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# Chapter 5:
# *Monte Carlo Modeling of Light Transport in Tissue (Steady State and Time of Flight)*

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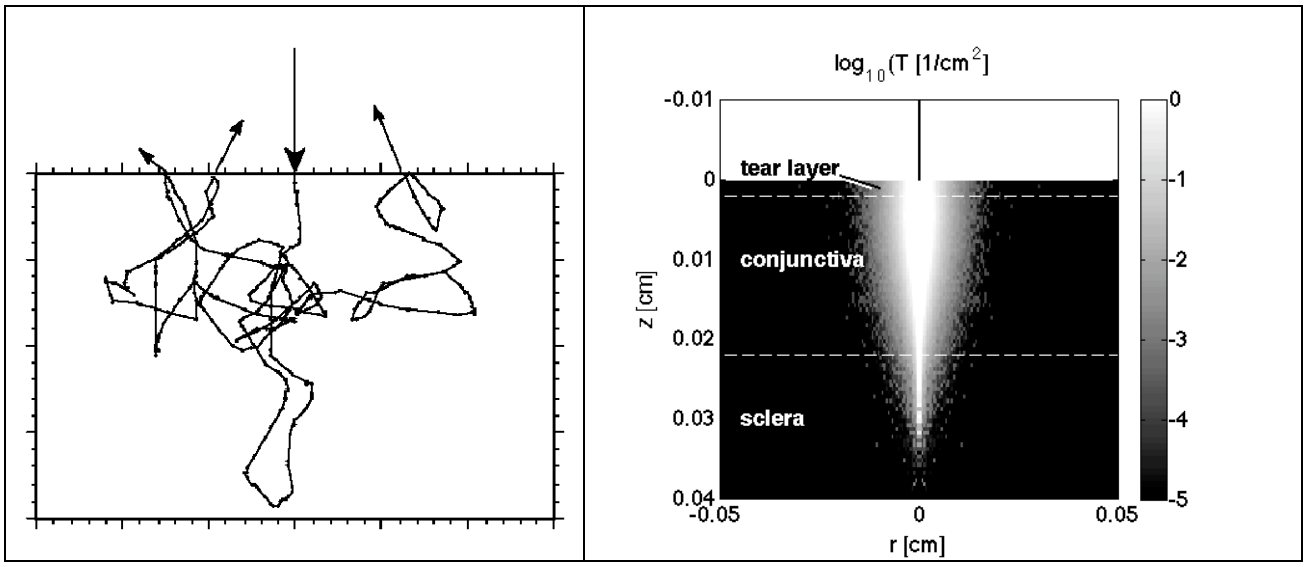
**Abstract**

This chapter introduces Monte Carlo simulations of light transport in light-scattering light-absorbing media such as biological tissues. Monte Carlo simulations provide a versatile method of predicting the distribution of light in biological tissues. The basic approach of Monte Carlo sampling is introduced, and illustrated by considering the variety of ways to launch photons, such as a collimated pencil beam, a uniform flat-field beam, a collimated or focused Gaussian beam, and as an isotropic point source. Steady-state Monte Carlo propagation of photons is first presented. Then, time-resolved propagation of photons is presented, along with its conversion to the frequency domain of modulated light. The chapter offers a basic introduction to Monte Carlo, providing a first step toward using and modifying Monte Carlo simulations for various light transport problems.

## 5.1 INTRODUCTION

Monte Carlo simulations are a fundamental and versatile approach toward modeling light transport in tissues. While diffusion theory for light transport is a fast and convenient way to model light transport, it fails when close to sources or boundaries and when absorption is strong compared to scattering, in other words whenever conditions cause the gradient of fluence rate (or photon concentration) to not be simply linear but to have some curvature. Monte Carlo steps in to treat problems when diffusion theory fails. Figure 5.1 illustrates a Monte Carlo simulation.




**A** **B**

**Figure 5.1**: A Monte Carlo simulation of photon transport. (A) Movement of a single photon in a light-scattering tissue. When the photon is totally internally reflected at the air/tissue surface, a fraction of the photon weight is allowed to escape as reflectance and the remaining photon weight continues to propagate in the tissue. In this example for the sake of illustration, the third time the photon encounters the surface, the photon is allowed to fully escape. (B) Superposition of millions of photons recorded as relative fluence rate, [W/cm$^2$] per W delivered, which is equivalently stated as transport $\boldsymbol{T}$ [1/cm$^2$]. The example is the penetration of a $CO_2$ laser (10.6 $\mu$m wavelength, $\mu_a$ = 500 cm$^{-1}$, $\mu_s$ = 10 cm$^{-1}$, g = 0.95 are approximate optical properties) into the conjunctiva of the eye, which illustrates how Monte Carlo can also describe the scattering in a situation where absorption dominates over scattering, a situation not well described by diffusion theory.

In the general Monte Carlo simulation, "photons" are inserted into tissue at a location defined by x,y,z coordinates with a trajectory defined by directional cosines (projection of trajectory onto x, y and z axes). The random distance traveled before the photon interacts with the tissue is based upon the selection of a random number [0,1] and the local attenuation coefficient of the medium. At the end of each photon step, the weight of the photon is reduced by absorption. The remaining non-absorbed weight is redirected according to a scattering (or "phase") function that

describes the angular dependence of single scattering by the particular tissue. Once a new trajectory is specified, the photon is again moved a random distance. The details of the photon path, absorption, scattering, reflection, and refraction are described in the following paragraphs.

Refraction at mismatched boundaries and even changes in local optical properties can be included in the simulation. The heat generated, $S$ [W/cm$^3$], within a small volume depends upon the total photon weight absorbed in the volume, the total number of photons, and power of the laser beam. Total energy absorbed [J/cm$^3$] can be computed when the energy [J] of the light source is given.

The Monte Carlo method is a widely used approach toward sampling probability density functions for simulating a wide range of problems. The first use of the Monte Carlo method for photon transport in biological materials was Adams and Wilson (1983), which considered isotropic scattering [1]. Keijzer *et al*. (1987) introduced anisotropic scattering into the Monte Carlo simulation of biological tissues, implementing a simulation that propagated photons using cylindrical coordinates, which introduced the Hop/Drop/Spin nomenclature for organizing the program [2]. Prahl et al. (1989) reformulated the program using photon propagation based on Cartesian coordinates, which made the program much simpler to convey in written form [3]. Wang and Jacques (1993) adapted and augmented the work of Keizer and Prahl to write the program Monte Carlo Multi-Layered (MCML) that considers tissues with many planar layers with different optical properties [4]. MCML is a well-organized program with a simple text input file that the user can modify to specify different problems, which allows various problems to be run without needing to re-compile the program each time. MCML has been widely promulgated via the web as source code [5-6], and modified by various groups to handle a variety of problems. Jacques (1998) reported on using Monte Carlo to specify the point spread function for light in tissue in planar, cylindrical and spherical coordinates from a plane source, line source or point source, respectively [7], using a minimal Monte Carlo program derived from MCML called mc321.c that is listed in the Appendix of this chapter for reference and is available on the web [8]. Students have usually modified mc321.c to build their own specialized programs. Jacques (2003) prepared a Monte Carlo subroutine, mcsub.c, which allows routine calls to Monte Carlo runs from other programs, discussed in [9], with updated versions listed on the web [10]. Ramella-Roman et al. (2005) modified mc321.c to simulate polarized light transport by propagating the Stokes Vector state of a photon [11], and posted the program on the web [12]. This paragraph does not offer a complete review of all contributions to Monte Carlo simulations, but provides a brief history of the programming code that is most widely used in biomedical optics and is freely available on the web.

A small note: throughout this chapter, simple math equations are mixed with programming language, and often an equal sign, "=", is used when an assignment, "←", is the appropriate symbol. The meaning will be obvious, but for those readers familiar with scientific grammar, the poor grammar is intentional.

## 5.2 BASIC MONTE CARLO SAMPLING

The Monte Carlo simulation of light propagation in tissue requires random selection of photon step size, scattering angle and reflection or transmission at boundaries. This is accomplished by a random number [0,1] assigned to the value of a random variable $x$, such as photon step size. The relationship is established through the density function $p(x)$ and distribution function $F(x)$ (see Chapter 3). Given $p(x)$, the value of the distribution function at a particular value $x_1$ of the random variable $x$ is

$$F(x_1) = \int_0^{x_1} p(x)\ dx = function(x_1) \tag{5.1}$$

This $F(x_1)$ is equated with a random number, $RND_1$, in the interval [0,1]:

$$RND_1 = F(x_1) \tag{5.2}$$

Then Equation 5.2 is rearranged to solve for $x_1$ in terms of $RND_1$. The resulting expression allows a series of values $RND_1$ to specify a series of values $x_1$. The histogram of $x_1$ values will conform to the probability density function p(x). Figure 5.2 illustrates the procedure.

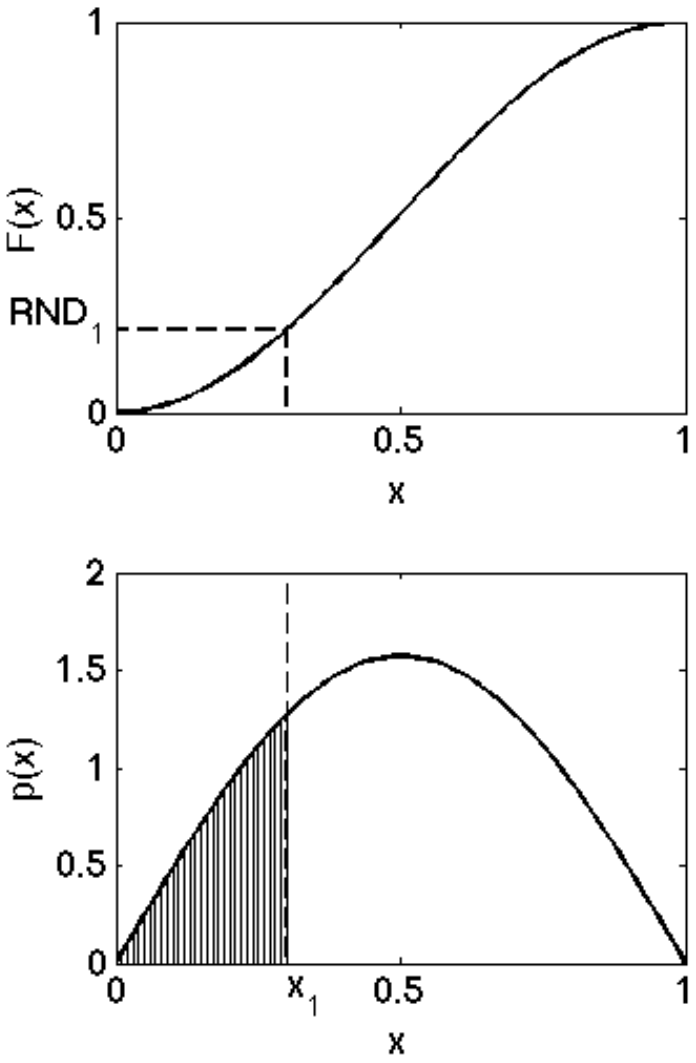



**Figure 5.2.** A random number generator [0,1] selects a value $RND_1$ which is set equal to the distribution function $F(x)$ which then specifies the value $x_1$. The cross hatched area is equal to $RND_1$.

This process is illustrated in the following section by the random selection of photon step size, $s$.

