled (second-order) Fokker-Planck equations or as a single Boltzmann (or BFP) equation with a special integral scattering operator. These two alternative formulations are mathematically equivalent. We have confirmed that by solving the Boltzmann form of the GFP equations using Monte Carlo and the differential form of the GFP equations using finite difference methods, one obtains the same numerical solution.

The GFP approximation is based on results in two earlier papers by Pomraning,[3,4] showing that an asymptotic expansion of the Boltzmann scattering operator in a small parameter ε, which scales the scattering operator in accordance with the previously stated four assumptions, yields an approximate scattering operator, having the form of an asymptotic power series in ε, in which the coefficient of ε^n contains the classical Fokker-Planck operator raised to the n'th power. If one retains just the first term in this asymptotic expansion, the classical Fokker-Planck result is obtained. If one retains terms including higher powers of ε, an equation is obtained that is asymptotically more accurate (at least formally). However, the higher-order correction terms contain higher-order differential operators in angle. Also, the resulting approximate equations can be unstable; they do not necessarily possess finite solutions. Thus, the direct application of Pomraning's asymptotic expansion is problematic.

In this paper, we show that if Pomraning's expansion is appropriately renormalized (to borrow a phrase from the physics community), a coupled system of second-order GFP equations is obtained that is robust and demonstrably more accurate than the classical Fokker-Planck approximation. The GFP equations are asymptotically equivalent to Pomraning's expansion and hence are valid asymptotic expansions of the Boltzmann equation in their own right. Moreover, the GFP equations can be written in different but mathematically equivalent forms—as coupled systems of second-order differential equations or as a single Boltzmann (or BFP) equation. Thus, they are amenable to different types of numerical treatment.

This paper presents the concepts underlying the GFP approach for monoenergetic transport problems. (Our main interest is with the Fokker-Planck approximation in angle, which does not describe large-angle scattering. We intend to treat energy dependence in future work.) In Sec. II, we present Pomraning's asymptotic theory applied to such problems. In Sec. III, we renormalize Pomraning's asymptotic result to obtain GFP approximations. In Sec. IV, we compare numerical solutions of the original Boltzmann equation, the classical Fokker-Planck approximation, and various GFP approximations, showing that the GFP solutions are consistently more accurate than the classical Fokker-Planck solution. We conclude in Sec. IV with a brief discussion.

II. POMRANING'S ASYMPTOTIC THEORY

We consider the monoenergetic linear Boltzmann equation

$$\frac{\partial \psi}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + \Sigma_t\psi(\underline{r},\underline{\Omega},s) = \int_{4\pi}\Sigma_s(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}',s)\,d\Omega' \ , \tag{1a}$$

where

$$\begin{aligned}
\underline{r} &= (x_1,x_2,x_3) = \text{spatial variable},\\
\underline{\Omega} &= (\Omega_1,\Omega_2,\Omega_3)\\
&= (\sqrt{1-\mu^2}\cos\phi,\sqrt{1-\mu^2}\sin\phi,\mu)\\
&= \text{direction variable},\\
s &= vt = \text{path length},\\
\psi(\underline{r},\underline{\Omega},s) &= \text{angular flux}.
\end{aligned}$$

Equation (1a) is prescribed in a spatial domain D, together with initial and boundary conditions:

$$\psi(\underline{r},\underline{\Omega},0) = \psi^i(\underline{r},\underline{\Omega}) \ , \quad \underline{r}\in D \ , \quad |\underline{\Omega}| = 1 \tag{1b}$$

and

$$\psi(\underline{r},\underline{\Omega},s) = \psi^b(\underline{r},\underline{\Omega},s) \ , \quad \underline{r}\in\partial D \ , \quad \underline{\Omega}\cdot\underline{n} < 0 \ , \quad s > 0 \ , \tag{1c}$$

where $\underline{n}$ is the unit outer normal vector on ∂D. With $\mu_0 = \underline{\Omega}\cdot\underline{\Omega}'$ = scattering cosine, the differential scattering cross section $\Sigma_s(\mu_0)$ has the familiar Legendre polynomial expansion[12]

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

with expansion coefficients

$$\Sigma_{sn} = 2\pi\int_{-1}^{1}\Sigma_s(\mu_0)P_n(\mu_0)\,d\mu_0 \ . \tag{2b}$$

We must also introduce the spherical harmonic functions and angular momentum operator and describe some of

their properties. First, the associated Legendre functions[12] are defined in terms of the Legendre polynomials by

$$P_{n,m}(\mu) = (1-\mu^2)^{m/2}\left(\frac{d}{d\mu}\right)^m P_n(\mu) \ , \qquad 0 \le m \le n \ . \tag{3}$$

The spherical harmonic functions[12] are now defined by

$$Y_{n,m}(\underline{\Omega}) = \left[\frac{2n+1}{4\pi}\frac{(n-|m|)!}{(n+|m|)!}\right]^{1/2} \times (-1)^{(m+|m|)/2} P_{n,|m|}(\mu) e^{im\phi} \ , \qquad 0 \le n < \infty \ , \quad -n \le m \le n \ . \tag{4}$$

These functions are orthonormal,

$$\int_{4\pi} Y_{j,k}(\Omega) Y^*_{n,m}(\Omega)\, d\Omega = \delta_{j,n}\delta_{k,m} \ , \tag{5}$$

and complete; any suitably smooth function $\psi(\underline{\Omega})$ has the spherical harmonic expansion

$$\psi(\underline{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} \psi_{n,m} Y_{n,m}(\underline{\Omega}) \ , \tag{6a}$$

with expansion coefficients,

$$\psi_{n,m} = \int_{4\pi} \psi(\underline{\Omega}') Y^*_{n,m}(\underline{\Omega}')\, d\Omega' \ . \tag{6b}$$

The spherical harmonic functions satisfy the addition theorem,

$$P_n(\underline{\Omega}\cdot\underline{\Omega}') = \frac{4\pi}{2n+1}\sum_{m=-n}^{n} Y_{n,m}(\underline{\Omega}) Y^*_{n,m}(\underline{\Omega}') \ , \tag{7}$$

and are eigenfunctions of the well-known angular momentum operator from quantum mechanics[13]:

$$LY_{n,m}(\underline{\Omega}) \equiv \left[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{1}{1-\mu^2}\frac{\partial^2}{\partial\phi^2}\right] \times Y_{n,m}(\underline{\Omega}) = -n(n+1) Y_{n,m}(\underline{\Omega}) \ . \tag{8}$$

(The operator L is the three-dimensional spherical-geometry Laplacian operator restricted to the unit sphere.)

Operating on Eq. (6a) by L and using Eq. (8), we obtain (for any sufficiently smooth ψ)

$$L\psi(\underline{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} [-n(n+1)]\psi_{n,m} Y_{n,m}(\underline{\Omega}) \ . \tag{9}$$

Also, introducing Eq. (6a) into the Boltzmann scattering operator embedded in Eq. (1a) and using the aforementioned identities, we easily obtain

$$L_{\mathrm{B}}\psi(\underline{\Omega}) \equiv \int_{4\pi} \Sigma_s(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{\Omega}')\, d\Omega' - \Sigma_{s0}\psi(\underline{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} [-(\Sigma_{s0}-\Sigma_{sn})]\psi_{n,m} Y_{n,m}(\underline{\Omega}) \ . \tag{10}$$

Thus, as is well-known, the spherical harmonic functions are eigenfunctions of both the angular momentum and the Boltzmann scattering operators, but with different eigenvalues:

$$LY_{n,m}(\underline{\Omega}) = -n(n+1) Y_{n,m}(\underline{\Omega}) \tag{11a}$$

and

$$L_{\mathrm{B}} Y_{n,m}(\underline{\Omega}) = -(\Sigma_{s0}-\Sigma_{sn}) Y_{n,m}(\underline{\Omega}) \ . \tag{11b}$$

