A Fast Algorithm to the Radiative Transport Equation and Implementation of Theory Into an Applet

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Abstract

In random media, such as clouds or biological tissue, light obeys the Radiative Transport Equation (RTE). Using the RTE, we developed a fast algorithm and implemented a Java applet to calculate the energy density of light in three dimensions.

1 Introduction

The radiative transport equation (RTE) has a connection to many interdisciplinary fields [1, 2, 3, 4]. In particular, light in random media is described by the RTE. For example, optical tomography is formulated as inverse problems of the RTE [5, 6].

A lot of numerical methods of solving the RTE have been developed [1, 2, 3, 4, 5, 6, 7], which include the Monte Carlo method, the finite element method, the P_L method, and the method of discrete ordinates. In 1960, Professor Kenneth Myron Case from University of Michigan published a paper on solving the one-dimensional RTE analytically [8]. Our theory in this report for the three-dimensional RTE is based on Case's method [9].

In this paper we will describe the theory for the three dimensional radiative transport equation. We will also delve into the implementation of a Java applet. The applet is programmed to graph the energy density of light in a three dimensional random medium.

2 Solving the Radiative Transport Equation

We consider the time-independent radiative transport equation (RTE) in three dimensions:

$$\hat{s} \cdot \nabla u + (\mu_a + \mu_s)u = \mu_s \int_{\mathbb{S}^2} p(\hat{s}, \hat{s}')u(\vec{r}, \hat{s})d\hat{s}' + S(\vec{r}, \hat{s}). \tag{1}$$

Here variables are defined as follows:

$\vec{r}$: The three dimensional position vector $\vec{r} = \langle x, y, z \rangle$.
$\hat{s}$: The three dimensional directional vector $\hat{s} = \langle \sin(\theta)\cos(\phi), \sin(\theta)sin(\phi), \cos(\theta) \rangle$.
∇: The three dimensional gradient vector $\nabla = \langle \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \rangle$.
$u(\vec{r}, \hat{s})$: The intensity of light dependent on position $\vec{r}$ and direction $\hat{s}$.
μ_a: The absorption constant proportional to the probability of absorption per unit length.
μ_s: The scattering constant proportional to the probability of scattering per unit length.
$S(\vec{r}, \hat{s})$: Source of light.
$p(\hat{s}, \hat{s}')$: The phase scattering function, modeling the probability of light being scattered from direction $\hat{s}'$ to direction $\hat{s}$.

Here we assume linear scattering

$$p(\hat{s}, \hat{s}') = \frac{1}{4\pi} + \frac{3g}{4\pi}(\hat{s} \cdot \hat{s}'), \quad g \in [0, 1]. \tag{2}$$

Note that g is the linear asymmetry parameter

$$g = \int_{\mathbb{S}^2} (\hat{s} \cdot \hat{s}')p(\hat{s}, \hat{s}')d\hat{s}'. \tag{3}$$

2.1 Specific Intensity

We define the total attenuation μ_t as

$$\mu_t = \mu_s + \mu_a. \tag{4}$$

Let us now introduce a constant c:

$$c = \frac{\mu_s}{\mu_a + \mu_s}. \tag{5}$$

By taking the unit of length to be $1/\mu_t$, we divide (1) by μ_t. Thus, we rewrite (1) into a more convenient form:

$$\hat{s} \cdot \nabla u + u = c \int_{\mathbb{S}^2} p(\hat{s}, \hat{s}')u(\vec{r}, \hat{s})d\hat{s}' + \frac{S(\vec{r}, \hat{s})}{\mu_t}. \tag{6}$$

We then obtain $u(\vec{r},\hat{s})$ as a superposition of elementary solutions $u_\nu(\vec{r},\hat{s};\vec{q})$, which obey

$$\hat{s}\cdot\nabla u_\nu + u_\nu = c\int_{\mathbb{S}^2} p(\hat{s},\hat{s}')u_\nu(\vec{r},\hat{s}')d\hat{s}'. \tag{7}$$

The elementary solutions are labeled by $\nu\in\mathbb{R}$ and $\vec{q}\in\mathbb{R}^2$ and are obtained by separation of variables [9].

