Monte Carlo Modeling of Light Transport in Multi-layered Tissues in Standard C

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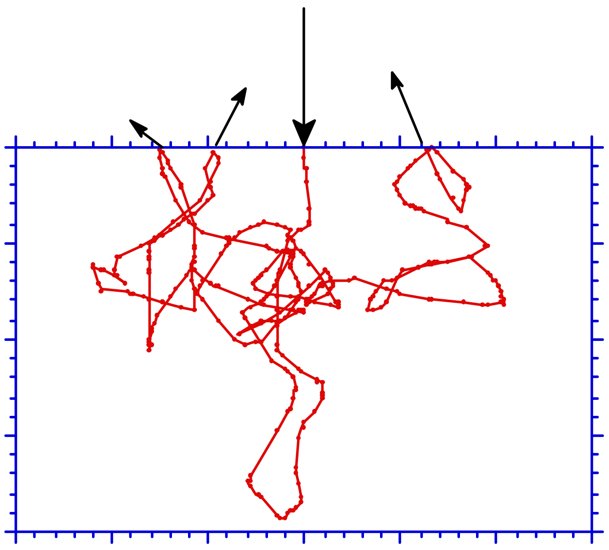

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Abstract

A Monte Carlo model of steady-state light transport in multi-layered tissue (mcml) and the corresponding convolution program (conv) have been coded in ANSI Standard C. The programs can therefore be executed on a variety of computers. Dynamic data allocation is used for mcml, hence the number of tissue layers and the number of grid elements of the grid system can be varied by users at run time as long as the total amount of memory does not exceed what the system allows. The principle and the implementation details of the model, and the instructions for using mcml and conv are presented here. We have verified some of the mcml and conv computation results with those of other theories or other investigators.

Acknowledgment

We would like to thank a group of people who have helped us with this package directly or indirectly. Massoud Motamedi (University of Texas Medical Branch, Galveston) has let us use his Sun SPARCstation 2. Scott A. Prahl (St. Vincent's Hospital, Oregon) and Thomas J. Farrell (Hamilton Regional Cancer Center, Canada) have helped us locate an insidious bug in the program. Craig M. Gardner (University of Texas, Austin) provided us his Monte Carlo simulation and convolution results of a multi-layered medium, which are compared with our results. We learned a lot from Marleen Keijzer and Steven L. Jacques's Monte Carlo simulation program in PASCAL on Macintoshes. Liqiong Zheng (University of Houston) has helped us greatly improve the speed of the convolution program. They all deserve our thanks.

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0. Introduction

Monte Carlo simulation has been used to solve a variety of physical problems. However, there is no succinct well-established definition. We would like to adopt the definition by Lux *et al*. (1991). In all applications of the Monte Carlo method, a stochastic model is constructed in which the expected value of a certain random variable (or of a combination of several variables) is equivalent to the value of a physical quantity to be determined. This expected value is then estimated by the average of multiple independent samples representing the random variable introduced above. For the construction of the series of independent samples, random numbers following the distribution of the variable to be estimated are used.

Monte Carlo simulations of photon propagation offer a flexible yet rigorous approach toward photon transport in turbid tissues. The method describes local rules of photon propagation that are expressed, in the simplest case, as probability distributions that describe the step size of photon movement between sites of photon-tissue interaction, and the angles of deflection in a photon's trajectory when a scattering event occurs. The simulation can score multiple physical quantities simultaneously. However, the method is statistical in nature and relies on calculating the propagation of a large number of photons by the computer. As a result, this method requires a large amount of computation time.

The number of photons required depends largely on the question being asked, the precision needed, and the spatial resolution desired. For example, to simply learn the total diffuse reflectance from a tissue of specified optical properties, typically about 3,000 photons can yield a useful result. To map the spatial distribution of photons, $\phi(r, z)$, in a cylindrically symmetric problem, at least 10,000 photons are usually required to yield an acceptable answer. To map spatial distributions in a more complex three-dimensional problem such as a finite diameter beam irradiating a tissue with a buried blood vessel, the required photons may exceed 100,000. The point to be remembered in these introductory remarks is that Monte Carlo simulations are rigorous, but necessarily statistical and therefore require significant computation time to achieve precision and resolution. Nevertheless, the flexibility of the method makes Monte Carlo modeling a powerful tool.

Another aspect of the Monte Carlo simulations presented in this paper deserves emphasis. The simulations described here do not treat the photon as a wave phenomenon, and ignore such features as phase and polarization. The motivation for these simulations is to predict radiant energy transport in turbid tissues. The photons are multiply scattered by most tissues, therefore phase and polarization are quickly randomized, and play little role in energy transport. Although the Monte Carlo simulations may be capable of bookkeeping phase and polarization and treating wave phenomena statistically, this manual will not consider these issues.

The Monte Carlo simulations are based on macroscopic optical properties that are assumed to extend uniformly over small units of tissue volume. Mean free paths between photon-tissue interaction sites typically range from 10-1000 μm, and 100 μm is a very typical value in the visible spectrum (Cheong *et al.,* 1990). The simulations do not treat the details of radiant energy distribution within cells, for example.

As a simple example of the Monte Carlo simulation. We would like to present a typical trajectory of a single photon packet in Fig. 0.1. Each step between photon positions (dots) is variable and equals $-\ln(\xi)/(\mu_a + \mu_s)$ where ξ is a random number and μ_a and μ_s are the absorption and scattering coefficients, respectively (in this example, μ_a = 0.5 cm^{-1}, μ_s = 15 cm^{-1}, g = 0.90). The value g is the anisotropy of scattering. The weight of the photon is decreased from an initial value of 1 as it moves through the tissue, and equals a^n after n steps, where a is the albedo ($a = \mu_s/(\mu_a + \mu_s)$). When the photon strikes the surface, a fraction of the photon weight escapes as reflectance and the remaining weight is internally reflected and continues to propagate. Eventually, the photon weight drops below a threshold level and the simulation for that photon is terminated. In this example, termination occurred when the last significant fraction of remaining photon weight escaped at the surface at the position indicated by the asterisk (*). Many photon trajectories (10^4 to 10^6) are typically calculated to yield a statistical description of photon distribution in the medium.

This manual is roughly divided into two major parts. Part I describes the principles of Monte Carlo simulations of photon transport in tissues, how to realize the simulation in ANSI Standard C, and some computation results and verifications. Part II provides users detailed instructions of using mcml and modifying mcml to suit special need, where mcml stands for Monte Carlo simulations for multi-layered tissues. The appendices furnish the flow graph and the whole source code of mcml, and some other useful information.

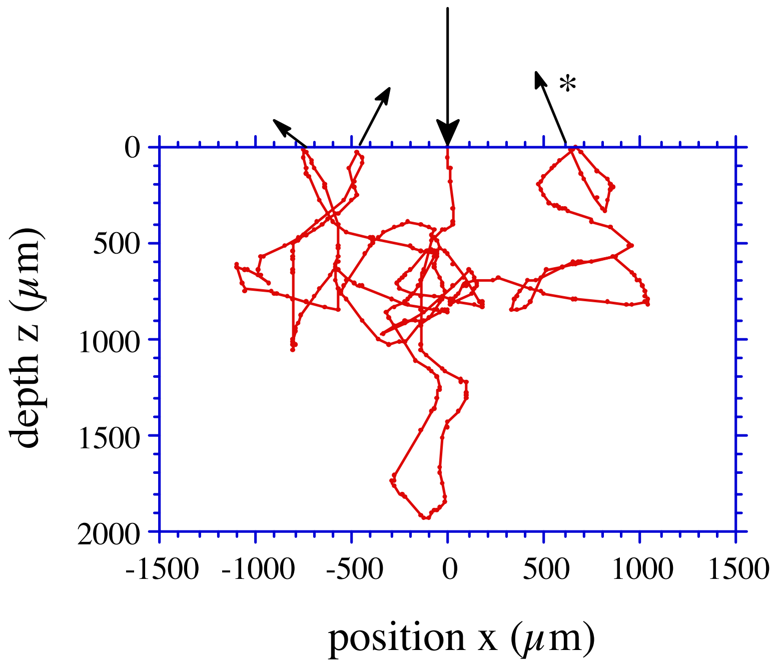

Figure 0.1. The movement of one photon through a homogenous medium, as calculated by Monte Carlo simulation.

Part I. Description of Monte Carlo Simulation

1. The Problem and Coordinate Systems

The Monte Carlo simulation described in this paper deals with the transport of an infinitely narrow photon beam perpendicularly incident on a multi-layered tissue. Each layer is infinitely wide, and is described by the following parameters: the thickness, the refractive index, the absorption coefficient μ_a, the scattering coefficient μ_s, and the anisotropy factor g. The refractive indices of the top ambient medium (e.g., air) and bottom ambient medium (if exists) have to be given as well. Although the real tissue can never be infinitely wide, it can be so treated if it is much larger than the spatial extent of the photon distribution. The absorption coefficient μ_a is defined as the probability of photon absorption per unit infinitesimal pathlength, and the scattering coefficient μ_s is defined as the probability of photon scattering per unit infinitesimal pathlength. For the simplicity of notation, the total interaction coefficient μ_t, which is the sum of the absorption coefficient μ_a and the scattering coefficient μ_s, is sometimes used. Correspondingly, the interaction coefficient means the probability of photon interaction per unit infinitesimal pathlength. The anisotropy g is the average of the cosine value of the deflection angle (see Section 3.5).

Photon absorption, fluence, reflectance and transmittance are the physical quantities to be simulated. The simulation propagates photons in three dimensions, records photon deposition, $A(x, y, z)$, (J/cm^3 per J of delivered energy or cm^{-3}) due to absorption in each grid element of a spatial array, and finally calculates fluence, $\phi(x, y, z)$, (J/cm^2 per J of delivered energy or cm^{-2}) by dividing deposition by the local absorption coefficient, μ_a in cm^{-1}: $\phi(x, y, z) = A(x, y, z)/\mu_a$. Since the photon absorption and the photon fluence can be converted back and forth through the local absorption coefficient of the tissue, we only report the photon absorption in mcml (see Section 4.2 and Section 9.3). The photon fluence can be obtained by converting the photon absorption in another program conv. The simulation also records the escape of photons at the top (and bottom) surface as local reflectance (and transmittance) (cm^{-2}sr^{-1}) (see Section 4.1).

In this first version of mcml, we consider cylindrically symmetric tissue models. Therefore, we chose to record photon deposition in a two-dimensional array, $A(r, z)$ although the photon propagation of this simulation is conducted in three-dimensions.

Three coordinate systems are used in the Monte Carlo simulation at the same time. A Cartesian coordinate system is used to trace photon packets. The origin of the coordinate system is the photon incident point on the tissue surface, the z-axis is always the normal of the surface pointing toward the inside of the tissue, and the xy-plane is therefore on the tissue surface (Fig. 1.1). A cylindrical coordinate system is used to score internal photon absorption A(r, z), where r and z are the radial and z axis coordinates of the cylindrical coordinate system respectively. The Cartesian coordinate system and the cylindrical coordinate system share the origin and the z axis. The r coordinate of the cylindrical coordinate system is also used for the diffuse reflectance and total transmittance. They are recorded on tissue surface in $R_d(r, \alpha)$ and $T_t(r, \alpha)$ respectively, where α is the angle between the photon exiting direction and the normal (–z axis for reflectance and z axis for transmittance) to the tissue surfaces. A moving spherical coordinate system, whose z axis is aligned with the photon propagation direction dynamically, is used for sampling of the propagation direction change of a photon packet. In this spherical coordinate system, the deflection angle θ and the azimuthal angle ψ due to scattering are first sampled. Then, the photon direction is updated in terms of the directional cosines in the Cartesian coordinate system (see Section 3.5).

For photon absorption, a two-dimensional homogeneous grid system is setup in z and r directions. The grid line separations are Δz and Δr in z and r directions respectively. The total numbers of grid elements in z and r directions are N_z and N_r respectively. For diffuse reflectance and transmittance, a two-dimensional homogeneous grid system is setup in r and α directions. This grid system can share the r direction with the grid system for photon absorption. Therefore, we only need to set up an extra one dimensional grid system for the diffuse reflectance and transmittance in the α direction. In our simulation, we always choose the range of α to be $[0, \pi/2]$, i.e., $0 \leq \alpha \leq \pi/2$. The total number of grid elements is N_α. Therefore the grid line separation is $\Delta\alpha = \pi/(2\ N_\alpha)$.

This is an appropriate time to mention that we always use cm as the basic unit of length throughout the simulation for consistency. For example, the thickness of each layer and the grid line separations in r and z directions are in cm. The absorption coefficient and scattering coefficient are in cm^{-1}.

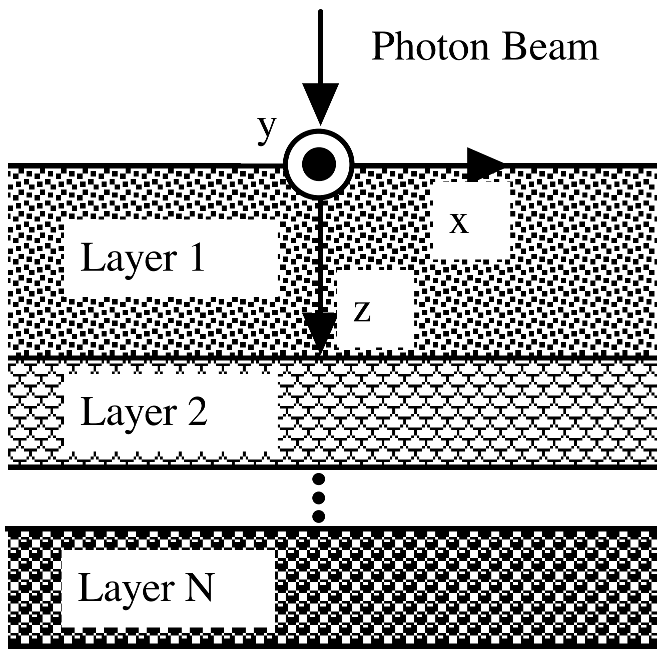

Fig. 1.1. A schematic of the Cartesian coordinate system set up on multi-layered tissues. The y-axis points outward.

In some of the discussions, the arrays will simply be referenced by the location of the grid element, e.g., (r, z) or (r, α), rather than by the indices of the grid element, although the indices are used in the program to reference array elements.

2. Sampling Random Variables

The Monte Carlo method, as its name implies ("throwing the dice"), relies on the random sampling of variables from well-defined probability distributions. Several books (Cashew *et al*., 1959; Lux *et al*., 1991; and Kalos *et al*., 1986) provide good references for the principles of Monte Carlo modeling. Let us briefly review the method for sampling random variables in a Monte Carlo simulation.

Consider a random variable χ, which is needed by the Monte Carlo simulation of photon propagation in tissue. This variable may be the variable step size a photon will take between photon-tissue interaction sites, or the angle of deflection a scattered photon may experience due to a scattering event. There is a probability density function that defines the distribution of χ over the interval (a, b). The probability density function is normalized such that:

$$\int_a^b p(\chi)\, d\chi = 1 \tag{2.1}$$

To simulate propagation, we wish to be able to choose a value for χ repeatedly and randomly based on a pseudo-random number generator. The computer provides a random variable, ξ, which is uniformly distributed over the interval (0, 1). The cumulative distribution function of this uniformly distributed random variable is:

$$F_\xi(\xi) = \begin{cases} 0 & \text{if } \xi \le 0 \\ \xi & \text{if } 0 < \xi \le 1 \\ 1 & \text{if } \xi > 1 \end{cases} \tag{2.2}$$

To sample a generally non-uniformly distributed function $p(\chi)$, we assume there exists a nondecreasing function $\chi = f(\xi)$ (Kalos *et al*., 1986), which maps $\xi \in (0, 1)$ to $\chi \in (a, b)$ (Fig. 2.1). The variable χ and variable ξ then have a one-to-one mapping. This subsequently leads to the following equality of probabilities:

$$P\{f(0) < \chi \le f(\xi_1)\} = P\{0 < \xi \le \xi_1\} \tag{2.3a}$$

or

$$P\{a < \chi \le \chi_1\} = P\{0 < \xi \le \xi_1\} \tag{2.3b}$$

According to the definition of cumulative distribution functions, Eq. 2.3b can be changed to an equation of cumulative distribution functions:

$$F_\chi(\chi_1) = F_\xi(\xi_1) \tag{2.4}$$

Expanding the cumulative distribution function $F_\chi(\chi_1)$ in terms of the corresponding probability density function for the left-hand side of Eq. 2.4 and employing Eq. 2.2 for the right-hand side, we convert Eq. 2.4 into:

$$\int_a^{\chi_1} p(\chi)\, d\chi = \xi_1 \quad \text{for } \xi_1 \in (0, 1) \tag{2.5}$$

Eq. 2.5 is then used to solve for χ_1 to get the function $f(\xi_1)$. If the function $\chi = f(\xi)$ is assumed nonincreasing, a similar derivation will lead to the counterpart of Eq. 2.5 as:

$$\int_a^{\chi_1} p(\chi)\, d\chi = 1 - \xi_1 \quad \text{for } \xi_1 \in (0, 1) \tag{2.6}$$

However, since $(1 - \xi_1)$ and ξ_1 have the same distribution, they can be interchanged. Therefore, Eq. 2.5 and Eq. 2.6 are equivalent. In the following chapter, Eq. 2.5 will be repeatedly invoked for sampling propagation variables.

The whole sampling process can be understood from Fig. 2.1. The key to the Monte Carlo selection of χ using ξ is to equate the probability that ξ is in the interval $[0, \xi_1]$ with the probability that χ is in the interval $[a, \chi_1]$. In Fig. 2.1, we are equating the shaded area depicting the integral of $p(\chi)$ over $[0, \chi_1]$ with the shaded area depicting the integral $p(\xi)$ over $[0, \xi_1]$. Keep in mind that the total areas under the curves $p(\chi)$ and $p(\xi)$ each equal unity, as is appropriate for probability density functions. The result is a one-to-one mapping between the upper boundaries ξ_1 and χ_1 based on the equality of the shaded areas in Fig. 2. In other words, we have equated $F_\chi(\chi_1)$ with $F_\xi(\xi_1)$ (Eq. 2.4) which is equivalent to Eq. 2.5. The transformation process $\chi_1 = f(\xi_1)$ is shown by the arrows. For each ξ_1, a χ_1 is chosen such that the cumulative distribution functions for ξ_1 and χ_1 have the same value. Correspondingly, the hatched areas are equal. It can also be seen in Fig. 2.1 that the monotonic function $f(\xi)$ always exists because both cumulative distribution functions of ξ and χ are monotonic.

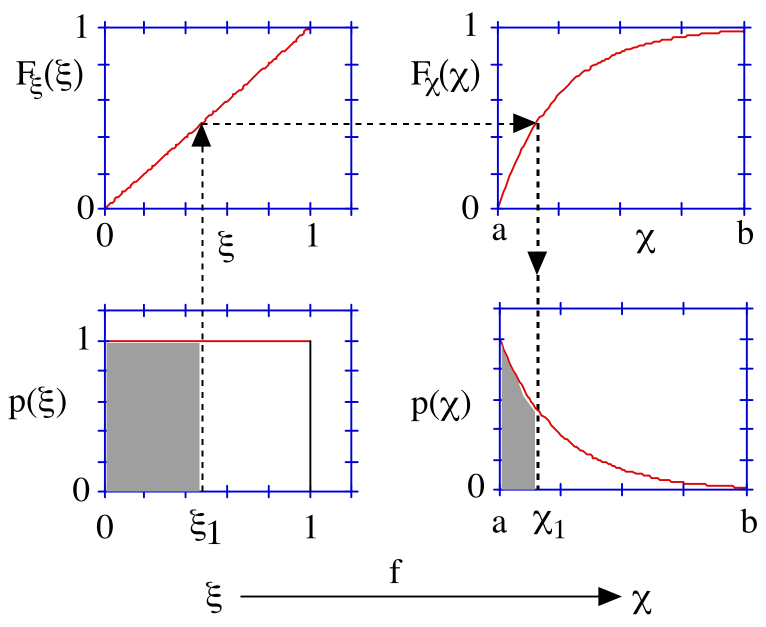

Fig. 2.1. Sampling a random variable χ based on a uniformly distributed random variable ξ.

For example, consider the sampling of the step size for photon movement, s, which is to be discussed fully in Section 3.2. The probability density function is given:

$$p(s) = \mu_t \exp(-\mu_t s) \tag{2.7}$$

where interaction coefficient μ_t equals $\mu_a + \mu_s$. Using this function in Eq. 2.5 yields an expression for a sampled value, s_1, based on the random number ξ:

$$\xi = \int_0^{s_1} p(s)\,ds = \int_0^{s_1} \mu_t \exp(-\mu_t s)\,ds = 1 - \exp(\mu_t s_1) \tag{2.8}$$

Solving for the value s_1:

$$s_1 = \frac{-\ln(1-\xi)}{\mu_t} \tag{2.9a}$$

As was explained in Eq. 2.6, the above expression is equivalent to:

$$s_1 = \frac{-\ln(\xi)}{\mu_t} \tag{2.9b}$$

3. Rules for Photon Propagation

This chapter presents the rules that define photon propagation in the Monte Carlo model as applied to tissues. The treatment is based upon Prahl *et al.* (1989) except that we deal with a multi-layered tissue instead of a semi-infinite tissue.

3.1 Launching a photon packet

A simple variance reduction technique, implicit photon capture, is used to improve the efficiency of the Monte Carlo simulation. This technique allows one to equivalently propagate many photons as a packet along a particular pathway simultaneously. Each photon packet is initially assigned a weight, W, equal to unity. The photon is injected orthogonally into the tissue at the origin, which corresponds to a collimated arbitrarily narrow beam of photons.

The current position of the photon is specified by the Cartesian coordinates (x, y, z). The current photon direction is specified by a unit vector, **r**, which can be equivalently described by the directional cosines (μ_x, μ_y, μ_z):

$$\begin{aligned}\mu_x &= \mathbf{r} \bullet \mathbf{x}\\ \mu_y &= \mathbf{r} \bullet \mathbf{y}\\ \mu_z &= \mathbf{r} \bullet \mathbf{z}\end{aligned} \tag{3.1}$$

where **x**, **y**, and **z** are unit vectors along each axis. The photon position is initialized to (0, 0, 0,) and the directional cosines are set to (0, 0, 1). This description of photon position and direction in a Cartesian coordinate system (Witt, 1977) turned out to be simpler than the counterpart in a cylindrical coordinate system (Keijzer *et al.*, 1989).

