Beam Propagation in Multiple Scattering Media*

Arnold D. Kim\textsuperscript{a}, Joseph B. Keller\textsuperscript{b} and Miguel Moscoso\textsuperscript{c}

\textsuperscript{a}Department of Mathematics
Stanford University, USA

\textsuperscript{b}Departments of Mathematics and Mechanical Engineering
Stanford University, USA

\textsuperscript{c}Departamento de Matemáticas, Escuela Politécnica Superior
Universidad Carlos III de Madrid, Spain

ABSTRACT

We examine optical beam propagation and scattering in random media using three equations: radiative transfer, Fokker-Planck and Leakeas-Larsen. The Fokker-Planck equation gives a good approximation to the radiative transfer equation for forward peaked scattering phase functions. The Leakeas-Larsen equation gives an even better approximation. The solutions for all three of these equations can be represented as expansions in plane wave modes. Using these plane wave modes, we can compute solutions to these equations in a stable and efficient way.

1. INTRODUCTION

Light propagating in a medium that scatters, emits and absorbs radiation is governed by the radiative transport equation. When scattering is sharply peaked in the forward direction, the Fokker-Planck\textsuperscript{1,2} and the Leakeas-Larsen\textsuperscript{3} equations approximate the radiative transport equation well. Kim and Keller\textsuperscript{4} studied these two equations in slab domains with normally incident plane waves. Here we use these equations to study beam propagation.

Numerical solution of the radiative transport equation for beams is difficult because of the many variables involved. Monte Carlo methods are often used (see Moscoso et al\textsuperscript{5} and references therein), but their convergence rates are slow for optically thick media. Kim and Moscoso\textsuperscript{6} used a Chebyshev spectral method to overcome this difficulty.

Recently we have solved all three equations using expansions in plane wave modes.\textsuperscript{7} These modes are solutions to an eigenvalue problem. This method is similar to that of Chang and Ishimaru.\textsuperscript{8} We review it and compare its results with Monte Carlo simulations.

2. MULTIPLE SCATTERING EQUATIONS

The fundamental quantity in multiple scattering equations for light is the radiance or specific intensity $\Psi(\omega, r)$ in the direction of the unit vector $\omega$ at position vector $r$. We consider equations of the form

$$\omega \cdot \nabla \Psi(\omega, r) + \Sigma_a \Psi(\omega, r) = L \Psi(\omega, r)$$

where $\Sigma_a$ is the absorption coefficient. The scattering operator $L$ determines the equation:

1. Radiative Transport

$$L \Psi = \Sigma_s \int_{\Omega} f(\omega \cdot \omega') \Psi(\omega', r) d\omega' - \Sigma_s \Psi(\omega, r)$$

The integral is over the unit sphere $\Omega$. The phase function $f(\omega \cdot \omega')$ gives the fraction of light scattered in direction $\omega'$ which is incident in direction $\omega$, and $\Sigma_s$ is the scattering coefficient.

* This paper is an abridgement of a paper by the authors with the same title [submitted to SIAM J. Sci. Comput.]. For author information: (Send correspondence to A.D.K.) A.D.K.: E-mail: adkim@math.stanford.edu, Telephone: 1 650 723 2975, Address: Department of Mathematics, Stanford University, Stanford, CA 94305-2125, USA
2. Fokker-Planck

\[ L\Psi = \frac{1}{2} \Sigma_{tr} \Delta \Psi \]  

(3)

The transport coefficient is \( \Sigma_{tr} = \Sigma_s (1 - g) \) where

\[ g = \int_{\Omega} f(\mathbf{\omega} \cdot \mathbf{\omega}') \mathbf{\omega} \cdot \mathbf{\omega}' d\mathbf{\omega}' \]  

(4)

is the anisotropy factor, and \( \Delta \) is the spherical laplacian or angular momentum operator.

3. Leakeas-Larsen

\[ L\Psi = \alpha \Delta [I - \beta \Delta]^{-1} \Psi \]  

(5)

The parameters \( \alpha \) and \( \beta \) are defined by the first three coefficients of the Legendre polynomial expansion of the phase function.