To proceed, Pomraning assumes that in Eq. (1a), the differential scattering cross section $\Sigma_s(\mu_0)$ is highly peaked near $\mu_0 = 1$. Physically, this assumption corresponds to a transport process with sufficiently forward-peaked scattering. To quantify this assumption of forward-peakedness, we define the positive constants

$$\xi_n \equiv 2\pi \int_{-1}^{1} (1-\mu_0)^n \Sigma_s(\mu_0)\, d\mu_0 \ , \quad n \ge 0 \ , \tag{12}$$

and assume

$$\xi_0 \gg \xi_1 \gg \xi_2 \cdots \ . \tag{13}$$

[Note: if $\Sigma_s(\mu_0)$ can be written as

$$\Sigma_s(\mu_0) = \frac{1}{\varepsilon^2} f\left(\frac{1-\mu_0}{\varepsilon}\right) \ , \tag{14a}$$

with $\varepsilon \ll 1$, then

$$\xi_n = 2\pi\int_{-1}^{1}(1-\mu_0)^n \frac{1}{\varepsilon^2} f\left(\frac{1-\mu_0}{\varepsilon}\right) d\mu_0 = \varepsilon^{n-1}\left(2\pi\int_0^{2/\varepsilon} t^n f(t)\, dt\right) = O(\varepsilon^{n-1}) \ , \tag{14b}$$

provided

$$\int_0^{\infty} t^n f(t)\, dt < \infty \ . \tag{14c}$$

For simplicity, we do not use the expression (14a) for $\Sigma_s(\mu_0)$ in our analysis. However, we do make use of the scaling implicit in Eq. (14b). That is, we assume that as n increases, the positive constants ξ_n decrease to zero in a manner consistent with Eq. (14b).]

Thus, the fundamental assumption of Pomraning's and our analysis is that in the linear Boltzmann Eq. (1a), the differential scattering cross section $\Sigma_s(\mu_0)$ satisfies Eqs. (12) and (13) [or (14b)]. In this paper, we make

explicit use of ξ_0, ξ_1, and ξ_2, which by Eqs. (2b) and (12) satisfy

$$\xi_0 = \Sigma_{s0} \ , \tag{15a}$$

$$\xi_1 = \Sigma_{s0} - \Sigma_{s1} = \Sigma_{a1} \ , \tag{15b}$$

$$\xi_2 = 2(\Sigma_{s0} - \Sigma_{s1}) - \tfrac{2}{3}(\Sigma_{s0} - \Sigma_{s2}) = 2\Sigma_{a1} - \tfrac{2}{3}\Sigma_{a2} \ , \tag{15c}$$

where for $n \geq 1$,

$$\Sigma_{an} \equiv \Sigma_{s0} - \Sigma_{sn} \ . \tag{16}$$

We now use Eq. (14b) to obtain an asymptotic expansion of the Legendre coefficients Σ_{sn} in Eq. (2b). By Taylor-expanding $P_n(\mu_0)$ in Eq. (2b) about $\mu_0 = 1$ and using[3,4]

$$P_n(1) = 1 \ , \tag{17a}$$

$$P_n'(1) = \frac{n(n+1)}{2} \ , \tag{17b}$$

and

$$P_n''(1) = [n(n+1) - 2]\,\frac{n(n+1)}{8} \ , \tag{17c}$$

we easily obtain for each n, and for $\varepsilon \approx 0$,

$$\Sigma_{sn} = \xi_0 - \frac{n(n+1)}{2}\,\xi_1 + [n(n+1) - 2] \times \frac{n(n+1)}{16}\,\xi_2 + O(\varepsilon^2) \ . \tag{18}$$

Introducing Eq. (18) into Eq. (10) and using Eq. (9), we obtain

$$L_{\rm B}\psi(\underline{\Omega}) = \frac{\xi_1}{2}\,L\psi(\underline{\Omega}) + \frac{\xi_2}{8}\left(L + \frac{1}{2}\,L^2\right)\psi(\underline{\Omega}) + O(\varepsilon^2) = \left(\frac{\xi_1}{2} + \frac{\xi_2}{8}\right)L\psi(\underline{\Omega}) + \frac{\xi_2}{16}\,L^2\psi(\underline{\Omega}) + O(\varepsilon^2) \ . \tag{19}$$

If we retain only $O(1)$ terms, Eq. (19) reduces to the standard Fokker-Planck approximation:

$$L_{\rm B}\psi(\underline{\Omega}) = L_{\rm FP}\psi(\underline{\Omega}) + O(\varepsilon) \ , \tag{20a}$$

where

$$L_{\rm FP} \equiv L_{P1} \equiv \frac{\xi_1}{2}\,L \ . \tag{20b}$$

If we retain $O(1)$ and $O(\varepsilon)$ terms, Eq. (19) reduces to the asymptotically improved result:

$$L_{\rm B}\psi(\Omega) = L_{P2}\psi(\Omega) + O(\varepsilon^2) \ , \tag{21a}$$

where

$$L_{P2} = \left(\frac{\xi_1}{2} + \frac{\xi_2}{8}\right)L + \frac{\xi_2}{16}\,L^2 \ . \tag{21b}$$

For general $n \geq 1$, if we retain only terms up to $O(\varepsilon^{n-1})$, Eq. (19) reduces to

$$L_{\rm B}\psi(\underline{\Omega}) = L_{Pn}\psi(\underline{\Omega}) + O(\varepsilon^n) \ , \tag{22a}$$

where

$$L_{Pn} = \sum_{m=1}^{n} a_{n,m}L^m \ , \tag{22b}$$

with coefficients

$$a_{n,m} = O(\xi_m) = O(\varepsilon^{m-1}) \ . \tag{22c}$$

Thus, Pomraning's result is that in the absence of large-angle scattering, for any positive integer n, an $O(\varepsilon^n)$ asymptotic approximation L_{Pn} to $L_{\rm B}$ exists as a polynomial of the angular momentum operator L, containing powers of L up to L^n. (L_{Pn} is a differential operator of order $2n$.) Thus, the angular momentum operator L is a building-block from which asymptotic polynomial approximations of $L_{\rm B}$ of arbitrarily high order can be constructed. The eigenfunctions of each of these asymptotic approximations are the spherical harmonics functions; the approximations differ in their definition of the eigenvalues.

III. GENERALIZED FOKKER-PLANCK THEORY

In the absence of absorption and space-dependence, Eq. (1a) reduces to

$$\frac{\partial\psi}{\partial s}\,(\underline{\Omega}, s) = L_{\rm B}\psi(\underline{\Omega}, s) \ , \tag{23a}$$

with $L_{\rm B}$ defined by Eq. (10). For solutions of Eq. (23a) to exist and remain finite for all $s > 0$, no eigenvalue of $L_{\rm B}$ can be positive. However, because $\Sigma_s(\mu_0)$ is a positive smooth function, one can easily show that its Legendre coefficients Σ_{sn} satisfy $\Sigma_{s0} > \Sigma_{sn}$ for all $n \geq 1$, and $\lim_{n\to\infty}\Sigma_{sn} = 0$. Thus, the eigenvalues

$$\lambda_{{\rm B},k} = -(\Sigma_{s0} - \Sigma_{sk}) \tag{23b}$$

of $L_{\rm B}$ [see Eq. (11b)] satisfy $\lambda_{{\rm B},0} = 0$, $\lambda_{{\rm B},k} < 0$ for $k \geq 1$, and $\lim_{k\to\infty}\lambda_{{\rm B},k} = -\Sigma_{s0}$. This assures the nonpositivity of $\lambda_{{\rm B},k}$.

The Fokker-Planck approximation to Eq. (23a) is

$$\frac{\partial\psi}{\partial s}\,(\underline{\Omega}, s) = L_{\rm FP}\psi(\underline{\Omega}, s) \ , \tag{24a}$$

with $L_{\rm FP}$ defined by Eqs. (20b) and (15b). The eigenvalues

$$\lambda_{{\rm FP},k} = -\Sigma_{a1}\,\frac{k(k+1)}{2} \tag{24b}$$

of L_{FP} satisfy

$$\lambda_{\mathrm{FP},k} = \lambda_{\mathrm{B},k} \ , \quad k = 0,1 \ , \tag{24c}$$

and

$$\lambda_{\mathrm{FP},k} < 0 \ , \quad k \geq 1 \ .$$

Thus, the first two eigenvalues of L_{FP} agree with those of L_{B}, and the remaining $\lambda_{\mathrm{FP},k}$ are negative.