When the photon is launched, if there is a mismatched boundary at the tissue surface, then some specular reflectance will occur. If the refractive indices of the outside medium and tissue are n_1 and n_2, respectively, then the specular reflectance, R_{sp}, is specified (Born *et al.,* 1986; Hecht, 1987):

$$R_{sp} = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} \tag{3.2a}$$

If the first layer is glass, which is on top of a layer of medium whose refractive index is n_3, multiple reflections and transmissions on the two boundaries of the glass layer are considered. The specular reflectance is then computed by:

$$R_{sp} = r_1 + \frac{(1-r_1)^2 \, r_2}{1-r_1 \, r_2} \tag{3.2b}$$

where r_1 and r_2 are the Fresnel reflectances on the two boundaries of the glass layer:

$$r_1 = \frac{(n_1 - n_2)^2}{(n_1 + n_2)^2} \tag{3.3}$$

$$r_2 = \frac{(n_3 - n_2)^2}{(n_3 + n_2)^2} \tag{3.4}$$

Note that if the specular reflectance is defined as the probability of photons being reflected without interactions with the tissue, then Eqs. 3.2a and 3.2b are not strictly correct although they may be very good estimates of the real specular reflectance for thick tissues. If we want to strictly distinguish the specular reflectance and the diffuse reflectance, we can keep track of the number of interactions experienced by a photon packet. When we score the reflectance, if the number of interactions is not zero, the reflectance is diffuse reflectance. Otherwise, it is specular reflectance. The transmittances can be distinguished similarly.

The photon weight is decremented by R_{sp}, and the specular reflectance R_{sp} will be reported to the file of output data.

$$W = 1 - R_{sp} \tag{3.5}$$

3.2 Photon's step size

The step size of the photon packet is calculated based on a sampling of the probability distribution for photon's free path $s \in [0, \infty)$, which means $0 \le s < \infty$. According to the definition of interaction coefficient μ_t, the probability of interaction per unit pathlength in the interval (s', s' + ds') is:

$$\mu_t = \frac{-\,dP\{s \ge s'\}}{P\{s \ge s'\}\, ds'} \tag{3.6a}$$

or

$$d(\ln(P\{s \geq s'\})) = -\mu_t \, ds' \qquad (3.6b)$$

The above Eq. 3.6b can be integrated over s' in the range (0, s_1), and lead to an exponential distribution, where $P\{s \geq 0\} = 1$ is used:

$$P\{s \geq s_1\} = \exp(-\mu_t s_1) \qquad (3.7)$$

Eq. 3.7 can be rearranged to yield the cumulative distribution function of free path s:

$$P\{s < s_1\} = 1 - \exp(-\mu_t s_1) \qquad (3.8)$$

This cumulative distribution function can be assigned to the uniformly distributed random number ξ as discussed in Chapter 2. The equation can be rearranged to provide a means of choosing step size:

$$s_1 = \frac{-\ln(1-\xi)}{\mu_t} \qquad (3.9a)$$

or substituting ξ for $(1-\xi)$:

$$s_1 = \frac{-\ln(\xi)}{\mu_t} \qquad (3.9b)$$

Eq. 3.9b gives a mean free path between photon-tissue interaction sites of $1/\mu_t$ because the statistical average of $-\ln(\xi)$ is 1, i.e., $\langle -\ln(\xi) \rangle = 1$. There is another approach to obtain Eq. 3.9b. Employing Eq. 3.8, the probability density function of free path s is:

$$p(s_1) = dP\{s < s_1\}/ds_1 = \mu_t \exp(-\mu_t s_1) \qquad (3.10)$$

$p(s_1)$ can be substituted into Eq. 2.5 to yield Eq. 3.9b, where the integration in Eq. 2.5 will be recovered to Eq. 3.8.

In multi-layered turbid media, the photon packet may experience free flights over multiple layers of media before an interaction occurs. In this case, the counterpart of Eq. 3.7 becomes:

$$P\{s \geq s_{sum}\} = \exp(-\sum_i \mu_{ti} s_i) \qquad (3.11)$$

where i is an index to a layer, the symbols μ_{ti} is the interaction coefficient for the ith layer, and s_i is the step size in the ith layer. The total step size s_{sum} is:

$$s_{sum} = \sum_i s_i \tag{3.12}$$

The summation is over all the layers in which the photon packet has traveled. Eq. 3.11 does not take photon reflection and transmission at boundaries into account because they are processed separately. The sampling equation is obtained by equating Eq. 3.11 to ξ:

$$\sum_i \mu_{ti} s_i = -\ln(\xi) \tag{3.13}$$

As you may have seen, Eq. 3.9b is just a special case of Eq. 3.13. The sampling can be interpreted as that the total dimensionless step size is –ln(ξ), where dimensionless step size is defined as the product of the dimensional step size s_i and the interaction coefficient μ_{ti}. Since the absorption coefficient and the scattering coefficient of a glass layer are zeros, it does not contribute to the left hand side of Eq. 3.13. The detailed process of Eq. 3.13 will be discussed in Section 3.6 and 3.7. Although Eq. 3.13 looks complicated, it is the theoretical ground for the process in Section 3.6 and 3.7 which looks simpler.

From now on, we will use step size s instead of s_1 or s_{sum} for simplicity. Note that this sampling method involves computation of a logarithm function, which is time-consuming. This is reflected in Section 5.7. Faster methods can be used to avoid the logarithmic computation (Ahrens *et al.*, 1972; Marsaglia, 1961; MacLaren *et al.*, 1964).

3.3 Moving the photon packet

Once the step size s is specified, the photon is ready to be moved in the tissue. The position of the photon packet is updated by:

$$\begin{aligned} x &\leftarrow x + \mu_x s \\ y &\leftarrow y + \mu_y s \\ z &\leftarrow z + \mu_z s \end{aligned} \tag{3.14}$$

The arrows indicate quantity substitutions. The variables on the left hand side have the new values, and the variables on the right hand side have the old values. In an actual program in C, an equal sign is used for this purpose. The simplicity of Eqs. 3.14 is a major reason for using Cartesian coordinates.

3.4 Photon absorption

Once the photon has taken a step, some attenuation of the photon weight due to absorption by the interaction site must be calculated. A fraction of the photon's current weight, W, will be deposited in the local grid element. The amount of deposited photon weight, ΔW, is calculated:

$$\Delta W = W \frac{\mu_a}{\mu_t} \tag{3.15}$$

The total accumulated photon weight A(r, z) deposited in that local grid element is updated by adding ΔW:

$$A(r, z) \leftarrow A(r, z) + \Delta W \tag{3.16}$$

The photon weight has to be updated as well by:

$$W \leftarrow W - \Delta W \tag{3.17}$$

The photon packet with the new weight W will suffer scattering at the interaction site (discussed later). Note that the whole photon packet experiences interaction at the end of the step, either absorption or scattering.

3.5 Photon scattering

Once the photon packet has been moved, and its weight decremented, the photon packet is ready to be scattered. There will be a deflection angle, $\theta \in [0, \pi)$, and an azimuthal angle, $\psi \in [0, 2\pi)$ to be sampled statistically. The probability distribution for the cosine of the deflection angle, cosθ, is described by the scattering function 1) that Henyey and Greenstein (1941) originally proposed for galactic scattering:

$$p(\cos\theta) = \frac{1 - g^2}{2\,(1 + g^2 - 2g\cos\theta)^{3/2}} \tag{3.18}$$

1) Note that the scattering function we defined here is a probability density function of cosθ. It has a difference of a constant 1/2 with the phase function defined by van de Hulst (1980).

where the anisotropy, g, equals <cosθ> and has a value between –1 and 1. A value of 0 indicates isotropic scattering and a value near 1 indicates very forward directed scattering. Jacques *et al*. (1987) determined experimentally that the Henyey-Greenstein function described single scattering in tissue very well. Values of g range between 0.3 and 0.98 for tissues, but quite often g is ~0.9 in the visible spectrum. Applying Eq. 2.5, the choice for cosθ can be expressed as a function of the random number, ξ:

$$\cos\theta = \begin{cases} \frac{1}{2g}\left\{1 + g^2 - \left[\frac{1 - g^2}{1 - g + 2g\,\xi}\right]^2\right\} & \text{if } g > 0 \\ 2\,\xi - 1 & \text{if } g = 0 \end{cases} \tag{3.19}$$

Next, the azimuthal angle, ψ, which is uniformly distributed over the interval 0 to 2π, is sampled:

$$\psi = 2\pi\,\xi \tag{3.20}$$

Once the deflection angle and azimuthal angle are chosen, the new direction of the photon packet can be calculated:

$$\begin{aligned} \mu'_x &= \frac{\sin\theta}{\sqrt{1-\mu_z^2}}\,(\mu_x\,\mu_z\cos\psi - \mu_y\sin\psi) + \mu_x\cos\theta \\ \mu'_y &= \frac{\sin\theta}{\sqrt{1-\mu_z^2}}\,(\mu_y\,\mu_z\cos\psi + \mu_x\sin\psi) + \mu_y\cos\theta \\ \mu'_z &= -\sin\theta\cos\psi\sqrt{1-\mu_z^2} + \mu_z\cos\theta \end{aligned} \tag{3.21}$$

If the angle of the photon packet is too close to normal of the tissue surfaces(e.g., $|\mu_z| > 0.99999$), then the following formulas should be used:

$$\begin{aligned} \mu'_x &= \sin\theta\cos\psi \\ \mu'_y &= \sin\theta\sin\psi \\ \mu'_z &= \mathrm{SIGN}(\mu_z)\cos\theta \end{aligned} \tag{3.22}$$

where SIGN(μ_z) returns 1 when μ_z is positive, and it returns –1 when μ_z is negative. Finally, the current photon direction is updated: $\mu_x = \mu'_x, \mu_y = \mu'_y, \mu_z = \mu'_z$.

In the sampling of the two angles θ and ψ and the updating of the directional cosines, trigonometric operations are involved. Because trigonometric operations are computation-intensive, we should try to avoid them whenever possible. The detailed process of the sampling can be found in the function `spin()` written in the file "mcmlgo.c" (See Appendix A and Appendix B.4).

3.6 Reflection or transmission at boundary

During a step, the photon packet may hit a boundary of the tissue, which is between the tissue and the ambient medium, where the step size s is computed by Eq. 3.9b. For example, the photon packet may attempt to escape the tissue at the air/tissue interface. If this is the case, then the photon packet may either escape as observed reflectance (or transmittance if a rear boundary is also included) or be internally reflected by the boundary. There are different methods of dealing with this problem when the step size is large enough to hit the boundary. Let us present one of the two approaches used in the program mcml first.

First, a foreshortened step size s_1 is computed:

$$s_1 = \begin{cases} (z - z_0)/\mu_z & \text{if } \mu_z < 0 \\ (z - z_1)/\mu_z & \text{if } \mu_z > 0 \end{cases} \tag{3.23}$$

where z_0 and z_1 are the z coordinates of the upper and lower boundaries of the current layer (See Fig. 1.1 for the Cartesian coordinate system). The foreshortened step size s_1 is the distance between the current photon location and the boundary in the direction of the photon propagation. Since the photon direction is parallel with the boundary when μ_z is zero, the photon will not hit the boundary. Therefore, Eq. 3.23 does not include the case when μ_z is zero. We move the photon packet s_1 to the boundary with a flight free of interactions with the tissue (see Section 3.3 for moving photon packet). The remaining step size to be taken in the next step is updated to $s \leftarrow s - s_1$. The photon packet will travel the remaining step size if being internally reflected.

Second, we compute the probability of a photon packet being internally reflected, which depends on the angle of incidence, α_i, onto the boundary, where $\alpha_i = 0$ means orthogonal incidence. The value of α_i is calculated:

$$\alpha_i = \cos^{-1}(|\mu_z|) \tag{3.24}$$

Snell's law indicates the relationship between the angle of incidence, α_i, the angle of transmission, α_t, and the refractive indices of the media that the photon is incident from, n_i, and transmitted to, n_t:

$$n_i \sin\alpha_i = n_t \sin\alpha_t \tag{3.25}$$

The internal reflectance, $R(\alpha_i)$, is calculated by Fresnel's formulas (Born *et al.,* 1986; Hecht, 1987):

$$R(\alpha_i) = \frac{1}{2}\left[\frac{\sin^2(a_i - a_t)}{\sin^2(a_i + a_t)} + \frac{\tan^2(a_i - a_t)}{\tan^2(a_i + a_t)}\right] \tag{3.26}$$

which is an average of the reflectances for the two orthogonal polarization directions.

Third, we determine whether the photon is internally reflected by generating a random number, ξ, and comparing the random number with the internal reflectance, i.e.:

$$\begin{aligned} &\text{If } \xi \le R(\alpha_i)\text{, then photon is internally reflected;} \\ &\text{If } \xi > R(\alpha_i)\text{, then photon escapes the tissue} \end{aligned} \tag{3.27}$$

If the photon is internally reflected, then the photon packet stays on the surface and its directional cosines (μ_x, μ_y, μ_z) must be updated by reversing the z component:

$$(\mu_x, \mu_y, \mu_z) \leftarrow (\mu_x, \mu_y, -\mu_z) \tag{3.28}$$

At this point, the remaining step size has to been checked again. If it is large enough to hit the other boundary, we should repeat the above process. If it hits a tissue/tissue interface, we will have to process it according to the following section. Otherwise, if the step size is small enough to fit in this layer of tissue, the photon packet will move with the small step size. At the end of this small step, the absorption and scattering are processed correspondingly.

On the other hand, if the photon packet escapes the tissue, the reflectance or transmittance at the particular grid element (r, α_t) must be incremented. The reflectance, $R_d(r, \alpha_t)$, or transmittance, $T_t(r, \alpha_t)$, is updated by the amount of escaped photon weight, W:

$$\begin{aligned} R_d(r, \alpha_t) &\leftarrow R_d(r, \alpha_t) + W \quad \text{if } z = 0 \\ T_t(r, \alpha_t) &\leftarrow T_t(r, \alpha_t) + W \quad \text{if } z = \text{the bottom of the tissue.} \end{aligned} \tag{3.29}$$

Since the photon has completely escaped, the tracing of this photon packet ends here. A new photon may be launched into the tissue and traced thereafter. Note that in our simulation, both unscattered transmittance, if any, and diffuse transmittance are scored into $T_t(r, \alpha_t)$ without distinction although they could be distinguished as we discussed in Section 3.1.

An alternative approach toward modeling internal reflectance deserves mention. Rather than making the internal reflection of the photon packet an all-or-none event, a partial reflection approach can be used each time a photon packet strikes the surface boundary. A fraction $1 - R(\alpha_i)$ of the current photon weight successfully escapes the tissue, and increments the local reflectance or transmittance array, e.g., $R_d(r, \alpha_t) \leftarrow R_d(r, \alpha_t) + W (1-R(\alpha_i))$. All the rest of the photon weight will be reflected, and the photon weight is updated as $W \leftarrow W R(\alpha_i)$.

Both approaches are available in the program mcml, and the users have the option to use either approach depending on the physical quantities that they want to score. A flag in the program can be changed to switch between these two approaches (see Section 5.2). The all-or-none approach is faster, but the partial reflection approach should be able to reduce the variance of the reflectance or transmittance. It is uninvestigated how much variance can be reduced by using the partial reflection approach.

Similar to Section 3.5, the number of trigonometric operations in Eqs. 3.24-3.26 should be minimized for the sake of computation speed. The detailed process of these computations can be found in the function `RFresnel()` written in the file "mcmlgo.c" (See Appendix A and Appendix B.4).

3.7 Reflection or transmission at interface

If a photon step size is large enough to hit a tissue/tissue interface, this step may cross several layers of tissue. Consider a photon packet that attempts to make a step of size s within tissue 1 with μ_{a1}, μ_{s1}, n_1, but hits an interface with tissue 2 with μ_{a2}, μ_{s2}, n_2 after a foreshortened step s_1. Similar to the discussion in the last section, the photon packet is first moved to the interface without interactions, and the remaining photon step size to be taken in the next step is updated to $s \leftarrow s - s_1$. Then, we have to determine statistically whether the photon packet should be reflected or transmitted according to the Fresnel's formulas. If the photon packet is reflected, it is processed the same way as in the last section. However, if the photon packet is transmitted to the next layer of tissue, it has to continue propagation instead of being terminated. Based on Eq. 3.13, the remaining step size has to be converted for the new tissue according to its optical properties:

$$s \leftarrow \frac{s\,\mu_{t1}}{\mu_{t2}} \tag{3.30}$$

where μ_{t1} and μ_{t2} are the interaction coefficients for tissue 1 and tissue 2 correspondingly. The current step size s is again checked for another boundary or interface crossing. The above process is repeated until the step size is small enough to fit in one layer of tissue. At the end of this small step, the absorption and scattering are processed correspondingly.

If the photon packet is in a layer of glass, the photons are moved to the boundary of the glass layer without updating the remaining photon step size because the path length in the glass layer does not contribute to the left hand side of Eq. 3.13. It is important to understand that if a photon packet traverses several layers of tissues, the use of Eq. 3.9b for the step size and the repetitive uses of Eq. 3.30 are based on Eq. 3.13.

3.8 Photon termination

After a photon packet is launched, it can be terminated naturally by reflection or transmission out of the tissue. For a photon packet that is still propagating inside the tissue, if the photon weight, W, has been sufficiently decremented after many steps of interaction such that it falls below a threshold value (e.g., Wth = 0.0001), then further propagation of the photon yields little information unless you are interested in the very late stage of the photon propagation. However, proper termination must be executed to ensure conservation of energy (or number of photons) without skewing the distribution of photon deposition. A technique called roulette is used to terminate the photon packet when W ≤ Wth. The roulette technique gives the photon packet one chance in m (e.g., m = 10) of surviving with a weight of mW. If the photon packet does not survive the roulette, the photon weight is reduced to zero and the photon is terminated.

$$W = \begin{cases} mW & \text{if } \xi \le 1/m \\ 0 & \text{if } \xi > 1/m \end{cases} \tag{3.31}$$

where ξ is the uniformly distributed pseudo-random number (see Chapter 2). This method conserves energy yet terminates photons in an unbiased manner. The combination of photon roulette and splitting that is contrary to roulette, may be properly used to reduce variance (Hendricks *et al*., 1985).

4. Scored Physical Quantities

As we mentioned earlier, we record the photon reflectance, transmittance, and absorption during the Monte Carlo simulation. In this chapter, we will discuss the process of these physical quantities in detail. The dimensions of some of the quantities are shown in square brackets at the end of their formulas.

The last cells in z and r directions require special attention. Because photons can propagate beyond the grid system, when the photon weight is recorded into the diffuse reflectance or transmittance array, or absorption array, the physical location may not fit into the grid system. In this case, the last cell in the direction of the overflow is used to collect the photon weight. Therefore, the last cell in the z and r directions do not give the real value at the corresponding locations. However, the angle α is always within the bound we choose for it, i.e., $0 \leq \alpha \leq \pi/2$, hence does not cause a problem in the scoring of diffuse reflectance and transmittance.

4.1 Reflectance and transmittance

When a photon packet is launched, the specular reflectance is computed immediately. The photon weight after the specular reflection is transmitted into the tissue. During the simulation, some photon packets may exit the media and their weights are accordingly scored into the diffuse reflectance array or the transmittance array depending on where the photon packet exits. After tracing multiple photon packets (N), we have two scored arrays $R_d(r, \alpha)$ and $T_t(r, \alpha)$ for diffuse reflectance and transmittance respectively. They are internally represented by $R_{d-r\alpha}[i_r, i_\alpha]$ and $T_{t-r\alpha}[i_r, i_\alpha]$ respectively in the program. The coordinates of the center of a grid element are computed by:

$$r = (i_r + 0.5)\ \Delta r \quad [\mathrm{cm}] \tag{4.1}$$

$$\alpha = (i_\alpha + 0.5)\ \Delta\alpha \quad [\mathrm{rad}] \tag{4.2}$$

where i_r and i_α are the indices for r and α. The raw data give the total photon weight in each grid element in the two-dimensional grid system. To get the total photon weight in the grid elements in each direction of the two-dimensional grid system, we sum the 2D arrays in the other dimension:

$$R_{d\text{-}r}[i_r] = \sum_{i_\alpha=0}^{N_\alpha-1} R_{d\text{-}r\alpha}\ [i_r, i_\alpha] \tag{4.3}$$

$$R_{d\text{-}\alpha}[i_\alpha] = \sum_{i_r=0}^{N_r-1} R_{d\text{-}r\alpha}\ [i_r, i_\alpha] \tag{4.4}$$

$$T_{t\text{-}r}[i_r] = \sum_{i_\alpha=0}^{N_\alpha-1} T_{t\text{-}r\alpha}\ [i_r, i_\alpha] \tag{4.5}$$

$$T_{t\text{-}\alpha}[i_\alpha] = \sum_{i_r=0}^{N_r-1} T_{t\text{-}r\alpha}\ [i_r, i_\alpha] \tag{4.6}$$

To get the total diffuse reflectance and transmittance, we sum the 1D arrays again:

$$R_d = \sum_{i_r=0}^{N_r-1} R_{d\text{-}r}\ [i_r] \tag{4.7}$$

$$T_t = \sum_{i_r=0}^{N_r-1} T_{t\text{-}r}\ [i_r] \tag{4.8}$$

All these arrays give the total photon weight per grid element, based on N initial photon packets with weight unity. To convert $R_{d\text{-}r\alpha}[i_r, i_\alpha]$ and $T_{t\text{-}r\alpha}[i_r, i_\alpha]$ into photon probability per unit area perpendicular to the photon direction per solid angle, they are divided by the projection of the annular area onto a plane perpendicular to the photon exiting direction ($\Delta a \cos\alpha$), the solid angle ($\Delta\Omega$) spanned by a grid line separation in the α direction around an annular ring, and the total number of photon packets (N):

$$R_{d\text{-}r\alpha}[i_r, i_\alpha] \leftarrow R_{d\text{-}r\alpha}[i_r, i_\alpha] \,/\, (\Delta\alpha \cos\alpha\ \Delta\Omega\ N) \ \ [\text{cm}^{-2}\ \text{sr}^{-1}] \tag{4.9}$$

$$T_{t\text{-}r\alpha}[i_r, i_\alpha] \leftarrow T_{t\text{-}r\alpha}[i_r, i_\alpha] \,/\, (\Delta\alpha \cos\alpha\ \Delta\Omega\ N) \ \ [\text{cm}^{-2}\ \text{sr}^{-1}] \tag{4.10}$$

where

$$\Delta\alpha = 2\ \pi\ r\ \Delta r = 2\ \pi\ (i_r + 0.5)\ (\Delta r)^2\ \ [cm^2] \tag{4.11}$$

$$\Delta\Omega = 4\ \pi\ \sin\alpha\ \sin(\Delta\alpha/2) = 4\ \pi\ \sin[(i_\alpha + 0.5)\ \Delta\alpha]\ \sin(\Delta\alpha/2)\ \ [sr] \tag{4.12}$$

where r and α are computed from Eq. 4.1 and Eq. 4.2 respectively. The radially resolved diffuse reflectance $R_{d\text{-}r}[i_r]$ and total transmittance $T_{t\text{-}r}[i_r]$ are divided by the area of the annular ring (Δa) and the total number of photon packets (N) to convert them into photon probability per unit area:

$$R_{d\text{-}r}[i_r] \leftarrow R_{d\text{-}r}[i_r]\ /\ (\Delta\alpha\ N)\ [cm^{-2}] \tag{4.13}$$

$$T_{t\text{-}r}[i_r] \leftarrow T_{t\text{-}r}[i_r]\ /\ (\Delta\alpha\ N)\ [cm^{-2}] \tag{4.14}$$

The angularly resolved diffuse reflectance $R_{d\text{-}\alpha}[i_\alpha]$ and total transmittance $T_{t\text{-}\alpha}[i_\alpha]$ are divided by the solid angle ($\Delta\Omega$) and the total number of photon packets (N) to convert them into photon probability per unit solid angle:

$$R_{d\text{-}\alpha}[i_\alpha] \leftarrow R_{d\text{-}\alpha}[i_\alpha]\ /\ (\Delta\Omega\ N)\ \ [sr^{-1}] \tag{4.15}$$

$$T_{t\text{-}\alpha}[i_\alpha] \leftarrow T_{t\text{-}\alpha}[i_\alpha]\ /\ (\Delta\Omega\ N)\ \ [sr^{-1}] \tag{4.16}$$

The total diffuse reflectance and transmittance are divided by the total number of photon packets (N) to get the probabilities:

$$R_d \leftarrow R_d\ /\ N\ \ [-] \tag{4.17}$$

$$T_t \leftarrow T_t\ /\ N\ \ [-] \tag{4.18}$$

where [–] means dimensionless units.