### 5.2.1 Predicting the step size of a photon

The first example is predicting the step size of a photon between interaction events (absorption or scattering) as the photon multiply scatters within a tissue. A photon takes a step (s [cm]) whose length is exponentially distributed, and depends on the value of the total attenuation coefficient $\mu_t$ [cm$^{-1}$] equal to $\mu_a + \mu_s$, where $\mu_a$ is the absorption coefficient and $\mu_s$ is the scattering coefficient. The value $1/\mu_t$ is the photon's mean free pathlength before either absorption or scattering occurs.

The first step is to specify a properly normalized probability density function that describes the probability of a particular step size $s$:

$$p(s) = \exp(-\mu_t s)/\mu_t \tag{5.3}$$

such that

$$\int_0^\infty p(s)ds = \int_0^\infty \frac{e^{-\mu_t s}}{\mu_t} ds = 1 \tag{5.4}$$

The second step is to determine the integral of $p(s)$ evaluated at a particular $s_1$, which defines the probability distribution function:

$$F(s_1) = \int_0^{s_1} p(s)ds = \int_0^{s_1} \frac{e^{-\mu_t s}}{\mu_t} ds = 1 - e^{-\mu_t s_1} \tag{5.5}$$

The third step is to set $F(x)$ equal to a random number $RND_1$.

$$RND_1 = F(s_1) = 1 - e^{-\mu_t s_1} \tag{5.6}$$

and solve for $s_1$:

$$s_1 = \frac{-\ln(1 - RND_1)}{\mu_t} = \frac{-\ln(RND_1)}{\mu_t} \tag{5.7}$$

The terms (1-RND$_1$) and (RND$_1$) are equal in a probabilistic sense because of the uniform distribution of the random number between [0,1]. This is the final answer. A series of random numbers $RND_1$ will generate a series of step sizes $s_1$ that follow the probability density function $p(s)$ of Eq. 5.3.

To illustrate, Figure 5.3 shows a histogram of $s_1$ values specified by 1000 $RND_1$ values. The value of $\mu_t$ is 1 cm$^{-1}$. The bin size of the histogram is $ds_1 = 0.275$ cm. Also plotted is the curve $N(s) = 1000\exp(-\mu_t s_1)ds_1$.

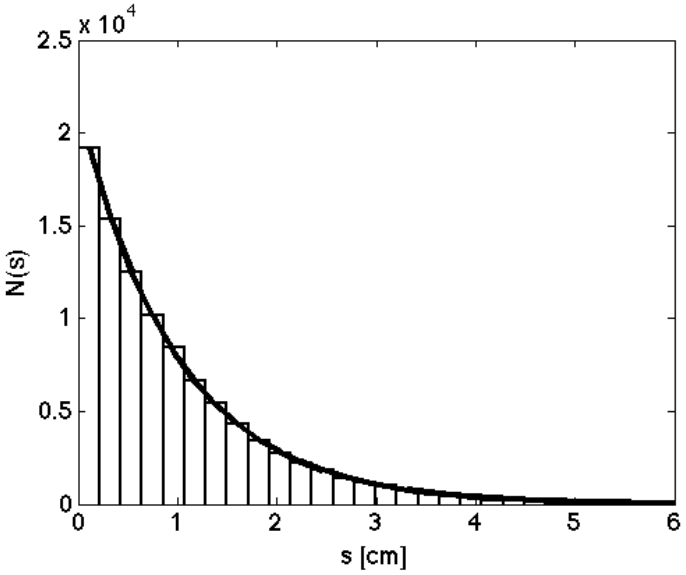



**Figure 5.3**: Histogram of step sizes predicted by 1000 random numbers using Monte Carlo sampling (Eq. 7). $N(s)$ is the number of step sizes per bin over a range of s value bins. The value of $\mu_t$ is 1 cm$^{-1}$. The bin size of the histogram is $ds_1 = 0.275$ cm. The curved line is $N(s) = 1000\exp(-\mu_t s_1)ds_1/\mu_t$.

### 5.2.2 Predicting the photon launch point for a circular flat-field beam

The second example is predicting where a photon should be launched at a tissue surface so as to mimic a circular flat-field (*i.e.*, a uniform irradiance) beam of light. Assume the beam of light is delivered perpendicular to the tissue surface. Also assume that we are working in cylindrically symmetric Cartesian coordinates. The Monte Carlo simulation will propagate the photon in 3D using $x$, $y$ and $z$ coordinates, but we will report out our results only as a function of $r$ and $z$. Therefore, we need only specify the radial distance $r$ from the center of the beam where a photon should enter the tissue, and the photon can be launched along the $x$ axis by letting $x = r$. Assume the beam of light has a radius $a$.

The number of photons per unit area should be constant. For each radial position $r$ there is an annular ring of area $(2\pi r\, dr)$. Therefore the number of photons to be launched at each choice of $r$ should vary as $(2\pi r\, dr)$. The total area of the light beam is $\pi a^2$. The first step is to specify the properly normalized probability density function $p(r)$:

$$p(r) = \frac{2\pi r}{\pi a^2} = \frac{2}{a^2} r \tag{5.8a}$$

such that

$$\int_0^a p(r)dr = \int_0^a \frac{2}{a^2} r dr = 1 \tag{5.8b}$$

The second step is to integrate this $p(r)$, evaluated for a specific $r_1$, and equate to $RND_1$.

$$\int_0^{r_1} \frac{2}{a^2} r dr = \frac{r_1^2}{a^2} = RND_1 \tag{5.9}$$

The third step is to solve for $r_1$ in terms of $RND_1$:

$$r_1 = a\sqrt{RND_1} \tag{5.10}$$

Now to illustrate, Figure 5.4 shows the histogram of 1000 $r_1$ values predicted by 1000 random numbers.

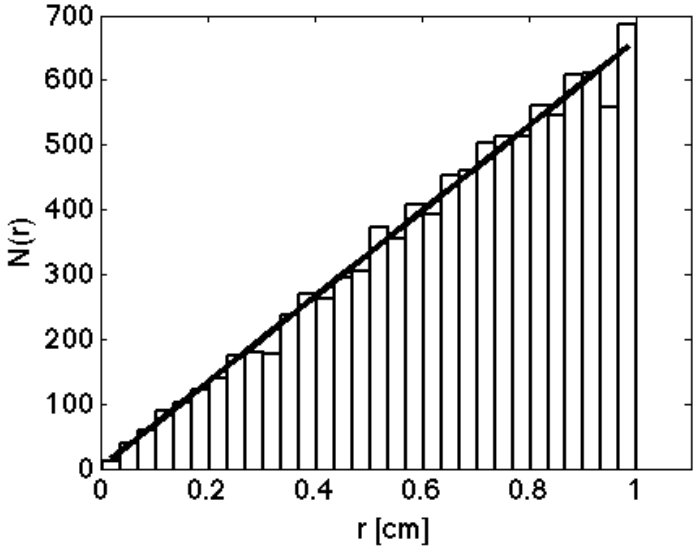



**Figure 5.4**: Histogram of radial position of photon launch to achieve a circular flat-field beam of light, perpendicularly illuminating a tissue surface. The histogram is predicted by 1000 random numbers using Monte Carlo sampling (Eq. 10). $N(r)$ is the number of predicted $r$ positions per bin over a range of $r$ value bins. The value of the beam radius $a$ is 1 cm. The bin size of the histogram is $ds_1 = 0.0327$ cm. The diagonal line is $N(s) = (1000\ 2r\ dr)/a^2$.

## 5.3 THE STEADY-STATE MONTE CARLO PROPAGATION OF PHOTONS IN A TISSUE

This section presents the basic form of the steady-state Monte Carlo simulation of photon propagation in tissues with optical scattering and absorption properties. The term steady-state

means that a stable distribution of light has been achieved, and there are no time dynamics. Section 5.4 will discuss time-resolved Monte Carlo.

It is convenient to consider the Monte Carlo simulation as yielding the fractional density matrix of incident light absorbed, $\boldsymbol{A}$ [1/cm$^3$], in response to one unit of delivered power or energy. The corresponding heat source matrix $\boldsymbol{S}$ [W/cm$^3$] or radiant energy density matrix $\boldsymbol{W}$ [J/cm$^3$] is obtained by scaling $\boldsymbol{A}$ by the beam power $P$ or radiant energy $Q$, respectively, such that

$$\boldsymbol{S} = P\boldsymbol{A} \tag{5.11a}$$

or

$$\boldsymbol{W} = Q\boldsymbol{A} \tag{5.11b}$$

where $\boldsymbol{S}(\boldsymbol{r})$ [W/cm$^3$] is the local density of power deposition at $r = (x, y, z)$ in response to a delivered power $P$ [W], and $\boldsymbol{W}(\boldsymbol{r})$ [J/cm$^3$] is the local density of energy deposition in response to a delivered energy $Q$ [J].

Also, the simulation keeps track of the escaping flux density out of the front surface to which light is delivered, $\boldsymbol{R}_r$ [1/cm$^2$], and out of the rear surface, $\boldsymbol{T}_r$ [1/cm$^2$]. The $\boldsymbol{A}$ [1/cm$^3$] is converted into the fractional transport $\boldsymbol{T}[iz][ir]$ [1/cm$^2$] within the tissue, such that the fluence rate $\boldsymbol{\phi}$ [W/cm$^2$] and the fluence $\boldsymbol{\psi}$ [J/cm$^2$] are

$$\boldsymbol{\phi}(\boldsymbol{r}) = P\boldsymbol{T}(\boldsymbol{r}) \tag{5.12a}$$

$$\boldsymbol{\psi}(\boldsymbol{r}) = Q\boldsymbol{T}(\boldsymbol{r}) \tag{5.12b}$$

The following sections will present the algorithm for implementing the Monte Carlo simulation. The overall algorithm is described by the flow diagram in Figure 5.5.

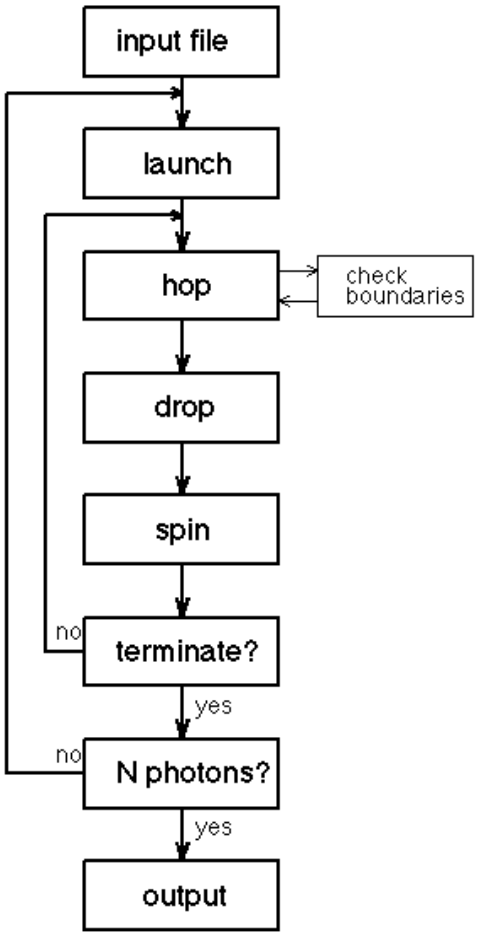



**Figure 5.**: The flow-diagram for a steady-state Monte Carlo simulation.

### 5.3.1 The input file

The parameters that govern a Monte Carlo simulation must be passed to the program before it can run. These parameters can be included in the programming at the beginning of a simple Monte Carlo code (as in `mc321.c`, see Appendix), or passed to a Monte Carlo subroutine from another program (as in `mcsub.c` [8,9]) or read from an input file (as in `MCML` [4-6]). In Fig. 5.5, these possibilities are referred to as the "input file".