Pomraning's $O(\varepsilon^2)$ approximation to Eq. (23a) is

$$\frac{\partial \psi}{\partial s}(\underline{\Omega}, s) = L_{P2}\psi(\underline{\Omega}, s) \ , \tag{25a}$$

with L_{P2} defined by Eqs. (21b) and (15). The eigenvalues

$$\lambda_{P2,k} = -\left(\frac{\xi_1}{2} + \frac{\xi_2}{8}\right)k(k+1) + \frac{\xi_2}{16}[k(k+1)]^2 \tag{25b}$$

of L_{P2} satisfy

$$\lambda_{P2,k} = \lambda_{\mathrm{B},k} \ , \quad k = 0,1,2 \ , \tag{25c}$$

$$\lambda_{P2,k} < 0 \quad \text{for } k(k+1) < 2 + \frac{8\xi_1}{\xi_2} \ ,$$

and

$$\lambda_{P2,k} > 0 \quad \text{for } k(k+1) > 2 + \frac{8\xi_1}{\xi_2} \ ,$$

$$\lim_{k\to\infty} \lambda_{P2,k} = +\infty \ .$$

Thus, the first three eigenvalues of L_{P2} agree with those of L_{B}. However, for large k, $\lambda_{P2,k}$ becomes positive and limits to $+\infty$. Thus, solutions of Eq. (25a) exist for all $s > 0$ only for special initial data ψ^i.

For general $n > 1$, Pomraning's $O(\varepsilon^n)$ approximation to Eq. (23a) is

$$\frac{\partial \psi}{\partial s}(\underline{\Omega}, s) = L_{Pn}\psi(\underline{\Omega}, s) \ , \tag{26a}$$

with L_{Pn} defined by Eq. (22b). The eigenvalues

$$\lambda_{Pn,k} = \sum_{m=1}^{n} a_{m,n}[-k(k+1)]^m \tag{26b}$$

of L_{Pn} satisfy

$$\lambda_{Pn,k} = \lambda_{\mathrm{B},k} \ , \quad 0 \leq k \leq n \ . \tag{26c}$$

Thus, the first $n+1$ eigenvalues of L_{Pn} agree with those of L_{B}. Unfortunately, there is no obvious way to determine whether the remaining $\lambda_{Pn,k}$ remain negative.

Thus, one is confronted with a dilemma. As n increases, the operators L_{Pn} formally become increasingly higher order asymptotic approximations to L_{B}. Also, the first $n+1$ eigenvalues of L_{Pn} agree with those of L_{B}. However, together with these good features are the bad features that L_{Pn} is a high-order differential operator of order $2n$, and the eigenvalues of L_{Pn} may eventually become positive.

The GFP solution to this difficulty is to replace L_{Pn} by an asymptotically equivalent representation that is simple and stable, and that preserves the first $n+1$ eigenvalues of L_{B} [Eq. (26c)]. For now, we focus on L_{P2}, defined by Eq. (21b). Let α and β be any two positive constants satisfying

$$\alpha = \frac{\xi_1}{2} + \frac{\xi_2}{8} + O(\varepsilon^2) \tag{27a}$$

and

$$\beta = \frac{\xi_2}{8\xi_1} + O(\varepsilon^2) \ . \tag{27b}$$

Then $\alpha = O(1), \beta = O(\varepsilon)$, and the operator L_{GFP_2}, defined by

$$\begin{aligned} L_{\mathrm{GFP}_2} &\equiv \alpha L(I - \beta L)^{-1} \\ &= \alpha L(I + \beta L) + O(\alpha\beta^2) \\ &= \alpha L + \alpha\beta L^2 + O(\varepsilon^2) \\ &= L_{P2} + O(\varepsilon^2) \\ &= L_{\mathrm{B}} + O(\varepsilon^2) \end{aligned} \tag{28a}$$

is, like L_{P2}, an asymptotic approximation to L_{B} with $O(\varepsilon^2)$ error. However, the eigenvalues of L_{GFP_2} are

$$\lambda_{\mathrm{GFP}_2,k} = \frac{-\alpha k(k+1)}{1 + \beta k(k+1)} \ , \tag{28b}$$

which are nonpositive for all k. Thus, if we replace L_{P2} by L_{GFP_2}, we eliminate the difficulties associated with the positive eigenvalues of L_{P2}.

Now, we must specify the constants α and β in Eqs. (27) and (28). Since the first three eigenvalues of L_{P2} agree with those of L_{B} [see Eq. (25c)], it is natural to try to choose α and β so that L_{GFP_2} preserves this property. The $k = 0$ eigenvalue is automatically preserved, and for $k = 0$ and 1 we obtain, from Eqs. (24b) and (28b),

$$\frac{2\alpha}{1 + 2\beta} = \Sigma_{a1}$$

and

$$\frac{6\alpha}{1 + 6\beta} = \Sigma_{a2} \ .$$

These equations imply

$$\beta = \frac{1}{6}\left(\frac{3\Sigma_{a1} - \Sigma_{a2}}{\Sigma_{a2} - \Sigma_{a1}}\right) \tag{29a}$$

and

$$\alpha = \frac{1}{3}\left(\frac{\Sigma_{a1}\Sigma_{a2}}{\Sigma_{a2}-\Sigma_{a1}}\right) = \frac{\Sigma_{a1}}{2}(1+2\beta) \ . \tag{29b}$$

Also, Eqs. (15) imply

$$\Sigma_{a1} = \xi_1 \tag{30a}$$

and

$$\Sigma_{a2} = 3\xi_1 - \frac{3}{2}\xi_2 \ . \tag{30b}$$

Introducing Eqs. (30) into Eqs. (29) and using the scaling of Eq. (14b), it is easy to show that α and β satisfy Eqs. (27). Thus, the aforementioned definitions of α and β ensure that

$$\lambda_{\mathrm{GFP}_2,k} = \lambda_{\mathrm{B},k} \ , \quad k = 0,1,2 \ , \tag{31}$$

and they also ensure that L_{GFP_2} is an $O(\varepsilon^2)$ asymptotic approximation to L_{B}, just like L_{P2}.

Finally, one can show that for the Henyey-Greenstein and screened Rutherford scattering cross sections, $\Sigma_{a2} > \Sigma_{a1}$ and $3\Sigma_{a1} > \Sigma_{a2}$. Hence, for these kernels, α and β in Eqs. (29) remain positive for all degrees of scattering anisotropy.

To summarize, the GFP_2 approximation to Eq. (1a) is

$$\frac{\partial\psi}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + \Sigma_a\psi(\underline{r},\underline{\Omega},s) = \alpha L(I-\beta L)^{-1}\psi(\underline{r},\underline{\Omega},s) \ , \tag{32}$$

where α and β are defined by Eqs. (29). Next, we discuss two alternative forms of Eq. (32).

First, if we define ψ_0 and ψ_1 by

$$\psi_0 = \psi$$

and

$$\psi_1 = (I-\beta L)^{-1}\psi_0 \ ,$$

then Eq. (32) can be written as

$$\frac{\partial\psi_0}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi_0(\underline{r},\underline{\Omega},s) + \Sigma_a\psi_0(\underline{r},\underline{\Omega},s) = \alpha L\psi_1(\underline{r},\underline{\Omega},s) \tag{33a}$$

and

$$(I-\beta L)\psi_1(\underline{r},\underline{\Omega},s) = \psi_0(\underline{r},\underline{\Omega},s) \ . \tag{33b}$$

This is a coupled system of (second-order differential) Fokker-Planck equations, with L the diffusion operator in the angular variable. The initial and boundary conditions for ψ are imposed on ψ_0. To discretize Eqs. (33) in space and angle, one can use the discrete ordinates approximation in angle with any sufficiently accurate spatial differencing scheme and Morel's[14] discretization of the angular momentum operator L. The standard concerns of accuracy of the discretized equations and solving the discretized equations efficiently are closely related to the issues of accurately discretizing and efficiently solving the linear Boltzmann equation. We will not discuss these concerns in depth in this paper.