4.2 Internal photon distribution

During the simulation, the absorbed photon weight is scored into the absorption array A(r, z). A(r, z) is internally represented by a 2D array $A_{rz}[i_r, i_z]$, where i_r and i_z are the indices for grid elements in r and z directions. The coordinates of the center of a grid element can be computed by Eq. 4.1 and the following:

$$z = (i_z + 0.5)\ \Delta z \tag{4.19}$$

The raw data $A_{rz}[i_r, i_z]$ give the total photon weight in each grid element in the two-dimensional grid system. To get the total photon weight in each grid element in the z direction, we sum the 2D array in the r direction:

$$A_z[i_z] = \sum_{i_r=0}^{N_r-1} A_{rz}\ [i_r, i_z] \tag{4.20}$$

The total photon weight absorbed in each layer $A_l[\text{layer}]$ and the total photon weight absorbed in the tissue A can be computed from $A_z[i_z]$:

$$A_l[\text{layer}] = \sum_{i_z \text{ in layer}} A_z\ [i_z] \tag{4.21}$$

$$A = \sum_{i_z=0}^{N_z-1} A_z\ [i_z] \tag{4.22}$$

where the summation range "i_z in layer" includes all i_z's that lead to a z coordinate in the layer. Then, these quantities are scaled properly to get the densities:

$$A_{rz}[i_r, i_z] \leftarrow A_{rz}[i_r, i_z] \,/\, (\Delta\alpha\ \Delta z\ N)\ \ [\text{cm}^{-3}] \tag{4.23}$$

$$A_z[i_z] \leftarrow A_z[i_z] \,/\, (\Delta z\ N)\ \ [\text{cm}^{-1}] \tag{4.24}$$

$$A_l[\text{layer}] \leftarrow A_l[\text{layer}] \,/\, N\ \ [-] \tag{4.25}$$

$$A \leftarrow A \,/\, N\ \ [-] \tag{4.26}$$

The quantity A gives the photon probability of absorption by the tissue. The 1D array $A_l[\text{layer}]$ gives the photon probability of absorption in each layer. At this point, $A_{rz}[i_r, i_z]$ gives the absorbed photon probability density (cm^{-3}), and can be converted into photon fluence, ϕ_{rz}, (cm^{-2}) by dividing it by the absorption coefficient μ_a (cm^{-1}) of the layer where the current location resides:

$$\phi_{rz}[i_r, i_z] = A_{rz}[i_r, i_z] / \mu_a \ \ [\text{cm}^{-2}] \tag{4.27}$$

The 1D array $A_z[i_z]$ gives the photon probability per unit length in the z direction (cm^{-1}). It can also be divided by the absorption coefficient μ_a (cm^{-1}) to yield a dimensionless quantity $\phi_z[i_z]$:

$$\phi_z[i_z] = A_z[i_z] / \mu_a \ \ [-] \tag{4.28}$$

This quantity may seem hard to understand or redundant at first glance. However, the summation of the raw data in Eq. 4.20 is equivalent to the convolution for an infinitely wide flat beam in Eq. 7.15 to be discussed in Chapter 7. The equivalence can be shown as follows. According to Eqs. 4.20, 4.23 and 4.24, the final converted $A_z[i_z]$ and $A_{rz}[i_r, i_z]$ have the following relation:

$$A_z[i_z] = \sum_{i_r=0}^{N_r-1} A_{rz} \ [i_r, i_z] \ \Delta\alpha(i_r) \tag{4.29}$$

where $\Delta a(i_r)$ is computed in Eq. 4.11, but we stress that it is a function of i_r in Eq. 4.29. Employing Eqs. 4.27 and 4.28, Eq. 4.29 can be converted to:

$$\phi_z[i_z] = \sum_{i_r=0}^{N_r-1} f_{rz} \ [i_r, i_z] \ \Delta\alpha(i_r) \tag{4.30}$$

This is a numerical solution of the following integral:

$$\phi_z(z) = \int_0^\infty f_{rz}(r, z) \ 2 \ \pi \ r \ dr \tag{4.31}$$

Eq. 4.31 is essentially Eq. 7.15 for an infinitely wide flat beam with a difference of constant S, where S is the power density of the infinitely wide flat beam. The equivalence between Eq. 4.31 and Eq. 7.15 can be seen after substituting $\phi_z(z)$ for F(r, z), $\phi_{rz}(r, z)$ for G(r'', z), and r for r''. Therefore, $\phi_z[i_z]$ gives the fluence for an infinitely wide flat beam with a difference of a constant which is the power density S.

The program mcml will only report $A_{rz}[i_r, i_z]$ and $A_z[i_z]$ instead of $\phi_{rz}[i_r, i_z]$ and $\phi_z[i_z]$. The program conv will be set up to convert $A_{rz}[i_r, i_z]$ and $A_z[i_z]$ into $\phi_{rz}[i_r, i_z]$ and $\phi_z[i_z]$.

4.3 Issues regarding grid system

In our Monte Carlo simulation, we always set up a grid system. The computation results will be limited by the finite grid size. This section will discuss what is the best that one can do.

Position of average value for each grid element

The simulation provides the average value of the scored physical quantities in each grid element. Now, the question is at what position should that averaged value be assigned? One can argue that there is no best point because the exact answer to the physical quantities is unknown. However, under linear approximations of the physical quantities in each grid element, we can find the best point for each grid point. The linear approximations can be justified for small grid size in most cases because the higher order terms are considerably less than the linear term. Some special occasions will be discussed subsequently.

Let us discuss the grid system in the r direction first because r is the variable over which the convolution for photon beams of finite size will be implemented (see Chapter 7). The grid system in the r direction uses Δr as the grid separation with a total of N grid elements. The index to each grid element is denoted by n. The center of each grid element is denoted by r_n:

$$r_n = (n + 0.5)\,\Delta r \qquad (4.32)$$

As we have mentioned, the Monte Carlo simulation actually approximates the average of the physical quantity Y(r) in each grid element, where Y(r) can be the diffuse reflectance, diffuse transmittance, and internal fluence $A_{rz}(r, z)$ for a particualr z value.

$$<Y(r)> = \frac{1}{2\,\pi\, r_n\, \Delta r} \int_{r_n - \Delta r/2}^{r_n + \Delta r/2} Y(r)\, 2\,\pi\, r\, dr \qquad (4.33)$$

where $2\,\pi\, r_n\, \Delta r$ is the area of the ring or the circle when n = 0.

If Y(r) in each grid element is approximated linearly, we can prove that there exists a best point r_b to satisfy:

$$<Y(r)> = Y(r_b) \tag{4.34}$$

where

$$r_b = r_n + \frac{\Delta r}{12\, r_n}\, \Delta r \tag{4.35}$$

Proof: Y(r) is approximated by a Taylor series about r_b expanded to the first order:

$$Y(r) = Y(r_b) + (r - r_b)\, Y'(r_b) \tag{4.36}$$

Substituting Eq. 4.36 into Eq. 4.33 yields:

$$<Y(r)> \;=\; \frac{1}{2\,\pi\, r_n\, \Delta r} \int_{r_n - \Delta r/2}^{r_n + \Delta r/2} [Y(r_b) + (r - r_b)\, Y'(r_b)]\; 2\,\pi\, r\, dr$$

$$= \frac{Y(r_b)}{2\,\pi\, r_n\, \Delta r} \int_{r_n - \Delta r/2}^{r_n + \Delta r/2} 2\,\pi\, r\, dr \;+\; \frac{Y'(r_b)}{2\,\pi\, r_n\, \Delta r} \int_{r_n - \Delta r/2}^{r_n + \Delta r/2} (r - r_b)\; 2\,\pi\, r\, dr$$

$$= \frac{Y(r_b)}{2\,\pi\, r_n\, \Delta r}\; [\pi\, r^2] \Bigg|_{r_n - \Delta r/2}^{r_n + \Delta r/2} + \frac{Y'(r_b)}{2\,\pi\, r_n\, \Delta r}\, (\pi/3)\;\; [2\, r^3 - 3\, r_b\, r^2] \Bigg|_{r_n - \Delta r/2}^{r_n + \Delta r/2}$$

$$= \frac{Y(r_b)}{2\,\pi\, r_n\, \Delta r}\; [2\,\pi\, r_n\, \Delta r] + \frac{Y'(r_b)}{2\,\pi\, r_n\, \Delta r}\, (\pi/3)\;\; [2\, \Delta r\, (3\, r_n^2 + \frac{(\Delta r)^2}{4} - 3\, r_b\, r_n)]$$

$$= Y(r_b) + Y'(r_b)\; [r_n + \frac{(\Delta r)^2}{12\, r_n} - r_b]$$

or

$$<Y(r)> = Y(r_b) + Y'(r_b)\; [r_n + \frac{(\Delta r)^2}{12\, r_n} - r_b] \tag{4.37}$$

If we set the term in the square bracket in Eq. 4.37 to zero, and solve for r_b, we obtain:

$$r_b = r_n + \frac{(\Delta r)^2}{12\, r_n} \qquad (4.38a)$$

and Eq. 4.37 becomes:

$$<Y(r)> = Y(r_b) \qquad (4.39)$$

Eq. 4.38a can be reformulated:

$$r_b = r_n + \frac{\Delta r}{12\, r_n}\ \Delta r \qquad (4.38b)$$

Q.E.D.

We can substitute Eq. 4.32 into the second term of Eq. 4.38b:

$$r_b = [(n + 0.5) + \frac{1}{12\,(n + 0.5)}\ ]\ \Delta r \qquad (4.38c)$$

When $n = 0$, $r_b = [0.5 + \frac{1}{6}\ ]\ \Delta r = \frac{2}{3}\ \Delta r$

When $n = 1$, $r_b = [1.5 + \frac{1}{18}\ ]\ \Delta r \approx 1.556\ \Delta r$

When $n = 2$, $r_b = [2.5 + \frac{1}{30}\ ]\ \Delta r \approx 2.533\ \Delta r$

When $n = 3$, $r_b = [3.5 + \frac{1}{42}\ ]\ \Delta r \approx 3.524\ \Delta r$

When $n = 4$, $r_b = [4.5 + \frac{1}{54}\ ]\ \Delta r \approx 4.519\ \Delta r$

...

It is observed that the best point deviates from the center of each grid element, and the smaller the index to the grid box, the larger the deviation. As the index n becomes large, the best point approaches the center of the grid element. This behavior is due to the $2\,\pi\, r$ factor in Eq. 4.33. A similar factor does not exist for the z direction, and the best points for the z direction should be the centers of each grid element.

The computation results of a Monte Carlo simulation with a selected grid system always have finite precision which is fundamentally limited by the finite grid size. The above theorem only gives the points where the function values are best represented by the simulated results.

<u>Effects of the first photon-tissue interaction</u>

The above theorem assumed differentiability of Y(r), where Y(r) can represent the diffuse reflectance $R_d(r)$, the diffuse transmittance $T_d(r)$, and the internal fluence $\phi_{rz}(r, z)$ at a particular z value. This assumption should hold for the diffuse reflectance and the diffuse transmittance. However, for the internal fluence, the on-z-axis fluence is a delta function for an impulse response (responses to an infinitely narrow photon beam). Therefore, you cannot assume the differentiability of the function $\phi_{rz}(r, z)$ at r equal zero, i.e., $\phi_{rz}(r=0, z)$. The best solution to this problem has been provided by Gardner *et al.* (1992b). They keep track of the first photon interactions with the medium, which are always on the z-axis, separately from the rest of the interactions. Therefore, the function $\phi_{rz}(r, z)$ will not include the first photon-tissue interaction which yield a delta function. This approach ensures a differentiable $\phi_{rz}(r, z)$ at r equal zero besides its better accuracy.

In the current version (version 1.0) of mcml, Gardner *et al.*'s approach is not yet implemented although we intend to add this in the later version. However, the result from mcml will still be correct within the spatial resolution of the grid size in the r direction. Although nobody will use Monte Carlo to simulate the responses in an absorption-only semi-infinite medium, let us use this simple example to illustrate what we mean. In this case, Gardner *et al.*'s approach will yield an exponentially decaying response on the z axis which is a delta function of r. The version 1.0 of mcml will yield the same exponentially decaying response in the first grid elements which is not a delta function because of the finite volume of the grid elements. However, as the grid separation Δr is made sufficiently small, the result approaches Gardner *et al.*'s.

So far the discussion has nothing to do with convolution for photon beams of finite size which will be discussed in Chapter 7. According to Gardner *et al.* (1992b), the error in the convolution caused by not scoring the first interactions separately will be small for Gaussian beams whose radius is at least three times larger than the grid separation Δr. As we will discuss in Section 7.4, our extended trapezoidal integration, instead of integrating over the original grid points, in the convolution program conv should further decrease the error. Of course, when the on-z-axis interactions are considered separately, our convolution program conv is not subject to this limitation on the radius of the Gaussian beam. In contrast, if the integration is approximated by computing the integrand over the original grid points, the radius of the photon beam should still be large enough to yield reasonable integration accuracy.

Since this theorem is a late development, it has not been implemented in the programs (mcml and conv) yet. We plan to implement it in the next release (see Appendix H).

5. Programming mcml

The simulation is written in ANSI Standard C (Plauger *et al*., 1989, Kelley *et al*., 1990), which makes it possible to execute the program on any computers that support ANSI Standard C. So far, the program has been successfully tested on Macintosh, IBM PC compatibles, Sun SPARCstation 2, IBM RISC/6000 POWERstation 320, and Silicon Graphics IRIS workstation. This chapter mainly describes several rules, the important constants and the data structures used in the program, the algorithm to trace photon packets, flow of the program, and the timing profile of the program. Prior knowledge of C is assumed to fully understand this chapter. The flow of the program is listed in detail in Appendix A. The complete source code is listed in Appendix B file by file. In Appendix C, we have provided a make file used by make utilities on UNIX machines. Appendix D and E are a template of input data file and a sample output data file respectively. Appendix F gives several C Shell scripts for UNIX users. The information needed to obtain the program is detailed in Appendix G.

5.1 Programming rules and conventions

When we write this program, we have followed the following rules and conventions:

1. Conform to ANSI Standard C so that the program can be executed on a variety of computers.

2. Avoid global variables whenever possible. This program has not defined any global variables so far.

3. Avoid hard limits on the program. For example, we removed the limits on the number of array elements by dynamic allocation at run time. This means that the program can accept any number of layers or gridlines as long as the memory permits.

4. Preprocessor names are all capital letters, e.g.,
   ```
   #define PREPROCESSORS
   ```

5. For global variables, function names, or data types, first letter of each word is capital, and words are connected without underscores, e.g.,

```
short GlobalVar;
```

6. For dummy variables, first letter of each word is capital, and words are connected by underscores, e.g.,

```
void NiceFunction(char Dummy_Var);
```

7. Local variables are all lower cases, and words are connected by underscores, e.g.,

```
short local_var;
```

5.2 Several constants

There are several important constants defined in the header file mcml.h or the source files mcmlmain.c and mcmlgo.c. They are listed in Table 5.1, and may be altered according to your special need.

The constant `STRLEN` is used in the program to define string length. `WEIGHT` is the threshold photon weight, below which the photon packet will go through a roulette. This photon packet with small weight W has a chance of `CHANCE` to survive with a new weight of W/`CHANCE`. `COSZERO` and `COS90D` are used for the computation of reflection with Fresnel's formulas, and for the computation of new photon directional cosines. When $|\cos\alpha| >$ `COSZERO`, α is considered very close to 0 or 180^o. When $|\cos\alpha| <$ `COS90D`, α is considered very close to 90^o.

When `THINKCPROFILER` is 1, the profiler of THINK C compiler (Symantec, 1991) on Macintosh can be used to monitor the timing profile of the program regarding each function (see Section 5.7). When `GNUCC` is 1, the code can be compiled with GNU C compiler (gcc) from the Free Software Foundation, which does not support several functions such as `difftime()` although being claimed to conform to ANSI C standards. Therefore, the timing modules in the program will not work when `GNUCC` is 1, although the program will otherwise operate normally. When `STANDARDTEST` is 1, the random number generator will generate a fixed sequence of random numbers after being fed a fixed seed. This feature is used to debug the program. `STANDARDTEST` should be set to 0 normally, which makes the random number generator use the current time as the seed. When `PARTIALREFLECTION` is set to 0, the all-or-none simulation mechanism of photon internal reflection at a boundary (e.g., air/tissue boundary) described in Section 3.6 is used, where the photon packet is either totally reflected or totally transmitted determined by the comparison of the Fresnel reflectance and a random number. Otherwise when `PARTIALREFLECTION` is set to 1, the photon packet will be partially reflected and transmitted. Normally we set `PARTIALREFLECTION` to 0 because the all-or-none simulation is faster.

Table 5.1. Important constants in the program mcml.

Constants	**File**	**Value**	**Meaning**
`WEIGHT`	mcml.h	1×10^{-4}	threshold weight
`CHANCE`	mcml.h	0.1	chance of surviving a roulette
`STRLEN`	mcml.h	256	string length
`COSZERO`	mcmlgo.c	$1 - 1 \times 10^{-12}$	cosine of ~ 0
`COS90D`	mcmlgo.c	1×10^{-6}	cosine of ~ 90^o
`THINKCPROFILER`	mcmlmain.c	1/0	switch for THINK C profiler on Macintosh
`GNUCC`	mcmlmain.c	1/0	switch for GNU C compiler
`STANDARDTEST`	mcmlgo.c	1/0	switch for fixed sequence of random numbers
`PARTIAL-REFLECTION`	mcmlgo.c	1/0	switch for partial internal reflection at boundary

5.3 Data structures and dynamic allocations

Data structures are an important part of the program. Related parameters are logically organized by structures such that the program is easier to write, read, maintain, and modify. The parameters for a photon packet are grouped into a single structure defined by:

```
typedef struct {
  double x, y, z;    /* Cartesian coordinates.[cm] */
  double ux, uy, uz;/* directional cosines of a photon. */
  double w;          /* weight. */
  Boolean dead;      /* 1 if photon is terminated. */
  short layer;       /* index to layer where the photon packet resides.*/
  double s;          /* current step size. [cm]. */
  double sleft;      /* step size left. dimensionless [-]. */
} PhotonStruct;
```

The location and the traveling direction of a photon packet are described by the Cartesian coordinates `x, y, z`, and the directional cosines (`ux, uy, uz`) respectively. The current weight of the photon packet is denoted by the structure member `w`. The member `dead`, initialized to be 0 when the photon packet is launched, represents the status of a photon packet. If the photon packet has exited the tissue or it has not survived a roulette when its weight is below the threshold weight, then the member `dead` is set to 1. It is used to signal the program to stop tracing the current photon packet. Note that the type `Boolean` is not an internal data type in ANSI Standard C. It is defined to be type char in our header file mcml.h. The member `layer` is the index to the layer where the photon packet resides. Type `short`, whose value ranges between –32768 (2^{15}) and +32768 (Plauger *et al.*, 1989), is used for the member `layer`. It is defined for computation efficiency although the layer can always be identified according to the Cartesian coordinates of the photon packet and the geometric structure of the media. The member `layer` is updated only when the photon packet crosses tissue/tissue interfaces. The member `s` is the step size in cm for the current step. The member `sleft` is used to store the unfinished step size in dimensionless units when a step size is large enough to hit a boundary or interface. For example, if a selected step size s is long enough to hit a boundary of the current layer with interaction coefficient μ_t as explained in Section 3.6, a foreshortened step size s_1 is chosen as the current step size, and the unfinished step size has to be stored. In the program, the following assignments are implemented: the member `s` = s_1 and the member `sleft` = $(s - s_1)\ \mu_t$. Note that we store the unfinished step size in dimensionless unit, therefore, we only need to know the interaction coefficient of the current layer to convert the step size back in cm when the photon packet crosses layers.

The parameters that are needed to describe a layer of tissue are grouped into one structure:

```
typedef struct {
  double z0, z1;     /* z coordinates of a layer. [cm] */
  double n;          /* refractive index of a layer. */
  double mua;        /* absorption coefficient. [1/cm] */
  double mus;        /* scattering coefficient. [1/cm] */
  double g;          /* anisotropy. */

  double cos_crit0, cos_crit1;
} LayerStruct;
```

The Cartesian coordinates of the top and bottom boundaries are denoted by `z0` and `z1` respectively. The refractive index, absorption coefficient, scattering coefficient, and anisotropy factor of a layer of medium are represented by the members `n`, `mua`, `mus`, and `g` respectively. The cosines of the critical angles are denoted by the members `cos_crit0` and `cos_crit1` respectively. They are computed with the relative refractive index of this layer with respect to the two neighbor layers.

