Stochastic View of Photon Migration in Turbid Media

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Abstract

Light propagation in an infinite uniform turbid medium is treated as a Markov stochastic process of photons to provide an intuitive framework for photon migration. The macroscopic physical quantities of photon migration are shown to be completely determined by the microscopic statistics of the photon propagation direction in direction space and a generalized Poisson distribution of the number of scattering events that includes an exponential decay absorption factor. A proper diffusion solution is derived with an exact time-dependent central position and half width of photon migration in this framework. The diffusion coefficient is found to be absorption-independent.
Propagation in a multiple scattering (turbid) medium such as the atmosphere is commonly treated by the theory of radiative transfer (see, for example, Chandrasekhar’s classic text[1]). Recent advances in ultrafast lasers and photon detectors for biomedical imaging and diagnostics have revitalized this field[2, 3, 4]. The basic equation of radiative transfer is the elastic Boltzmann equation, a non-separable integro-differential equation of first order for which an exact closed form solution is not known except for the case for isotropic scatterers as far as the authors know[5]. Solutions are often based on truncation of the spherical harmonics expansion of the photon distribution function or resort to numerical calculation including Monte Carlo simulation[6, 7]. Cai et. al.[8] recently used truncation of a cumulant expansion of the photon distribution function to solve the elastic Boltzmann equation.

In this Letter, photon migration in an infinite uniform medium is treated as a Markov stochastic process. The solution to the elastic Boltzmann equation with a point source propagating initially along the positive $z$-axis from the origin of space and time is interpreted as the probability of finding a photon at any specified location, direction and time.

In the stochastic picture of photon migration in turbid media, photons take a random walk in the medium and may get scattered or absorbed according to the scattering coefficient $\mu_s$ and the absorption coefficient $\mu_a$ of the medium. A normalized phase function, $f(s \cdot s')$, describes the probability of scattering a photon from direction $s$ to $s'$. The free path (step-size) between consecutive events (either scattering or absorbing) has an exponential distribution $\mu_T \exp(-\mu_T d)$ characterized by the total attenuation $\mu_T = \mu_s + \mu_a$. At an event, photon scattering takes place with probability $\mu_s/\mu_T$ (the albedo) and absorption with probability $\mu_a/\mu_T$. This picture forms the basis for Monte Carlo simulation of photon migration.

Here we will show that this simple picture of a Markov stochastic process of photons can be utilized to compute analytically macroscopic quantities such as the average central position and half width of the photon distribution. The microscopic statistics of the photon propagation direction in direction space (solely determined by the phase function and the incident direction) provides a basis for computing the macroscopic quantities at any specified time and position. The bridge between them is a generalized Poisson distribution $p_n(t)$, the probability that a photon has endured exactly $n$ scattering events before time $t$ (solely determined by the scattering and absorption coefficients of the medium).

Denote the $i$th propagation position, direction and step-size of a photon as $x^{(i)}$, $s^{(i)}$ and
Figure 1: A photon moving along $\mathbf{n}$ is scattered to $\mathbf{n}'$ with a scattering angle $\theta$ and an azimuthal angle $\phi$ in a photon coordinate system $xyz$ whose $z$-axis coincides with the photon’s propagation direction prior to scattering. $XYZ$ is the laboratory coordinate system.

The initial condition is $\mathbf{x}^{(0)} = (0, 0, 0)$ for the starting point and $\mathbf{s}^{(0)} = s_0 = (0, 0, 1)$ for the incident direction. The laboratory Cartesian components of $\mathbf{x}^{(i)}$ and $\mathbf{s}^{(i)}$ are $x^{(i)}_\alpha$ and $s^{(i)}_\alpha$ ($\alpha = 1, 2, 3$). The photon is incident at time $t_0 = 0$. For simplicity the speed of light is taken as the unit of speed and the mean free path $\mu_{\text{T}}^{-1}$ as the unit of length.