In this simple summary of a generic Monte Carlo simulation, a simple homogeneous tissue is specified. The tissue parameters to be specified are:

| | | | |
|---|---|---|---|
| $\mu_a$ | [cm$^{-1}$] | absorption coefficient of tissue | |
| $\mu_s$ | [cm$^{-1}$] | scattering coefficient of tissue | (5.13) |
| $g$ | [-] | anisotropy of scattering of tissue | |
| $n$ | [-] | refractive index of tissue | |

where [-] denotes [dimensionless]. The above parameters specify an infinite optically homogeneous medium, and the simulation will track the 3D movement of a photon over an infinite spatial range. To specify boundaries, for example the front and rear surfaces of a slab of tissue, the following parameters should be specified:

| | | | |
|---|---|---|---|
| $D$ | [cm] | thickness of the tissue slab | |
| $n_f$ | [-] | refractive index of external medium outside front of tissue | (5.14) |
| $n_r$ | [-] | refractive index of external medium outside rear of tissue | |

The position $z = 0$ is aligned with the front surface of the tissue slab, and the rear surface is aligned with $z = D$. As the program runs, the history of the photon is recorded by deposition of "photon weight" into spatially distributed bins, either $\boldsymbol{A}(x, y, z)$ for full 3-D accumulations or $\boldsymbol{A}(r, z)$ for circular symmetric laser beams. In the example of this chapter, the bins are denoted $\boldsymbol{A}[iz][ir]$ [photon weight/bin], where *iz* and *ir* are the indices of the array $\boldsymbol{A}$. The grid of bins for recording this $\boldsymbol{A}$ is independent of the photon propagation, which is implemented in *x, y,* z coordinates. Once a photon is absorbed at *x, y, z*, its position in this example is recorded as $z, r = \sqrt{x^2 + y^2}$, and some "photon weight" is deposited in *A[iz][ir]*. The parameters to be specified for recording output are:

| | | | |
|---|---|---|---|
| $N_z$ | [-] | number of $z$ bins (depth) | |
| $N_r$ | [-] | number of $r$ bins (radial position) | (5.15) |
| $dz$ | [cm] | size of $z$ bins | |
| $dr$ | [cm] | size of $r$ bins | |

where the bins cover the extent of the tissue,

$$dz = \frac{D}{N_z} \tag{5.16}$$

Finally, the number of photons that will be launched must be specified,

| | | | |
|---|---|---|---|
| $N_{\text{photons}}$ | [-] | number of photons to be launched | (5.17) |

Typically about $10^4$ to $10^8$ photons are launched, depending on how much computation time is appropriate or available. The run time will vary with the optical properties. As will be discussed in later sections, each photon will take an average step size of $1/(\mu_s + \mu_a)$ and at each step the photon weight will drop via multiplication by the fraction $\mu_s/(\mu_s + \mu_a)$ called the albedo.

The weight is initially 1 upon launching the photon and drops until it reaches a threshold value, THRESHOLD, which is typically $10^{-4}$. The time required to reach THRESHOLD is proportional to the number of steps, $N_{\text{steps}}$, taken by the photon

$$\text{THRESHOLD} = \left( \frac{\mu_s}{\mu_s + \mu_a} \right)^{N_{\text{steps}}} \tag{5.18}$$

and the number of steps required for each photon is

$$N_{\text{steps}} = \frac{\ln(\text{THRESHOLD})}{\ln\left( \frac{\mu_s}{\mu_s + \mu_a} \right)} \tag{5.19}$$

As the absorption $\mu_a$ decreases, $N_{\text{steps}}$ increases. As the scattering $\mu_s$ increases, $N_{\text{steps}}$ increases. The values of $g$ and $n$ have no effect. Therefore, the time required to run $N_{\text{photons}}$ is

$$t = N_{\text{photons}}\, t_{\text{per.step}}\, N_{\text{steps}} \tag{5.20}$$

where $t_{\text{per.step}}$ is the time required per photon step in the simulation. One may run several example simulations with known values of THRESHOLD, $\mu_s$, $\mu_a$, and $N_{\text{photons}}$, and record the time required for each simulation. Then fit the data to solve for $t_{\text{per.step}}$:

$$t_{\text{per.step}} = \frac{t}{N_{\text{photons}} N_{\text{steps}}} \tag{5.21}$$

For example, if it takes 23.0 s to run $10^5$ photons with optical properties $\mu_a = 1$ cm$^{-1}$, $\mu_s = 100$ cm$^{-1}$, using THRESHOLD = $10^{-4}$, then $t_{\text{per.step}}$ is 249 ns. Now, if one desires a simulation that takes exactly $t$ =10 min (600 s) for properties $\mu_a = 0.4$ cm$^{-1}$ and $\mu_s = 65$ cm$^{-1}$, then the choice of $N_{\text{photons}}$ is

$$N_{\text{photons}} = \frac{t}{t_{\text{per.step}} N_{\text{steps}}} = \frac{t}{t_{\text{per.step}}} \frac{\ln\left( \frac{\mu_s}{\mu_s + \mu_a} \right)}{\ln(\text{THRESHOLD})} = \frac{600s}{249 \times 10^{-9}} \frac{\ln\left( \frac{65}{65 + 0.4} \right)}{\ln\left(10^{-4}\right)} = 1.60 \times 10^6 \tag{5.22}$$

So one would launch 1.60 million photons for a 10-min simulation using the above optical properties. In this manner, the choice of $N_{\text{photons}}$ for a given simulation can be made on the basis of available time, regardless of the optical properties in the simulation.

Now the Monte Carlo simulation can proceed to run.

### 5.3.1 Launching photons

Photons are launched with an initial weight (w) set to 1.0. As the photon propagates, this weight will be decremented as "photon weight" is "dropped" into the bins $A[iz][ir]$, where $iz$ and $ir$ are index pointers to the bins for the depth $z$ and radial position $r$, respectively. A large number of photons will be launched ($N_{photons}$) and later at the end of the program all the weight deposited in $A[iz][ir]$, as well as any weight that escaped the tissue as transmission or reflectance, will be normalized by $N_{photons}$, such that the final results are reported as the fraction of all delivered light that is either absorbed, reflected or transmitted.

The position of the photon is specified in Cartesian coordinates, $(x,y,z)$, and all the propagation is done in full 3D. The recording of $A[iz][ir]$ is in cylindrical coordinates, but one could implement $A[iz][ix][iy]$ if desired. If one is using 100x100 bins for $A[iz][ir]$, one needs only to fill $10^4$ bins with photon weight. If one is using 100x100x100 bins for $A[iz][ix][iy]$, one needs to fill $10^6$ bins with photon weight. Since the signal-to-noise in any bin is roughly proportional to $\sqrt{(A)/A}$, it takes many more photons to attain good signal-to-noise filling $A[iz][ix][iy]$ than filling $A[iz][ir]$. This is why cylindrical coordinates are often chosen for use. But there is no reason not to record data as $A[iz][ix][iy]$. The choice of recording does not affect the photon propagation.

The trajectory of the photon will be specified by the trajectory cosines $(ux,uy,uz)$:

$$\begin{aligned} ux &= \cos\theta\cos\phi \\ uy &= \cos\theta\sin\phi \\ uz &= \cos\theta \end{aligned} \tag{5.23}$$

where $\theta$ is the angle that the trajectory makes with respect to the $z$ axis, and $\phi$ is the angle that the trajectory makes with the $x$ axis.

So let's launch some photons.

#### 5.3.1.1 Collimated launch

In this example, photons are launched perpendicular to the tissue and enter the tissue exactly at the origin $(x,y,z) = (0,0,0)$. The photon position and trajectory are

$$\begin{aligned} x &= 0 \\ y &= 0 \\ z &= 0 \end{aligned} \tag{5.24a}$$

and

$$\begin{aligned} ux &= 0 \\ uy &= 0 \\ uz &= 1 \end{aligned} \tag{5.24b}$$

The photon is directed straight downward, so *uz* = 1. The values of *ux* and *uy* are zero because no component of the trajectory is directed in the *x* or *y* directions.

The case of collimated launch as a flat-field beam, *i.e.*, uniform irradiance, where the beam has a radius a, was discussed in 5.2.2. Photons can be placed along the *x* axis according to Eq. (10) with *y* = 0, *z* = 0.

**5.3.1.2 Isotropic point source**

To launch a photon isotropically, *i.e.*, with no preferential direction, at a position located within the tissue, for example at *x* = 0, *y* = 0, and *z* = 0.1 cm, the launch specification is:

$$\begin{aligned} x &= 0 \\ y &= 0 \\ z &= 0.1 \end{aligned} \tag{5.25a}$$

and

$$\begin{aligned} &\cos\theta = 2\ RND - 1 \\ &\sin\theta = \sqrt{(1 - \cos\theta)} \\ &\varphi = 2\,\pi\ RND \\ &\text{if } (\varphi < \pi) \\ &\quad \sin\varphi = \sqrt{(1 - \cos^2\varphi)} \\ &\text{else} \\ &\quad \sin\varphi = -\sqrt{(1 - \cos^2\varphi)} \end{aligned} \tag{5.25b}$$

such that

$$\begin{aligned} ux &= \sin\theta\cos\varphi \\ uy &= \sin\theta\sin\varphi \\ uz &= \cos\theta \end{aligned} \tag{5.25c}$$

The *z* position is 0.1 cm. The trajectory (*ux*,*uy*.*uz*) is randomly selected such that

$$\sqrt{ux^2 + uy^2 + uz^2} = 1 \tag{5.26}$$

It is necessary for the total length of the trajectory vector to be unity.

The photon is launched at *x* = 0 and *y* = 0 because we wish to retain cylindrical symmetry. If one launched at any other *x,y* position the cylindrical symmetry would be broken. Then the results would have to be recorded as ***A***[*iz*][*ix*][*iy*]. The results recorded as ***A***[*iz*][*ir*] would respond as if photons were launched in a ring of radius $\sqrt{x^2 + y^2}$ .

**5.3.1.4 Collimated Gaussian beam**

Consider a collimated Gaussian beam that irradiates a tissue, which has a 1/*e* radius of *b*. The probability density function for the radial position of launch is

$$p(r) = \frac{e^{-(r/b)^2}\, 2\pi r}{\pi b^2} \tag{5.27}$$

which can be sampled using the Monte Carlo sampling method by

$$r = b\sqrt{-\ln(RND)} \tag{5.28}$$

To launch a Gaussian beam when using cylindrically symmetric results, one can launch the photon at $x = r$. The launch parameters are:

(29a)

$$\begin{aligned} x &= b\sqrt{-\ln(RND)} \\ y &= 0 \\ z &= 0 \end{aligned} \tag{5.29a}$$

and

$$\begin{aligned} ux &= 0 \\ uy &= 0 \\ uz &= 1 \end{aligned} \tag{5.29b}$$

**5. 3.1.5 Focused Gaussian beam**

Consider the same Gaussian beam but focused to a focal point within the tissue at depth $z_{\text{focus}}$. Let the focus have a radial Gaussian distribution with a 1/*e* radius of *w*. Then the launch parameters are calculated:

$$\begin{aligned} x &= b\sqrt{-\ln(RND)} \\ y &= 0 \\ z &= 0 \end{aligned} \tag{5.30a}$$

and

$$\begin{aligned} x_{\text{focus}} &= w\sqrt{-\ln(RND)}(2RND - 1) \\ \text{temp} &= \sqrt{((x - x_{\text{focus}})^2 + z_{\text{focus}}^2)} \\ \sin\theta &= -(x - x_{\text{focus}})/\text{temp} \\ \cos\theta &= z_{\text{focus}}/\text{temp} \end{aligned} \tag{5.30b}$$

such that

$$ux = \sin\theta$$
$$uy = 0 \qquad (5.30c)$$
$$uz = \cos\theta$$

There is a tendency in Monte Carlo simulations using cylindrical coordinates to not get sufficient photons in the bins along the $z$ axis, because the size of each bin is ($2\pi r\, dr\, dz$), so the size of bins near $r = 0$ is very small, and the likelihood of photon deposition in such a small bin is quite low. During this focused Gaussian launch, one should launch toward both $+x_{\text{focus}}$ and $-x_{\text{focus}}$ positions, which forces the photons to cross the $z$ axis. Doing this causes the bins along the central axis to not be so neglected, and is accomplished by the extra term (2 *RND* - 1) in the expression for $x_{\text{focus}}$.