All the input parameters are defined in the following structure. Most of the members of the structure are provided by the user before the simulation.

```
typedef struct {
  char   out_fname[STRLEN]; /* output filename. */
  char   out_fformat;       /* output file format. */
                            /* 'A' for ASCII, */
                            /* 'B' for binary. */
  long   num_photons;       /* to be traced. */
  double Wth;               /* play roulette if photon */
                            /* weight < Wth.*/

  double dz;                /* z grid separation.[cm] */
  double dr;                /* r grid separation.[cm] */
  double da;                /* alpha grid separation. */
                            /* [radian] */
  short nz;                 /* array range 0..nz-1. */
  short nr;                 /* array range 0..nr-1. */
  short na;                 /* array range 0..na-1. */

  short num_layers;         /* number of layers. */
  LayerStruct * layerspecs; /* layer parameters. */
} InputStruct;
```

The filename for data output is `out_fname`, and its format (`out_fformat`) can be A for ASCII or B for binary. Currently, only ASCII format is supported. The number of photon packets to be simulated is denoted by the member `num_photons`. Since larger number of photon packets may be simulated, type `long int`, whose value ranges between –2,147,483,648 (2^{31}) and +2,147,483,648 (Plauger *et al*, 1989), is used for the member `num_photons`. The threshold weight is denoted by the member `Wth`. The photon packet with weight less than `Wth` will experience a roulette. The grid line separations Δz, Δr, and $\Delta\alpha$ are represented by members `dz`, `dr`, and `da` respectively. The numbers of grid elements N_z, N_r, and N_α are represented by `nz`, `nr`, and `na` respectively. The total number of layers is represented by the member `num_layers`. The member `layerspecs` is a pointer to the structure `LayerStruct`. This pointer can be dynamically allocated with an array of structures, in which each structure represents a layer, or the top ambient medium, or the bottom ambient medium (e.g., air). Therefore, there are (`num_photons` + 2) elements in the array, where the element 0 and element (`num_photons` + 1) store the refractive indices for the top ambient medium and bottom ambient medium respectively. The dynamic allocation will be discussed subsequently.

All the output data are organized into one structure too:

```
typedef struct {
  double    Rsp;    /* specular reflectance. [-] */
  double ** Rd_ra;  /* 2D distribution of diffuse */
                    /* reflectance. [1/(cm2 sr)] */
  double *  Rd_r;   /* 1D radial distribution of diffuse */
                    /* reflectance. [1/cm2] */
  double *  Rd_a;   /* 1D angular distribution of diffuse */
                    /* reflectance. [1/sr] */
  double    Rd;     /* total diffuse reflectance. [-] */

  double ** A_rz;   /* 2D probability density in turbid */
                    /* media over r & z. [1/cm3] */
  double *  A_z;    /* 1D probability density over z. */
                    /* [1/cm] */
  double *  A_l;     /* each layer's absorption */
                     /* probability. [-] */
  double    A;       /* total absorption probability. [-] */

  double ** Tt_ra;   /* 2D distribution of total */
                     /* transmittance. [1/(cm2 sr)] */
  double *  Tt_r;    /* 1D radial distribution of */
                     /* transmittance. [1/cm2] */
  double *  Tt_a;    /* 1D angular distribution of */
                     /* transmittance. [1/sr] */
  double    Tt;      /* total transmittance. [-] */
} OutStruct;
```

The member `Rsp` is the specular reflectance. The pointer `Rd_ra` will be allocated dynamically, and used equivalently as if it is a 2D array over r and α. `Rd_ra` is the internal representation of diffuse reflectance $R_d(r, \alpha)$ discussed in Section 4.1. The members `Rd_r` and `Rd_a` are the 1D diffuse reflectance distributions over r and α respectively. The member `Rd` is the total diffuse reflectance R_d. The member `A_rz` is the representation of the 2D internal photon distribution A(r, z) (see Section 4.2). The members `A_z` and `A_l` are the corresponding 1D internal photon distributions with respect to z and layers respectively. The member `A` is the probability of photon absorption by the whole tissue. The members for transmittance are analogous to these for reflectance except that there is no distinction between unscattered transmittance and diffuse transmittance. All the transmitted photon weight is scored into the arrays.

In the above defined structures, pointers are used to denote the 2D or 1D arrays. These pointers are dynamically allocated at run time according to user's specifications. Therefore, the user can use different numbers of layers or numbers of grid elements without changing the source code of the program. This provides the flexibility of the program and the efficiency of memory utilization. The dynamic allocation procedures are modified from Press (1988). Only 1D array allocation will be presented here, and the matrix allocation can be found in Appendix B.5 -- "mcmlnr.c".

```
double *AllocVector(short nl, short nh)
{
  double *v;
  short i;

  v=(double *)malloc((unsigned) (nh-nl+1)*sizeof(double));
  if (!v) nrerror("allocation failure in vector()");

  v -= nl;
  for(i=nl;i<=nh;i++) v[i] = 0.0;   /* init. */
  return v;
}
```

This function returns a pointer, which points to an array of elements. Each element is a double precision floating point number. The index range of the array is from nl to nh inclusive. In our simulation, nl is always 0, which is the default value in C. This function also initializes all the elements equal to zero.

5.4 Flowchart of photon tracing

Fig. 5.1 indicates the basic flowchart for the photon tracing part of the Monte Carlo calculation as described in Chapter 3. Many boxes in the flowchart are direct implementations of the discussions in Chapter 3. This chart also includes the situation where the photon packet is in a glass, in which absorption and scattering do not exist. In this case, the photon packet will be moved to the boundary of the glass layer in the current photon direction. Then, we have to determine statistically whether the photon packet will cross the boundary or be reflected according to the Fresnel's formulas.

The box "Launch photon" initializes the photon packet position, direction, weight, and several other structure members including ds and dsleft in PhotonStruct. The flow control box "Photon in glass?" determines whether the current layer is a glass layer or tissue layer.

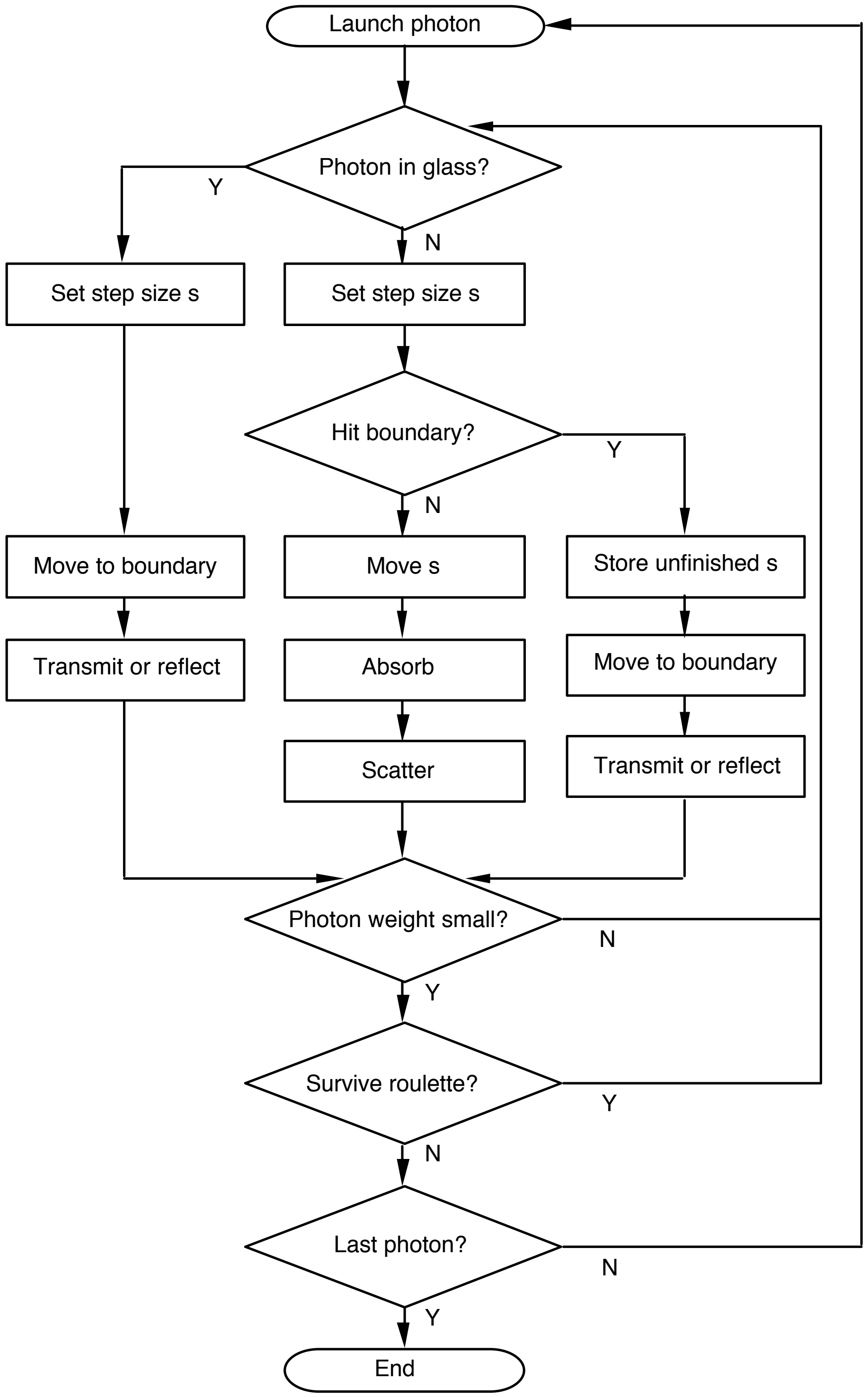

Fig. 5.1. Flowchart for Monte Carlo simulation of multi-layered tissue.

When the photon packet is in glass layers, which have no absorption or scattering, the box "Set step size s" chooses the distance between the current photon position and the boundary in the direction of the photon movement as the step size. The box "Move to boundary" updates the position of the photon packet. Now, as the photon packet is on the boundary, two approaches of processing photon transmission and reflection are supported in the box "Transmit or reflect" as discussed in Section 3.6. If the constant `PARTIALREFLECTION` is zero, the box determines whether the photon packet should cross the boundary or be reflected according to the Fresnel reflectance in an all-or-none fashion. If the photon packet is reflected, the propagation direction should be updated. Otherwise, if the photon packet crosses the interface into another layer of tissue, the propagation direction and the index to the layer are updated. If the photon packet crosses the boundary and moves out of the medium, the photon packet is terminated and the photon weight is scored into the array for reflectance or transmittance depending on where the photon packet exits. If the constant `PARTIALREFLECTION` is one, the box "Transmit or reflect" deals with ambient medium/tissue interface differently. Part of the photon weight is transmitted to the ambient medium as reflectance or transmittance, and the rest of the weight will be reflected and continue propagation. Normally we set `PARTIALREFLECTION` to 0 because the all-or-none simulation is faster (see Section 3.6).

In tissue layers, the box "Set step size s" sets the step size to the unfinished step size according to the structure member `sleft` if `sleft` is not zero. Otherwise, it sets the step size according to the interaction coefficient of the medium. With the chosen step size s, the box "Hit boundary?" identifies whether the step size is long enough to hit the boundary of the current layer.

If the step does not hit the boundary, then the box "Move s" will update the position of the photon packet. Then, the box "Absorb" will deposit a portion of the photon packet weight in the local grid element, and the box "Scatter" will determine the new traveling direction for the rest of the photon packet after absorption.

If the step hits the boundary, then the step size s is foreshortened. The foreshortened step size is the distance between the photon position and the boundary in the direction of the photon movement, and the unfinished step size is stored by the box "Store unfinished s". The stored unfinished step size in dimensionless units will be used by the box "Set step size s" for tissue layers to generate the next step size. The next two boxes "Move to boundary" and "Transmit or reflect" function the same as for the glass layer.

At this point, the photon weight and the structure member `dead` are checked in the box "Photon weight small?". If the photon packet is dead, it will jump to the box "Last photon?" (transition not shown in the flowchart). If the photon packet is still alive and its weight exceeds `Wth`, it will start the next step of propagation. If the photon packet is still alive and its weight is lower than `Wth`, it has to experience a roulette in the box "Survive roulette?". If the photon packet survives the roulette, it will start the next step of propagation. Otherwise, the photon packet is terminated and the box "Last photon?" determines whether to end the simulation or to start tracing a new photon packet.

5.5 Flow of the program mcml

A flow graph of the mcml source code has been generated using the UNIX command cflow under SunOS. Each line of output begins with a reference number, i.e., a line number, followed by a suitable number of tabs indicating the level, then the name of the global (normally only a function not defined as an external or beginning with an underscore), a colon, and its definition. The definition consists of an abstract type declaration (for example, char *), and delimited by angle brackets, the name of the source file and the line number where the definition was found.

Once a definition of a name has been printed, subsequent references to that name contain only the reference number of the line where the definition may be found. For undefined references, only <> is printed.

The list in Fig. 5.2 is generated by command: `cflow -d2 mcml*.c`. The option "-d2" limits the nesting depth to 2. The command output with all the nesting levels is shown in Appendix A.

```
1   main: char(), <mcmlmain.c 198>
2       ShowVersion: void*(), <mcmlio.c 49>
3           CenterStr: char*(), <mcmlio.c 28>
4           puts: <>
5       GetFnameFromArgv: void*(), <mcmlmain.c 150>
6           strcpy: <>
7       GetFile: struct*(), <mcmlio.c 94>
8           printf: <>
9           scanf: <>
10          strlen: <>
11          exit: <>
12          fopen: <>
13      CheckParm: void*(), <mcmlio.c 514>
14          ReadNumRuns: short(), <mcmlio.c 205>
15          printf: 8
16          ReadParm: void*(), <mcmlio.c 425>
17          FnameTaken: char(), <mcmlio.c 487>
18          sprintf: <>
19          free: <>
20          nrerror: void*(), <mcmlnr.c 19>
21          FreeFnameList: void*(), <mcmlio.c 500>
22          rewind: <>
23      ReadNumRuns: 14
24      ReadParm: 16
25      DoOneRun: void*(), <mcmlmain.c 163>
26          InitOutputData: void*(), <mcmlio.c 546>
27          Rspecular: double(), <mcmlgo.c 117>
28          PunchTime: long(), <mcmlmain.c 60>
29          ReportStatus: void*(), <mcmlmain.c 122>
30          LaunchPhoton: void*(), <mcmlgo.c 143>
31          HopDropSpin: void*(), <mcmlgo.c 726>
32          ReportResult: void*(), <mcmlmain.c 133>
33          FreeData: void*(), <mcmlio.c 581>
34      fclose: <>
```

Fig. 5.2. Flow of mcml.

The names of most functions well describe what they do. The function `ShowVersion()` prints the name of the program, the names and address of the authors of the program, and the version of the program. The function `GetFnameFromArgv()` get an input data filename from the command line input for UNIX users or DOS users. Macintosh OS does not allow command line input. The function `GetFile()` is used to get the pointer to the file stream for the input data file. The function `CheckParm()` checks the input parameters. If the `CheckParm()` detects an error, it will exit the program. Otherwise, if all the input parameters pass the error check by the function `CheckParm()`, independent simulation runs will be implemented one by one. For each independent run, the function `ReadParm()` obtains the input parameters, and the function `DoOneRun()` does the simulation and reports the results to the output data file.

After all the input parameters are checked by `CheckParm()`, the file pointer is rewound to the beginning of the file stream so that the input parameters can be read again by the functions `ReadNumRuns()` and `ReadParm()`. The function `ReadNumRuns()` gets how many independent simulations are to be specified in this input data file. The function `ReadParm()` only reads the input parameters for one independent run.

Under the function `DoOneRun()`, the function `PunchTime()` provides the user time and the real time used so far by the current simulation run. The function `ReportStatus()` fetches the real time and predicts when the current simulation run will finish. However, these timing functions will not work if the source code is compiled by a GNU C compiler. The function `LaunchPhoton()` initializes a photon packet. The function `HopDropSpin()` moves the photon packet, deposits some photon packet weight, scatters the packet, and deals with the boundary. After the given number of photon packets are traced, the results are properly processed (see Chapter 4) and then written to an output file by the function `ReportResult()`.

5.6 Multiple simulations

The program can do any number of independent simulations sequentially without being subject to memory limit. It checks the parameters of one simulation after another before starting the simulation. If it detects an error in the input data file, the program stops the execution. Otherwise, it reads in the parameters of one independent simulation at a time and starts the simulation. At the end of the simulation, it writes the results to the output data file whose name is specified by the input data file. The next independent run will be processed thereafter. The users should try to make sure not to use the same output filenames for different simulations, although the program checks against duplicated output filenames.

To check against duplicated filenames specified in an input data file, we set up a linear linked list to store the filenames specified in the input data file. Each new filename is compared with every node of the filename list. If the name is already taken, the program notifies the user of the name, and exits to the system. Otherwise, if no filename is duplicated, the program deletes the filename list to release the memory, and continues execution.

5.7 Timing profile of the program

The timing profile of the program mcml indicates how to improve the efficiency of the program by logging how much time the program spends on each function. Profilers are available in a few compilers including C compilers of UNIX operating systems, and

THINK C compiler on Macintosh. We used the THINK C 5.0.1 profiler here (Symantec, 1991). To log the timings, we turn on the flag `THINKCPROFILER` to 1 in mcmlmain.c, and check the "Generate profiler calls" check box in the Debugging page of the "Options..." dialog box in the THINK C compiler.

The following input file is used (see Section 9.1 for how to name the input file) to test the profile, where only 100 photon packets are traced. The optical parameters of the tissue are: refractive index n = 1.37, absorption coefficient μ_a = 1 cm^{-1}, scattering coefficient μ_s = 100 cm^{-1}, anisotropy factor g = 0.9, and thickness d = 0.1 cm.

```
1.0                                     # file version
1                                       # number of runs

prof.mco      A                         # output filename, ASCII/Binary
100                                     # No. of photons
1E-2   1E-2                             # dz, dr
100    100    1                         # No. of dz, dr & da.

1                                       # No. of layers
# n    mua    mus    g      d           # One line for each layer
1.0                                     # n for medium above.
1.37   1      100    0.90   0.1         # layer 1
1.0                                     # n for medium below.
```

The profiler output is listed in Table 5.2. The heading "Function" gives the name of a function. The headings "Minimum", "Maximum" and "Average" give the minimum, maximum and average time spent in a routine respectively. The unit of time here is a unit of the VIA 1 timer. Each unit is 1.2766 μsec (approximately 780,000 in a second). The heading "%" is the percentage of profiling period spent in the routine, where the profiling period is the accumulated time spent in routines that were compiled with the "Generate profiler calls" options on. The heading "Entries" is the number of times the routine was called.

Table 5.2. Timing profile of the program mcml.

Function	Minimum	Maximum	Average	%	Entries
AllocMatrix	2507	134153	46662	0	3
AllocVector	65	319	169	0	6
CrossDnOrNot	53	670	145	0	95
CrossOrNot	40	631	66	0	175
CrossUpOrNot	53	635	144	0	80
Drop	166	887	245	5	3554
HitBoundary	38	622	62	1	3729
Hop	40	595	59	1	3729
HopDropSpin	52	711	74	1	3729
HopDropSpinInTissue	111	815	242	5	3729
InitOutputData	314	314	314	0	1
LaunchPhoton	35	123	59	0	100
PredictDoneTime	56472	61201	58638	3	9
PunchTime	76	116	104	0	10
RFresnel	300	905	411	0	105
RandomNum	37	735	67	4	10937
RecordR	1099	2293	1690	0	46
RecordT	1363	2396	1761	0	54
ReportStatus	19	790	90	0	100
Rspecular	58	58	58	0	1
Spin	914	2157	1412	**33**	3554
SpinTheta	72	665	102	2	3554
StepSizeInTissue	36	2094	1378	**33**	3729
ran3	27	1187	44	3	10938

From the percentage column, we observe that the functions `Spin()` and `StepSizeInTissue()` take most of the computation time. They are the primary places to modify if we need to improve the efficiency. The function `StepSizeinTissue()` takes a long time because of the logarithmic operation. The function `PredictDoneTime()` apparently takes much computation time too. This is because we simulated only 100 photon packets. This function will be called for a fixed number of times (10 times) for a simulation no matter how many photon packets are simulated. Therefore, its percentage will decrease linearly with the number of photon packets to be simulated. Note that we made the profiler include only the main part of the simulation (See file mcmlmain.c in Appendix B). Therefore, the functions for input or output of data are not included since they do not scale up as the number of photon packets to be simulated increases.

6. Computation Results of mcml and Verification

Some computation results are described in this chapter as examples, and some of them are compared with the results from other theory or with the Monte Carlo simulation results from other investigators to verify the program.

6.1 Total diffuse reflectance and total transmittance

We computed the total diffuse reflectance and total transmittance of a slab of turbid medium with the following optical properties: relative refractive index n = 1, absorption coefficient $\mu_a = 10\ \text{cm}^{-1}$, scattering coefficient $\mu_s = 90\ \text{cm}^{-1}$, anisotropy factor g = 0.75, and thickness d = 0.02 cm. Ten Monte Carlo simulations of 50,000 photon packets each are completed. Then, the averages and the standard errors of the total diffuse reflectance and total transmittance are computed (Table 6.1). The table also lists the results from van de Hulst's table (van de Hulst, 1980) and from Monte Carlo simulations by Prahl *et al*. (1989). All results agree with each other.

Table 6.1. Verification of the total diffuse reflectance and the total transmittance in a slab with a matched boundary.

Source	**R_d Average**	**R_d Error**	**T_t Average**	**T_t Error**
van de Hulst, 1980	0.09739		0.66096	
mcml	0.09734	0.00035	0.66096	0.00020
Prahl *et al*., 1989	0.09711	0.00033	0.66159	0.00049

The columns "R_d Average" and "R_d Error" are the average and the standard error of the total diffuse reflectance respectively, while the columns "T_t Average" and "T_t Error" are the average and the standard error of the total transmittance.