The scattering of photons takes a simple form in an orthonormal coordinate system $(\frac{\mathbf{m} - (\mathbf{n} \cdot \mathbf{m}) \mathbf{n}}{|\mathbf{n} \times \mathbf{m}|}, \frac{\mathbf{n} \times \mathbf{m}}{|\mathbf{n} \times \mathbf{m}|}, \mathbf{n})$ attached to the moving photon itself where $\mathbf{n}$ is the photon’s propagation direction prior to scattering and $\mathbf{m}$ is an arbitrary unit vector not parallel to $\mathbf{n}$[see Fig. 1]. The distribution of scattering angle $\theta \in [0, \pi]$ is given by the phase function of the medium and the azimuthal angle $\phi$ is uniformly distributed over $[0, 2\pi)$. For one realization of the scattering event of angles $(\theta, \phi)$ in the photon coordinate system, the outgoing propagation direction $\mathbf{n}'$ of the photon will be:

$$
\mathbf{n}' = \frac{\mathbf{m} - (\mathbf{n} \cdot \mathbf{m}) \mathbf{n}}{|\mathbf{n} \times \mathbf{m}|} \sin \theta \cos \phi + \frac{\mathbf{n} \times \mathbf{m}}{|\mathbf{n} \times \mathbf{m}|} \sin \theta \sin \phi + \mathbf{n} \cos \theta.
$$

(1)

The freedom of choice of the unit vector $\mathbf{m}$ reflects the arbitrariness of the $xy$ axes of the...
s_0=1 \quad <s_2>=g^2 \quad \frac{1}{1-g} 

<s_1>=g \quad <s_3>=g^3

Figure 2: The average photon propagation direction (vector) decreases as \( g^n \) where \( g \) is the anisotropy factor and \( n \) is the number of scattering events.

photon coordinate system. For example, taking \( \mathbf{m} = (0, 0, 1) \), Eq. (1) gives

\[
\begin{align*}
\langle s_{1}^{(i+1)} \rangle &= - \frac{\sin \theta}{\sqrt{1 - (s_{3}^{(i)})^2}} \left( s_{1}^{(i)} s_{3}^{(i)} \cos \phi - s_{2}^{(i)} \sin \phi + s_{1}^{(i)} \cos \theta \right) \\
\langle s_{2}^{(i+1)} \rangle &= - \frac{\sin \theta}{\sqrt{1 - (s_{3}^{(i)})^2}} \left( s_{2}^{(i)} s_{3}^{(i)} \cos \phi + s_{1}^{(i)} \sin \phi + s_{2}^{(i)} \cos \theta \right) \\
\langle s_{3}^{(i+1)} \rangle &= \sqrt{1 - (s_{3}^{(i)})^2} \sin \theta \cos \phi + s_{3}^{(i)} \cos \theta.
\end{align*}
\]

Here \( s_{\alpha}^{(i)} \) etc are stated in the laboratory coordinate system.

The ensemble average of the propagation direction over all possible realizations of (\( \theta, \phi \)) and then over all possible \( s_{\alpha}^{(i)} \) in Eq. (2) turns out to be \( \langle s_{\alpha}^{(i+1)} \rangle = \langle s_{\alpha}^{(i)} \rangle \langle \cos \theta \rangle \) because \( \theta \) and \( \phi \) are independent and \( \langle \cos \phi \rangle = \langle \sin \phi \rangle = 0 \). By recursion,

\[
\langle s_{\alpha}^{(n)} \rangle = \langle s_{\alpha}^{(0)} \rangle \langle \cos \theta \rangle^n = \hat{z} g^n = \hat{z} (1 - g_1)^n
\]

where \( g = \langle \cos \theta \rangle = 1 - g_1 \) is the anisotropy factor [see Fig. 2].