2.2 Eigenvalues

In the case of linear scattering (2), the index ν which labels u_ν, is either $\pm\nu_0$ where ($\nu_0>1$), or any value on $(-1,1)$. We can calculate ν_0 as follows [9, 10]. Let us expand u_ν with Legendre polynomials.

$$u_\nu(\vec{r},\hat{s};\vec{q}) = \sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\hat{s}\cdot\hat{k})e^{-\hat{k}\cdot\vec{r}/\nu}, \tag{8}$$

where the vector $\hat{k}$ is given by [9]

$$\hat{k} = \begin{pmatrix} -i\nu\vec{q} \\ Q(\nu q)\end{pmatrix}, \quad Q(\nu q) = \sqrt{1+\nu^2 q^2}, \quad q = |\vec{q}|\,. \tag{9}$$

Here Legendre polynomials are recursively computed as

$$P_0 = 1, \quad P_1 = \mu, \qquad P_{l+1} = \frac{(2l+1)\mu P_l - lP_{l-1}}{l+1}. \tag{10}$$

Moreover, spherical harmonics are given by

$$Y_{lm}(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\phi}. \tag{11}$$

By plugging (8) into (7), we end up with the following equation.

$$\begin{aligned}\hat{s}\cdot\nabla\sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\hat{s}\cdot\hat{k})e^{-\hat{k}\cdot\vec{r}/\nu} \quad &+ \quad \sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\hat{s}\cdot\hat{k})e^{-\hat{k}\cdot\vec{r}/\nu} \\ &= \quad c\int_{\mathbb{S}^2} p(\hat{s},\hat{s}')\sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\hat{s'}\cdot\hat{k})e^{-\hat{k}\cdot\vec{r}/\nu}d\hat{s}'.\end{aligned} \tag{12}$$

We write

$$p(\hat{s},\hat{s}') = \sum_{lm} p_l Y_{lm}(\hat{s}\cdot\hat{k}) Y^*_{lm}(\hat{s}'\cdot\hat{k}), \tag{13}$$

where $p_0 = 1$, $p_1 = g$, $p_2 = p_3 = \cdots = 0$. We now have

$$-\frac{\mu}{\nu}\sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\mu) + \sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\mu) = c\sum_l p_l\sqrt{\frac{2l+1}{4\pi}}C_l P_l(\mu). \tag{14}$$

We then multiply $P_{l_0}(\mu)$ and integrate both sides over μ. Note that

$$\int_{-1}^{1} P_l(\mu)P_{l'}(\mu)d\mu = \frac{2}{2l+1}\delta_{ll'}, \tag{15}$$

where $\delta_{ll'}$ is the Kronecker's delta function (if $l = l'$, then $\delta_{ll'} = 1$ and if $l \neq l'$, then $\delta_{ll'} = 0$). After some calculations, (14) reduces to the following equation:

$$\begin{aligned}\sum_{l=0}^{\infty}\left[\frac{l+1}{\sqrt{[4(l+1)^2-1](\sigma_{l+1})(\sigma_l)}}\delta_{l_0,l+1} \right. &+ \left.\frac{l}{\sqrt{(4l^2-1)(\sigma_{l-1})(\sigma_l)}}\delta_{l_0,l-1}\right]C_l\sqrt{2l+1}\sqrt{\sigma_l} \\ &= \nu C_{l_0}\sqrt{2l_0+1}\sqrt{\sigma_{l_0}},\end{aligned} \tag{16}$$

where $\sigma_l = (1 - cp_l)$.