**5. 3.2 Hop**

Now the photon is launched along a trajectory, and takes a step along this trajectory. The standard procedure for taking the step is described as the "Standard Hop" in 5.3.2.1. But if the tissue has a front and/or rear boundary, then a second step to "Check boundaries" is taken, as described in 5.3.2.2, and if the photon is attempting to escape the tissue, a procedure is used to decide whether the photon escapes or is reflected back into the tissue.

**5.3.2.1 Standard Hop**

The step size of the photon's step (or hop) must be determined. The step size is calculated:

$$s = -\ln(RND)/\mu_t \qquad (5.31)$$

as was described in section 3.2.1. Now the position of the photon is updated:

$$x = x + s\, ux$$
$$y = y + s\, uy \qquad (5.32)$$
$$z = z + s\, uz$$

**5.3.2.2 Check boundaries**

As part of the Hop step, there is a side box labeled "check boundaries" in Fig. 5.5, which is used when there are front and surface boundaries in the problem. This boundary check is denoted by a side box to emphasize that it is part of the Hop step.

As the photon moves toward the front surface of the tissue and attempts to cross the boundary to escape the tissue, there is a possibility that the photon will be reflected by the surface boundary where the air/tissue interface (or *external medium*/tissue interface) presents a mismatch in refractive indices ($n_f \neq n$ or $n_r \neq n$, for front and rear boundaries, respectively). The method chosen here for handling the boundary is to let a fraction of the photon weight escape the tissue as observable reflectance, and let the remaining fraction of photon weight reflect back into the tissue and continue to propagate.

After taking the step, the position of the photon is checked to see if the photon is still within the tissue or has escaped the tissue:

If $z < 0$
    photon is trying to escape
else
    photon still within tissue (5.33)

If the photon is trying to escape, then a partial step is taken along the escaping trajectory that will just reach the boundary surface. The size of the partial step $s_1$ is

$$s_1 = \text{abs}(z/uz) \tag{5.34}$$

where abs() denotes the absolute value function. First, the photon retracts the full step it took in Hop, which led to escape,

$$\begin{aligned} x &= x - s\,ux \\ y &= \text{y} - s\,uy \\ z &= z - s\,uz \end{aligned} \tag{5.35a}$$

and then the photon takes the partial step $s_1$,

$$\begin{aligned} x &= x + s_1\,ux \\ y &= \text{y} + s_1\,uy \\ z &= z + s_1\,uz \end{aligned} \tag{5.35b}$$

Now the photon is located at the boundary surface. Next, a decision is made about how much of the photon weight escapes or how much is reflected.

The probability of reflectance at the boundary is a function of the angle of incidence, encoded as the value *uz*, and the refractive indices $n_1$ and n, where $n_1$ denotes the external medium and equals either $n_f$ or $n_r$ for the front and rear boundaries, respectively. Consider a photon striking the front surface. The internal reflectance, $\boldsymbol{R}_i$, is calculated using the Fresnel equation:

$$R_i = \frac{\sin\theta^2\left(\sin\theta_1\cos\theta_2 - \cos\theta_1\sin\theta_2\right)^2}{2} \frac{\left(\left(\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\right)^2 + \left(\cos\theta_1\cos\theta_2 - \sin\theta_1\sin\theta_2\right)^2\right)}{\left(\left(\sin\theta_1\cos\theta_2 + \cos\theta_1\sin\theta_2\right)^2\left(\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\right)^2\right)} \tag{5.36}$$

where

| | | |
|---|---|---|
| $n_1$ | refractive index of incident medium | $= n_{\text{tissue}}$ |
| $n_2$ | refractive index of transmitted medium | $= n_f$ |
| $\cos\theta_1$ | incident trajectory | = uz |
| $\sin\theta_1$ | incident trajectory | $= (1 - uz^2)^{1/2}$ |
| $\sin\theta_2$ | transmitted trajectory | $= \sin\theta_1(n_1/n_2)$ |

$\cos\theta_2$ transmitted trajectory $= (1 - \sin\theta_1^2)^{1/2}$

Once the reflectance $\boldsymbol{R}_i$ is computed, a fraction (1-$\boldsymbol{R}_i$) of the current photon weight is allowed to escape and the remaining fraction of weight is reflected back into the tissue to continue propagating. The escape is recorded by placing its remaining weight in the reflectance array bin, $\boldsymbol{R}[ir]$,

$$\boldsymbol{R}r[ir] = \boldsymbol{R}r[ir] + (1\text{-}\boldsymbol{R}_i)w \tag{5.37}$$

where the radial position of escape is $r$:

$$\begin{aligned} r &= \sqrt{x^2 + y^2} \\ ir &= \text{round}(r/dr) + 1 \end{aligned} \tag{5.38}$$

The function round($r/dr$) denotes taking the integer value of the value $r/dr$, rounding down, such that a photon somewhere within the location of one bin will be assigned to that particular bin. (Note: In this summary, ir extends from 1 to $N_z$, and $ir$ is not allowed to equal zero. Sometimes, programs let $ir$ extend from 0 to $N_z$-1. Not mentioned here but important in programming is that a check should be made that $ir$ does not exceed $Nr$, the allocated size of $\boldsymbol{R}r[ir]$.)

The remaining fraction of the photon weight is reflected by the boundary,

$$w = \boldsymbol{R}_i w \tag{5.39}$$

and the trajectory with respect to the $z$ axis is reversed,

$$uz = -uz \tag{5.40}$$

The $ux$ and $uy$ components of the trajectory are not changed. Then the photon position is updated by taking the remaining portion of the original step, which equals $s - s_1$:

$$\begin{aligned} y &= (s - s_1)ux \\ y &= (s - s_1)uy \\ z &= (s - s_1)uz \end{aligned} \tag{5.41}$$

Some of the photon weight has escaped the boundary and some has been reflected by the boundary back into the tissue to continue propagating.

The procedure for testing if the photon is attempting to escape the tissue through its rear surface boundary and contributing to $\boldsymbol{T}[iz][ir]$ and for modifying the position and trajectory accordingly, is very similar to the above procedure for the front surface, and is not outlined here. If one wished to place other boundaries in the problem, like a lateral cylindrical boundary as if

the tissue were held within a tube (*e.g.*, a glass test tube, or a pipe), this "check boundaries" box is the proper place within the program to implement such special boundaries.

**5. 3.3 Drop**

Arriving at its new position, the photon must interact with the tissue. Upon interaction, a fraction $\mu_a / \mu_t$ of the photon's weight is absorbed and the remaining $\mu_s / \mu_t$ fraction of the photon's weight is scattered and continues to propagate. The absorbed fraction is placed in the bin that encloses the current photon position. This process is summarized by the following calculation steps:

$$\begin{aligned} r &= \sqrt{x^2 + y^2} \\ ir &= \text{round}(r/dr) + 1 \\ iz &= \text{round}(z/dz) + 1 \end{aligned} \qquad (5.42)$$

$$\begin{aligned} \boldsymbol{A}[iz][ir] &= \boldsymbol{A}[iz][ir] + \text{W}(\mu_a / \mu_t) \\ w &= w(\mu_s / \mu_t) \end{aligned}$$

where *ir* and *iz* are index values and *dr* and *dz* are bin width and depth, respectively. This finishes the absorption event.

Note that *ir* and *iz* should not be allowed to exceed $N_r$ and $N_z$, respectively, lest one exceed the allocated size of $\boldsymbol{A}[iz][ir]$. Always check this. Often, the last bin is used as an overflow bin and any photon weight that is deposited outside the array is simply accumulated in the last *iz,ir* bin. At the end of the simulation, the values of weigth in $\boldsymbol{Rr}[ir]$, $\boldsymbol{Tr}[ir]$ and $\boldsymbol{A}[iz][ir]$ are the fraction of total delivered photon weight. The sum of $\boldsymbol{Rr}[ir]$, $\boldsymbol{Tr}[ir]$ and $\boldsymbol{A}[iz][ir]$ over all bins divided by $N_{photons}$ will equal unity. In section 5.3.6, the proper normalization of these fractional weights by the size of the bins will convert ***Rr*** and ***Tr*** into the fraction of delivered power or energy escaping per unit surface area and convert ***A*** into the fraction of delivered power or energy deposited per unit volume. But the values of ***Rr***, ***Tr*** and ***A*** determined from the overflow bins are meaningless after normalization.

Next, is the scattering event.

**5. 3.4 Spin**

The photon is scattered into a new trajectory according to some scattering function. The two angles of scatter are $\theta$ and $\varphi$, the deflection and azimuthal scattering angles, respectively. This section describes how to calculate the new trajectory after sampling the probabilities for $\theta$ and $\varphi$.

The most commonly used function for the deflection angle $\theta$ is the Henyey-Greenstein (HG) function (1941), which was proposed for describing the scattering of light from distant galaxies by galactic dust. The original paper does not offer any explanation for the function, but simply asserts it use. But the HG function is actually very interesting. The function is here expressed as a function of the angle of deflection, $\theta$, and the anisotropy of scattering, $g$:

$$p(\cos\theta) = \frac{1}{4\pi}\frac{1-g^2}{\left(1+g^2-2g\cos\theta\right)^{3/2}} \tag{5.43}$$

which has the properties that

$$2\pi\int_0^{\pi} p(\theta)\sin\theta\, d\theta = 1 \tag{5.44a}$$

and

$$2\pi\int_0^{\pi} p(\theta)\cos\theta\,\sin\theta\, d\theta = \mathrm{g} \tag{5.44b}$$

The last equation is the definition of *g*. Hence, the HG function is an identity with respect to the definition of *g*. If you choose a value *g* to define $p(\theta)$ using Eq. 43, the definition of *g* in Eq. 44b will yield exactly *g*.

The Monte Carlo sampling of the HG function is specified by the following sequence of calculations:

$$\cos(\theta) = \frac{1+g^2-\left(\dfrac{1-g^2}{\left(1-\mathrm{g}+2g\mathrm{RND}\right)^{3/2}}\right)^2}{2g} \tag{5.45}$$

If g is 0, then use $\cos\theta = 2\,RND - 1$. If *g* is 1.0, then simply let $\cos\theta = 1.0$. Otherwise, use the Monte Carlo sampling in Eq. (5.45).