Kim and Keller\(^4\) give a summary of the derivations for (3) and (5) as approximations of (2) for sharply forward peaked scattering.

3. NUMERICAL METHOD

Using the polar angle \( \theta \) with respect to the \( z \)-axis and azimuthal angle \( \phi \) to parameterize \( \mathbf{\omega} \), we write (1) as

\[
\cos \theta \frac{\partial \Psi}{\partial z} + \sin \theta \left[ \cos \phi \frac{\partial \Psi}{\partial x} + \sin \phi \frac{\partial \Psi}{\partial y} \right] + \Sigma_a \Psi = L\Psi. 
\]

(6)

We wish to solve (6) with \( L \) given by (2), (3) or (5) in the slab \( 0 < z < z_0 \) containing a uniform medium for which \( \Sigma_a \) and \( \Sigma_s \) are constant. A Gaussian beam of width \( W_0 \) impinges on the boundary \( z = 0 \) in the \( \theta = 0 \) direction. No other sources of light are present. Hence, we impose the boundary conditions:

\[
\Psi(\theta, \phi, z, x, y) = B(x, y) \frac{\delta(\theta)}{2\pi \sin \theta} \quad \text{for } 0 \leq \theta < \pi/2 \text{ and } -\pi \leq \phi < +\pi, 
\]

(7a)

\[
\Psi(\theta, \phi, z_0, x, y) = 0 \quad \text{for } \pi/2 < \theta \leq \pi \text{ and } -\pi \leq \phi < +\pi, 
\]

(7b)

with

\[
B(x, y) = e^{-(x^2+y^2)/W_0^2}. 
\]

(8)

Assuming that Fourier transformation with respect to \( x \) and \( y \)

\[
\hat{\Psi}(\theta, \phi, z, k, \varphi) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \Psi(\theta, \phi, z, x, y) \exp[-ikx \cos \varphi - iky \sin \varphi] \, dx \, dy. 
\]

(9)

is applicable, we transform (6) to

\[
\cos \theta \frac{\partial \hat{\Psi}}{\partial z} + ik \sin \theta \cos(\varphi - \phi) \hat{\Psi} + \Sigma_a \hat{\Psi} = L\hat{\Psi}. 
\]

(10)

The polar coordinates of the transform variables are \( (k, \varphi) \). The boundary conditions (7) transform to

\[
\hat{\Psi}(k, \varphi, 0, \theta, \phi) = \hat{B}(k) \frac{\delta(\theta)}{2\pi \sin \theta} \quad \text{for } 0 \leq \theta < \pi/2 \text{ and } -\pi \leq \phi < +\pi, 
\]

(11a)

\[
\hat{\Psi}(k, \varphi, z_0, \theta, \phi) = 0 \quad \text{for } \pi/2 < \theta \leq \pi \text{ and } -\pi \leq \phi < +\pi, 
\]

(11b)

with

\[
\hat{B}(k) = \frac{W_0^2}{2} e^{-W_0^2 k^2/4}. 
\]

(12)

Because \( L \) and the boundary conditions (11) are invariant with respect to azimuthal rotations, \( \hat{\Psi} \) involves only the relative azimuthal angle \( \varphi = \varphi - \phi \). Furthermore, it depends only parametrically on \( k \).
3.1. Plane Wave Mode Expansions

Plane wave modes are solutions of (10) of the form

$$\tilde{\Psi} = e^{\lambda z} V(\theta, \varphi)$$  \hspace{1cm} (13)

with $\varphi = \tilde{\varphi} - \phi$. Both $\lambda$ and $V$ depend on $k$. Substituting (13) into (10) yields the eigenvalue problem

$$\lambda \cos \theta V + ik \sin \theta \cos \varphi V + \Sigma_n V = LV.$$  \hspace{1cm} (14)

Kim and Keller showed that if $[\lambda, V(\theta, \varphi)]$ is a solution pair of (14) with $L$ given by (2), (3) or (5), then so is $[-\lambda, V(\pi - \theta, \varphi)]$.