Upon rewriting (14) in the form of a matrix-vector equation $Bx = \nu x$, we can solve for eigenvalues ν and ν_0 as explained below.

$$B = \begin{bmatrix} B_{00} & B_{01} & B_{02} & . & . & B_{0n} \\ B_{10} & B_{11} & B_{12} & . & . & B_{1n} \\ B_{20} & B_{21} & B_{22} & . & . & B_{2n} \\ . & . & . & . & . & . \\ . & . & . & . & B_{n-1n-1} & . \\ B_{n0} & B_{n1} & B_{n3} & . & . & B_{nn} \end{bmatrix}.$$

Note that from (16) we have

$$B_{l_0 l} = \left[\frac{l+1}{\sqrt{[4(l+1)^2-1](\sigma_{l+1})(\sigma_l)}}\delta_{l_0,l+1} + \frac{l}{\sqrt{(4l^2-1)(\sigma_{l-1})(\sigma_l)}}\delta_{l_0,l-1}\right]. \tag{17}$$

That is,

$$B = \begin{bmatrix} 0 & \frac{1}{\sqrt{3\sigma_1\sigma_0}} & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{3\sigma_1\sigma_0}} & 0 & \frac{2}{\sqrt{15\sigma_2\sigma_1}} & 0 & 0 & 0 \\ 0 & \frac{2}{\sqrt{15\sigma_2\sigma_1}} & 0 & . & . & 0 \\ 0 & 0 & . & 0 & . & 0 \\ 0 & 0 & 0 & . & 0 & \frac{n}{\sqrt{(4n^2-1)\sigma_n\sigma_{n-1}}} \\ 0 & 0 & 0 & 0 & \frac{n}{\sqrt{(4n^2-1)\sigma_n\sigma_{n-1}}} & 0 \end{bmatrix}.$$

Hence, diagonalizing the symmetric matrix B will yield real eigenvalues $\nu \in (0,1)$ and $\nu_0 > 1$, where ν_0 is the largest eigenvalue. These eigenvalues can later be used to solve for constants N_0 and $N(\nu)$.

3 Finding Energy Density $U(z)$

The Green's function $G(\vec{r}, \hat{s}; \vec{r_0}, \hat{s}_0)$ for the radiative transport equation satisfies

$$\hat{s} \cdot \nabla G + G = c \int_{\mathbb{S}^2} p(\hat{s}, \hat{s}')G(\vec{r}, \hat{s}')d\hat{s}' + \delta(\vec{r} - \vec{r_0})\delta(\hat{s} - \hat{s}_0), \qquad (18)$$

where $\delta(\vec{r} - \vec{r_0}), \delta(\hat{s} - \hat{s}_0)$ are the Dirac delta functions with properties:

$$\int_{-\infty}^{\infty} \delta(x)dx = 1, \qquad (19)$$

$$\int_{-\infty}^{\infty} f(x)\delta(x - x_0)dx = f(x_0). \qquad (20)$$

We obtain G in (18) using u_ν in (7), which we write as $u_\nu(\vec{r}, \hat{s}; \vec{q}) = \phi_\nu(\mu(\hat{k}))e^{-\hat{k}\cdot\vec{r}/\nu}$, where $\mu(\hat{k}) = \hat{s} \cdot \hat{k}$. We can write G as

$$G_+ = A_+\phi_{\nu_0}(\mu(\hat{k}))e^{i\vec{q}\cdot\vec{\rho}}e^{-Q(\nu_0 q)z/\nu_0} + \int_0^1 A(\nu)\phi_\nu(\mu(\hat{k}))e^{i\vec{q}\cdot\vec{\rho}}e^{-Q(\nu q)z/\nu}d\nu \qquad (21)$$

for $z > z_0$,

$$G_- = -A_-\phi_{-\nu_0}(\mu(\hat{k}))e^{i\vec{q}\cdot\vec{\rho}}e^{Q(\nu_0 q)z/\nu_0} - \int_{-1}^0 A(\nu)\phi_\nu(\mu(\hat{k}))e^{i\vec{q}\cdot\vec{\rho}}e^{-Q(\nu q)z/\nu}d\nu \qquad (22)$$

for $z < z_0$, where $\vec{\rho} = \langle x, y \rangle$. Moreover, A_+, A_-, and $A(\nu)$ are functions of $\vec{q}$ that we must solve for. To solve for A_+, A_-, and $A(\nu)$, we integrate (18) with respect to z as $\int_{z_0-\epsilon}^{z_0+\epsilon}(18)dz$ for $\epsilon \approx 0$. Then we use the orthogonality relations for $\phi_\nu(\mu)$:

$$\int_{-1}^{1} \mu \phi_{\nu_0}^2(\mu) d\mu = N_0, \tag{23}$$

$$\int_{-1}^{1} \mu \phi_\nu(\mu) \phi_\nu'(\mu) d\mu = N(\nu)\delta(\nu - \nu'), \tag{24}$$

$$\int_{-1}^{1} \mu \phi_\nu(\mu) \phi_\nu'(\mu) d\mu = 0, \tag{25}$$

if $\nu \neq \nu'$. Here N_0 and $N(\nu)$ are given by

$$\begin{aligned} N_0 &= \frac{c\nu_0^3}{2}\gamma(\nu_0)\left[\frac{c}{\nu_0^2 - 1}\gamma(1) - \frac{\frac{1}{\nu_0^2}(3\gamma(\nu_0) - 2)(1 - c + c\gamma(\nu_0))}{\gamma(\nu_0)}\right. \\ &+ \left. 3c(\gamma(1) - 1)\right], \end{aligned} \tag{26}$$

$$N(\nu) = \nu\left[(1 - c + c\gamma(\nu) - c\nu\gamma(\nu)\tanh^{-1}(\nu))^2 + (\frac{\pi c \nu}{2}\gamma(\nu))^2\right], \tag{27}$$

where $\gamma(\nu) = 1 + 3g\sigma_0\nu^2$. Using the orthogonality relations and some Dirac delta function relations we obtain:

$$A_+(\vec{q_0}) = \frac{1}{2\pi Q(\nu_0 q_0) N_0} e^{-i\vec{q_0}\cdot\vec{\rho_0}} e^{Q(\nu_0 q_0) z_0/\nu_0} \phi_{\nu_0}^*(\mu_0(\hat{k})), \tag{28}$$

$$A_-(\vec{q_0}) = \frac{-1}{2\pi Q(\nu_0 q_0) N_0} e^{-i\vec{q_0}\cdot\vec{\rho_0}} e^{-Q(\nu_0 q_0) z_0/\nu_0} \phi_{-\nu_0}^*(\mu_0(\hat{k})), \tag{29}$$

$$A(\nu) = \frac{1}{2\pi Q(\nu q_0) N(\nu)} e^{-i\vec{q_0}\cdot\vec{\rho_0}} e^{Q(\nu q_0) z_0/\nu} \phi_\nu^*(\mu_0(\hat{k})). \tag{30}$$

We can then include A_+, A_-, and $A(\nu)$ in (21) and (22) and combining (21) and (22) will yield:

$$\begin{aligned} G(\vec{\rho}, z, \hat{s}; \vec{\rho_0}, z_0, \hat{s}_0) &= \frac{1}{(2\pi)^3}\int_{\mathbb{R}^2} e^{i\vec{q}\cdot(\vec{\rho}-\vec{\rho_0})}\left[\frac{\phi_{\pm\nu_0}(\mu(\hat{k}))\phi_{\pm\nu_0}^*(\mu_0(\hat{k}))}{Q(\nu_0 q)N_0} e^{\frac{-Q(\nu_0 q)|z-z_0|}{\nu}}\right. \\ &+ \left.\int_0^1 \frac{\phi_{\pm\nu_0}(\mu(\hat{k}))\phi_{\pm\nu_0}^*(\mu_0(\hat{k}))}{Q(\nu q)N(\nu)} e^{\frac{-Q(\nu q)|z-z_0|}{\nu}} d\nu\right] d\vec{q}. \end{aligned} \tag{31}$$

We now recover the dimension. Let us consider a point source

$$S(\vec{r}, \hat{s}) = \delta(\vec{r}). \tag{32}$$

We obtain u as

$$u(\vec{\rho}, z, \hat{s}) = \mu_t^2 \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} G(\vec{\rho}, z, \hat{s}; \vec{\rho}_0, z_0, \hat{s}_0) \delta(\vec{\rho_0}) \delta(z_0) d\vec{\rho}_0 dz_0 d\hat{s}_0. \tag{33}$$

We calculate the energy density U of light defined as

$$U = \frac{1}{v} \int u(\vec{r}, \hat{s}) d\hat{s}, \tag{34}$$

where v is the speed of light in the medium. Since U is spherically symmetric, we measure it along the z-axis as

$$U(z) = \frac{\mu_t}{vz} \left[\frac{e^{\left(\frac{-\mu_t z}{\nu_0}\right)}}{\nu_0 N_0} + \int_0^1 \frac{e^{\left(\frac{-\mu_t z}{\nu}\right)}}{\nu N(\nu)} d\nu \right], \quad z > 0. \tag{35}$$

We conclude the theory for our algorithm by plotting $U(z)$ in Figure 1.