Second, if we use

$$\alpha L(I-\beta L)^{-1} = \frac{\alpha}{\beta}[I-(I-\beta L)](I-\beta L)^{-1} = \frac{\alpha}{\beta}[(I-\beta L)^{-1} - I] \ ,$$

then Eq. (32) can be written as

$$\frac{\partial\psi}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + (\Sigma_a+\bar{\Sigma}_s)\psi(\underline{r},\underline{\Omega},s) = \bar{\Sigma}_s(I-\beta L)^{-1}\psi(\underline{r},\underline{\Omega},s) \ , \tag{34a}$$

where

$$\bar{\Sigma}_s = \frac{\alpha}{\beta} = \frac{2\Sigma_{a1}\Sigma_{a2}}{3\Sigma_{a1}-\Sigma_{a2}} \ . \tag{34b}$$

To interpret the right side of Eq. (34a), we must return to the definitions of the spherical harmonics functions. Introducing Eq. (6b) into Eq. (6a), we obtain

$$\psi(\underline{\Omega}) = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_{n,m}(\underline{\Omega})\int_{4\pi} Y^*_{n,m}(\underline{\Omega}')\psi(\underline{\Omega}')\,d\Omega' = \int_{4\pi}\frac{\delta(\underline{\Omega}\cdot\underline{\Omega}'-1)}{2\pi}\psi(\underline{\Omega}')\,d\Omega' \ , \tag{35}$$

where

$$\frac{\delta(\underline{\Omega}\cdot\underline{\Omega}'-1)}{2\pi} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} Y_{n,m}(\underline{\Omega})Y^*_{n,m}(\underline{\Omega}') \tag{36}$$

is the delta function defined on the unit sphere. Equations (36), (11a), and (7) now give

$$(I-\beta L)^{-1}\frac{\delta(\underline{\Omega}\cdot\underline{\Omega}'-1)}{2\pi} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n}\frac{Y_{n,m}(\underline{\Omega})Y^*_{n,m}(\underline{\Omega}')}{1+\beta n(n+1)} = \sum_{n=0}^{\infty}\frac{2n+1}{4\pi}\frac{P_n(\underline{\Omega}\cdot\underline{\Omega}')}{1+\beta n(n+1)} \equiv G(\underline{\Omega}\cdot\underline{\Omega}') \ . \tag{37}$$

Hence, the function $G(\mu_0)$ is the Green's function for the angular diffusion operator $I-\beta L$. It is also the probability distribution function for neutrons scattering from $\underline{\Omega}'$ into $\underline{\Omega}$. [It can be proved[15] that $G(\mu_0) > 0$.]

Operating on Eq. (35) by $(I - \beta L)^{-1}$ and using Eq. (37), we easily obtain

$$(I - \beta L)^{-1}\psi(\underline{\Omega}) = \int_{4\pi} G(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{\Omega}')\, d\Omega' \quad . \tag{38}$$

Hence, Eq. (34a) may be written as

$$\frac{\partial\psi}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + (\Sigma_a + \bar{\Sigma}_s)\psi(\underline{r},\underline{\Omega},s)$$

$$= \bar{\Sigma}_s \int_{4\pi} G(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}',s)\, d\Omega' \quad . \tag{39}$$

Thus, Eq. (32) is mathematically equivalent to the system of Fokker-Planck differential Eqs. (33), and to Eq. (39), a linear Boltzmann equation with scattering cross section $\bar{\Sigma}_s$ and differential scattering cross section $\bar{\Sigma}_s G(\underline{\Omega}\cdot\underline{\Omega}')$. Equation (39) can be solved by any deterministic or stochastic technique for solving the conventional linear Boltzmann equation.

A logical (and even necessary at this point) question is: What is the possible benefit of replacing the exact Boltzmann equation [Eq. (1a)] by the approximate Boltzmann equation [Eq. (39)]? This question has at least two answers. First, Eq. (39) is mathematically equivalent to Eq. (32) and Eqs. (33). Thus, one has the option of discretizing the integrodifferential Eq. (39) or discretizing the simpler differential Eqs. (33). This option does not exist with the original Boltzmann Eq. (1a). Second, Eq. (39) is easier to work with than Eq. (1a) because Eq. (39) usually has a much larger mean-free-path and a smaller mean scattering cosine than Eq. (1a). Deterministic methods for Eq. (39) are more efficient because the physical system is less optically thick and scattering is less forward-peaked, enabling one to use coarser space-angle grids. Stochastic methods are more efficient because the distance between collisions is much larger, making particle histories much shorter. [In effect, a Monte Carlo simulation of Eq. (39) amounts to a form of condensed history simulation[16–18] of Eq. (1a). Other methods, employing Radau quadrature sets, also yield condensed history approximations to the Boltzmann equation.[19,20] However, these methods do not involve representations of the scattering operator in terms of the angular momentum operator L and will not be discussed further in this paper.]

Next, we discuss two other important features of the GFP approximation.

III.A. Preservation of Space-Angle Moments

It does not seem to be widely appreciated that the Fokker-Planck approximation preserves certain properties of Boltzmann Eq. (1a): In an infinite homogeneous medium, the zeroth and first-order space-angle moments of the Boltzmann and Fokker-Planck solutions are identical for all $s > 0$. Also, in the same infinite homogeneous medium, the zeroth, first- and second-order space-angle moments of the Boltzmann and GFP_2 equations are identical for all $s > 0$. These properties follow easily from old results of Lewis,[21] Spencer,[22] and Schultis and Faw,[23] which we state in a form that is relevant to our analysis:

Lewis' Result: For $j = 1$ and 2, let $\psi^{(j)}(\underline{r},\underline{\Omega},s)$ be solutions of the homogeneous, infinite-medium problems

$$\frac{\partial\psi^{(j)}}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi^{(j)}(\underline{r},\underline{\Omega},s) + \Sigma_a\psi^{(j)}(\underline{r},\underline{\Omega},s)$$

$$= L^{(j)}\psi^{(j)}(\underline{r},\underline{\Omega}',s) \quad , \tag{40a}$$

$$\psi^{(j)}(\underline{r},\underline{\Omega},0) = \psi^{i}(\underline{r},\underline{\Omega}) \quad , \quad \text{all } \underline{r},\underline{\Omega} \quad , \tag{40b}$$

and

$$\psi^{(j)}(\underline{r},\underline{\Omega},s) \to 0 \quad \text{as } |\underline{r}| \to \infty \quad . \tag{40c}$$

Here, $L^{(j)}$ are two scattering operators whose eigenfunctions are the spherical harmonics functions

$$L^{(j)}Y_{n,m}(\underline{\Omega}) = \lambda_n^{(j)}Y_{n,m}(\underline{\Omega}) \quad ,$$

and whose eigenvalues satisfy

$$\lambda_n^{(j)} \le 0 \quad .$$

[Note that for $j = 1$ and 2, Eqs. (40) differ only in their specification of $L^{(j)}$; the initial conditions are the same.] Then the following results hold:

1. If $\lambda_0^{(1)} = \lambda_0^{(2)}$, then for all $s \ge 0$,

$$\iint \psi^{(1)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r = \iint \psi^{(2)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r \quad . \tag{41}$$

[The zeroth space-angle moments of $\psi^{(1)}(\underline{r},\underline{\Omega},s)$ and $\psi^{(2)}(\underline{r},\underline{\Omega},s)$ are identical for all $s > 0$.]

2. If $\lambda_m^{(1)} = \lambda_m^{(2)}$ for $m = 0$ and 1, then Eq. (41) and

$$\iint \Omega_i\psi^{(1)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r = \iint \Omega_i\psi^{(2)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r \tag{42a}$$

and

$$\iint x_i\psi^{(1)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r = \iint x_i\psi^{(2)}(\underline{r},\underline{\Omega},s)\, d\Omega d^3r \tag{42b}$$

hold for $1 \le i \le 3$. [The zeroth and first space-angle moments of $\psi^{(1)}(\underline{r},\underline{\Omega},s)$ and $\psi^{(2)}(\underline{r},\underline{\Omega},s)$ are identical for all $s > 0$.]

3. If $\lambda_m^{(1)} = \lambda_m^{(2)}$ for $m = 0$, 1, and 2, then Eqs. (41), (42), and

$$\iint \Omega_i \Omega_j \psi^{(1)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r = \iint \Omega_i \Omega_j \psi^{(2)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r \ , \tag{43a}$$

$$\iint \Omega_i x_j \psi^{(1)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r = \iint \Omega_i x_j \psi^{(2)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r \ , \tag{43b}$$

and

$$\iint x_i x_j \psi^{(1)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r = \iint x_i x_j \psi^{(2)}(\underline{r}, \underline{\Omega}, s)\, d\Omega d^3 r \tag{43c}$$

hold for $1 \le i, j \le 3$. [The zeroth, first, and second space-angle moments of $\psi^{(1)}(\underline{r}, \underline{\Omega}, s)$ and $\psi^{(2)}(\underline{r}, \underline{\Omega}, s)$ are identical for all $s > 0$.]