In terms of the $[\lambda_n, V_n(\theta, \varphi)]$ pairs for which $\text{Re}[\lambda_n] > 0$, the general solution of (10) is

$$\tilde{\Psi}(\theta, \varphi, z, k) = \sum_{\text{Re}[\lambda_n]>0} \left\{ a_n e^{\lambda_n(z-z_0)} V_n(\theta, \varphi) + b_n e^{-\lambda_n z} V_n(\pi - \theta, \varphi) \right\}.$$  \hspace{1cm} (15)

The factor $e^{-\lambda_n z_0}$ has been introduced to keep the coefficients $a_n$ and $b_n$ from being too small. These expansion coefficients are determined by imposing the boundary conditions (7a) and (7b) which give, respectively:

$$\sum_{\text{Re}[\lambda_n]>0} \left\{ a_n e^{-\lambda_n z_0} V_n(\theta, \varphi) + b_n V_n(\pi - \theta, \varphi) \right\} = \tilde{B}(k) \frac{\delta(\theta)}{2\pi \sin \theta} \text{ for } 0 \leq \theta < \pi/2 \text{ and } -\pi \leq \varphi < +\pi, \hspace{1cm} (16a)$$

$$\sum_{\text{Re}[\lambda_n]>0} \left\{ a_n V_n(\theta, \varphi) + b_n e^{-\lambda_n z_0} V_n(\pi - \theta, \varphi) \right\} = 0 \text{ for } \pi/2 < \theta \leq \pi \text{ and } -\pi \leq \varphi < +\pi. \hspace{1cm} (16b)$$

The solution $\Psi$ in the physical domain is given by the inverse transform

$$\Psi(\theta, \varphi, z, y) = \frac{1}{(2\pi)^2} \int_0^\infty \int_{-\pi}^\pi \tilde{\Psi}(\theta, \varphi - \phi, z, k) \exp[ikx \cos \varphi + iky \sin \varphi] k d\phi dk.$$  \hspace{1cm} (17)

We solve (14) numerically. For (2) we approximate $L$ using a Gauss-Legendre quadrature for $\mu = \cos \theta$ and an extended trapezoid rule for $\varphi$ (see Appendix A). For (3) we use a second-order finite difference approximation for the spherical laplacian (see Appendix B). For (5) we also use this finite difference approximation and some additional matrix algebra to construct $L$. By replacing $L$ in (14) by one of these numerical approximations, we obtain a matrix eigenvalue problem. Each of the three matrix eigenvalue problems maintains the symmetry mentioned above. Kim et al give details of the numerical approximations used and their implementation.

3.2. The Transmitted Flux

The magnitude of the flux at $z = z_0$ is given by

$$F(z_0, x, y) = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi/2} \Psi(\theta, \phi, z_0, x, y) \cos \theta \sin \theta d\theta d\phi.$$  \hspace{1cm} (18)

By using (17) in (18), we find that this flux is axi-symmetric and is given by an inverse Hankel transform

$$F(z_0, \rho) = \frac{1}{2\pi} \int_0^\infty \tilde{F}(z, k) J_0(k\rho) k dk.$$  \hspace{1cm} (19)

Here $J_0(k\rho)$ is the Bessel function of order zero, $\rho = \sqrt{x^2 + y^2}$, and

$$\tilde{F}(z, k) = \int_{-\pi}^{\pi} \int_{-\pi}^{\pi/2} \tilde{\Psi}(\theta, \varphi, z, k) \cos \theta \sin \theta d\theta d\varphi.$$  \hspace{1cm} (20)

To evaluate the integral in (19), we use the FFTLog package. This algorithm requires samples of the functions $\tilde{F}(z, k)$ over a discrete set of $k$ values evenly spaced in $\log(k)$. With this choice of sample points, the Hankel transform is a Fourier convolution which can be approximated by discrete Fourier transforms.
4. RESULTS

In the results that follow, we used 32 points in $\mu$ and 8 points in $\varphi$ leading to eigenvalue problems with matrices of size $256 \times 256$. We replaced the delta function in $\mu$ given in (11a) by a normalized Gaussian of width $\theta_0 = 0.1 \text{ rad} \approx 5.7 \text{ deg}$. These eigenvalue problems were solved for each of the 256 points in $k$ that evenly sample the domain $-16 \leq \log(k) \leq +16$ on a logarithmic scale, for use in the discrete Hankel transforms. The same set of eigenvalues and eigenvectors are used for different slab thicknesses. Hence they only need to be computed once and stored in memory.