Using Eq. (2) and recognizing the symmetry obeyed by the \( x, y \) and \( z \) components of \( s_{\alpha}^{(i)} \), the correlations between the propagation directions are given by

\[
\langle s_{\beta}^{(i+1)} s_{\alpha}^{(i+1)} \rangle = \frac{g_2}{3} \delta_{\alpha \beta} + (1 - g_2) \langle s_{\beta}^{(i)} s_{\alpha}^{(i)} \rangle
\]

where \( g_2 = \frac{3}{2} \langle \sin^2 \theta \rangle \). On the other hand, the correlation between \( s_{\beta}^{(j)} \) and \( s_{\alpha}^{(i)} \) (\( j > i \)) can be reduced to a correlation of the form of Eq. (4) due to the following observation

\[
\begin{align*}
\langle s_{\beta}^{(j)} s_{\alpha}^{(i)} \rangle &= \int ds^{(j)} ds^{(i)} s_{\beta}^{(j)} p(s^{(j)}|s^{(i)}) s_{\alpha}^{(i)} p(s^{(i)}|s^{(0)}) \\
&= \int ds^{(j-1)} ds^{(i)} \left[ \int ds^{(j)} s_{\beta}^{(j)} p(s^{(j)}|s^{(j-1)}) \right] p(s^{(j-1)}|s^{(i)}) s_{\alpha}^{(i)} p(s^{(i)}|s^{(0)})
\end{align*}
\]
where \( p(s^{(j)}|s^{(i)}) \) means the conditional probability that a photon jumps from \( s^{(i)} \) to \( s^{(j)} \). Eq. (5) is a result of the Markov property of the process \( p(s^{(j)}|s^{(i)}) = \int ds^{(j-1)} p(s^{(j-1)}|s^{(i)}) p(s^{(i)}|s^{(0)}) \) and the fact \( \int ds^{(j)} s_{\beta}^{(j)} p(s^{(j)}|s^{(j-1)}) = g_{\beta}^{(j-1)} \) from Eq. (2). Combining Eqs. (4) and (5), and using the initial condition of \( s^{(0)} \), we conclude

\[
\langle s_{\beta}^{(j)} s_{\alpha}^{(i)} \rangle = \frac{\delta_{\beta\alpha}}{3} g^{j-i} \left[ 1 + f_\alpha (1 - g_2)^j \right], \quad j \geq i
\]

where constants \( f_1 = f_2 = -1 \) and \( f_3 = 2 \). Here we see that the auto-correlation of the \( x, y, \) or \( z \) component of the photon propagation direction approaches \( 1/3 \), i.e., scattering uniformly in all directions, after a sufficient large number of scattering (\( \alpha = \beta \) and \( j = i \to \infty \)), and the cross-correlation between them is zero (\( \alpha \neq \beta \)).

The connection between the macroscopic physical quantities about the photon distribution and the microscopic statistics of the photon propagation direction is made by the probability \( p_n(t) \) that the photon has taken exactly \( n \) scattering events before time \( t \) (the \( (n+1) \)-th event comes at \( t \)). We claim \( p_n(t) \) obeys the generalized Poisson distribution [14]

\[
p_n(t) = \frac{(\mu_s t)^n \exp(-t)}{n!} = \frac{(\mu_s t)^n \exp(-\mu_s t)}{n!} \exp(-\mu_a t)
\]

which is the Poisson distribution of times of scattering with the expected rate occurrence of \( \mu_s^{-1} \) multiplied by an exponential decay factor due to absorption. Here we have used \( \mu_T^{-1} = 1 \) as the unit of length. This form of \( p_n(t) \) can be easily verified by recognizing first that \( p_0(t) = \exp(-t) \) equals the probability that the photon experiences no events within time \( t \) (and the first event occurs at \( t \)); and second that the probability \( p_{n+1}(t) \) is given by

\[
p_{n+1}(t) = \int_0^t p_n(t-t') \frac{\mu_s}{\mu_T} p_0(t') dt' = \int_0^t \left[ \frac{(\mu_s t-t')^n \exp[-(t-t')] \mu_s}{\mu_T} \exp(-t') dt' \right] = \frac{(\mu_s t)^{n+1} \exp(-t)}{(n+1)!},
\]