These results follow from Lewis's analysis and the following facts:

1. A constant can be represented in terms of the spherical harmonic function of order 0.

2. Each Ω_i can be represented as a linear combination of spherical harmonic functions of order 1.

3. Each $\Omega_i \Omega_j$ can be represented as a linear combination of spherical harmonic functions of order 0 and 2; etc.

These results generalize in the obvious way for higher values of m.

Because of Eq. (24c), Lewis's result guarantees that all the zeroth and first space-angle moments of the Boltzmann and Fokker-Planck solutions agree for all $s \ge 0$. Because of Eq. (31), Lewis's result guarantees that all the zeroth, first, and second space-angle moments of the Boltzmann and GFP solutions agree for all $s \ge 0$. Hence, the GFP equation is not only a higher-order asymptotic approximation to the Boltmann equation than the Fokker-Planck equation, but it also preserves more exact transport physics. (However, this latter result requires a homogeneous medium and does not hold when a particle crosses a material boundary.)

III.B. Higher-Order Generalized Fokker-Planck Theory

It is possible to extend the GFP_2 result to more accurate approximations of the Boltzmann equation that retain the relatively simple nature of the GFP_2 approximation. For example, one can consider approximations to L_B of the form

$$L_{GFP_3} \equiv \alpha_1 L(I - \beta_1 L)^{-1} + \alpha_2 L \ , \tag{44}$$

in which the constants α_1, β_1, and α_2 are chosen to be positive, such that the first four eigenvalues of L_{GFP_3} agree with those of L_B. (In the Appendix, we show how to derive α_1, β_1; and α_2 explicitly.)

The GFP_3 transport equation is

$$\frac{\partial \psi}{\partial s} \psi(\underline{r}, \underline{\Omega}, s) + \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}, s) + \Sigma_a \psi(\underline{r}, \underline{\Omega}, s) = [\alpha_1 L(I - \beta_1 L)^{-1} + \alpha_2 L] \psi(\underline{r}, \underline{\Omega}, s) \ . \tag{45}$$

This equation can be written either as a system of two coupled Fokker-Planck equations:

$$\frac{\partial \psi_0}{\partial s} (\underline{r}, \underline{\Omega}, s) + \underline{\Omega} \cdot \underline{\nabla} \psi_0(\underline{r}, \underline{\Omega}, s) + \Sigma_a \psi_0(\underline{r}, \underline{\Omega}, s) = \alpha_1 L \psi_1(\underline{r}, \underline{\Omega}, s) + \alpha_2 L \psi_0(\underline{r}, \underline{\Omega}, s) \ , \tag{46a}$$

$$(I - \beta_1 L) \psi_1(\underline{r}, \underline{\Omega}, s) = \psi_0(\underline{r}, \underline{\Omega}, s) \ , \tag{46b}$$

or as a single BFP equation:

$$\frac{\partial \psi}{\partial s} (\underline{r}, \underline{\Omega}, s) + \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}, s) + (\Sigma_a + \bar{\Sigma}_{s1}) \psi(\underline{r}, \underline{\Omega}, s) = \bar{\Sigma}_{s1} \int_{4\pi} G_1(\underline{\Omega} \cdot \underline{\Omega}') \psi(\underline{r}, \underline{\Omega}', s)\, d\Omega' + \alpha_2 L \psi(\underline{r}, \underline{\Omega}, s) \ . \tag{47}$$

In an infinite homogeneous medium, the space-angle moments up to order 3 of the GFP_3 solution agree with those of the Boltzmann solution for all $s > 0$.

One can also consider approximations to L_B of the form

$$L_{GFP_4} \equiv \alpha_1 L(I - \beta_1 L)^{-1} + \alpha_2 L(I - \beta_2 L)^{-1} \ , \tag{48}$$

in which the constants α_1, β_1, α_2, and β_2 are chosen to be positive, such that the first five eigenvalues of L_{GFP_4} agree with those of L_B. (In the Appendix, we show how to derive α_1, β_1, α_2, and β_2 explicitly.) The GFP_4 transport equation is

$$\frac{\partial \psi}{\partial s} \psi(\underline{r}, \underline{\Omega}, s) + \underline{\Omega} \cdot \underline{\nabla} \psi(\underline{r}, \underline{\Omega}, s) + \Sigma_a \psi(\underline{r}, \underline{\Omega}, s) = [\alpha_1 L(I - \beta_1 L)^{-1} + \alpha_2 L(I - \beta_2 L)^{-1}] \psi(\underline{r}, \underline{\Omega}, s) \ . \tag{49}$$

This equation can be written either as a system of three coupled Fokker-Planck equations:

$$\frac{\partial \psi_0}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi_0(\underline{r},\underline{\Omega},s) + \Sigma_a\psi_0(\underline{r},\underline{\Omega},s) = \alpha_1 L\psi_1(\underline{r},\underline{\Omega},s) + \alpha_2 L\psi_2(\underline{r},\underline{\Omega},s) \ , \quad (50a)$$

$$(I-\beta_1 L)\psi_1(\underline{r},\underline{\Omega},s) = \psi_0(\underline{r},\underline{\Omega},s) \ , \quad (50b)$$

$$(I-\beta_2 L)\psi_2(\underline{r},\underline{\Omega},s) = \psi_0(\underline{r},\underline{\Omega},s) \ , \quad (50c)$$

or as a single linear Boltzmann equation:

$$\frac{\partial \psi}{\partial s}(\underline{r},\underline{\Omega},s) + \underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega},s) + (\Sigma_a + \bar{\Sigma}_{s1} + \bar{\Sigma}_{s2})\psi(\underline{r},\underline{\Omega},s) = \int_{4\pi}[\bar{\Sigma}_{s1}G_1(\underline{\Omega}\cdot\underline{\Omega}') + \bar{\Sigma}_{s2}G_2(\underline{\Omega}\cdot\underline{\Omega}')] \times \psi(\underline{r},\underline{\Omega}',s)\,d\Omega' \ . \quad (51)$$

In an infinite homogeneous medium, the space-angle moments up to order 4 of the GFP_4 solution agree with those of the Boltzmann solution for all $s > 0$.

In the GFP_4 approximation to the Boltzmann equation, the total cross section and mean scattering cosine are usually greater than in the GFP_2 approximation. Thus, the computational efficiencies of the GFP_2 approximation are somewhat lessened in the GFP_4 approximation. However, because the GFP_4 equations are a more accurate representation of L_B, their solutions are more accurate than the GFP_2 solutions.

It is quite possible that other approximations to L_B, having the form of simple rational functions of L, can be constructed that are more advantageous than the ones presented in this paper. We do not claim that the particular GFP_n approximations that we discuss are best, but rather, that they should be (a) systematically more accurate than the standard Fokker-Planck approximation and (b) very similar to it in mathematical form. In considering other possible approximations, the main things to keep in mind are the following:

1. They should be simple.

2. They should have only nonpositive eigenvalues.

3. They should preserve as many of the first n eigenvalues of the Boltzmann operator as is practical.

4. The condition (3) should lead to easily solved equations for α_n and β_n (see the Appendix).

IV. NUMERICAL COMPARISONS

We have performed numerous deterministic and Monte Carlo numerical comparisons between the linear Boltzmann, Fokker-Planck, and GFP equations.[15] Here, we report some typical results.

First, in one-dimensional planar geometry, we implemented in a test code the differential GFP_2 equations [(33) and (29)] and GFP_4 equations [(50)], using the discrete ordinates approximation in angle, the linear-discontinuous spatial differencing scheme in space,[24] and Morel's[14] angular differencing approximation of the angular momentum operator. We also implemented the Boltzmann GFP_2 equations [(39), (37), (34b), and (29)] and GFP_4 equations [(51)] using the conventional analog Monte Carlo scheme. To accelerate the convergence of the deterministic equations, we used conventional transport sweeps in combination with the modified source iteration scheme.[25] [In this procedure, when one sweeps from left to right across the system, a spatial cell calculation couples all discrete angles $\mu_m > 0$, and when one sweeps from right to left, one couples all discrete angles $\mu_m < 0$.]