We compare results computed by this spectral method with those from Monte Carlo simulations. Monte Carlo simulations involve tracing individual photons as they propagate in and interact with the medium, and recording a score each time a photon encounters the scoring region. The scoring method we have used is a ring detector technique that is valid for normally incidence beams. Because this problem is symmetric, the ring detector estimates the average flux on a ring rather than the flux at the surface of a real detector. Since the score converges to the expected value at the rate $\text{const.}/\sqrt{N}$, where $N$ is the number of scores, the ring detector technique gives lower variance estimates. Particularly important is the fact that the ring detector has finite variance even in a scattering medium. For a more detailed discussion of Monte Carlo methods for photon transport problems, we refer to Moscoso et al\textsuperscript{5} and references therein.

4.1. The Radiative Transport Equation

We first compare results between the plane wave mode expansion method for the radiative transport equation and Monte Carlo simulations. For these comparisons, we use the Henyey-Greenstein scattering phase function

$$f(\theta, \varphi, \theta', \varphi') = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos \Theta)^{3/2}}$$

with

$$\cos \Theta = \cos \theta \cos \theta' + \sin \theta \sin \theta' \cos(\varphi - \varphi').$$

This phase function is parameterized only by the anisotropy factor $g$.

In Figs. 1–3, we plot the radial dependence of the transmitted flux (19) computed by Monte Carlo simulations (solid curves) and the plane wave mode expansion solution (dotted curves) of the radiative transport equation. In Fig. 1, the slab has optical thickness $\tau_o = (\Sigma_a + \Sigma_s)z_0 = 1$. For Figs. 2 and 3, the slab has optical thickness 5 and 10, respectively. Within the slab, the ratio of the absorption coefficient to the scattering coefficient is $\Sigma_a/\Sigma_s = 0.01$. The anisotropy factor is $g = 0.2$. The radial distance is normalized by the scattering mean free path $l_o/2$. In all of these results, we see excellent agreement between the two methods, since the two curves are nearly indistinguishable.

4.2. The Fokker-Planck and Leakeas-Larsen Equations

To solve the radiative transport equation with forward peaked scattering in which $g \sim 1$, one needs many more angle points to resolve the $L$ properly. This requirement leads to large matrix eigenvalue problems which increase the computational time significantly. Instead, we propose replacing the radiative transport equation by the Fokker-Planck and Leakeas-Larsen equations. These equations treat forward peaked scattering analytically and therefore do not require large numbers of angle points for numerical computations.

To compare solutions of the radiative transport equation to those of the Fokker-Planck and Leakeas-Larsen equations, we use the exponential phase function

$$f(\theta, \varphi, \theta', \varphi') = \frac{1}{2\pi \epsilon} \frac{\exp\left[-(1 - \cos \Theta)/\epsilon\right]}{1 - \exp[-2/\epsilon]}.$$  

The dimensionless parameter, $\epsilon$ controls the anisotropy. As $\epsilon \to 0$, the radiative transport equation with this phase function is asymptotic to the Fokker-Planck and Leakeas-Larsen equations.\textsuperscript{4}
Because (23) depends only on $\cos \Theta$, it can be expanded in Legendre functions

\[ f(\mu) = \sum_{n=0}^{\infty} (2n+1) f_n P_n(\cos \Theta) \]  

(24)

with

\[ f_n = \frac{1}{2} \int_{-1}^{+1} f(\cos \Theta) P_n(\cos \Theta) d(\cos \Theta). \]  

(25)

The first three coefficients are

\[ f_0 = 1, \]  

(26a)

\[ f_1 = \coth(\epsilon^{-1}) - \epsilon, \]  

(26b)

\[ f_2 = 1 - 3\epsilon \coth(\epsilon^{-1}) + 3\epsilon^2. \]  

(26c)