in which the first event occurred at \( t' \) is scattering and followed by \( n \) scattering events up to but not including time \( t \), that confirms Eq. (7) at \( n+1 \) if Eq. (7) is valid at \( n \). The total probability of finding a photon at time \( t \)

\[
\sum_{n=0}^{\infty} p_n(t) = \exp(-\mu_a t)
\]

decreases with time due to the annihilation of photons due to absorption.
The average propagation direction \( \langle s(t) \rangle \) at time \( t \) is then,
\[
\langle s(t) \rangle = \frac{\sum_{n=0}^{\infty} \langle s_n \rangle p_n(t)}{\sum_{n=0}^{\infty} p_n(t)}. \tag{10}
\]
Plug Eqs. (3) and (7) into Eq. (10), we obtain
\[
\langle s(t) \rangle = \hat{z} \exp(-\mu_s g_1 t) = \hat{z} \exp(-t/l_t). \tag{11}
\]
Here \( l_t = \mu_s^{-1}/(1 - g) \) is usually called the transport mean free path which is the randomization distance of the photon propagation direction.

The first moment of the photon density with respect to position is thus
\[
\langle x(t) \rangle = \int_0^t \langle s(\tau) \rangle d\tau = \hat{z} l_t [1 - \exp(-t/l_t)], \tag{12}
\]
revealing that the center of the photon cloud moves along the incident direction for one transport mean free path \( l_t \) before it stops [see Fig. 3].

The second moment of the photon density is calculated as follows. Assume \( p(s_2, t_2|s_1, t_1) \) is the conditional probability that a photon jumps from a propagation direction \( s_1 \) at time \( t_1 \) to a propagation direction \( s_2 \) at time \( t_2 \) \( (t_2 \geq t_1 \geq 0) \), the conditional correlation of the photon propagation direction subject to the initial condition is given by
\[
\langle s_\beta(t_2)s_\alpha(t_1) \rangle = \frac{\int ds_2 ds_1 s_\beta s_\alpha p(s_2, t_2|s_1, t_1)p(s_1, t_1|s_0, t_0)}{\int ds_2 ds_1 p(s_2, t_2|s_1, t_1)p(s_1, t_1|s_0, t_0)}. \tag{13}
\]
Denote the number of scattering events encountered by the photon at states \((s_1, t_1)\) and \((s_2, t_2)\) as \( n_1 \) and \( n_2 \) respectively. Here \( n_2 \geq n_1 \) since the photon jumps from \((s_1, t_1)\) to \((s_2, t_2)\). Eq. (13) can be rewritten as
\[
\langle s_\beta(t_2)s_\alpha(t_1) \rangle = \frac{\sum_{n_2 \geq n_1} \langle s_\beta^{(n_2)} s_\alpha^{(n_1)} \rangle p_{n_2-n_1}(t_2-t_1)p_{n_1}(t_1)}{\sum_{n_2 \geq n_1} p_{n_2-n_1}(t_2-t_1)p_{n_1}(t_1)}. \tag{14}
\]
After a straightforward calculation by utilizing Eq. (6) and (7), we obtain
\[
\langle s_\beta(t_2)s_\alpha(t_1) \rangle = \frac{\delta_{\alpha\beta}}{3} [1 + f_\alpha \exp(-\mu_s g_2 t_1)] \exp \mu_s g_1 (t_1 - t_2). \tag{15}
\]
The second moment is then
\[
\langle x_\alpha^2(t) \rangle = 2 \int_0^t dt_2 \int_0^{t_2} dt_1 \langle s_\alpha(t_2) s_\alpha(t_1) \rangle. \tag{16}
\]
The diffusion coefficient is obtained from \( \left( \langle x^2 \rangle - \langle x \rangle^2 \right)/2t \), i.e.,
\[ D_{xx} = D_{yy} = \frac{1}{3t} \left\{ \frac{t}{\mu_s g_1} + \frac{g_2 (1 - \exp(-\mu_s g_1 t))}{\mu_s^2 g_1^2 (g_1 - g_2)} - \frac{1 - \exp(-\mu_s g_2 t)}{\mu_s^2 g_2 (g_1 - g_2)} \right\} \]