The azimuthal angle is calculated:

$$\varphi = 2\pi\, RND \tag{5.46}$$

To update the trajectory based on the values of $\cos\theta$ and $\varphi$ specified using random numbers, use the following calculations:

$$\begin{aligned}
&\sin\theta = \sqrt{\left(1-\cos^2\theta\right)}\\
&\mathrm{temp} = \sqrt{\left(1-uz^2\right)}\\
&uxx = \sin\theta\,(ux\;uz\cos\varphi - uy\sin\varphi)/\mathrm{temp} + ux\cos\theta\\
&uyy = \sin\theta\,(uy\;uz\cos\varphi + ux\sin\varphi)/\mathrm{temp} + uy\cos\theta\\
&uzz = -\sin\theta\cos\varphi\;\mathrm{temp} + uz\cos\theta
\end{aligned} \tag{5.47a}$$

If the trajectory is extremely close to alignment with the $z$ axis, *i.e.* nearly ($uz$,$uy$,$uz$) = (0,0,±1), do not use Eq. (5.24) above, but instead use:

$$\begin{aligned} &uxx = \sin\theta\cos\varphi \\ &uyy = \sin\theta\sin\varphi \\ &\text{if } uz \geq 0 \\ &\quad uzz = \cos\theta \\ &\text{else} \\ &\quad uzz = -\cos\theta \end{aligned} \tag{5.47b}$$

Finally, one updates the trajectory:

$$\begin{aligned} ux &= uxx \\ uy &= uyy \\ uz &= uzz \end{aligned} \tag{5.48}$$

The photon is now oriented along a new trajectory, and ready to take a new step s (see Figure 5.5).

There are alternative scattering functions. Mie theory is an important scattering function to consider. Perhaps an experiment has yielded a particular scattering function, and one wishes to run a simulation using this function. This chapter will not discuss these alternatives, but as long as the criteria of Eqs. 44ab are followed, most any scattering function for the deflection angle $\theta$ can be used. Sometimes the scattering function does not lend itself to a solution of $\cos\theta$ in terms of a random number, as in Eq. 3. Also, sometimes one wishes to consider an azimuthal scattering angle $\varphi$ that depends on the deflection angle $\theta$, as in Mie scattering of polarized light. In such cases, the "rejection method" is a useful approach [10].

**5. 3.5 Terminate?**

The photon will continue propagating as its weight becomes progressively smaller. How can one stop the photon yet properly conserve energy? The "Roulette Method" is used to terminate the photon. A threshold value (THRESHOLD) is chosen, typically $10^{-4}$. When the photon's weight drops below this threshold value, the roulette procedure is employed. A random number (*RND*) is generated and if this random number is less than a small fraction called CHANCE, typically 0.10, then the photon weight is increased by dividing $W$ by CHANCE. For CHANCE = 0.10, this would be a 10-fold increase in $W$. Otherwise, the photon is terminated. Consequently, 9 out 10 times the photon is terminated, but 1 out of 10 times the photons weight is increased 10–fold and the photon continues to propagate. The result is that photons are usually terminated, but energy is conserved by the occasional surviving photon being given extra weight. Since millions of photons are run, the statistically averaged result is correct. In summary, the roulette method is implemented by the following:

```
if (w < THRESHOLD)
        if (RND <= CHANCE)
                w = w/CHANCE                                    (5.49)
        else
                terminate the photon
```

Once the photon is terminated, a new photon can be launched. One checks to see if the total number of photons has already reached the maximum number ($N_{photons}$) requested by the input file. If not, then a new photon is launched. If yes, the simulation is complete, and it is time to prepare the results for output.

**5. 3.6 Normalizing results for output**

Now, all the photons ($N_{photons}$) have been run, and it is time to save the output of the simulation. The data has been stored in the array $\boldsymbol{A}$, as $\boldsymbol{A}[iz][ir]$ or perhaps $\boldsymbol{A}[iz][ix][iy]$, in units of [photon weight/bin]. Either way, the key parameter is the volume $V$ [cm$^3$] associated with each bin. For $\boldsymbol{A}[iz][ir]$, the volumes vary with the value of $ir$,

$$V = 2\pi(ir - 0.5)dr^2dz \tag{5.50a}$$

and for $\boldsymbol{A}[iz][ix][iy]$, the volumes are all equal,

$$V = dx\ dy\ dz \tag{50b}$$

Then the values $\boldsymbol{A}$ [photon weight/bin] are normalized by the appropriate $V$ and by the value $N_{photons}$ to yield the absorbed fraction, $\boldsymbol{A}$ [1/cm$^3$], for each pixel:

$$\boldsymbol{A}[iz,ir] = \frac{\boldsymbol{A}[ir,iz]}{V[ir,iz]N_{photons}} \tag{5.51}$$

The fractional transport, $\boldsymbol{T}$ [1/cm$^2$], is then calculated as

$$\boldsymbol{T} = \frac{\boldsymbol{A}}{\mu_a} \tag{5.52}$$

Recall from Eqs. (5.12ab) that fluence rate $\phi$ [W/cm$^2$] equals the incident power $P$ [W] times $\boldsymbol{T}$, $\phi = P\boldsymbol{T}$, and the fluence $\psi$ [J/cm$^2$] equals the incident energy $Q$ [J] ] times $\boldsymbol{T}$, $\psi = Q\boldsymbol{T}$.

Keep in mind that the values of $\boldsymbol{A}$, $V$ and $\mu_a$ are specific to each bin, when calculating $\boldsymbol{T}[iz][ir]$ or $\boldsymbol{T}[iz][ix][iy]$. In this summary of a simple implementation of the Monte Carlo method, the $\mu_a$ was assumed to be uniform, as well as the scattering properties, so every bin had

the same value of $\mu_a$. But in MCML, for example, bins at different depths can have different values of $\mu_a$.

The light fluxes that have escaped at the front and rear surface boundaries are similarly normalized, but in this case the surface area AREA rather than the volume V is used. The value of AREA[ir] is $2\pi(ir\text{-}0.5)dr^2$. The array of escaping photons, $\boldsymbol{R}_r[ir]$ [photon weight/bin], is converted to the fractional escaping flux density, $\boldsymbol{R}_r[ir]$ [1/cm$^2$], by the expression:

$$\boldsymbol{R}_r = \frac{\boldsymbol{R}_r}{AREA\, N_{\text{photons}}} \tag{5.53}$$

This completes the discussion of the steady-state Monte Carlo simulation. The output is the fractional transport, $\boldsymbol{T}[iz][ir]$ [1/cm$^2$], and the fractional escaping flux densities, $\boldsymbol{R}_r[ir]$ [1/cm$^2$] and $\boldsymbol{T}_r[ir]$ [1/cm$^2$]. This discussion ends with one example calculation shown in Figure 5.6, showing $\boldsymbol{T}$, $\boldsymbol{R}_r$ and $\boldsymbol{T}_r$ for a 1-mm-thick slab of tissue, with light delivered as a pencil beam of collimated light at the origin: $(x,y,z) = (0,0,0)$, $(ux,uy,uz) = (0,0,1)$.

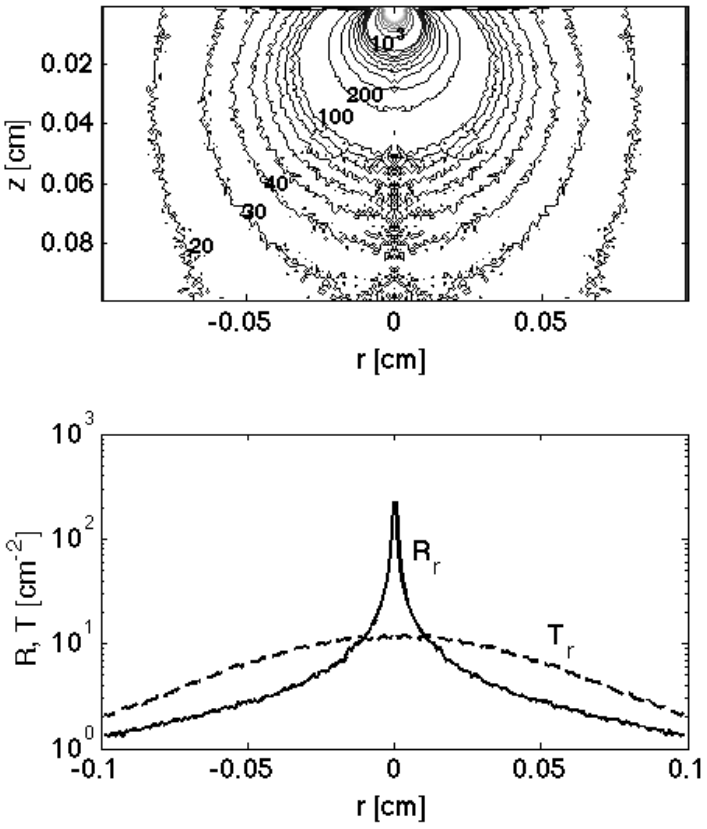



**Figure 5.6.** Example steady-state Monte Carlo simulation. The optical properties were $\mu_a$ = 1 cm$^{-1}$, $\mu_s$ = 100 cm$^{-1}$, $g$ = 0.90, n = 1.4, for a 1-mm-thick tissue slab with air/tissue boundaries at

front and rear surfaces. There were $10^6$ photons propagated during a run time of 3 min 49 s on a laptop computer (2 GHz processor). (A) Iso-$\boldsymbol{T}$ contours for 20, 30, 40, 100, 200 and $10^3$ 1/cm$^2$], $\boldsymbol{T}$ denotes the fractional transport. The noise is evident along the central axis near $r = 0$ because the bins are smaller and collect less photons. Running more photons improves the signal-to-noise. (B) The reflectance ($\boldsymbol{R}_r$) and transmission ($\boldsymbol{T}_r$) as flux densities of escape [1/cm$^2$] versus radial position r at front and rear surfaces, respectively.

**5.4 Time resolved Monte Carlo propagation**

Time-resolved Monte Carlo simulation is almost identical to the steady-state simulation discussed above, except for some minor changes. There are actually several ways to implement time-resolved Monte Carlo, and this section show one approach that illustrates the basic idea.

In this example, the photon is allowed to propagate with no absorption, and the total path of the photon is accumulated after each step s throughout the propagation:

$$L = L + s \tag{5.54}$$

Since there is no absorption, $\mu_a = 0$ and $\mu_t = \mu_s$. Since the speed of light is $c/n$, the time duration of the propagation is:

$$t = \frac{L}{c} \tag{5.55}$$

where $c$ is the speed of light in the tissue, $c = c_o/n$ where $c_o$ is the speed of light *in vacuo*. The time for a photon to escape out the front surface is determined from its total pathlength $L$ at the moment of escape divided by $c$.

Assume that one is interested in a set of 10 time-points, $t[it]$, where $it = 1$ to 10 is an index that refers to the desired time-point. Let the first time-point, $t[1]$, be 100 ps. Propagation is allowed to continue until the next photon step causes $L$ to exceed the pathlength corresponding to 100 ps,

$$L + s > t[it]/c \tag{5.56}$$

where $t\,[1] = 100$ ps for this example. At this point, a partial step size, $s_1$, is taken,

$$s_1 = t[it]/c - L \tag{5.57}$$

The photon is now located exactly at the time-point of 100 ps. The current photon weight $W$ is deposited in the bin $\boldsymbol{A}[iz][ir][it]$, where $[it]$ selects a full 2-D $\boldsymbol{A}[iz][ir]$ array associated with each particular time point. The entire photon weight ($w = 1$) is placed in the local bin, but the weight of the photon is not decremented. The bin $\boldsymbol{A}[iz][ir][it]$ takes a snapshot of the photon's location and weight, but does not affect the photon. There is no absorption. The photon is allowed to continue propagating. The remainder of the step size, $s - s_1$, is taken by the photon. The photon continues to propagate as usual, until a next step causes $L$ to exceed the 2$^{nd}$ time

point, $t$[2]. The process of taking a partial step, depositing $W$ into $\boldsymbol{A}[ir][iz][it]$ without changing the $W$ of the photon, completing the step, and resuming propagation is executed. The process continues until $L$ passes the last desired time point, then the photon is terminated and a second photon is launched.