For a semi-infinite turbid medium that has mismatched refractive index with the ambient medium, the average and the standard error of the total diffuse reflectance are computed similarly, and compared in Table 6.2 with Giovanelli's (1955) results and Monte Carlo simulation results by Prahl *et al*. (1989). The medium has the following optical properties: relative refractive index n = 1.5, $\mu_a = 10\ \text{cm}^{-1}$, $\mu_s = 90\ \text{cm}^{-1}$, g = 0 (isotropic scattering). Ten Monte Carlo simulations of 5,000 photon packets each are completed to compute the average and the standard error of the total diffuse reflectance.

Table 6.2. Verification of the total diffuse reflectance in a semi-infinite medium with a mismatched boundary.

Source	**R_d Average**	**R_d Error**
Giovanelli, 1955	0.2600	
mcml	0.25907	0.00170
Prahl *et al.*, 1989	0.26079	0.00079

6.2 Angularly resolved diffuse reflectance and transmittance

We used mcml to compute the angularly resolved diffuse reflectance and transmittance of a slab of turbid medium with the following optical properties: relative refractive index n = 1, absorption coefficient μ_a = 10 cm^{-1}, scattering coefficient μ_s = 90 cm^{-1}, anisotropy factor g = 0.75, and thickness d = 0.02 cm. In the simulation, 500,000 photon packets are used, and the number of angular grid elements is 30. The results are compared with the data from van de Hulst's table (van de Hulst, 1980) as shown in Figs. 6.2a and b.

Since mcml also scores the unscattered transmittance into the transmittance array, we have to subtract it from the first element of the array to obtain the diffuse transmittance. In this case, the unscattered transmittance is $\exp(-(\mu_a+\mu_s)\ d) = \exp(-2) \approx 0.13534$, which is only scored into the first grid element in the α direction. The solid angle spanned by the first grid element is $\Delta\Omega \approx 2\ \pi\ \sin(\Delta\alpha/2)\ \Delta\alpha$, where $\Delta\alpha = \pi/(2\times30)$. Therefore, the contribution of the unscattered transmittance to the first element of the array $T_t(\alpha)$ is $\exp(-2)/\Delta\Omega \approx 15.68$. After the subtraction, we get the adjusted first element of transmittance array being 0.765 sr^{-1}, which is the diffuse transmittance. Note that the variance in Fig. 6.2a for diffuse reflectance is larger than that in Fig. 6.2b for diffuse transmittance. This is because the total diffuse reflectance is much less than the total diffuse transmittance (0.09739 vs 0.66096–0.13534 = 0.52562, as shown in Table 6.1).

Since van de Hulst used a different definition of reflectance and transmittance, and a normalization to incident flux π, we multiplied van de Hulst's data by the cosine of the exiting angle from the normal to the surface, then divided by π.

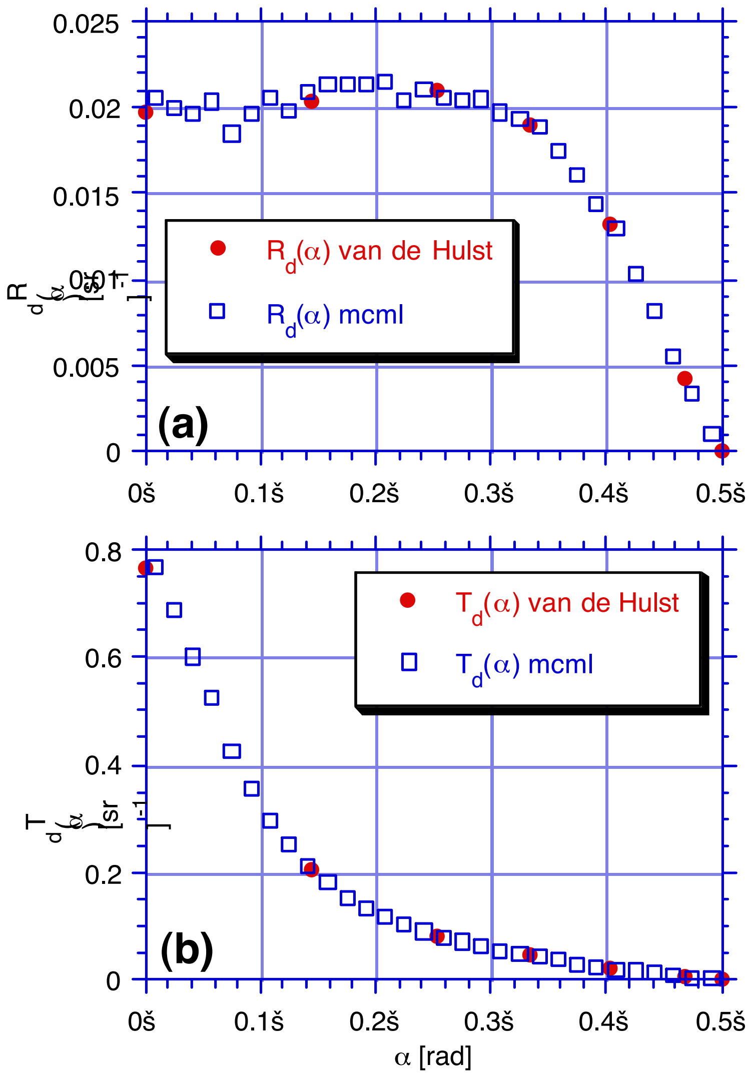

Fig. 6.2. Angularly resolved (a) diffuse reflectance $R_d(\alpha)$ and (b) diffuse transmittance $T_d(\alpha)$ vs the angle between the photon exiting direction and the normal to the medium surface α. Solid circles are from van de Hulst's table, and the open square boxes are from mcml simulation. The optical parameters are: relative refractive index n = 1.0, μ_a = 10 cm^{-1}, μ_s = 90 cm^{-1}, g = 0, thickness d = 0.02 cm.

6.3 Radially resolved diffuse reflectance

As an example of the simulation of radially resolved diffuse reflectance, we compare the diffuse reflectances of two semi-infinite media whose optical properties are governed by similarity relations (Wyman *et al.*, 1989a and 1989b). The two sets of optical parameters share the same absorption coefficient μ_a and transport scattering coefficient $\mu_s(1-g)$. These two media should give approximately the same diffuse reflectances if the similarity relations are valid. The results (Fig. 6.3) confirmed that the similarity relations do not apply for photon sources near the media boundary as Wyman *et al.* expected. The relative difference between two diffuse reflectances is very large when the radius r is small, and becomes smaller when r becomes larger. We have also confirmed that the similarity relations work very well when the photon source is deep inside the media using a modified mcml (see Chapter 11).

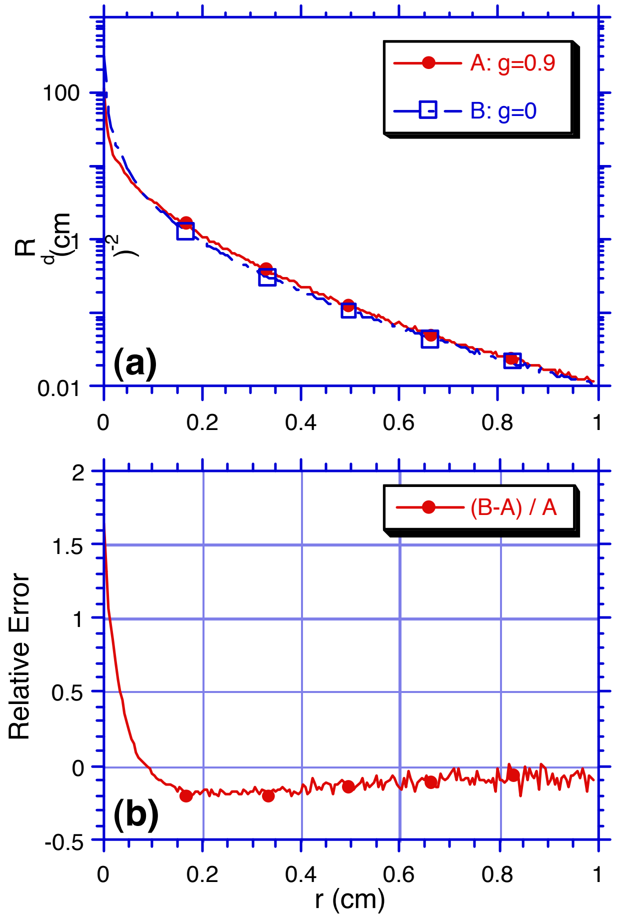

Fig. 6.3. (a) Comparison and (b) the relative difference of diffuse reflectances as a function of radius r for two semi-infinite media whose optical properties are "equivalent" according to similarity relations.

In Fig. 6.3., The optical properties for curve A are: $\mu_a = 0.1$ cm^{-1}, $\mu_s = 100$ cm^{-1}, g = 0.9, $n_{rel} = 1$, and the optical properties for curve B are: $\mu_a = 0.1$ cm^{-1}, $\mu_s = 10$ cm^{-1}, g = 0, $n_{rel} = 1$. The two curves A and B are results from pure Monte Carlo simulations of 1 million photon packets. The grid line separation in the r direction is 0.005 cm, and number of grid elements is 200.

<u>6.4 Depth resolved internal fluence</u>

As an example of simulation of the depth resolved internal fluence, we show the results for two semi-infinite media with matched and mismatched boundaries respectively

(Fig. 6.4). The dimensionless internal fluence as a function of depth z, $\phi_z[i_z]$ in Section 4.2, is computed from the response to an infinitely narrow photon beam normally incident on a semi-infinite medium. However, it can be equivalently considered as the response of an infinitely wide photon beam perpendicularly incident on a semi-infinite medium with a difference of a constant S (see Section 4.2), where S is the power density. Since the direction output of the program mcml gives $A_z[i_z]$ instead of $\phi_z[i_z]$, we divided $A_z[i_z]$ by the absorption coefficient of the semi-infinite medium to get $\phi_z[i_z]$. Although the response of an infinitely narrow photon beam is dimensionless (Fig. 6.4), if the input photon beam is measured in W/cm^2 or J/cm^2 as the power density of energy density, the unit of fluence is also in the unit of W/cm^2 or J/cm^2 correspondingly. Since we only consider steady-state responses, we can discuss either energy density or power density because they can be converted back and forth.

Note that the fluence near the surface is larger than 1 because the back scattered light augments the fluence. Furthermore, the internal fluence for the medium with a mismatched boundary is higher than that for the medium with a matched boundary. This is due to the internal reflection by the mismatched boundary, therefore the photons that would escape from the boundary of the boundary-matched medium may be reflected back into the medium by the mismatched boundary and hence have a greater chance to be absorbed. Also note that when z is sufficiently deep, the two curves are parallel. This confirms the valid range of diffusion theory. For z larger than the penetration depth δ, diffusion theory predicts that the internal fluence distribution should be (Wilson *et al.*, 1990):

$$\phi(z) = \phi_0 \, k \exp(-z/\delta) \tag{6.1}$$

where k is a scalar that depends on the amount of back scattered reflectance, and ϕ_0 is the incident irradiance, which is 1 in our mcml simulation. The scalar k is obviously a function of the relative index of refraction. Therefore, the matched boundary and the mismatched boundary will have different k. The penetration depth δ is computed:

$$\delta = 1/\sqrt{3\,\mu_a\,(\mu_s + \mu_s\,(1-g))} \quad = 1/\sqrt{3(0.1)(0.1+100(1-0.9))} \quad \approx 0.57 \text{ cm} \tag{6.2}$$

which is independent of relative index of refraction. Therefore, the two curves in Fig. 6.4 should be off just by a factor due to different k values when $z > \delta$, which means the curves are parallel in log-linear scale when $z > \delta$. The two curves shown here are parallel even when $z > 1$ mfp' $= 1/(\mu_s + \mu_s\,(1-g)) \approx 0.1$ cm, where mfp' is the transport mean free path.

One mfp' may be a better criterion for valid application of diffusion theory than the penetration depth. Further supporting evidence can be found in Chapter 11 and Wang *et al*. (1992).

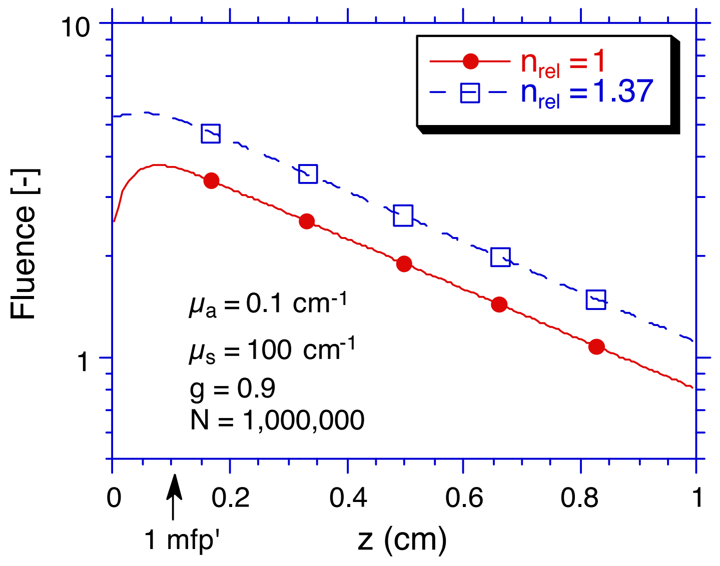

Fig. 6.4. Comparison of internal fluences as a function of depth z for two semi-infinite media with a matched boundary and a mismatched boundary respectively. The results are from Monte Carlo simulations with 1 million photon packets each using mcml. The grid line separation in the z direction is 0.005 cm, and number of grid elements is 200.

We fit the parallel part of the two curves with exponential functions. The damping constants for the curves are approximately 1.73 cm^{-1} for the matched boundary and 1.74 cm^{-1} for the mismatched boundary respectively. The reciprocals of the damping constants are 0.578 cm for the matched boundary and 0.575 cm for the mismatched boundary respectively. They are very close to the penetration depth (0.57 cm, Eq. 6.2) predicted from diffusion theory.

6.5 Computation times vs optical properties

We completed multiple Monte Carlo simulations with mcml for semi-infinite media with various optical properties, and fitted the user times as a function of the ratio between scattering coefficient and absorption coefficient μ_s/μ_a and anisotropy g. The situations for media with matched boundaries (relative refractive index is 1) and mismatched boundaries (relative refractive index is not 1) will be presented separately. Note that the user time is whatever the system allocates to the running of the program, as opposed to the real time which is wall-clock time. In a time-shared system, they need not be the same, and the real time of the same run may not be reproduced depending on the status of the system. In mcml, the user time is reported to the output data file, and the real time is used to predict when the simulation finishes during the simulation.

Before starting multiple mcml simulations for various optical properties, we know that the time required to finish tracing a photon packet is proportional to the number of steps that a photon packet takes until being terminated. According to the rules for photon propagation described in Chapter 3, this number of steps should not be dependent on the absolute values of scattering coefficient μ_s and absorption coefficient μ_a, but their ratio. Therefore, we keep one of the two parameters constant (e.g., μ_s = 100 cm^{-1}), and vary the other one (e.g., μ_a).

Matched boundary

For media with matched boundaries (relative refractive index n_{rel} is 1), we finished multiple mcml simulations of 10,000 photon packets each for various absorption coefficients μ_a and anisotropy factors while keeping the scattering coefficient μ_s fixed to 100 cm^{-1}. The results are listed in Table 6.3, where the ratios between the scattering coefficient and the absorption coefficient are tabulated, instead of the two coefficients themselves separately, and the user

Table. 6.3. Computation times for various media with matched boundaries. The column "Predicted User Time" is the computed values using Eqs. 6.1-6.3 presented later. The column "Error" is equal to (Predicted User Time – User Time)/(User Time)*100.

μ_s/μ_a	**g**	**User Time (sec./1000 photons)**	**Predicted User Time (sec./1000 photons)**	**Error (%)**
0.2	0	0.43	0.36	–16.15
1	0	0.78	0.81	3.58
2	0	1.10	1.15	4.42
10	0	2.59	2.56	–0.99
20	0	3.66	3.62	–0.97
100	0	8.46	8.10	–4.23
200	0	12.27	11.46	–6.64
1000	0	29.61	25.61	–13.49
0.2	0.1	0.40	0.38	–5.04
1	0.1	0.80	0.86	7.19
2	0.1	1.10	1.22	10.70
10	0.1	2.80	2.75	–1.82
20	0.1	3.90	3.90	0.10
100	0.1	9.80	8.81	–10.07
200	0.1	13.20	12.52	–5.19
1000	0.1	28.60	28.25	–1.21
0.2	0.5	0.50	0.45	–9.54
1	0.5	1.00	1.08	7.71
2	0.5	1.40	1.57	11.80
10	0.5	3.50	3.73	6.49
20	0.5	5.30	5.42	2.19
100	0.5	12.10	12.90	6.60
200	0.5	17.90	18.74	4.71
1000	0.5	40.60	44.63	9.93
0.2	0.9	0.50	0.49	–1.83
1	0.9	1.20	1.35	12.74
2	0.9	1.90	2.09	10.20
10	0.9	6.30	5.77	–8.39
20	0.9	9.80	8.93	–8.86
100	0.9	25.80	24.62	–4.58
200	0.9	38.10	38.10	0.00
1000	0.9	95.30	105.02	10.20
0.2	0.99	0.50	0.42	–16.18
1	0.99	1.20	1.42	18.68
2	0.99	2.10	2.41	14.85
10	0.99	8.80	8.20	–6.87
20	0.99	16.50	13.88	–15.89
100	0.99	60.60	47.16	**–22.18**
200	0.99	97.20	79.86	–17.84
1000	0.99	248.80	271.37	9.07

times are converted to seconds per 1000, instead of 10,000, photon packets. The columns "Predicted User Time" and "Error" will be discussed subsequently

We plotted the user times as a function of the ratio between the scattering coefficient and the absorption coefficient for each anisotropy factor g in a log-log scale (Fig. 6.5). For each anisotropy factor g, the higher the ratio between the scattering coefficient and the absorption coefficient, the longer the user time. This is because the photon packets in media of higher ratio μ_s/μ_a, compared with media of lower ratio, can jump more steps before reaching the threshold weight and hence having a chance to be terminated. Therefore, the Monte Carlo simulation of low absorbing medium is very slow. If the diffuse reflectance as a function of r in a low absorption semi-infinite turbid medium is the only physical quantity to be computed, a hybrid model of pure Monte Carlo simulation and diffusion theory (Wang *et al*., 1992) is a much faster model than pure Monte Carlo simulations. The speed of the hybrid model is not so sensitive to the ratio between the scattering coefficient and the absorption coefficient.

For the same ratio between the scattering coefficient and the absorption coefficient, the larger the anisotropy factor g, the longer the user time. This is because that the photon packets in media of larger anisotropy factors g have less chance to be reflected out of the media because the scatterings are more forward directed, and hence to be terminated.

For each anisotropy factor g, the data points are well aligned in the log-log plot. This means that we can fit the data points for each anisotropy factor g with a power function. The fitted lines are presented in Fig. 6.5.

The two fitting coefficients $C_1(g)$ and $C_2(g)$ are dependent on the anisotropy factor g. The fitting coefficients $C_1(g)$ are plotted against the anisotropy factor g in a log-linear scale (Fig. 6.6a), and can be fitted with an exponential function. Similarly, the fitting coefficients $C_2(g)$ are plotted against $(1 - g)$ in a linear-log scale (Fig. 6.6b), and can be fitted with a logarithmic function. These three fittings are summarized as the following empirical formulas:

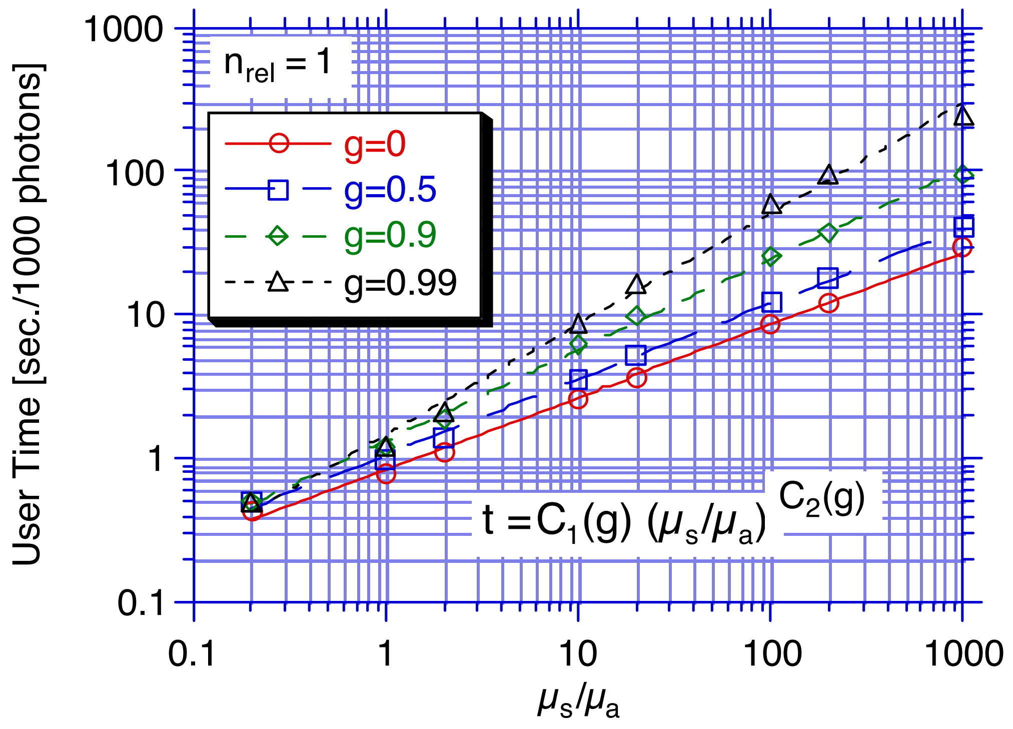

Fig. 6.5. The user times vs the ratio between the scattering coefficient μ_s and the absorption coefficient μ_a for different anisotropy factors g of media with matched boundaries.

$$C_1(g) = 0.81 \exp(0.57\ g) \tag{6.3}$$

$$C2(g) = 0.50 - 0.13 \log(1-g) \tag{6.4}$$

$$t = C_1(g)\ (\mu_s/\mu_a)^{C_2(g)} \quad \text{[sec./1000 photons]} \tag{6.5}$$

where t is the user time in seconds per 1000 photon packets for semi-infinite media with matched boundaries.