\[ D_{zz} = \frac{1}{3t} \left\{ \frac{t}{\mu_s g_1} - \frac{(3g_1 - g_2) [1 - \exp(-\mu_s g_1 t)]}{\mu_s^2 g_1^2 (g_1 - g_2)} + \frac{2 [1 - \exp(-\mu_s g_2 t)]}{\mu_s^2 g_2 (g_1 - g_2)} - \frac{3 [1 - \exp(-\mu_s g_1 t)]^2}{2 \mu_s^2 g_1^2} \right\} \]

after integration. This exact result does not depend on absorption and agrees with our previous independently calculated work [Eq. (21) in Ref. 8].

The general form of the photon distribution depends on all moments of the distribution. However, after a sufficient large number of scattering events have taken place, the photon distribution approaches a Gaussian distribution over space according to the central limit theorem [9]. This asymptotic Gaussian distribution, characterized by its central position and half width \((2Dt)\), is then

\[ G(x, t) = C(t) \frac{1}{(4\pi D_{zz} t)^{1/2}} \frac{1}{4\pi D_{xx} t} \exp \left[ -\frac{x^2 + y^2}{4D_{xx} t} - \frac{(z - \langle z(t) \rangle)^2}{4D_{zz} t} \right] \]  

where the normalizing factor \( C(t) = \exp(-\mu_a t) \) owing to Eq. (9). This provides a “proper” diffusion solution to radiative transfer, revealing a behavior of light propagation that photons migrate with a center that advances in time, and with an ellipsoidal contour that grows and changes shape [see Fig. 3].

It is also worth mentioning that the absorption coefficient only appears in the generalized Poisson distribution \( p_n(t) \) through an exponential decay factor \( \exp(-\mu_a t) \). This exponential factor will be canceled in the evaluation of the conditional moments of the photon distribution [see Eqs. (13) and (14)]. Hence, the sole role played by absorption is to annihilate photons and affects neither the shape of the distribution function nor the diffusion coefficient [10, 11].

The results, except for the Gaussian photon distribution Eq. (18), are exact under the sole assumption of a Markov random process of photon migration. The deviation from a Poisson distribution of scattering or absorption events can be dealt with by modifying \( p_n(t) \). The Markov random process is usually a good description of scattering due to short-range forces such as photon migration in turbid media. In situations where interference of light is appreciable, the phase of photon, which depends on its full past history, must be considered and this is non-Markovian. One well-known example is weak localization of light [12]. Non-Markov processes may also occur in scattering involving long-range forces such as Coulomb
Figure 3: The center of a photon cloud approaches $l_t$ along the incident direction and the diffusion coefficient approaches $l_t/3$ with increase of time.

interaction between charged particles in which the many-body effect can not be ignored. However, the idea presented here may still be helpful.

In summary, the macroscopic physical property of photon migration in turbid medium has its root in the microscopic statistics of photon propagation direction in direction space which is solely determined by the phase function. A generalized Poisson distribution function determined by the scattering and absorption coefficients of the medium serves as a bridge to connect the microscopic statistics to the macroscopic property. This provides us a clear and comprehensive physical picture of photon migration in turbid medium.

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[13] For example, squaring the third equation in Eq. (2) and then taking an ensemble average, yields \( \left( s_3^{(i+1)} \right)^2 = \frac{1}{2} \left( s_3^{(i)} \right)^2 / 2 + \frac{1}{2} \left( s_3^{(i)} \right)^2 / 2 = g_2 / 3 + (1 - g_2) \left( s_3^{(i)} \right)^2 \) as \( \langle \sin^2 \phi \rangle = \langle \cos^2 \phi \rangle = \frac{1}{2} \). Similar equalities are obtained for \( x \) and \( y \) components as the label is rotated.

[14] Note added in review: The generalized Poisson distribution Eq. (7) was previously proven in Lihong Wang and S. L. Jacques, Phys. Med. Biol. 39, 2349 (1994).