During propagation, when a photon strikes one of the boundaries, a fraction $(1-\boldsymbol{R}_i)$ of the current photon weight will escape, and the photon weight will decrement. The new photon weight, $\boldsymbol{R}_i W$, will internally reflect and continue propagating. The escaping photon weight will be placed in the bin $\boldsymbol{R}_r[ir][jt]$,

$$\boldsymbol{R}_r[ir][jt] = \boldsymbol{R}_r[ir][jt] + (1-\boldsymbol{R}_i)W \tag{5.58}$$

where $jt$ is an index that encodes the time of escape, and may be divided into equal time steps, $dt$ [$s$], that cover the time duration of interest. The current $jt$ is computed:

$$jt = \text{round}(t/dt) + 1 \tag{5.59}$$

As an example of evenly divided time bins, if the time duration of interest was from 10 ps to 1 ns, then $dt$ would be 10 ps and $jt$ would extend from 1 to 100. An alternative approach is to have progressively larger $dt$ bin sizes, so the time base can extend from very short times to very long times, which is not discussed here.

Finally, after $N_{\text{photons}}$ have been launched and terminated, it is time to normalize the bins $\boldsymbol{A}$ and $\boldsymbol{R}_r$ for final output. For each time point, [$it$], conservation of energy in terms of photon weight is summarized:

$$\frac{1}{N_{\text{photons}}}\left(\sum_{iz}\sum_{ir}\boldsymbol{A}[iz][ir][it] + \sum_{jt=1}^{it} R_r[ir][jt]\right) = 1 \tag{5.60}$$

The above calculation is not routinely needed, but is only a check that energy is conserved. The final normalization is

$$\boldsymbol{T} = c\frac{\boldsymbol{A}}{V\,N_{\text{photons}}} \tag{5.61}$$

which has units of [1/(cm$^2$ s)]. The time-resolved fluence rate, [W/cm$^2$] in response to an impulse of energy $Q$ [J] delivered at time zero is:

$$\phi(t) = Q\boldsymbol{T} \tag{5.62}$$

The escaping flux density, $\boldsymbol{R}_r$ [1/(cm$^2$ s)], is normalized:

$$\boldsymbol{R}_r = \frac{\boldsymbol{R}_r}{\text{AREA } N_{\text{photons}}\ dt} \tag{5.63}$$

Both ***A[iz][ir][it]*** and $\boldsymbol{R}_r[ir][it]$ will have good signal-to-noise in regions near the source where most photons spend their time, and poor signal-to-noise in regions far from the source. It is difficult to get good results far from the source even when a large number of photons are launched. Usually, time-resolved Monte Carlo simulation is used to specify results close to a source, and time-resolved diffusion theory is used to specify results at far distances from the source.

Now that the Monte Carlo simulation is completed, absorption can be added to the problem. The attenuation due to absorption is specified by Beer's law which says that photon survival equals $\exp(-\mu_a ct)$, since the ct equals the photon's total pathlength $L$ at any particular time $t$. Therefore,

$$\phi(t) = Q\boldsymbol{T}(t)e^{-\mu_a ct} \tag{5.64}$$

and

$$\boldsymbol{R}_r(t) = \frac{\boldsymbol{R}_r(t)}{\text{AREA } N_{\text{photons}}\ dt}\ e^{-\mu_a ct} \tag{5.65}$$

In this way, any value of $\mu_a$ can be introduced to learn its influence on the time-resolved distribution of $\boldsymbol{T}(t)$ or $\boldsymbol{R}_r(t)$.

To illustrate time-resolved Monte Carlo, an example of snapshots of $\boldsymbol{T}[iz][ir]$ at 4 time-points is presented in Figure 5.7, which illustrates the early movement of an incident laser pulse into a tissue. The narrow beam laser pulse broadens with time due to scattering.

Figure 5.8 shows an optical fiber embedded within a tissue and terminating at a depth of 500 $\mu$m, delivering light toward the surface. As the light reaches the surface, the time-resolved escape of fractional flux density, $\boldsymbol{R}_r(t,r)$ [1/(cm$^2$ s)] is shown.

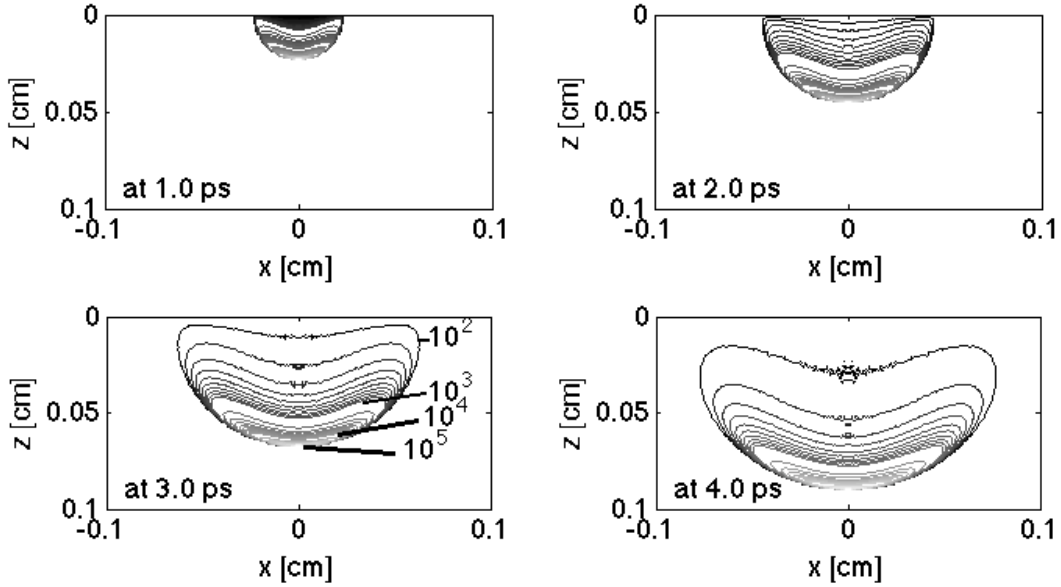



**Figure 5.7.** Time-resolved propagation of a collimated laser impulse launched at $r = 0$, $z = 0$ into a 1-mm thickness of a standard tissue. The thickness represents ~10 optical depths for optical properties of $\mu_a = 1$ cm$^{-1}$, $\mu_s = 100$ cm$^{-1}$, $g = 0.90$, $n = 1.4$. The four time points are 1, 2, 3 and 4 ps. The maps are iso-$\boldsymbol{T}$ contours, where $\boldsymbol{T}$ is the time-resolved fractional transport [1/(cm$^2$ s)]. The influence of $\mu_a$ is minor, for example, $\exp(-\mu_a ct)$ is only 0.92 when $t = 4$ ps.

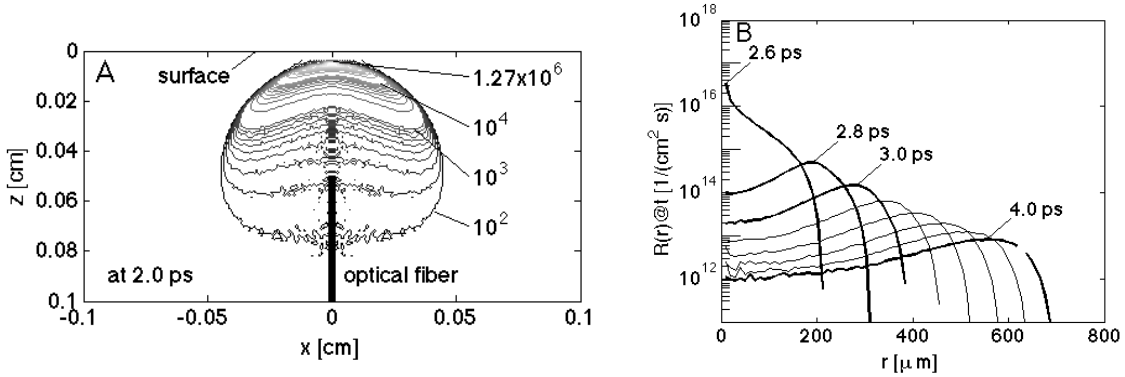



**Figure 5.8.** Time-resolved escape of a laser pulse from within tissue. The optical properties were $\mu_s = 100$ cm$^{-1}$, $g = 0.90$, $n_{\text{tissue}} = 1.33$. The impulse is delivered toward the surface from an optical fiber terminated at a depth of 500 $\mu$m within the tissue and pointed toward the surface. (A) Impulse at time 2 ps, shown as $\boldsymbol{T}$ [1/(cm$^2$ s)], maximum is 1.27x10$^6$. (B) The escaping fractional flux density versus radial position at different times, $\boldsymbol{R}_r(t,r)$ [1/(cm$^2$ s)].

### 5.5 Converting time-resolved results to frequency-domain

When the intensity of a light source is modulated at very high frequencies, the ability of the frequency of modulation to transport to some position of observation is described as *frequency*

*domain* light transport. Time-resolved information generated by a time-resolved Monte Carlo simulation can be converted by Fourier Transform into frequency domain information.

Consider the time-resolved escape of fractional flux density, $\boldsymbol{R_r}(t,r)$ [1/(cm$^2$ s)], when light is delivered as a collimated impulse to position $(r,z) = (0,0)$ on a tissue surface. The light enters the tissue, but due to scattering begins to escape from the tissue after some delay. This time-resolved $\boldsymbol{R_r}(t,r)$ is shown in Figure 5.9A, for a typical tissue. As the position of observation moves from 1 mm to 6 mm distance from the source, the time delay before onset of escaping flux increases, and the amount of light escaping decreases.

The corresponding frequency domain information is obtained by using a Fast Fourier Transform (*fft*) to convert the time-resolved $\boldsymbol{R_r}(t,r)$ escaping at a particular radial position $r$, denoted as $R_r(t)$, into the frequency domain:

$$F(f) = \text{abs}(fft(\boldsymbol{R_r}(t)dt)\ ) \tag{5.66}$$

where $dt$ is the time-step of the time-resolved data. The absolute value converts the imaginary values generated by the *fft*() into real values that correspond to the power spectrum, expressed as the fractional power $F$ [1/cm$^2$]. In other words, if the source was modulated at a frequency f [1/s], the function $F$ would specify the fractional escaping flux, $\boldsymbol{R_r}$ [1/cm$^2$], that was still modulated at frequency $f$. Figure 5.9B shows this power spectrum. The limiting values toward low frequencies of modulation correspond to the steady-state reflectance $\boldsymbol{R_r}(r)$ [1/cm$^2$], which is why the factor $dt$ was included in the above equation.

To illustrate the above equation more specifically, the equivalent programming code written in MATLAB$^{TM}$ notation is listed:

```
mua = 1;    % absorption coefficient [cm^-1]
mus = 100;  % scattering coefficient [cm^-1]
g   = 0.90; % anisotropy of scattering [dimensionless]
n   = 1.5;  % refractive index [dimensionless]
dt = 1e-12; % time step of time-resolved data [s], in this case dt = 1 ps.
t = (1:100)'*dt;       % time base of Monte Carlo data [s], up to 100 ps
r = (1:100)'/100*1.0;  % radial position of Monte Carlo data [cm], up to 1 cm
Rr = getRrMonteCarlo(t,r,mua,mus,g,n); % get Monte Carlo data [1/cm2/s], not shown
N = 2048;  % adds zeros to end of time-resolved data, for padding the transform
f = (1:N/2)'/N/dt; % the x-axis frequency of the power spectrum
ir = 10;   % selects one radial position r(ir)
F = abs(fft(Rr(:,ir)*dt, N));  % Rr(:,ir) is the time-resolved Rr(t) at r(ir)
plot(f, F)  % the plot command yields the power spectrum in [1/cm^2]
```

The original data $\boldsymbol{R_r}(t,r)$ has 100 time-points, but the fft() operates best when the number of data points is a multiple of 2. Therefore, zeros are added to the end of the data, which is called *padding*. Adding more zeros causes the result to have more points, so the curves look smoother. In this case 1948 zeros were added to yield a final 2048 data points. The above program yielded Figure 5.9B. Figure 5.9C normalizes the data by the DC value of $\boldsymbol{R_r}$, so as to emphasize the shape of the power spectra.