These simulations showed that the deterministic GFP_2 and Monte Carlo GFP_2 solutions agree to within truncation and statistical errors, and the same holds for the GFP_4 simulations. This confirms the theoretical prediction that the differential and Boltzmann forms of the GFP equations are equivalent.

To assess the accuracy of the GFP equations, we performed analog Monte Carlo simulations of the linear Boltzmann, Fokker-Planck,[7] GFP_2, and GFP_4 equations for three-dimensional monoenergetic pencil beam problems in planar-geometry systems. By using sufficiently many particles, we ensure that the resulting solutions determine the accuracy of the Fokker-Planck and GFP solutions in the absence of truncation errors and in the near-absence of statistical errors.

We considered pencil beam problems of the form

$$\underline{\Omega}\cdot\underline{\nabla}\psi(\underline{r},\underline{\Omega}) + \Sigma_t\psi(\underline{r},\underline{\Omega}) = \int_{4\pi}\Sigma_s(\underline{\Omega}\cdot\underline{\Omega}')\psi(\underline{r},\underline{\Omega}')\,d\Omega' \ , \quad 0 < z < Z \ , \quad (52a)$$

$$\psi(x,y,0,\underline{\Omega}) = \delta(x)\delta(y)\frac{\delta(\mu-1)}{2\pi} \ , \quad 0 < \mu \le 1 \ , \quad (52b)$$

and

$$\psi(x,y,Z,\underline{\Omega}) = 0 \ , \quad -1 \le \mu < 0 \ . \quad (52c)$$

These problems contain no absorption ($\Sigma_a = 0$, $\Sigma_t = \Sigma_s$) and employ the screened Rutherford scattering kernel,[3] which is commonly used for nonrelativistic electrons:

$$\Sigma_s(\mu_0) = \Sigma_s\frac{\eta(1+\eta)}{\pi(1+2\eta-\mu_0)^2} \ , \quad (53)$$

with η the screening parameter. If $\eta \approx 0$, scattering is highly forward-peaked. However, the screened Rutherford kernel has an asymptotically valid Fokker-Planck approximation only when η takes unphysically small values.[3,7] For physically meaningful values of η, the screened

Rutherford kernel contains sufficient large-angle scattering that the Fokker-Planck approximation is not accurate for many problems. (The pencil beam problems considered here are highly singular in both space and angle and provide a rigorous test of an approximate transport theory to a physically relevant problem.)

The problems defined by Eqs. (52) contain radial symmetry about the z axis. (In effect, they are r, z–geometry problems.) In our numerical experiments, we calculated the radial scalar flux as a function of radius r and depth z,

$$\phi(r,z) = \int_{4\pi} \psi(r,z,\underline{\Omega})\, d\Omega \ , \tag{54}$$

and the transversely integrated scalar flux as a function of z,

$$\phi(z) = 2\pi \int_0^\infty \phi(r,z)\, r dr \ . \tag{55}$$

Figures 2 and 3 describe the transversely integrated scalar flux and the radial flux at depth $z = 0.8$ cm for a typical two-region problem defined in Fig. 1.

Figure 2 shows that the transversely integrated Fokker-Planck result has errors of ~10% near the material interface, and of ~50% near the far edge of the slab. To the eye, it is difficult to see any error at all in the GFP_2 and GFP_4 solutions; the errors in these quantities are at least one order of magnitude less than those of the Fokker-Planck solution for all depths z.

Figure 3 displays the radial profile at depth $z = 0.8$ cm, just past the material interface. This figure shows that the GFP radial fluxes are significantly more accurate than the Fokker-Planck fluxes away from the central axis of the beam but that significant errors in the GFP solutions do exist near the central axis ($r \approx 0$). This is because the mean-free-paths (mfp's) of the GFP_2 and GFP_4 equations are much larger than the true mfp. While this allows Monte Carlo GFP calculations to run very quickly, it also introduces an artificial uncollided flux that can be very prominent in pencil beam problems. This effect is more noticeable in the GFP_2 simulation because it has a larger mfp than the GFP_4 simulation. In typical calculations of dose, the errors in all of the approximate solutions near $r \approx 0$ are suppressed because of the factor r in Eq. (55). Thus, the errors in calculated dose near $r \approx 0$ shown in Fig. 2 become very minor. These errors also tend to zero with increasing depth into the slab.

The results shown in Figs. 1 and 2 are typical of results for other problems,[15] with $10^{-6} \le \eta \le 10^{-2}$ and varying values of Σ_t. In all the problems we simulated, the Fokker-Planck solution is more accurate for very small values of η than for larger values, but it always has at least 10% errors. The GFP_2 and GFP_4 solutions always yield very accurate transverse-integrated fluxes for all depths, and the GFP_4 solution has very accurate radial fluxes for all r. The GFP_2 radial flux is least accurate near the central axis of the beam but becomes much more accurate than the Fokker-Planck result away from the central axis.

In problems with less-severe space-angle singularities, both the Fokker-Planck and GFP solutions become more accurate, as expected. However, the GFP solutions remain more accurate than the Fokker-Planck solutions, presumably because they contain more transport physics.

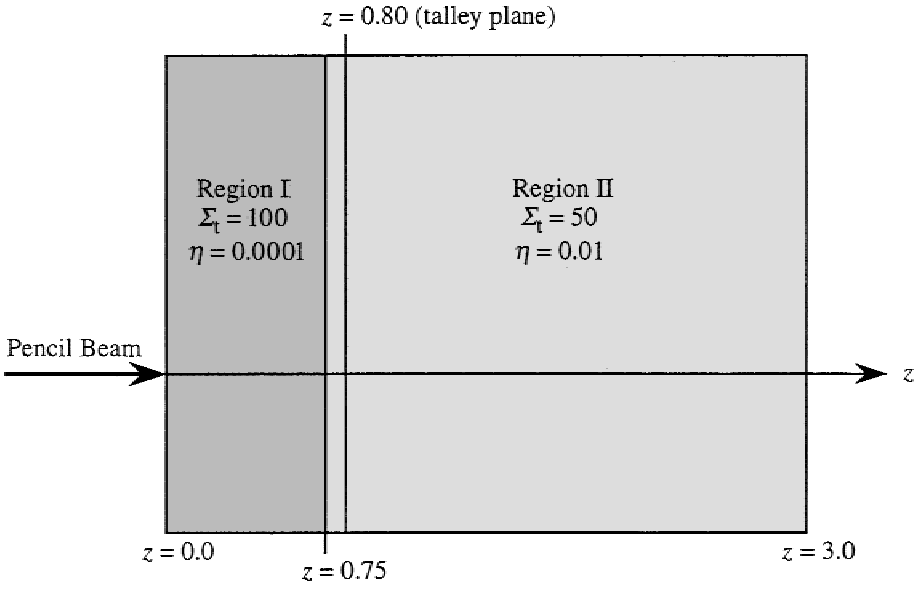

Fig. 1. Two-region pencil beam problem.