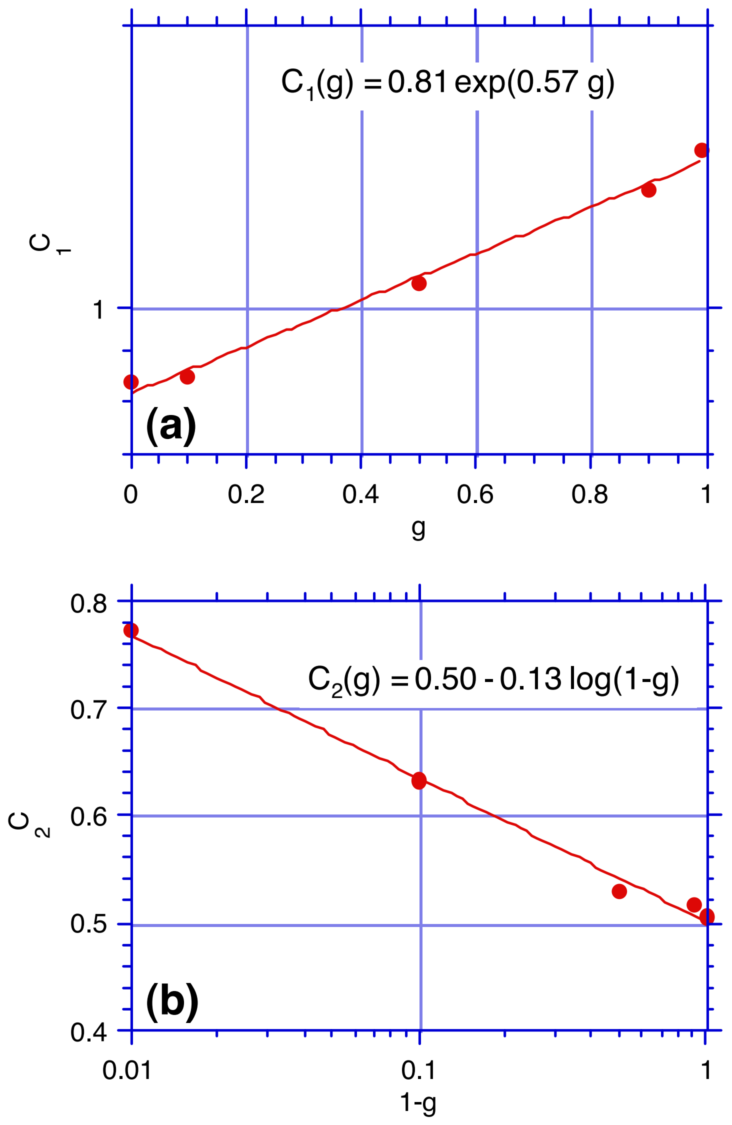

Fig. 6.6. The fitting coefficients (a) $C_1(g)$ and (b) $C_2(g)$ vs the anisotropy factor g of media with matched boundaries.

To test how good Eqs. 6.3-6.5 are, we use them to compute the user times for the optical properties given in Table 6.3, and presented the computed user times in Table 6.3 as the column "Predicted User Time". The relative errors are within 20% as shown in the column "Error" in Table 6.3 for all rows in the table except one of them (in bold face).

The Eqs. 6.3-6.5 can be used generally to predict user time of a medium with a matched boundary. However, several limitations and notes have to be mentioned. First, the anisotropy factor g is limited to less than 0.99, and the accuracy is unknown for $g > 0.99$ because the fitting coefficient $C_2(g)$ approaches infinity when g approaches 1. Second, these equations are based on mcml simulations on a Sun SPARCstation 2. Therefore, we expect a scale factor for Eq. 6.5 or the values in Table 6.3 on a different computer system. This scale factor can be determined by simulating one or several media with optical properties in Table 6.3 using mcml running on your computer system and taking the ratio between the user time on your machine and the user time in Table 6.3. Third, the speed of mcml is related to the threshold weight in the program mcml (`WEIGHT` in Table 5.1), which is normally 1×10^{-4} (See Table 5.1), and the chance of surviving a roulette (`CHANCE` in Table 5.1), which is normally 0.1 (See Table 5.1). If these two parameters are changed, Eqs. 6.3-6.5 are no longer valid. It is unexplored yet how these two parameters will affect the user times.

Mismatched boundary

We repeat the above process to media with mismatched boundaries (relative refractive index n_{rel} 1). We finished multiple mcml simulations of 1,000 (instead of 10,000 for matched boundaries) photon packets each for various absorption coefficients and anisotropy factors while keeping the scattering coefficient fixed to 100 cm^{-1} and the relative refractive index to 1.37, which is typical for human tissues in visible or infrared wavelength. The results are listed in Table 6.4.

We plotted the user times as a function of the ratio between the scattering coefficient and the absorption coefficient for each anisotropy factor g in a log-log scale (Fig. 6.7). Then, the fitting coefficients $C_1(g)$ and $C_2(g)$ are plotted with respect to g and (1–g) respectively (Fig. 6.8a and b), and fitted with an exponential function and a logarithmic function correspondingly. The fittings give the following empirical formulas:

Table 6.4. Computation times for various media with mismatched boundaries. The column "Predicted User Time" is the computed values using Eqs. 6.4-6.6 presented later. The column "Error" is equal to (Predicted User Time – User Time)/(User Time)*100.

μ_s/μ_a	g	User Time (sec./1000 photons)	Predicted User Time (sec./1000 photons)	Error (%)
0.2	0	0.48	0.43	–9.74
1	0	0.98	1.05	7.14
2	0	1.42	1.54	8.26
10	0	3.67	3.73	1.51
20	0	5.47	5.45	–0.28
100	0	13.43	13.22	–1.57
200	0	18.67	19.35	3.66
1000	0	50.50	46.90	–7.13
0.2	0.1	0.50	0.44	–11.03
1	0.1	1.00	1.09	8.85
2	0.1	1.50	1.60	6.68
10	0.1	3.83	3.92	2.23
20	0.1	5.90	5.76	–2.44
100	0.1	15.95	14.08	–11.70
200	0.1	22.55	20.71	–8.18
1000	0.1	42.38	50.66	19.54
0.2	0.5	0.53	0.49	–8.10
1	0.5	1.13	1.26	11.25
2	0.5	1.73	1.89	9.31
10	0.5	4.87	4.88	0.22
20	0.5	7.63	7.34	–3.77
100	0.5	19.53	18.95	–2.97
200	0.5	27.08	28.51	5.28
1000	0.5	77.96	73.58	–5.62
0.2	0.9	0.55	0.49	–11.64
1	0.9	1.27	1.45	14.31
2	0.9	2.03	2.33	14.58
10	0.9	7.28	6.95	–4.55
20	0.9	12.10	11.13	–7.99
100	0.9	35.98	33.26	–7.56
200	0.9	55.05	53.28	–3.21
1000	0.9	133.06	159.18	19.63
0.2	0.99	0.55	0.41	**–25.96**
1	0.99	1.28	1.50	17.16
2	0.99	2.10	2.63	**25.19**
10	0.99	8.82	9.68	9.77
20	0.99	16.82	16.97	0.92
100	0.99	69.55	62.51	–10.12
200	0.99	120.56	109.60	–9.09
1000	0.99	366.45	403.62	10.14

$$C_1(g) = 1.05 \exp(0.36\ g) \tag{6.6}$$

$$C2(g) = 0.55 - 0.13 \log(1-g) \tag{6.7}$$

$$t = C_1(g)\ (\mu_s/\mu_a)^{C_2(g)} \quad \text{[sec./1000 photons]} \tag{6.8}$$

where t is the user time in seconds per 1000 photon packets for semi-infinite media with mismatched boundaries (n_{rel} = 1.37).

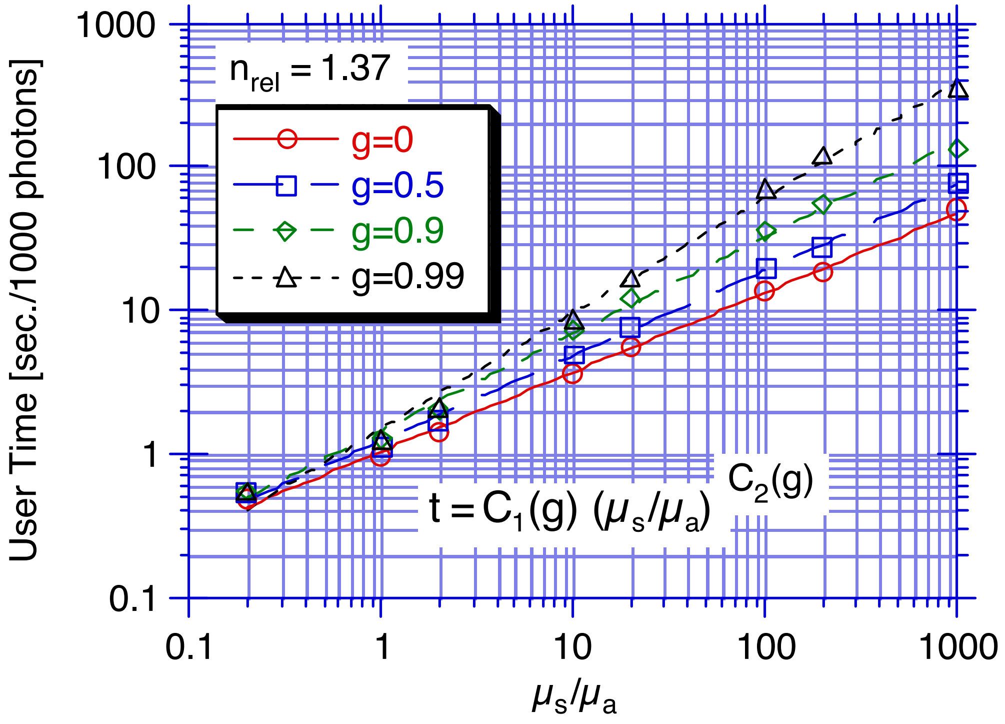

Fig. 6.7. The user times vs the ratio between the scattering coefficient μ_s and the absorption coefficient μ_a for different anisotropy factors g in media with relative refractive index 1.37.

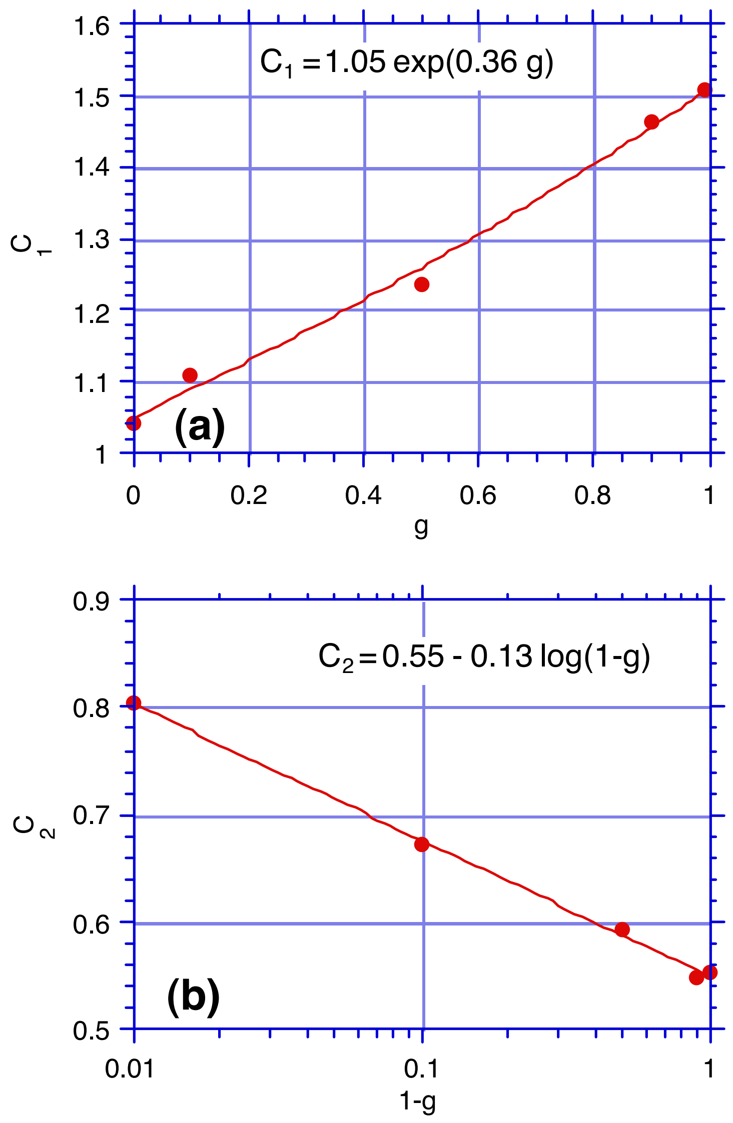

Fig. 6.8. The fitting coefficients (a) C_1 and (b) C_2 vs the anisotropy factor g of media with relative refractive index 1.37.

To test how good Eqs. 6.6-6.8 are, we use them to compute the user times for the optical properties in Table 6.4, and presented the computed user times in Table 6.4 in the column "Predicted User Time". For all rows in the table except two of them (in bold face), the relative errors are within 20%. The cautions made for media with matched boundaries apply here as well.

To summarize the empirical formulas for both matched and mismatched boundaries, we list the formulas in Table 6.5.

Table 6.5. Empirical formulas of user times for matched and mismatched boundaries.

Items	**Matched (n_{rel} = 1)**	**Mismatched (n_{rel} = 1.37)**
$C_1(g)$	0.81 exp(0.57 g)	1.05 exp(0.36 g)
$C_2(g)$	0.50 – 0.13 log(1–g)	0.55 – 0.13 log(1–g)
t [sec./1000 photons]	$C_1(g)\ (\mu_s/\mu_a)^{C_2(g)}$	$C_1(g)\ (\mu_s/\mu_a)^{C_2(g)}$

6.6 Scored Physical Quantities of Multi-layered Tissues

For multi-layered tissues, we have not found computation results based on other theories to compare with our computation. However, thanks to Gardner's cooperation (Gardner *et al*., 1992), we compared our Monte Carlo simulation results of multi-layered tissues with their results of an independently written Monte Carlo simulation. The comparison includes the diffuse reflectance versus radius, $R_d(r)$, where the radius r is the distance between the photon incident point and the observation point, the transmittance versus radius, $T_t(r)$, and the internal fluence versus z, $\phi_z(z)$, and the internal fluence versus r and z, $\phi_{rz}(r, z)$. This comparison can at least greatly reduce the chance of programming errors.

We chose a three-layer tissue for the simulation. The optical properties of each layer are shown in Table 6.6.

Table 6.6. The optical properties of the three-layer tissue.

Layer	**Refractive Index n**	**Absorption Coeff. (cm^{-1})**	**Scattering Coeff. (cm^{-1})**	**Anisotropy Factor g**	**Thickness (cm)**
1	1.37	1	100	0.9	0.1
2	1.37	1	10	0	0.1
3	1.37	2	10	0.7	0.2

The refractive indices of the top and bottom ambient media are both set to 1.0. The grid separations in z and r directions are both 0.01 cm. The number of grid elements in z and r directions are 40 and 50 respectively. We do not want to resolve the exiting angles of reflected or transmitted photons, therefore we set the number of grid elements in the angle α direction to 1. The number of photon packets traced is 1,000,000. The actual input file for the program mcml is as follows.

```
1.0                                         # file version
1                                           # number of runs

### Specify data
comp.mco     A                              # output filename, ASCII/Binary
1000000                                     # No. of photons
.01    .01                                  # dz, dr
40     50     1                             # No. of dz, dr & da.

3                                           # No. of layers
# n    mua    mus    g      d               # One line for each layer
1.0                                         # n for medium above.
1.37   1      100    0.90   0.1             # layer 1
1.37   1      10     0      0.1             # layer 2
1.37   2      10     0.70   0.2             # layer 3
1.0                                         # n for medium below.
```

Craig Gardner set up the same run for his simulation code except he used only 100,000 photons (Gardner *et al.*, 1992). The total diffuse reflectance and transmittance from the two simulations are compared in Table 6.7.

Table 6.7. Comparison of total diffuse reflectances and transmittances.

Source	**Diffuse Reflectance R_d**	**Transmittance T_t**
Gardner *et al.*, 1992	0.2381	0.0974
mcml	0.2375	0.0965

The comparison between the diffuse reflectances and transmittances are shown in Figs. 6.9 and 6.10 respectively. The comparison between fluences $\phi_{rz}(r, z)$, as an impulse response, as a function of radius r for several given z coordinates is shown in Fig. 6.11. The comparison between fluences $\phi_z(z)$ as a function of z as described in Section 4.2 is subsequently given in Fig. 6.12. All of the comparisons have shown agreement between the two independent simulations.

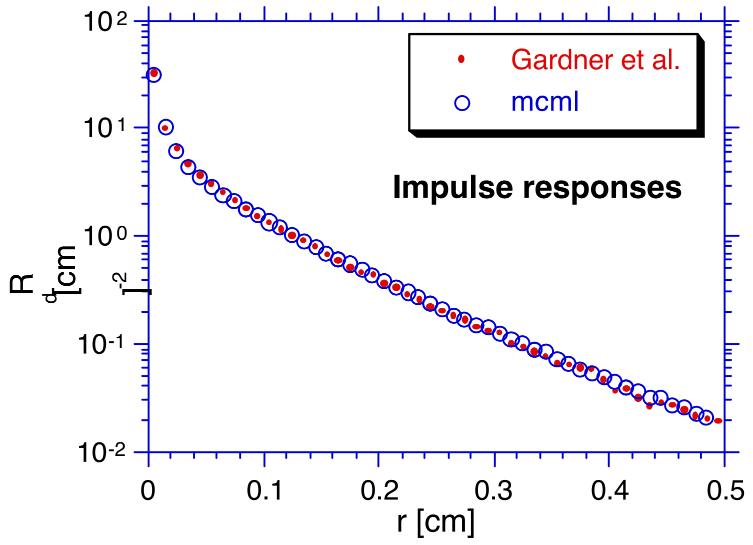

Fig. 6.9. Comparison between diffuse reflectances as a function of radius based on Gardner's computation (Gardner *et al.*, 1992) and mcml simulation.

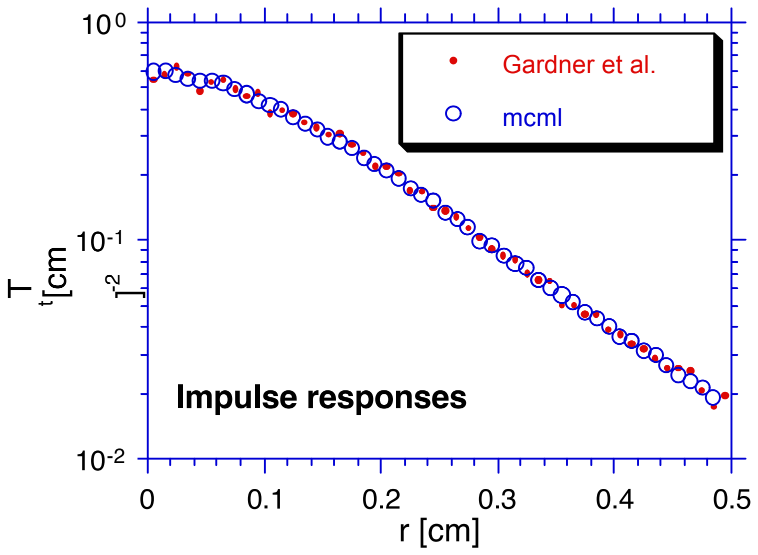

Fig. 6.10. Comparison between transmittances as a function of radius based on Gardner's computation (Gardner *et al.*, 1992) and mcml simulation.

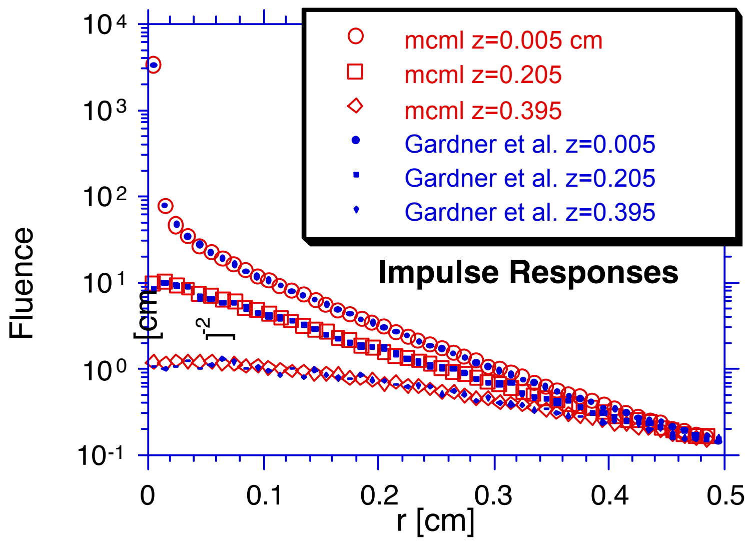

Fig. 6.11. Comparison between fluences as a function of radius r for several z coordinates based on Gardner's computation (Gardner *et al.*, 1992) and mcml simulation.

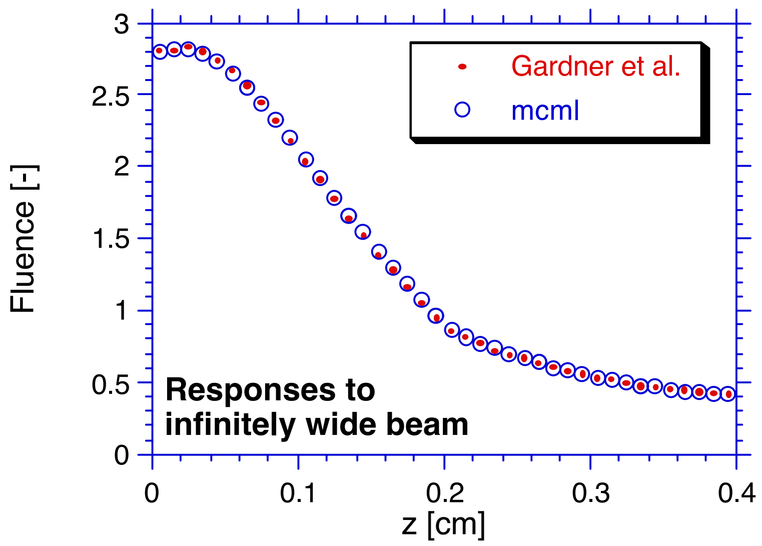

Fig. 6.12. Comparison between fluences as a function of z based on Gardner's computation (Gardner *et al.*, 1992) and mcml simulation.