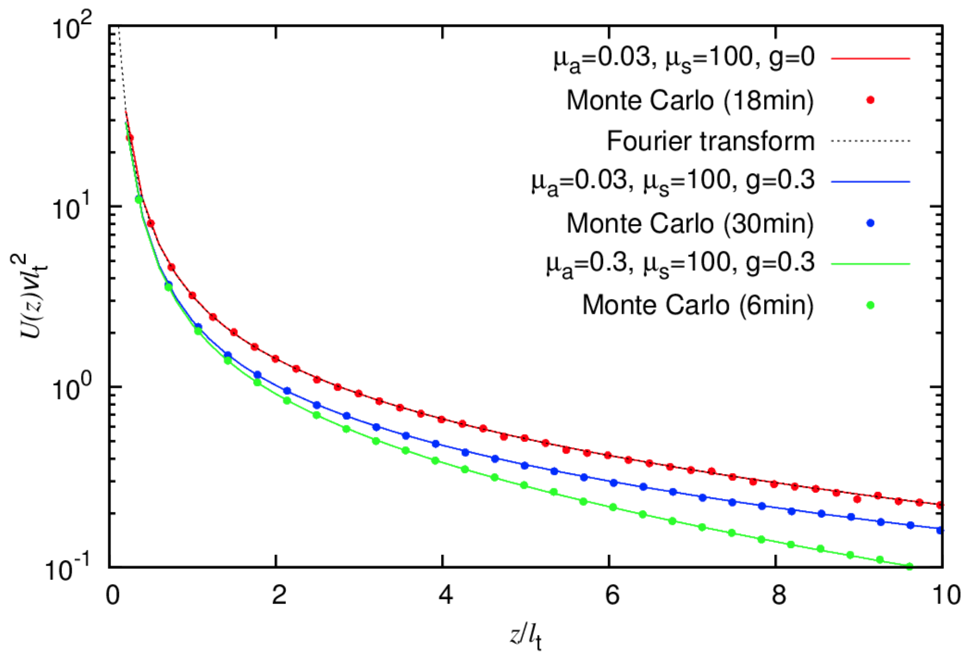

Figure 1: Energy density $U(z)$ in (35) for different optical parameters compared with results from Monte Carlo simulations [13]. For isotropic scattering, $U(z)$ can also be obtained analytically with the Fourier transform.

4 Implementation of the Applet

We aspired to create an applet, in the programming language Java, which can graph the intensity of light depending on a point in three dimensional space.

A snippet of our applet can be seen below:

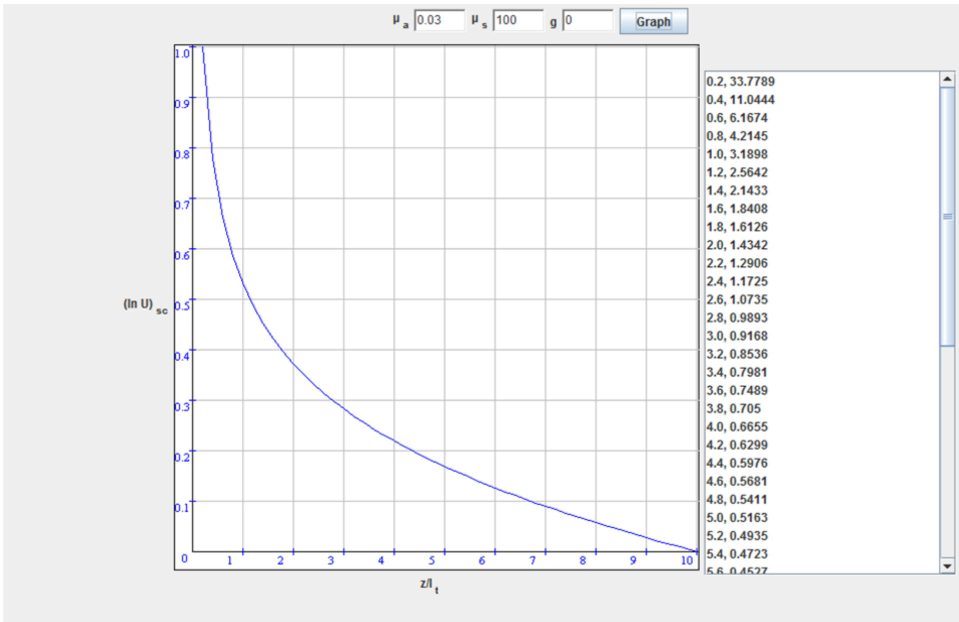

Figure 2: Java Applet Using Quick RTE Algorithm.

The applet simply takes the user input: μ_a, μ_s, and g (see page 2 of this report) which are the absorption constant, scattering constant, and scattering asymmetry parameter, respectively. Upon invoking the "Graph" button, a list of $[z, U(z)]$ coordinates appear on the list to the right of the graphic, and a density line is drawn on the graph. The coordinates in the list are exact measures of intensity accurate to $\frac{1}{1000}$th of a decimal.

In the graph, the vertical axis shows $(\ln U)_{sc}$, which is given below, and the horizontal axis is z/l_t.

We discretize z as

$$z_i = i\Delta z, \quad i = 1, 2, ..., N, \quad N = 50, \quad N\Delta z = 10 l_t, \tag{36}$$

where $l_t = 1/\mu_t$. We then define $(\ln U)_{sc}$ as

$$(\ln U)_{sc} = \frac{\ln U(z_i) - \ln U(z_N)}{\ln U(z_1) - \ln U(z_N)}, \tag{37}$$

This scaling prevents the graph from digressing from the viewing window of $z/l_t \in [0, 10]$ and $(\ln U)_{sc} \in [0, 1]$ in our applet.

5 Summary

In this report we illustrated the theory for solving the three dimensional radiative transport equation. Moreover, we implemented a Java applet which is formulated to graph the energy density of light in a three dimensional random medium. The URL for the Java applet can be found below.
URL: https://sites.google.com/site/ezrte13/

References

[1] S. Chandrasekhar, *Radiative Transfer* (Dover, 1960).

[2] K. M. Case and P. F. Zweifel, *Linear Transport Theory* (Addison-Wesley, 1967).

[3] A. Ishimaru *Wave Propagation and Scattering in Random Media* (Academic Press, 1978).

[4] L. A. Apresyan and Y. A. Kravtsov, *Radiation Transfer: Statistical and Wave Aspects* (Gordon and Breach Publishers, 1996).

[5] S. R. Arridge "Optical tomography in medical imaging," Inverse Problems **15** (1999) R41–R93.

[6] S. R. Arridge and J.C. Schotland, "Optical Tomography: Forward and Inverse Problems," Inverse Problems **25** (2009) 123010 (pp. 59).

[7] K. Ren, "Recent Developments in Numerical Techniques for Transport-Based Medical Imaging Methods," Commun. Comput. Phys. **8** (2010) 1–50.

[8] K. M. Case "Elementary Solutions of the Transport Equation and Their Applications," Ann. Phys. **9** (1960) 1–23.

[9] M. Machida, "The three-dimensional radiative transport equation with Case's method and rotated reference frames," arXiv:1304.1941.

[10] M. Machida, "Case's Eigenvalues by Markel's Matrix," arXiv:1304.5207.

[11] V. A. Markel, "Modified spherical harmonics method for solving the radiative transport equation," Waves in Random Media **14** (2004) L13–L19.

[12] G. Panasyuk, J. C. Schotland, and V. A. Markel, "Radiative transport equation in rotated reference frames," J. Phys. A: Math. Gen. **39** (2006) 115–137.

[13] The Monte Carlo package MC written by Vadim A. Markel was used after implementing linear scattering.