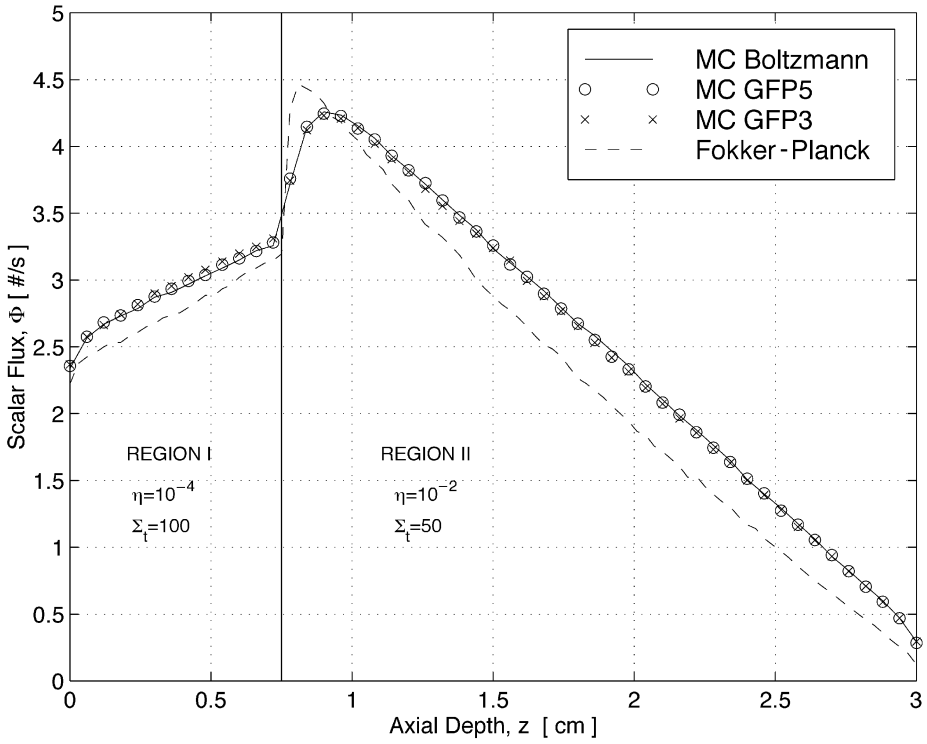

Fig. 2. Transversely integrated scalar flux.

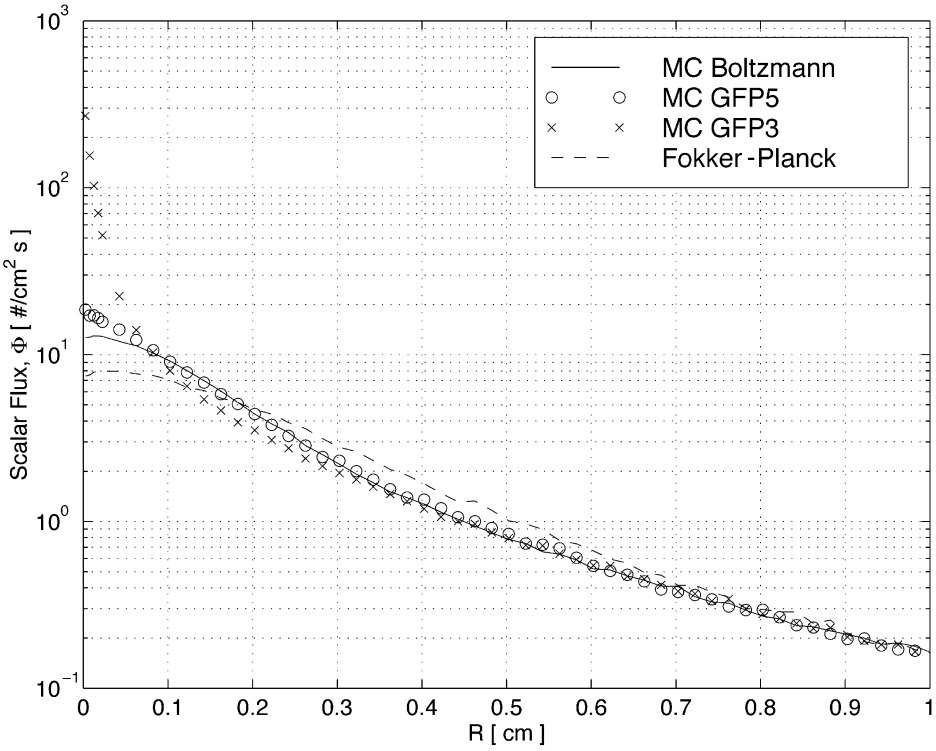

Fig. 3. Radial scalar flux at $z = 0.80$ cm.

In a different test of accuracy, we implemented one-dimensional deterministic simulations of the Boltzmann GFP equations using the standard discrete ordinates approximation in angle and linear-discontinuous approximation in space. These approximations have the property that the discretized scattering operator preserves a large number of eigenvalues of the analytic scattering operator, due to the ability of Gauss-Legendre quadrature sets to integrate high-order polynomials. However, Morel's discretization of the angular momentum operator preserves only the first two eigenvalues of the scattering operator. Thus, it might be anticipated that discretizations of the Boltzmann GFP equations using standard discrete ordinates would be more accurate than discretizations of the differential GFP equations using Morel's discretization of L. However, our numerical results showed that this is not the case for pencil beam problems. This may be due to the severe space-angle coupling that exists in these problems and the fact that the spatial differencing schemes do not enable higher-order Lewis space-angle moments to be preserved exactly; thus, the theoretical gain in preserving more angular moments may be lost. This reasoning suggests that for infinite-medium problems with no space dependence, discrete solutions of the Boltzmann GFP equations might be more accurate than discrete solutions of the differential GFP equations. However, such problems are of narrow physical interest. Generally, we observed no advantage in accuracy in deterministic solutions of the Boltzmann GFP equations over deterministic solutions of the differential GFP equations.

V. DISCUSSION

We have developed accurate generalizations of the classical Fokker-Planck approximation to the monoenergetic linear Boltzmann equation for problems with highly forward-peaked scattering. Our analysis is based on earlier work of Pomraning,[3,4] who showed that for highly forward-peaked transport problems, the Boltzmann scattering operator can be asymptotically approximated as a polynomial in the angular momentum operator L. Pomraning's expansion is not directly useful for two reasons: It is a high-order differential operator, and some of its eigenvalues may be positive. In the GFP method, we replace Pomraning's polynomial expansion in L by an asymptotically equivalent rational function of L, chosen so that the first n eigenvalues of the approximation agree with those of the Boltzmann scattering operator and so that the remaining eigenvalues are negative. Our choices of rational functions of L lead to GFP approximations that can either be written as coupled systems of second-order differential (Fokker-Planck) equations or as a single Boltzmann (or BFP) equation. The nature of the differential (Fokker-Planck) form of these equations is (a) first-order transport in the spatial variable $(\underline{\Omega}\cdot\underline{\nabla})$ and (b) second-order diffusion in the angular variable L. Because these Fokker-Planck equations do not involve diffusion in the spatial variable, the well-known difficulties of discretizing the spatial diffusion operator on unstructured spatial grids do not arise. Also, if a Gauss-Legendre quadrature set is used, then Morel's accurate discretization of L can be employed. (However, Morel's discretization method is not available for certain other types of quadrature sets, and this might pose difficulties not addressed in this paper.) Our numerical results confirm that the Fokker-Planck and Boltzmann forms of the GFP equations are indeed equivalent and that the resulting GFP solutions can be significantly more accurate than classical Fokker-Planck solutions.

Our results are applicable to many charged-particle transport problems in which scattering is forward-peaked, but not sufficiently forward-peaked that the classical Fokker-Planck approximation is sufficiently accurate. Such problems include any particle transport problem in which the BFP approximation is viewed as a sufficiently accurate correction to the Fokker-Planck approximation.

The asymptotic validity of the GFP results presented in this paper relies on the asymptotic validity of Pomraning's results—because we derived the GFP equations from Pomraning's results. However, Pomraning himself has shown that his high-order polynomial expansions are not applicable to such commonly used scattering kernels as the screened Rutherford kernel. This is because the Boltzmann equation with the screened Rutherford kernel is not sufficiently forward-peaked to possess a high-order asymptotic polynomial expansion in L. [The screened Rutherford kernel does not satisfy Eq. (14c) for $n = 1$.] Since Pomraning's high-order expansion is not valid for screened Rutherford scattering, our GFP result may not be asymptotic to L_B for screened Rutherford scattering. In fact, recent work by Larsen[26] suggests that more complicated operators may be required to achieve a true asymptotic expansion of L_B for screened Rutherford scattering. In spite of this doubt concerning the asymptotic pedigree of the GFP approximation, Lewis's theory gives confidence that the GFP equations are more accurate than the Fokker-Planck equations because they preserve more space-angle moments of the transport solution. It still may be that in some meaningful but not-yet-understood sense, the L_{GFP} operators are asymptotic to L_B for screened Rutherford scattering. However, the analysis in this paper does not clearly establish this.