For 2D arrays such as the fluence as a function of r and z, conv has the ability to output the data in contour format (see Sections 10.9 and 10.10). The fluence as a function of r and z of the impulse response is shown in contour lines in Fig. 6.13.

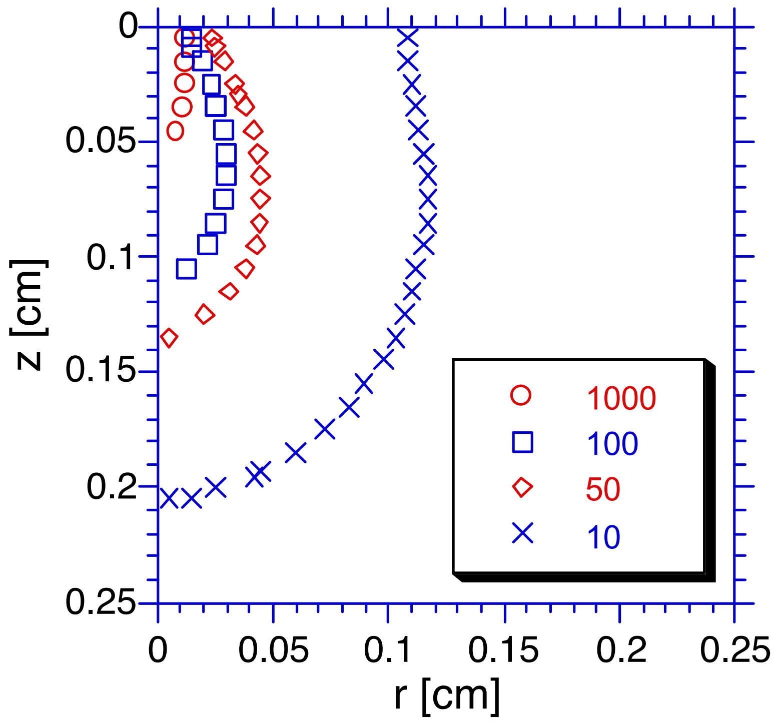

Fig. 6.13. Contour plot of the fluence as a function of r and z of impulse response based on mcml simulation.

7. Convolution for Photon Beams of Finite Size

This chapter will discuss the principles and implementation of convolving Monte Carlo simulation results for an infinitely narrow photon beam to yield the responses to photon beams of finite size. Gaussian beams and circularly flat beams are considered as special cases.

7.1 Principles of convolution

So far we have only dealt with the response to an infinitely narrow photon beam normally incident on the surface of a multi-layered tissue. This response is also called the impulse response. However, all photon beams have finite size in reality. Theoretically, we can use the Monte Carlo simulation to compute the response to a finite size photon beam directly by distributing the initial positions of the launched photon packets. The only problem is that it requires a larger number of photon packets to be traced to get acceptable variance than simulating the responses of an infinitely narrow photon beam. Therefore, this method is not efficient although sometimes it might be the only approach for some types of tissue configurations which can not be convolved, such as a tissue with an irregular buried object.

Fortunately, the system we are dealing with is linear and invariant. The linearity means that if the input intensity of the infinitely narrow photon beam is multiplied by a factor, the responses will be multiplied by the same factor. It also means that the response to two photon beams is the sum of the responses to each photon beam. The invariance means that when the infinitely narrow photon beam is shifted horizontally by a distance in a certain direction, the responses will be shifted also horizontally by the same distance in the same direction. Therefore, if we assume the photon beam of finite size is collimated, the response of an infinitely narrow photon beam will be a Green's function of the tissue system, and the response of the finite size photon beam can be computed from the convolution of the Green's function according to the profile of the finite size photon beam.

Note that the responses mentioned above can be the internal absorption distribution, or the reflectance or transmittance distributions. We denote the responses generally as C(x, y, z) although it may not be a three-variable function of all three coordinates. Such degeneracy due to the symmetry will be discussed subsequently. We denote the Green's function corresponding to the type of response under consideration as

G(x, y, z). Since the photon beam is normally incident on the tissue surface, the function G(x, y, z) possesses cylindrical symmetry. If the collimated photon beam as the source has the intensity profile S(x, y), the responses can be obtained through convolution (Prahl, 1988; Prahl *et al.*, 1989):

$$C(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x-x', y-y', z)\, S(x', y')\, dx'\, dy' \qquad (7.1a)$$

or through variable transformation with x'' = x – x' and y'' = y – y':

$$C(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(x'', y'', z)\, S(x-x'', y-y'')\, dx''\, dy'' \qquad (7.1b)$$

In Eq. 7.1a the Green's function is a function of the distance between the source point (x', y') and the observation point (x, y), where the distance is:

$$d' = \sqrt{(x-x')^2 + (y-y')^2} \qquad (7.2)$$

If the intensity profile S(x', y') of the source also has cylindrical symmetry, S(x', y') is only a function of the radius of the source point (x', y') with respect to the origin point of the coordinate system, where the radius is:

$$r' = \sqrt{x'^2 + y'^2} \qquad (7.3)$$

Therefore, Eq. 7.1a can be reformulated considering these symmetries:

$$C(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\sqrt{(x-x')^2 + (y-y')^2}\ , z)\, S(\sqrt{x'^2 + y'^2})\, dx'\, dy' \qquad (7.4a)$$

Similarly, Eq. 7.1b can also be reformulated with these symmetries:

$$C(x, y, z) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} G(\sqrt{x''^2 + y''^2}\ , z)\, S(\sqrt{(x-x'')^2 + (y-y'')^2})\, dx''\, dy'' \qquad (7.4b)$$

Since the response C(x, y, z) will have the same cylindrical symmetry, the problem can be more easily handled in a cylindrical coordinate system, where Eqs. 7.4a and 7.4b can be written:

$$C(r, z) = \int_0^\infty S(r')\, r' \left[\int_0^{2\pi} G(\sqrt{r^2 + r'^2 - 2rr'\cos\theta'}\ , z)\ d\theta' \right] dr' \tag{7.5a}$$

$$C(r, z) = \int_0^\infty G(r'', z)\, r'' \left[\int_0^{2\pi} S(\sqrt{r^2 + r''^2 - 2rr''\cos\theta''})\ d\theta'' \right] dr'' \tag{7.5b}$$

Eq. 7.5b is more advantageous than Eq. 7.5a in computation because the integration over θ'' is independent of z. This integration hence need only be computed once for all depths z. In some cases as presented subsequently, the integral over θ'' can be expressed analytically, therefore the two-dimensional integral is converted into a one dimensional integral.

The transformation of variables is illustrated in Fig. 7.1. The first coordinate system (r', θ', z) has its origin at the center of the source, as in Fig. 7.1A and Eq. 7.5a. The point of observation is at (r, 0). An incremental region of source is located at (r', θ') and has a value S(r'). The distance between the source point and the observation point is d' equal $\sqrt{r^2 + r'^2 - 2rr'\cos\theta'}$.

The second coordinate system (r", θ", z) has its origin at the center of the point of observation, as in Fig. 7.1B and Eq. 7.5b. The source is centered at (r, 0). The incremental region of source is located at (r", θ") and has a value S(d"), where d" equals $\sqrt{r^2 + r''^2 - 2rr''\cos\theta''}$. The distance between the source point and the observation point is r".

In the following sections, we will consider a Gaussian beam and a circularly flat beam as examples of cylindrical symmetry to further simplify Eq. 7.5b.

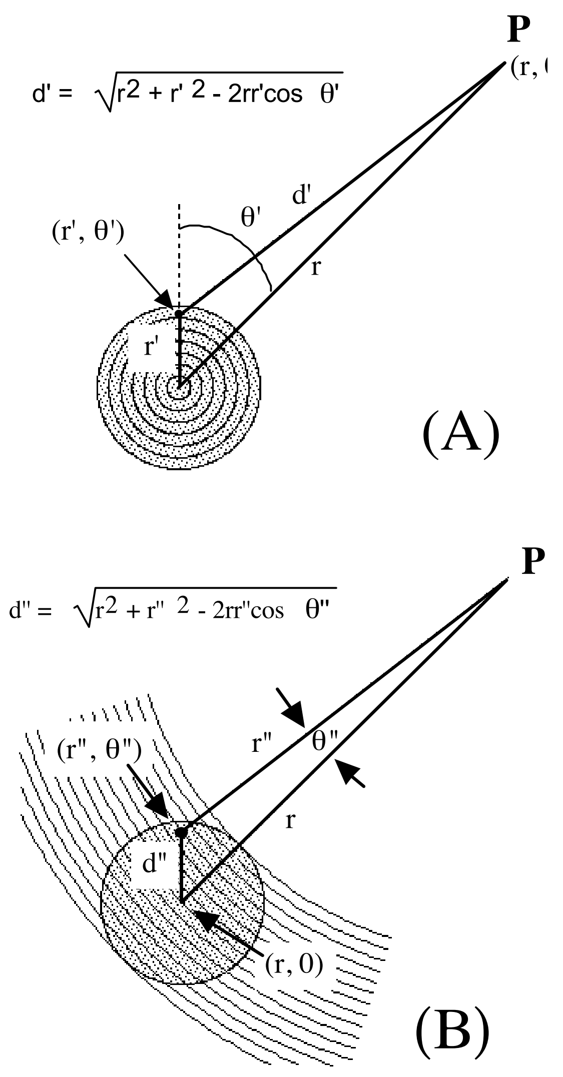
P
(r,
d' = $\sqrt{r^2 + r'^2 - 2rr'\cos\theta'}$
d'
θ'
(r', θ')
r
r'
(A)
P
d'' = $\sqrt{r^2 + r''^2 - 2rr''\cos\theta''}$
r''
θ''
(r'', θ'')
r
d''
(r, 0)
(B)

Fig. 7.1. Illustration of the transform between two coordinate systems. The stippled circle is the laser source and P is the point of observation. The circular lines schematically represent the integration of Eq. 7.5a (A) and Eq. 7.5b (B).

7.2 Convolution over Gaussian beams

In the case of a Gaussian beam, if the divergence is ignored, the above convolution can be applied. If the $1/e^2$ radius of the Gaussian beam is denoted by R, the beam intensity profile is:

$$S(r') = S_0 \exp(-2\,(r'/R)^2) \tag{7.6}$$

where the intensity in the center (r=0), S_0, is related to the total power P by:

$$S_0 = 2\,P\,/\,(\pi\,R^2) \tag{7.7}$$

Substituting Eq. 7.6 into Eq. 7.5b, the convolution becomes:

$$C(r, z) = S(r) \int_0^{\infty} G(r'', z)\exp(-2\,(r''/R)^2)\left[\int_0^{2\pi} \exp(4rr''\cos\theta''/R^2)\, d\theta''\right] r''dr'' \tag{7.8}$$

The integration in the square brackets resembles the integral representation of the modified Bessel function (Spiegel, 1968):

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \exp(x\,\sin\theta)\, d\theta \tag{7.9a}$$

which can be reformatted to be:

$$I_0(x) = \frac{1}{2\pi}\int_0^{2\pi} \exp(x\,\cos\theta)\, d\theta \tag{7.9b}$$

Eq. 7.8 can be written by substituting Eq. 7.9b into it:

$$C(r, z) = S(r) \int_0^{\infty} G(r'', z)\, \exp(-2\,(r''/R)^2)\, I_0(4rr''/R^2)\; 2\,\pi\, r''\, dr'' \tag{7.10}$$

where I_0 is the zero order modified Bessel function.

7.3 Convolution over circularly flat beams

If the photon beam is homogeneous within a radius R and collimated, the source function becomes:

$$S(r') = \begin{cases} P/(\pi R^2) & \text{if } r' \le R \\ 0 & \text{if } r' > R \end{cases} \tag{7.11}$$

where P is the total power of the beam. Substituting Eq. 7.11 into Eq. 7.5b, the convolution becomes:

$$C(r, z) = P/(\pi R^2) \int_0^\infty G(r'', z)\, I_\theta(r, r'')\, 2\, \pi\, r''\, dr'' \tag{7.12}$$

where the function $I_\theta(r, r'')$ is:

$$I_\theta(r, r'') = \begin{cases} 1 & \text{if } R \ge r + r'' \\ \frac{1}{\pi} \cos^{-1}((r^2 + r''^2 - R^2)/(2rr'')) & \text{if } |r - r''| \le R < r + r'' \\ 0 & \text{if } R < |r - r''| \end{cases} \tag{7.13}$$

From Eq. 7.13 and Fig. 7.1B, the limits of integration in Eq. 7.12 can be changed to a finite region:

$$C(r, z) = P/(\pi R^2) \int_a^{r+R} G(r'', z)\, I_\theta(r, r'')\, 2\, \pi\, r''\, dr'' \tag{7.14a}$$

where

$$a = \text{Max}(0, r - R) \tag{7.14b}$$

where the function Max takes the larger of the two arguments.

The circular lines in Fig. 7.1B illustrated the second case in Eq. 7.13 when the observation point P is outside of the source. When the point P is outside the source, the first case of Eq. 7.13 is never satisfied. Readers can similarly draw the pictures for the case where the point P is inside the source. Note that much of the region of integration lies outside the source and therefore the value of S in the integrand is zero.

As a special case of a circularly flat beam, we let the radius R approach infinity, which represents an infinitely wide flat beam. In this case the total power P also approaches infinity, but we can use the power density to describe the intensity of the beam. The convolution for this case can be accomplished by simply letting $R \rightarrow \infty$ and $P/(\pi R^2) \rightarrow S$, where S is the power density or irradiance (W/cm^2), in Eq. 7.14. $I_\theta(r, r'')$ will be 1 constantly. Eq. 7.14 becomes:

$$C(r, z) = S \int_0^\infty G(r'', z)\, 2\pi r''\, dr'' \tag{7.15}$$

7.4 Numerical solution to the convolution

In these two special cases of photon beams, the two-dimensional integrations are converted into one-dimensional integrations, which are significantly faster in numerical computation. Since the Monte Carlo simulation scores physical quantities to discrete grid points, the best choice of integration algorithm is the extended trapezoidal rule, which is written in C called `qtrap()` by Press *et al.* (1988). "Increased sophistication will usually translate into a higher order method whose efficiency will greater only for sufficiently smooth integrands. qtrap is the method of choice, e.g., for an integrand which is a function of a variable that is linearly interpolated between measured data points." Press *et al.* (1988) state.

The simplest choice of the integration is the summation of the integrand values at the original grid points multiplied by the grid separation. However, this approach does not have any control over the integration accuracy. For a given accuracy, sometimes this approach gives more accuracy than required, which is a waste of computation time, and sometimes it gives less accuracy, which does not meet the expectation. For example, the number of original grid elements in the r direction is 50, and we want to convolve the responses over a circularly flat beam with a radius of R which is about 5 Δr, where Δr is the grid separation in the r direction. To compute C(0, z) in Eq. 7.14a, the integral range, from 0 and R, only covers 5 Δr. This means only 5 function evaluations will be completed, which may yield unacceptable answer. On the contrary, the extended trapezoidal rule does the right amount of computation until it reaches the user specified accuracy.

We have slightly modified the original function `qtrap()` so that it takes the required degree of accuracy as an argument. Therefore, the users of the program `conv` can change the allowed error at run time (the program `conv` is to be discussed in the next section).

The sequence of integrand evaluations used in the extended trapezoidal integration is shown in Fig. 7.2. (Press *et al.*, 1988) If we are integrating f(x) over [a, b], we evaluate f(a) and f(b) in the first step as noted by 1 and 2 in Fig. 7.2. This step will not give sufficient accuracy unless the function if linear. To refine the grid, we evaluate f((a+b)/2) in the second step as noted by 3. We continue this process until the integration evaluation reaches the specified accuracy.

Note that the sequence of integrand evaluation after the third evaluation in Fig. 7.2 resembles a perfectly balanced binary tree. If we want to store the evaluated function values, it is natural to store them in a binary tree for speed retrieval (to be discussed subsequently).

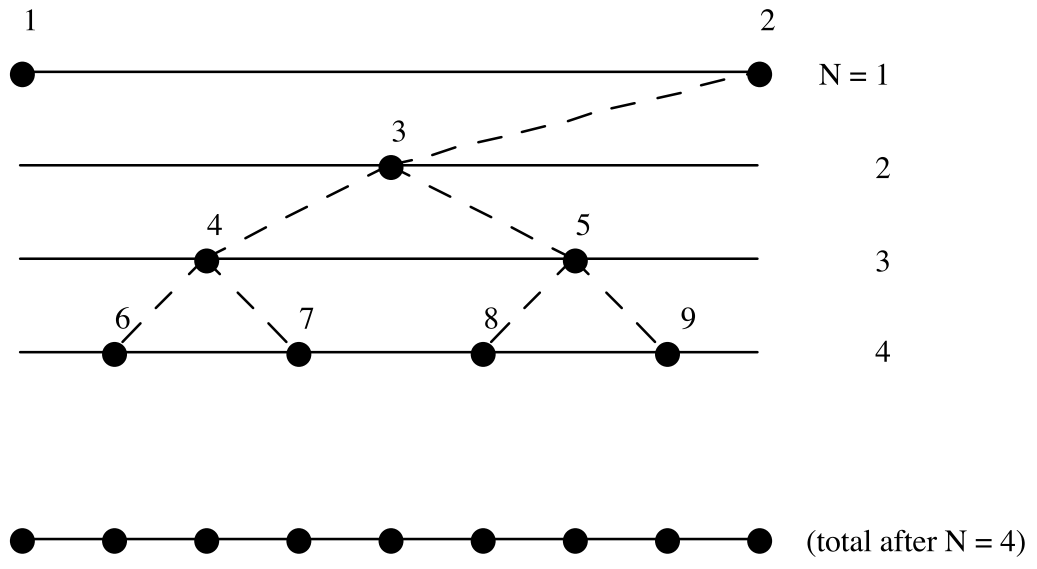

Fig. 7.2. Illustration of integrand evaluation sequence in trapzd() called by qtrap(). "Sequential calls to the routine trapzd() incorporate the information from previous calls and evaluate the integrand only at those new points necessary to refine the grid. The bottom line shows the totality of function evaluations after the fourth call." (Press *et al.*, 1988) The sequence of integrand evaluation after the third evaluation resembles a perfectly balanced binary tree.

Interpolation and extrapolation of physical quantities

As shown in Fig. 7.2, the function `qtrap()` will need to evaluate the integrand,

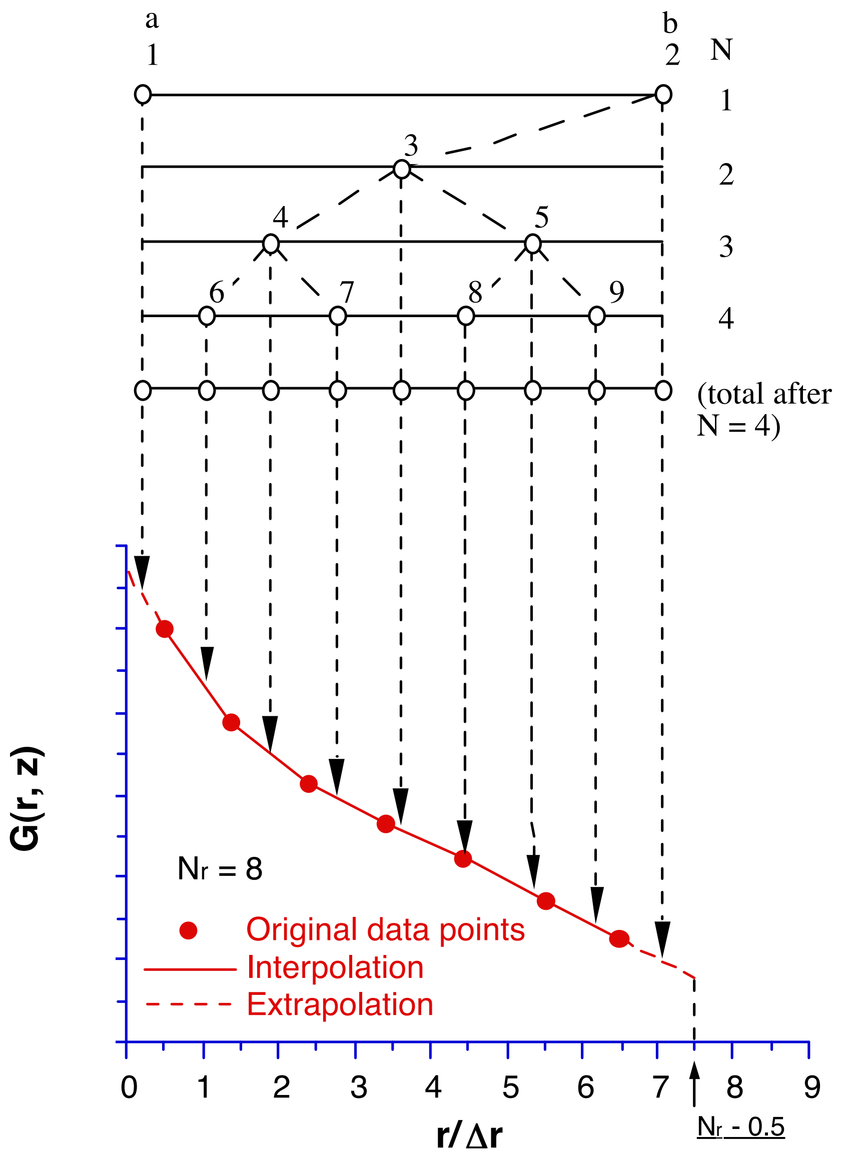

Fig. 7.3. Illustration of the interpolation and extrapolation of the physical quantities. As an example, the number of grid elements in the r direction N_r is set to 8. Δr is the grid separation in the r direction. The integral limits are a and b (see Eqs. 7.21 & 7.22). The arrows point to the places where the integrand is evaluated.

hence the physical quantities, at points which may not be the original grid points. Linear interpolations are used for those points that fall between two original grid points. Linear extrapolations are used for those points that fall beyond the original grid system. The interpolation and extrapolation are illustrated in Fig. 7.3. The solid circles represent the original score values at the grid points. The solid lines and the dashed lines represent the interpolation and extrapolation respectively. For a given number of grid elements in the r direction (e.g., $N_r = 8$ in this picture), the extrapolation is only computed up to $(N_r - 0.5)$ because the linear extrapolation can be unreliable for points beyond $(N_r - 0.5)$. Therefore, the physical quantity is set to zero beyond $(N_r - 0.5)$. Sometimes, the data may be so noisy that the function at the last point is even higher than the function at the second to the last point. In this case, the extrapolation is not used. Instead, we simply set the function values to zero. Note that as we mentioned in the beginning of Chapter 4, the last cells in the r direction are used to collect the photons that do not fit into the grid system. Therefore, the values in the last cell are usually much higher than the values in the second to the last cells, and hence are not used in the convolution process. In a word, the physical quantities are non-zero in the interval $[0, r_{max}]$, where r_{max} is:

$$r_{max} = (N_r - 0.5)\,\Delta r \tag{7.16}$$

where Δr is the grid separation in the r direction.