Note in this example that light escaping at 1 mm from the source has higher frequency content than light escaping at 6 mm from the source. In practical frequency domain measurements, the detection of light transport is usually made at least 10 mm from the source, where diffusion theory suffices to describe light transport, and the frequency content of interest is in the 100's of MHz [1/s]. This example shows how time-resolved Monte Carlo data can be converted to the frequency domain to address questions where diffusion theory is inadequate.

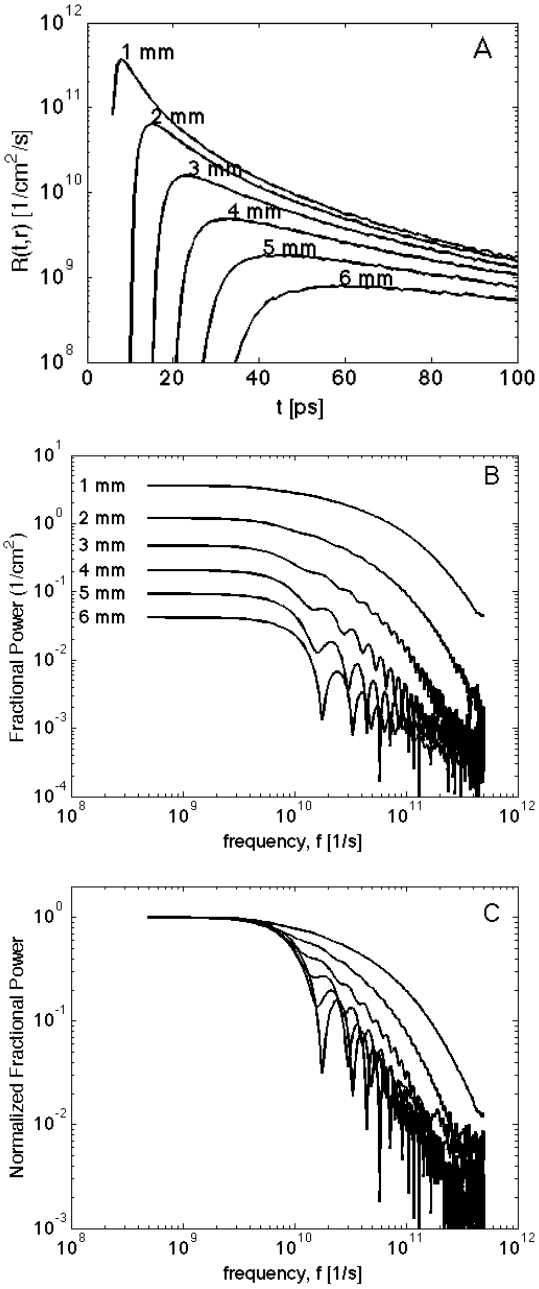



**Figure 5.9.** Frequency domain light transport, showing how light modulated at different frequencies and delivered as a collimated beam to position $(r,z) = (0,0)$, will escape from the

tissue as a function of radial position. (A) The time-resolved escape of light from the tissue, $\boldsymbol{R_r}$ [1/(cm$^2$ s)] for r = 1 to 6 mm. (B) The fractional power spectrum [1/cm$^2$] versus frequency f [1/s]. The optical properties of the tissue were $\mu_a$ = 1 cm$^{-1}$, $\mu_s$ = 100 cm$^{-1}$, $g$ = 0.90, $n$ = 1.4, and $10^7$ photons were launched during a 35-min simulation. The data at the higher frequencies for the most distant radial positions were based on low photon weights and show artifactual oscillations.

### 5.6 Summary

Monte Carlo simulations are a relatively simple and flexible method for exploring the behavior of light transport in biological tissues or other media with average absorption and scattering properties. The simulations are like experiments involving a number of photons ($N_{photons}$) and hence the simulations take time to execute. Some simulations take only a minute, and others take hours or even days. If you are trying to fill small bins with rare photons, the simulations take a lot of time. But common problems take about 10 min or less to get a good result.

The strength of Monte Carlo simulations is to treat situations where diffusion theory, or some other analytic expression of light transport, fails. It is not the proper tool for every job.

### 5.7 References

1. B. C. Wilson and G. Adam: "A Monte Carlo model for the absorption and flux distributions of light in tissue," *Med. Phys.* 10:824–830, 1983.

2. Keijzer M, SL Jacques, SA Prahl, AJ Welch: Light distributions in artery tissue: Monte Carlo simulations for finite-diameter laser beams. *Lasers Surg.Med.* 9:148-154, 1989

3. Prahl, S.A., M. Keijzer, S.L. Jacques, A.J. Welch: A Monte Carlo model of light propagation in tissue. In *Dosimetry of Laser Radiation in Medicine and Biology*, G. Müller, D. Sliney, Eds., SPIE Series Vol IS 5:102-111, 1989.

4. L.-H. Wang, S. L. Jacques, L.-Q. Zheng: MCML - Monte Carlo modeling of photon transport in multi-layered tissues. *Computer Methods and Programs in Biomedicine*, 47, 131-146, 1995.

5. http://omlc.ogi.edu/software/mc/mcml. This site includes a 178-page manual on MCML. Also, a convolution program, CONV, is available for convolving the point spread functions generated by MCML.

6. http://labs.seas.wustl.edu/bme/Wang/mc.html. Alternative site for obtaining MCML, CONV and the manual.

7. S. L. Jacques: Light distributions from point, line, and plane sources for photochemical reactions and fluorescence in turbid biological tissues. *Photochem. Photobiol.* 67:23-32, 1998.

8. http://omlc.ogi.edu/software/mc/mc321. This site lists the minimal Monte Carlo program mc321.m, used in Ref. 7.

9. Jacques SL, Monte Carlo simulations of fluorescence in turbid media, Ch. 6 in *Handbook of Biomedical Fluorescence,* M.A. Mycek, B.W. Pogue, publ. Marcel-Dekker, New York, NY, 2003.

10. http://omlc.ogi.edu/software/mc/mcsub. This site lists the subroutine mcsub() that can be called by c programs to run a Monte Carlo simulation.

11. JC Ramella-Roman, SA Prahl, SL Jacques, Three Monte Carlo programs of polarized light transport into scattering media: part I. *Optics Express* 13(12):4420-4438, 2005.

12. http://omlc.ogi.edu/software/mc/polarizedlight. This site lists the program for Monte Carlo simulation of polarized light, reported in Ref. 11.

### 5.8 Appendix: mc321.c

A simplest version of a Monte Carlo simulation, called `mc321.c`, is listed below. The program can be downloaded from the web [8], but since websites may change, the program is listed here as an archival example, and as an easy reference while reading this chapter. This program does not consider escape across boundaries, but shows the basic format of photon propagation, recording and normalization. The output of this program is plotted in Figure 5.10:

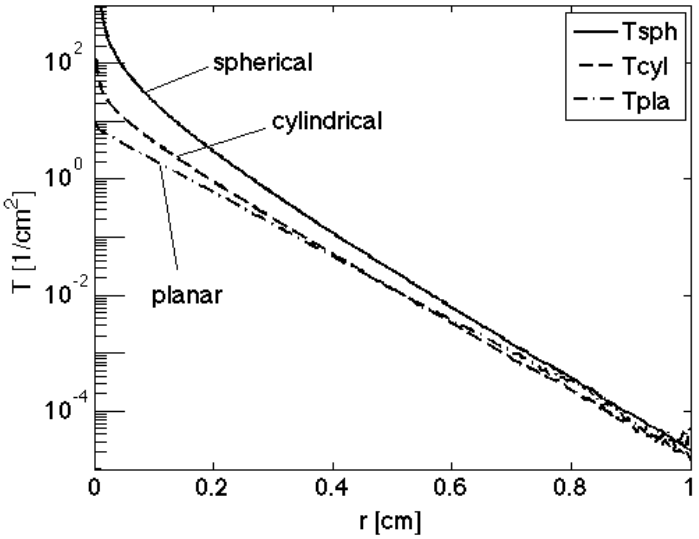



**Figure 5.10.** The data in `mc321.out`, produced by `mc321.c`, plotted using a separate graphics program. The spherical transport from a point source, the cylindrical transport from a line source, and the planar transport from a planar source are shown versus the distance, *r*, from the source.

```
/****************************************
 *  mc321.c    , in ANSI Standard C programming language
 *
 *  Monte Carlo simulation yielding spherical, cylindrical, and planar
 *    responses to an isotropic point source (equivalent to a plane source,
 *    line source, and point source, respectively) in an infinite homogeneous
 *    medium with no boundaries. This program is a minimal Monte Carlo
 *    program scoring photon distributions in spherical, cylindrical,
 *    and planar shells.
 *
 *  by Steven L. Jacques based on prior collaborative work
 *    with Lihong Wang, Scott Prahl, and Marleen Keijzer.
 *    partially funded by the NIH (R29-HL45045, 1991-1997) and
 *    the DOE (DE-FG05-91ER617226, DE-FG03-95ER61971, 1991-1999).
 *
 *  A published report illustrates use of the program:
 *    S. L. Jacques: "Light distributions from point, line, and plane
 *    sources for photochemical reactions and fluorescence in turbid
 *    biological tissues," Photochem. Photobiol. 67:23-32, 1998.
 **********/

#include <math.h>
#include <stdio.h>

#define Nbins          500
#define Nbinsp1        501
#define   PI          3.1415926
#define   LIGHTSPEED   2.997925E10 /* in vacuo speed of light [cm/s] */
#define ALIVE       1               /* if photon not yet terminated */
#define DEAD        0               /* if photon is to be terminated */
#define THRESHOLD   0.01            /* used in roulette */
#define CHANCE      0.1             /* used in roulette */
#define COS90D      1.0E-6
     /* If cos(theta) <= COS90D, theta >= PI/2 - 1e-6 rad. */
#define ONE_MINUS_COSZERO 1.0E-12
     /* If 1-cos(theta) <= ONE_MINUS_COSZERO, fabs(theta) <= 1e-6 rad. */
     /* If 1+cos(theta) <= ONE_MINUS_COSZERO, fabs(PI-theta) <= 1e-6 rad. */
#define SIGN(x)           ((x)>=0 ? 1:-1)
#define InitRandomGen    (double) RandomGen(0, 1, NULL)
     /* Initializes the seed for the random number generator. */
#define RandomNum        (double) RandomGen(1, 0, NULL)
     /* Calls for a random number from the randum number generator. */

/* DECLARE FUNCTION */
double RandomGen(char Type, long Seed, long *Status);
     /* Random number generator */


main() {

/* Propagation parameters */
double    x, y, z;    /* photon position */
double    ux, uy, uz; /* photon trajectory as cosines */
double  uxx, uyy, uzz;  /* temporary values used during SPIN */
double    s;          /* step sizes. s = -log(RND)/mus [cm] */
double    costheta;   /* cos(theta) */
double  sintheta;   /* sin(theta) */
double    cospsi;     /* cos(psi) */
double  sinpsi;     /* sin(psi) */
double    psi;        /* azimuthal angle */
double    i_photon;   /* current photon */
```

```
    double    W;          /* photon weight */
    double    absorb;     /* weighted deposited in a step due to absorption */
    short   photon_status;  /* flag = ALIVE=1 or DEAD=0 */

    /* other variables */
    double    Csph[Nbinsp1];  /* spherical   photon concentration CC[ir=0..100] */
    double    Ccyl[Nbinsp1];  /* cylindrical photon concentration CC[ir=0..100] */
    double    Cpla[Nbinsp1];  /* planar      photon concentration CC[ir=0..100] */
    double    Fsph;       /* fluence in spherical shell */
    double    Fcyl;       /* fluence in cylindrical shell */
    double    Fpla;       /* fluence in planar shell */
    double    mua;        /* absorption coefficient [cm^-1] */
    double    mus;        /* scattering coefficient [cm^-1] */
    double    g;          /* anisotropy [-] */
    double    albedo;     /* albedo of tissue */
    double    nt;         /* tissue index of refraction */
    double    Nphotons;   /* number of photons in simulation */
    short     NR;         /* number of radial positions */
    double    radial_size;  /* maximum radial size */
    double    r;          /* radial position */
    double  dr;         /* radial bin size */
    short     ir;         /* index to radial position */
    double  shellvolume;  /* volume of shell at radial position r */
    double    CNT;        /* total count of photon weight summed over all bins */

    /* dummy variables */
    double  rnd;        /* assigned random value 0-1 */
    short     i, j;       /* dummy indices */
    double    u, temp;    /* dummy variables */
    FILE*     target;     /* point to output file */


    /**** INPUT
       Input the optical properties
       Input the bin and array sizes
       Input the number of photons
    *****/

    mua         = 1.673;     /* cm^-1 */
    mus         = 312.0;  /* cm^-1 */
    g           = 0.90;
    nt          = 1.33;
    Nphotons    = 10000; /* set number of photons in simulation */
    radial_size = 2.0;   /* cm, total range over which bins extend */
    NR          = Nbins;    /* set number of bins.  */
    /* IF NR IS ALTERED, THEN USER MUST ALSO ALTER THE ARRAY DECLARATION TO A SIZE =
NR+1. */
    dr          = radial_size/NR;  /* cm */
    albedo      = mus/(mus + mua);


    /**** INITIALIZATIONS
    *****/
    i_photon = 0;
    InitRandomGen;
    for (ir=0; ir<=NR; ir++) {
       Csph[ir] = 0;
       Ccyl[ir] = 0;
       Cpla[ir] = 0;
       }
```

```
/**** RUN
   Launch N photons, initializing each one before progation.
*****/
do {


/**** LAUNCH
   Initialize photon position and trajectory.
   Implements an isotropic point source.
*****/
i_photon += 1;   /* increment photon count */
if ( fmod(i_photon, Nphotons/10)  == 0)
   printf("%0.0f%% done\n", i_photon/Nphotons*100);


W = 1.0;                    /* set photon weight to one */
photon_status = ALIVE;      /* Launch an ALIVE photon */

x = 0;                      /* Set photon position to origin. */
y = 0;
z = 0;

/* Randomly set photon trajectory to yield an isotropic source. */
costheta = 2.0*RandomNum - 1.0;
sintheta = sqrt(1.0 - costheta*costheta);  /* sintheta is always positive */
psi = 2.0*PI*RandomNum;
ux = sintheta*cos(psi);
uy = sintheta*sin(psi);
uz = costheta;


/* HOP_DROP_SPIN_CHECK
   Propagate one photon until it dies as determined by ROULETTE.
*******/
do {


/**** HOP
   Take step to new position
   s = step size
   ux, uy, uz are cosines of current photon trajectory
*****/
  while ((rnd = RandomNum) <= 0.0);   /* yields 0 < rnd <= 1 */
  s = -log(rnd)/(mua + mus);          /* Step size.  Note: log() is base e */
  x += s * ux;                        /* Update positions. */
  y += s * uy;
  z += s * uz;


/**** DROP
   Drop photon weight (W) into local bin.
*****/
   absorb = W*(1 - albedo);      /* photon weight absorbed at this step */
   W -= absorb;                  /* decrement WEIGHT by amount absorbed */

   /* spherical */
   r = sqrt(x*x + y*y + z*z);    /* current spherical radial position */
   ir = (short)(r/dr);           /* ir = index to spatial bin */
   if (ir >= NR) ir = NR;        /* last bin is for overflow */
   Csph[ir] += absorb;           /* DROP absorbed weight into bin */
```

```
      /* cylindrical */
      r = sqrt(x*x + y*y);          /* current cylindrical radial position */
      ir = (short)(r/dr);           /* ir = index to spatial bin */
      if (ir >= NR) ir = NR;        /* last bin is for overflow */
      Ccyl[ir] += absorb;           /* DROP absorbed weight into bin */

      /* planar */
      r = fabs(z);                  /* current planar radial position */
      ir = (short)(r/dr);           /* ir = index to spatial bin */
      if (ir >= NR) ir = NR;        /* last bin is for overflow */
      Cpla[ir] += absorb;           /* DROP absorbed weight into bin */


   /**** SPIN
      Scatter photon into new trajectory defined by theta and psi.
      Theta is specified by cos(theta), which is determined
      based on the Henyey-Greenstein scattering function.
      Convert theta and psi into cosines ux, uy, uz.
   *****/
     /* Sample for costheta */
     rnd = RandomNum;
        if (g == 0.0)
           costheta = 2.0*rnd - 1.0;
        else {
           double temp = (1.0 - g*g)/(1.0 - g + 2*g*rnd);
           costheta = (1.0 + g*g - temp*temp)/(2.0*g);
           }
     sintheta = sqrt(1.0 - costheta*costheta); /* sqrt() is faster than sin(). */

     /* Sample psi. */
     psi = 2.0*PI*RandomNum;
     cospsi = cos(psi);
     if (psi < PI)
       sinpsi = sqrt(1.0 - cospsi*cospsi);     /* sqrt() is faster than sin(). */
     else
       sinpsi = -sqrt(1.0 - cospsi*cospsi);

     /* New trajectory. */
     if (1 - fabs(uz) <= ONE_MINUS_COSZERO) {      /* close to perpendicular. */
       uxx = sintheta * cospsi;
       uyy = sintheta * sinpsi;
       uzz = costheta * SIGN(uz);   /* SIGN() is faster than division. */
       }
     else {                              /* usually use this option */
       temp = sqrt(1.0 - uz * uz);
       uxx = sintheta * (ux * uz * cospsi - uy * sinpsi) / temp + ux * costheta;
       uyy = sintheta * (uy * uz * cospsi + ux * sinpsi) / temp + uy * costheta;
       uzz = -sintheta * cospsi * temp + uz * costheta;
       }

     /* Update trajectory */
     ux = uxx;
     uy = uyy;
     uz = uzz;


   /**** CHECK ROULETTE
      If photon weight below THRESHOLD, then terminate photon using Roulette
technique.
      Photon has CHANCE probability of having its weight increased by factor of
1/CHANCE,
```

```
      and 1-CHANCE probability of terminating.
   *****/
   if (W < THRESHOLD) {
      if (RandomNum <= CHANCE)
         W /= CHANCE;
      else photon_status = DEAD;
      }


   } /* end STEP_CHECK_HOP_SPIN */
   while (photon_status == ALIVE);

     /* If photon dead, then launch new photon. */
   } /* end RUN */
   while (i_photon < Nphotons);


   /**** SAVE
      Convert data to relative fluence rate [cm^-2] and save to file called
"mcmin321.out".
   *****/
   target = fopen("mc321.out", "w");

   /* print header */
   fprintf(target, "number of photons = %f\n", Nphotons);
   fprintf(target, "bin size = %5.5f [cm] \n", dr);
   fprintf(target, "last row is overflow. Ignore.\n");

   /* print column titles */
   fprintf(target, "r [cm] \t Fsph [1/cm2] \t Fcyl [1/cm2] \t Fpla [1/cm2]\n");

   /* print data:  radial position, fluence rates for 3D, 2D, 1D geometries */
   for (ir=0; ir<=NR; ir++) {
      /* r = sqrt(1.0/3 - (ir+1) + (ir+1)*(ir+1))*dr; */
      r = (ir + 0.5)*dr;
      shellvolume = 4.0*PI*r*r*dr; /* per spherical shell */
       Fsph = Csph[ir]/Nphotons/shellvolume/mua;
      shellvolume = 2.0*PI*r*dr;   /* per cm length of cylinder */
       Fcyl = Ccyl[ir]/Nphotons/shellvolume/mua;
      shellvolume = dr;            /* per cm2 area of plane */
       Fpla =Cpla[ir]/Nphotons/shellvolume/mua;
      fprintf(target, "%5.5f \t %4.3e \t %4.3e \t %4.3e \n", r, Fsph, Fcyl, Fpla);
      }

   fclose(target);


   } /* end of main */



   /* SUBROUTINES */

   /*****************************************************************************
    * RandomGen
    *      A random number generator that generates uniformly
    *      distributed random numbers between 0 and 1 inclusive.
    *      The algorithm is based on:
    *      W.H. Press, S.A. Teukolsky, W.T. Vetterling, and B.P.
    *      Flannery, "Numerical Recipes in C," Cambridge University
    *      Press, 2nd edition, (1992).
```

```
 *      and
 *      D.E. Knuth, "Seminumerical Algorithms," 2nd edition, vol. 2
 *      of "The Art of Computer Programming", Addison-Wesley, (1981).
 *
 *      When Type is 0, sets Seed as the seed. Make sure 0<Seed<32000.
 *      When Type is 1, returns a random number.
 *      When Type is 2, gets the status of the generator.
 *      When Type is 3, restores the status of the generator.
 *
 *      The status of the generator is represented by Status[0..56].
 *
 *      Make sure you initialize the seed before you get random
 *      numbers.
 ****/
#define MBIG 1000000000
#define MSEED 161803398
#define MZ 0
#define FAC 1.0E-9

double RandomGen(char Type, long Seed, long *Status){
  static long i1, i2, ma[56];   /* ma[0] is not used. */
  long        mj, mk;
  short       i, ii;

  if (Type == 0) {              /* set seed. */
    mj = MSEED - (Seed < 0 ? -Seed : Seed);
    mj %= MBIG;
    ma[55] = mj;
    mk = 1;
    for (i = 1; i <= 54; i++) {
      ii = (21 * i) % 55;
      ma[ii] = mk;
      mk = mj - mk;
      if (mk < MZ)
        mk += MBIG;
      mj = ma[ii];
    }
    for (ii = 1; ii <= 4; ii++)
      for (i = 1; i <= 55; i++) {
        ma[i] -= ma[1 + (i + 30) % 55];
        if (ma[i] < MZ)
          ma[i] += MBIG;
      }
    i1 = 0;
    i2 = 31;
  } else if (Type == 1) {       /* get a number. */
    if (++i1 == 56)
      i1 = 1;
    if (++i2 == 56)
      i2 = 1;
    mj = ma[i1] - ma[i2];
    if (mj < MZ)
      mj += MBIG;
    ma[i1] = mj;
    return (mj * FAC);
  } else if (Type == 2) {       /* get status. */
    for (i = 0; i < 55; i++)
      Status[i] = ma[i + 1];
    Status[55] = i1;
    Status[56] = i2;
  } else if (Type == 3) {       /* restore status. */
```

```
    for (i = 0; i < 55; i++)
      ma[i + 1] = Status[i];
    i1 = Status[55];
    i2 = Status[56];
  } else
    puts("Wrong parameter to RandomGen().");
  return (0);
}
#undef MBIG
#undef MSEED
#undef MZ
#undef FAC
```