With (26) we define $\alpha$ and $\beta$ in (5) for the Leakeas-Larsen equation as

\[ \beta = \frac{2 - 3f_1 + f_2}{6(f_1 - f_2)} \]  

(27a)

\[ \alpha = \frac{\Sigma_a}{2} (1 - f_1)(1 + 2\beta) \]  

(27b)

In Figs. 4–6, we plot the radial dependence of the transmitted flux (19) computed by Monte Carlo simulations of the radiative transport equation (solid curves), and the plane wave mode expansion solutions of the Fokker-Planck (dotted curves) and Leakeas-Larsen (dashed curves) equations. In Fig. 4, the slab has optical thickness $\tau_o = 1$. In Figs. 5 and 6, the slab has optical thickness 5 and 10, respectively. The ratio of the absorption coefficient to the scattering coefficient is $\Sigma_a/\Sigma_s = 0.01$ and $\epsilon = 0.1$. Thus, the anisotropy factor is $g = 0.9$. The beam width is one half of a scattering mean free path $W_0 = l_o/2$.

Overall, the results for the Fokker-Planck and Leakeas-Larsen equations agree well with those of Monte Carlo simulations of the radiative transport equation. The largest error incurred by the Fokker-Planck equation occurs for the slab with $\tau_o = 1$ shown in Fig. 4. Since $g = 0.9$, the slab thickness is only $0.1l_{tr}$ where the transport mean free path is $l_{tr} = \Sigma_{tr}^{-1}$. It is too thin for the Fokker-Planck equation to provide a good approximation. As the thickness of the slab increases, the Fokker-Planck equation provides a better approximation. The Leakeas-Larsen equation results are nearly indistinguishable from the Monte Carlo results for all cases, so it yields a better approximation for thin slabs.

5. CONCLUSIONS

Plane wave modes can be used to solve the radiative transport, Fokker-Planck and Leakeas-Larsen equations. For media with strong forward scattering, the solutions of the Fokker-Planck and Leakeas-Larsen equations are close to those of the radiative transport equation, and they are easier to solve.

Acknowledgments

A. D. Kim was supported by a National Science Foundation Mathematical Sciences Postdoctoral Fellowship (DMS-0071578). J. B. Keller was supported in part by the Air Force Office of Scientific Research. M. Moscoso was supported from Dirección General de Enseñanza Superior grant PB98-0142-C04-01 from the Autonomous Region of Madrid (Strategic Groups Action) and by grant RTN2-2001-00349 from the European Union.
Figure 1. Transmitted flux computed by Monte Carlo simulations (solid curve) and by the plane wave mode expansion solution (dotted curve) of the radiative transport equation. The optical thickness of the slab is \( \tau_0 = 1.0 \) with \( \Sigma_s/\Sigma_a = 0.01 \) and has Henyey-Greenstein scattering with \( g = 0.2 \).

Figure 2. Same as Fig. 1 but for \( \tau_0 = 5 \). The right plot is a detail of the left one near the beam center.

Figure 3. Same as Fig. 1 but for \( \tau_0 = 10 \). The right plot is a detail of the left one near the beam center.
Figure 4. Transmitted flux computed by Monte Carlo simulations of the radiative transport equation (solid curve), the Fokker-Planck equation (dotted curve) and the Leakeas-Larsen equation (dashed curve). The optical thickness of the slab is $\tau_0 = 1.0$ with $\Sigma_s/\Sigma_a = 0.01$ and has exponential scattering with $g = 0.9$.

Figure 5. Same as Fig. 4 but for $\tau_0 = 5$. The right plot is a detail of the left one near the beam center.