One aspect of the theory presented in this paper may be applicable to BFP simulations. Currently, in the construction of approximate BFP operators, the differential scattering cross section $\Sigma_s(\mu_0)$ is written as a sum of two nonnegative functions:

$$\Sigma_s(\mu_0) = \Sigma_1(\mu_0) + \Sigma_2(\mu_0) \ ,$$

where $\Sigma_1(\mu_0)$ depends smoothly on μ_0 for $-1 \leq \mu_0 \leq 1$, and $\Sigma_2(\mu_0)$ is very peaked at $\mu_0 = 1$ [and,

typically, $\Sigma_2(\mu_0) = 0$ for $-1 \le \mu_0 \le 1 - \epsilon$ with ϵ small]. This decomposition is not unique. After it is made, the scattering operator involving $\Sigma_2(\mu_0)$ is replaced by a Fokker-Planck operator that preserves Σ_{a0} and Σ_{a1}. Thus, particles and the scattering power are preserved. However, no attempt is usually made to preserve Σ_{a2} or any higher moments, perhaps by introducing a correction to $\Sigma_1(\mu_0)$. The results of Lewis discussed in this paper suggest that if moments Σ_{an} higher than $n = 1$ are preserved in BFP simulations, greater accuracy should result.

In this paper, we have not numerically compared the new GFP approximation to previous BFP approximations. It is virtually certain that BFP solutions will be more accurate than the conventional Fokker-Planck solutions for pencil beam problems and that GFP and BFP methods should be viewed as alternate methods for enhancing the accuracy of Fokker-Planck calculations. The possible advantages of the GFP method over the BFP method are the existence of the differential form of the GFP equations, and the fact that the GFP equations preserve more space-angle moments than the BFP equations (but, as described in the preceding paragraph, it may be possible to modify the BFP approximations to preserve extra moments as well). Further development and testing are required to clarify these issues.

For the GFP equations to become broadly applicable, certain aspects of the work presented in this paper must be developed more fully. First, GFP theory must be extended to include energy dependence. Second, it is important to establish whether there is a meaningful sense in which the GFP results are asymptotic for realistic scattering kernels. Third, an exploration of deterministic numerical methods for the GFP equations should be undertaken to understand more completely the relative advantages and disadvantages of the differential and integrodifferential forms of these equations. There are at least three important issues that should be examined:

1. Discretizations of the differential GFP equations yield larger linear systems of equations than discretizations of the integral GFP equations because there are more underlying differential equations. However, the discretized differential GFP equations are much sparser because these equations are differential (requiring only local angular coupling) rather than integral (requiring global angular coupling).

2. Highly forward-peaked scattering kernels often require very high order Legendre polynomial expansions in order to yield accurate, positive numerical results. This often places severe demands on the order and accuracy of the angular quadrature sets in discretizations of the integrodifferential transport and GFP equations. However, the differential GFP equations contain no highly peaked differential scattering cross sections that require a Legendre-polynomial expansion.

3. The continuous differential GFP equations always yield a positive solution. If accurate, diagonally dominant discretizations of the angular momentum operator L can be developed that preserve this positivity for general angular quadrature sets, then the process of angularly discretizing the differential GFP equations in a way that retains positivity of the solution will become very simple.

Also, there is the issue of whether an efficient technique exists to sample from the function $G(\mu_0)$, defined in Eq. (37). If such a technique can be found, then Monte Carlo simulations of Eq. (39) or (51) would be very efficient.

APPENDIX

DETERMINATION OF α_n AND β_n

In the GFP_3 method, constants α_1, β_1, and α_2 must be chosen so that the first three nonzero eigenvalues of L_{GFP_3} [Eq. (44)] equal the first three nonzero eigenvalues of L_B [Eq. (10)]. This yields the following nonlinear equations for α_1, β_1, and α_2:

$$\Sigma_{an} = \frac{\alpha_1 n(n+1)}{1+\beta_1 n(n+1)} + \alpha_2 n(n+1) \ , \quad 1 \le n \le 3 \ .$$

Multiplying these equations by $1 + \beta_1 n(n+1)$ and rearranging, we obtain

$$(\alpha_1 + \alpha_2) - \Sigma_{an}(\beta_1) + n(n+1)(\alpha_2\beta_1) = \frac{\Sigma_{an}}{n(n+1)} \ , \quad 1 \le n \le 3 \ . \qquad \text{(A.1)}$$

If we define

$$u_1 = \alpha_1 + \alpha_2 \ , \qquad \text{(A.2a)}$$

$$u_2 = \beta_1 \ , \qquad \text{(A.2b)}$$

$$u_3 = \alpha_2\beta_1 \ , \qquad \text{(A.2c)}$$

then Eqs. (A.1) become

$$u_1 - \Sigma_{an} u_2 + n(n+1)u_3 = \frac{\Sigma_{an}}{n(n+1)} \ , \quad 1 \le n \le 3 \ ,$$

which is a linear system of three equations for u_1, u_2, and u_3. This system can be solved uniquely, and then α_1, β_1, and α_2 can be determined uniquely from Eqs. (A.2a), (A.2b), and (A.2c). For screened Rutherford scattering, the resulting values of α_1, β_1, and α_2 are positive for all screening parameters satisfying (approximately) $0.0 < \eta < 0.1$. For electrons in water, this range of η corresponds to 10 keV $< E < \infty$. Therefore, the GFP_3 scheme applied to electrons in water breaks down only for electron energies less than ~10 keV.

In the GFP_4 method, constants α_1, β_1, α_2, and β_2 must be chosen so that the first four nonzero eigenvalues of L_{GFP_4} [Eq. (48)] equal the first four nonzero eigenvalues of L_B [Eq. (10)]. This yields the following nonlinear equations for α_1, β_1, α_2, and β_2:

$$\Sigma_{an} = \frac{\alpha_1 n(n+1)}{1+\beta_1 n(n+1)} + \frac{\alpha_2 n(n+1)}{1+\beta_2 n(n+1)} \ ,$$

$$1 \le n \le 4 \ .$$

Multiplying these equations by $[1 + \beta_1 n(n + 1)][1 + \beta_2 n(n + 1)]$ and rearranging, we obtain

$$(\alpha_1+\alpha_2) - \Sigma_{an}(\beta_1+\beta_2) - n(n+1)\Sigma_{an}(\beta_1\beta_2) + n(n+1)(\alpha_1\beta_2+\alpha_2\beta_1) = \frac{\Sigma_{an}}{n(n+1)} \ ,$$

$$1 \le n \le 4 \ . \qquad \text{(A.3)}$$

If we define

$$u_1 = \alpha_1 + \alpha_2 \ , \qquad \text{(A.4a)}$$

$$u_2 = \beta_1 + \beta_2 \ , \qquad \text{(A.4b)}$$

$$u_3 = \beta_1\beta_2 \ , \qquad \text{(A.4c)}$$

$$u_4 = \alpha_1\beta_2 + \alpha_2\beta_1 \ , \qquad \text{(A.4d)}$$

then Eq. (A.3) becomes

$$u_1 - \Sigma_{an}u_2 - n(n+1)\Sigma_{an}u_3 + n(n+1)u_4 = \frac{\Sigma_{an}}{n(n+1)} \ ,$$

$$1 \le n \le 4 \ ,$$

which is a linear system of four equations for u_1, u_2, u_3, and u_4. This system can be solved uniquely, and then α_1, β_1, α_2, and β_2 can be determined from Eqs. (A.4a) through (A.4d). For screened Rutherford scattering, the resulting values of α_1, β_1, α_2, and β_2 are positive for all screening parameters satisfying (approximately) $0.0 < \eta < 0.1$. (This is the same range of validity as for the GFP_3 method.) Therefore, for electrons in water, the GFP_4 scheme breaks down only for electron energies less than ~10 keV.

Hence, the GFP_3 and GFP_4 equations for α_n and β_n can be explicitly solved without the need to determine an approximate iterative solution. There is no general guarantee that the resulting values of α_n and β_n are positive, but our experience with screened Rutherford scattering is that α_n and β_n are positive for sufficiently small η, and in the GFP_2 method, α_n and β_n are positive for all values of η. Thus, one could employ a higher-order GFP method for fast electrons until they lose enough energy that this description is no longer valid. At this point, a lower-order GFP method, such as GFP_2, could be employed. Alternatively, an S_N method could be used directly because the scattering is now much more isotropic, so the use of a very high-order angular quadrature set is not required.

POSTSCRIPT

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