Figure 6. Same as Fig. 4 but for $\tau_0 = 10$. The right plot is a detail of the left one near the beam center.
APPENDIX A. QUADRATURE RULES FOR THE RADIATIVE TRANSPORT EQUATION

The radiative transport scattering operator is

\[ Lu(\mu, \varphi) = -\Sigma_s u(\mu, \varphi) + \Sigma_s \int^{+\pi}_{-\pi} f(\mu, \varphi; \mu', \varphi') u(\mu', \varphi') d\mu' d\varphi' \]  \tag{28}

with \( \mu = \cos \theta \). To compute a numerical approximation to \( L \), we use the two dimensional quadrature rule

\[ Lu(\mu_i, \varphi_j) \approx -\Sigma_s \left[ u(\mu_i, \varphi_j) - \sum_{m=1}^{M} \sum_{n=1}^{N} u(\mu_m, \varphi_n) w_m \Delta \varphi \right]. \]  \tag{29}

We use an N-point extended trapezoid rule for the \( \varphi \) integration. The \( \varphi \) quadrature points are

\[ \varphi_j = -\pi + (j-1) \Delta \varphi \quad \text{for} \quad j = 1, \ldots, N, \]  \tag{30}

with \( \Delta \varphi = 2\pi/N \). For the \( \mu \) integration we use an M-point Gauss-Legendre quadrature rule\(^\text{12}\) with quadrature points \( \mu_i \) and quadrature weights \( w_i \). This approximation yields an \( MN \times MN \) matrix that is dense.

APPENDIX B. FINITE DIFFERENCE APPROXIMATION FOR THE SPHERICAL LAPLACIAN

The spherical laplacian operator \( \Delta \) is defined by

\[ \Delta u(\theta, \varphi) = \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left[ \sin \theta \frac{\partial u}{\partial \theta} \right] + \frac{1}{\sin^2 \theta} \frac{\partial^2 u}{\partial \varphi^2}. \]  \tag{31}

To compute numerical approximations of \( \Delta u \), we use finite difference methods. We sample \( u \) at discrete values \( u_{i,j} = u(\theta_i, \varphi_j) \) where

\[ \theta_i = \left( i - \frac{1}{2} \right) \Delta \theta \quad \text{for} \quad i = 1, \ldots, M \]  \tag{32}

with \( \Delta \theta = \pi/M \) and \( \varphi_j \) defined in (30). The \( \theta_i \) points avoid the numerical singularities \( \theta = 0 \) and \( \theta = \pi \). With these points and \( \theta_{i \pm 1/2} = \theta_i \pm \Delta \theta/2 \), the centered second order finite difference scheme is

\[ \Delta u_{i,j} \approx \frac{1}{\sin \theta_i} \frac{1}{\Delta \theta} \left[ \sin \theta_{i+1/2} \frac{u_{i+1,j} - u_{i,j}}{\Delta \theta} - \sin \theta_{i-1/2} \frac{u_{i,j} - u_{i-1,j}}{\Delta \theta} \right] + \frac{1}{\sin^2 \theta_i} \left[ \frac{u_{i,j+1} - 2u_{i,j} + u_{i,j-1}}{(\Delta \varphi)^2} \right]. \]  \tag{33}

The function \( u(\theta, \varphi) \) is \( 2\pi \)-periodic in \( \varphi \) so that

\[ u(\theta, \varphi) = u(\theta, \varphi + 2\pi). \]  \tag{34}

Therefore \( u_{i,0} = u_{i,N} \), and \( u_{i,N+1} = u_{i,1} \). To obtain numerical boundary conditions for the \( \theta \) variable, we recognize that

\[ u(-\Delta \theta, \varphi) = u(+\Delta \theta, \varphi \pm \pi), \]  \tag{35}

\[ u(\pi + \Delta \theta, \varphi) = u(\pi - \Delta \theta, \varphi \pm \pi). \]  \tag{36}

Therefore

\[ u_{0,j} = \begin{cases} u_{1,j+N/2} & \text{for} \quad j = 1, \ldots, N/2, \\ u_{1,j-N/2} & \text{for} \quad j = N/2 + 1, \ldots, N, \end{cases} \]  \tag{37}

and

\[ u_{M+1,j} = \begin{cases} u_{M,j+N/2} & \text{for} \quad j = 1, \ldots, N/2, \\ u_{M,j-N/2} & \text{for} \quad j = N/2 + 1, \ldots, N. \end{cases} \]  \tag{38}

The approximation (33) to \( \Delta \) yields an \( MN \times MN \) banded matrix of upper and lower bandwidth \( N \).
REFERENCES