<u>Integrand evaluation for Gaussian beams</u>

As shown in Eq. 7.10, the evaluation of the physical quantities is only part of the integrand evaluation for convolution over the Gaussian beam. Although the integration has to converge due to physical reasons, the form of Eq. 7.10 may not be directly computed numerically because the modified Bessel function increases rapidly as the argument increases, and it can exceed the limit which the computer can hold (e.g., 10^{+38} for some computers). Therefore, a proper reformulation is required to compute Eq. 7.10. We note that the modified Bessel function in the region where the argument is large has the following approximation:

$$I_0(x) \approx \exp(x) / \sqrt{2\,\pi\,x} \qquad \text{for large x} \tag{7.17}$$

Therefore, if we extract the exponential term from $I_0()$, we can make sure the modified Bessel function decreases as the argument increases. We define the following new function based on $I_0()$:

$$I_{0e}(x) = I_0(x)\exp(-x) \tag{7.18a}$$

or

$$I_0(x) = I_{0e}(x)\exp(x) \tag{7.18b}$$

$I_{0e}()$ should always be bounded. Note that Eq. 7.17 is presented just to show the asymptotic behavior of the function $I_0()$. Eq. 7.18a by no means carries any approximations. Substituting Eqs. 7.6, 7.7 and 7.18b into Eq. 7.10, it becomes:

$$C(r, z) = \frac{4P}{R^2}\int_0^{\infty} G(r'', z)\exp\left[-2\left(\frac{r''-r}{R}\right)^2\right] I_{0e}\left(\frac{4rr''}{R^2}\right) r''\,dr'' \tag{7.19}$$

Since both the exponential term and the $I_{0e}()$ term decrease, the integrand can be computed without being out of bound.

Up to now, we have just solved the problem of how to compute the convolution without overflow. However, the computation speed is another issue. We found that the evaluation of the exp() $I_{0e}()$ in Eq. 7.19 is a major part of the computation for each integration, which can be up to 90% depending on the specific problem being solved. For multi-variant physical quantities (e.g., A(r, z)), the convolution may repeatedly evaluate the exp() $I_{0e}()$ in Eq. 7.19 at the same point as the integration is computed for different z coordinates.

Therefore, if we can save the function evaluations, i.e. the computations of exp() $I_{0e}()$ in Eq. 7.19, for one z coordinate, then we can save a lot computation time. However, the integration is executed iteratively until a given precision is reached. Hence, the number of function evaluations is unknown in advance. We can only save the function evaluations with dynamic data allocation. Furthermore, since the evaluation sequence of the trapezoidal integration `qtrap()` resembles a binary tree as in Fig. 7.2., a well-balanced binary tree can be used to store the function evaluations for searching speed.

Integral Limits for Gaussian beams

Since the integral limits in Eq. 7.14a for circularly flat beams are finite, the integration can be computed directly using the function `qtrap()`. In contrast, the upper integral limit in Eq. 7.19 for Gaussian beams is infinity. This problem can be solved using variable transformation and the integration can be computed by the routine `midexp()` (Press *et al*., 1988). However, we found this approach is not computationally efficient. We can reduce the upper limit to a finite value by properly truncating the exponential term in Eq. 7.19. When

$$|r'' - r| \le K\,R \qquad (7.20a)$$

or

$$r - K\,R \le r'' \le r + K\,R \qquad (7.20b)$$

where K is a constant which can be set in the convolution program `conv`, we compute the integrand, otherwise we think the integrand negligible. For example, if we choose K equal to 4 (which is actually used in the program), the exponential term in Eq. 7.19 is about $1\text{x}10^{-14}$ whose order of magnitude is considerable larger than the dynamic range of the order of magnitude of the scored physical quantities.

As we discussed in the beginning of this section, we only compute the physical quantities in the interval $[0, r_{max}]$, where r_{max} is given by Eq. 7.16. Combining this limit and Eq. 7.20b, Eq. 7.19 becomes:

$$C(r, z) = \frac{4\,P}{R^2} \int_a^b G(r'', z) \exp[-2\,(\frac{r''- r}{R})^2]\; I_{0e}(\frac{4rr''}{R^2})\; r''\, dr'' \qquad (7.21a)$$

$$a = \text{Max}(0,\; r - K\,R) \qquad (7.21b)$$

$$b = \text{Min}(r_{max},\; r + K\,R) \qquad (7.21c)$$

where the functions Max() and Min() take the greater and the lesser of the two arguments respectively.

<u>Integrand evaluation for circularly flat beams</u>

The integrand evaluation for circularly flat beams is much simpler than that for Gaussian beams. However, the evaluation of $I_\theta()$ in Eq. 7.14a is time-consuming. Similar to the integrand evaluation for Gaussian beams, a binary tree is used to store the evaluated $I_\theta()$ to speed up the integration (see the discussion for Gaussian beams).

Integral Limits for circularly flat beams

Since the integral limits in Eq. 7.14a for circularly flat beams are finite, the integration can be computed directly using the function `qtrap()`. As we discussed in the beginning of this section, we only compute the physical quantities in the interval $[0, r_{max}]$, where r_{max} is given by Eq. 7.16. Considering this limit, Eq. 7.14a becomes:

$$C(r, z) = P/(\pi R^2) \int_a^b G(r'', z)\, I_\theta(r, r'')\, 2\, \pi\, r''\, dr'' \qquad (7.22a)$$

$$a = \mathrm{Max}(0,\ r - R) \qquad (7.22b)$$

$$b = \mathrm{Min}(r_{max},\ r + R) \qquad (7.22c)$$

where the functions Max() and Min() take the greater and the lesser of the two arguments respectively.

Source of error in convolution

In Eqs. 7.21c and 7.22c, the upper limit of the integration may be limited by r_{max} which is the grid limit in the r direction during the Monte Carlo simulation. The physical quantities beyond the original grid limit in the r direction do not contribute to the convolution, which leads an error.

Let us discuss the case for circularly flat beams first because it is easier. From Eq. 7.22c, we know that when

$$r_{max} \geq r + R \qquad (7.23a)$$

or

$$r \leq r_{max} - R \qquad (7.23b)$$

the limited grid in the r direction does not affect the convolution. Otherwise, the convolution is truncated by the limited grid in the r direction. This effect can be see in the next section. Therefore, we should not trust the convolution data for $r \geq r_{max} - R$. In other words, if you want to observe the physical quantity at r in response to a circularly flat beam of radius R, the grid limit in the r direction should be large enough so that Eq. 7.23a holds when you perform the Monte Carlo simulation with mcml.

For Gaussian beams, there are no clean formulas like Eqs. 7.23 to describe the valid range because the Gaussian beams theoretically extend to infinity in the r direction. However, the convolution results of a Gaussian beam with a $1/e^2$ radius of R is so close to those of a circularly flat beam with a radius of R for r >> R (shown in the next section). Therefore, we can use the same criteria for circularly flat beams (Eqs. 7.23) for Gaussian beams to certain precision.

The other source of error is due to the Monte Carlo simulation by mcml 1.0. This version of mcml does not score the first interactions separately (see Section 4.3) as Gardner *et al*. (1992b) did. This may make considerable error if the radius of the Gaussian beam is less than three times the grid separation Δr. In other words, the following equation should be satisfied to get reliable convolution:

$$R \geq 3\ \Delta r \tag{7.24}$$

In summary, when Eqs. 7.23 and 7.24 hold, the convolution should be reliable.

7.5 Computation results of conv and verification

The convolution process of the Monte Carlo simulation results from mcml is implemented in another program called "conv". Like the program mcml, it is written in ANSI Standard C, hence it can be executed on a variety of computers.

Convolution results of Gaussian beams

We do not have any standard data to verify the convolution program. However, Craig Gardner kindly provided some convolution results using his convolution program (Gardner *et al*., 1992). The impulse responses are based on the simulation discussed in Section 6.6 where we have used the same turbid media and grid system. He computed his convolution on his Monte Carlo simulation results, and we did it on ours after we compared the Monte Carlo simulation results in Section 6.6.

The incident photon beam is a Gaussian beam with total energy of 1 J and radius of 0.1 cm. The convolved diffuse reflectances and transmittance are compared in Figs. 7.4 and 7.5 respectively. The convolved fluences are compared in Fig. 7.6. Note that the curves in Figs. 7.4-6 bend down faster near r equal 0.5 cm. This can be explained by the integrations in Eqs. 7.21. Due to the spatially limited range of the grid system (50 radial grids of 0.01 cm spacing, or r_{max} = 0.5 cm), the upper limit of the integration is cut by r_{max} more and more as the observation point r approaches r_{max}. Therefore, the integration underestimates the true value.

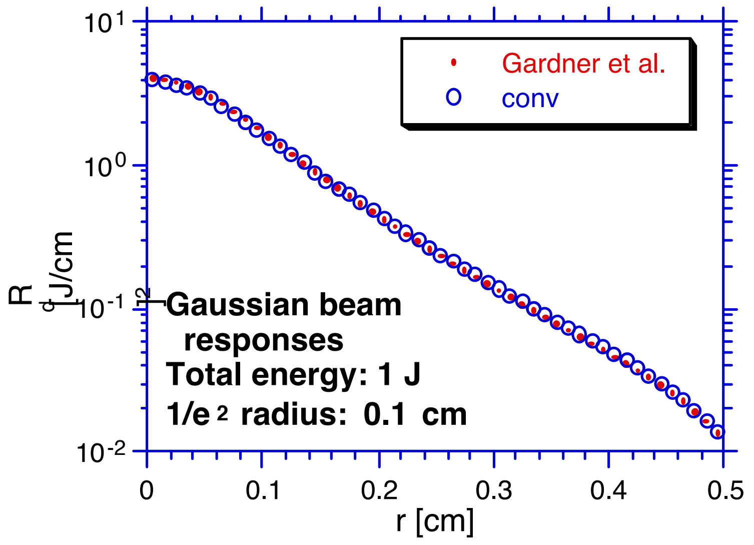

Fig. 7.4. Comparison between diffuse reflectances as a function of r based on conv and Gardner's computation (Gardner *et al*., 1992).

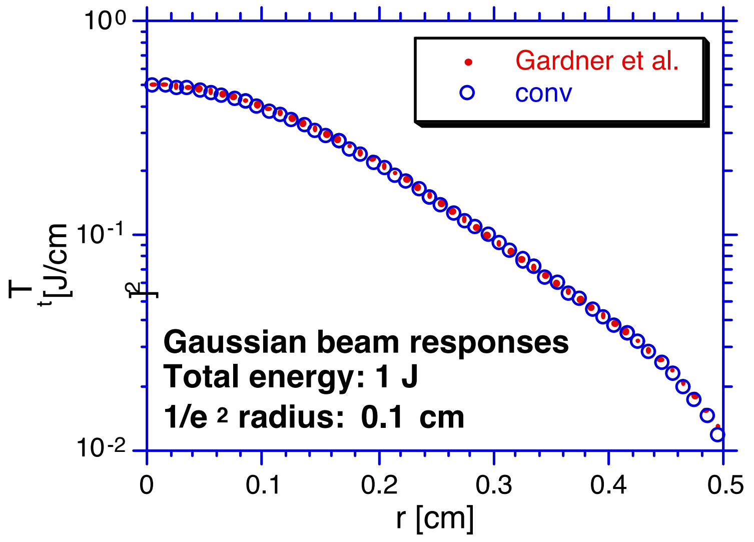

Fig. 7.5. Comparison between transmittances as a function of r based on conv and Gardner's computation (Gardner *et al.*, 1992).

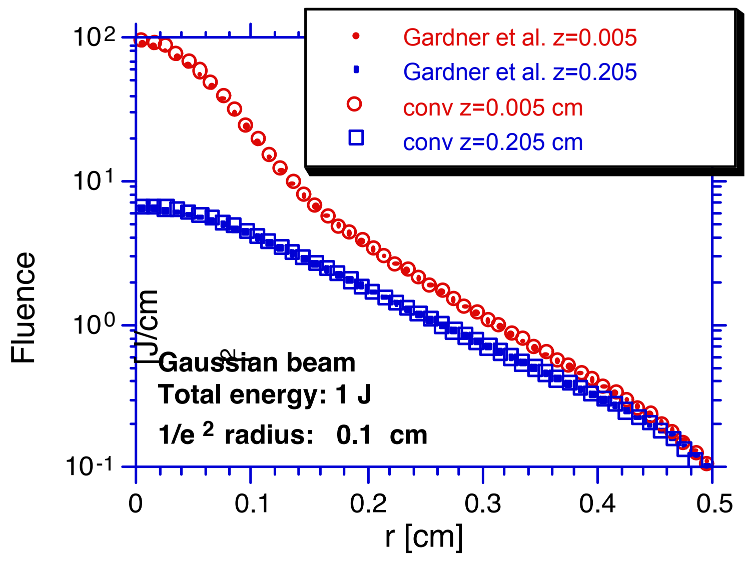

Fig. 7.6. Comparison between fluences as a function of r for given z coordinates based on conv and Gardner's computation (Gardner *et al.*, 1992).

For 2D arrays such as the fluence as a function of r and z, conv has the ability to output the data in contour format (see Sections 10.9 and 10.10). The fluence as a function of r and z of the Gaussian beam is shown in contour lines in Fig. 7.7.

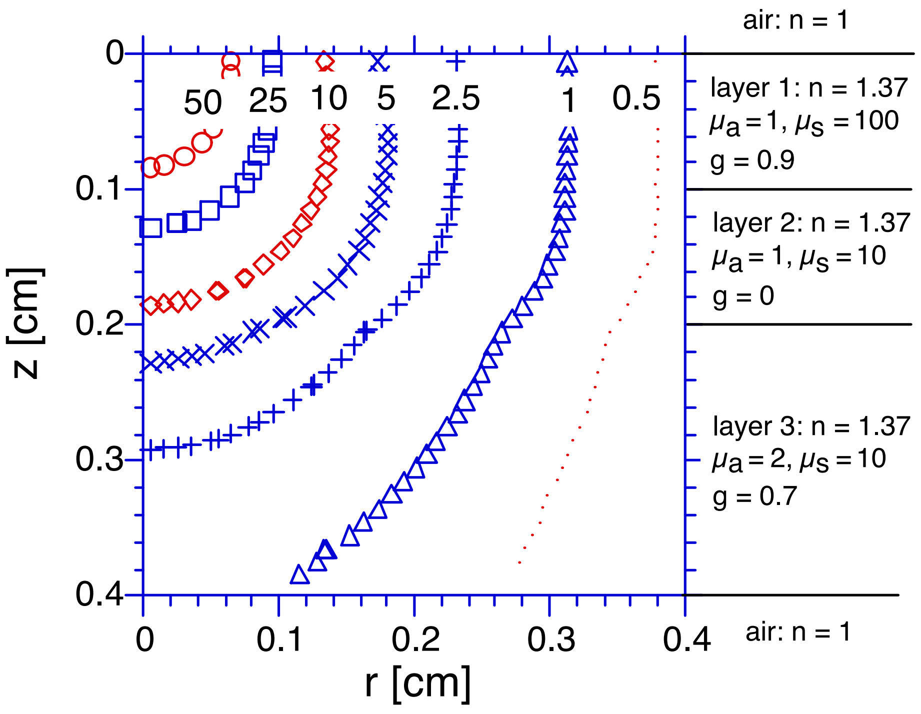

Fig. 7.7. Contour plot of the fluence [J cm^{-2}] as a function of r and z based on conv for a Gaussian beam. The Gaussian beam has total energy of 1 J and 1/e^2 radius of 0.1 cm. The Monte Carlo simulation is for a three-layer tissue of Table 6.6. The absorption coefficient μ_a and scattering coefficient μ_s are in cm^{-1}.

Convolution results of circularly flat beams

For circularly flat photon beams, we do not have other results for comparison. However, we would like to compare the results of circularly flat photon beams with that of Gaussian beams. The results of Gaussian beams are taken from the above computations. The circularly flat beam has 1 J of total energy and 0.1 cm of radius. The diffuse reflectances, transmittances and fluences are compared respectively in Figs. 7.8, 7.9, and 7.10.

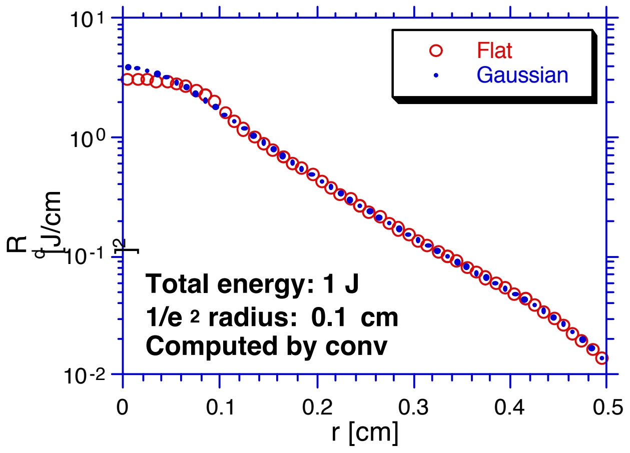

Fig. 7.8. Comparison between diffuse reflectances as a function of r convolved over a Gaussian beam and a flat beam using conv. Both beams have total energy of 1 J and radii of 0.1 cm.

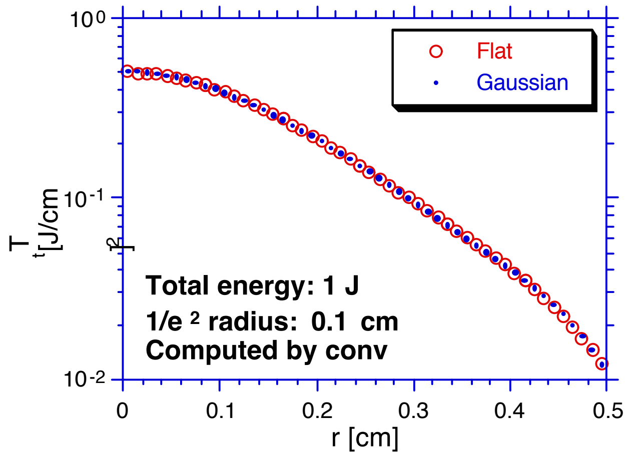

Fig. 7.9. Comparison between transmittances as a function of r convolved over a Gaussian beam and a flat beam using conv. Both beams have total energy of 1 J and radii of 0.1 cm.

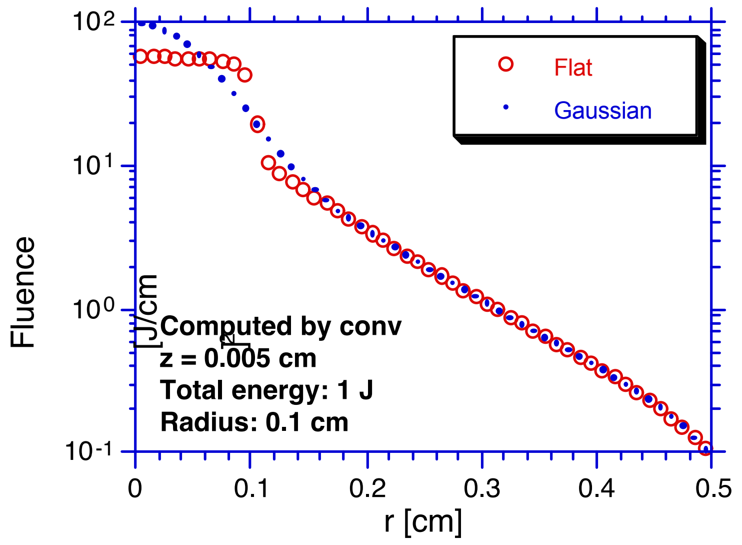

Fig. 7.10. Comparison between fluences as a function of r at z equal 0.005 cm convolved over a Gaussian beam and a flat beam using conv. Both beams have total energy of 1 J and radii of 0.1 cm.

It is observed that the Gaussian beam and the flat beam give nearly the same results when r is larger than about 2 R, where R is the radius of the beams. Furthermore, both kinds of responses bend down when r approaches 0.5 cm which is the grid limit in the r direction as discussed in last section.

Convolution error

The convolution integration is computed iteratively. The iteration stops when the difference between the new estimate and the old estimate of the integration is a small part of the new estimate. This small ratio can be controlled by users using command "e". It ranges between 0 to 1. Small values would give better precision but longer computation time and vice versa. Normally, 0.001 to 0.1 is recommended. Sometimes, a high allowed error can cause some discontinuity in the convolved results. If this happens, choose a lower allowed convolution error and redo the convolution. For example, the convolution over a Gaussian beam in Fig. 7.10 has been done with an allowed convolution error of 0.001. If we choose the allowed convolution error to be 0.01, we can see the discontinuity in the fluence distribution (Fig. 7.11).

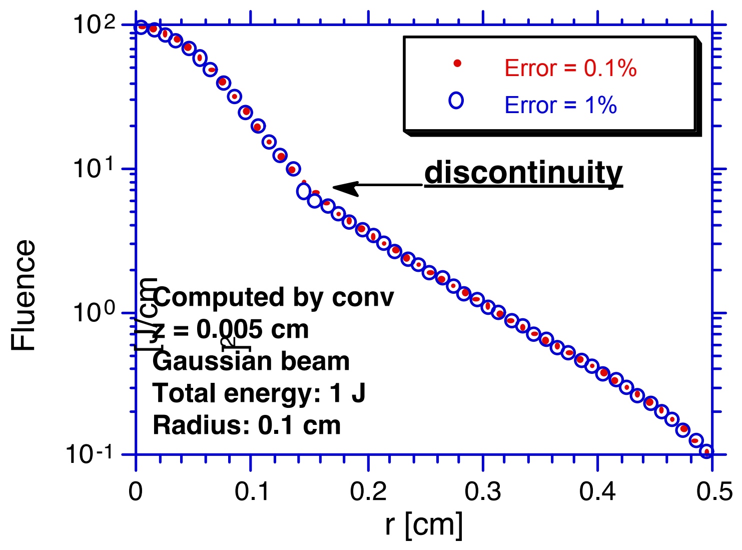

Fig. 7.11. Comparison between fluences as a function of r at z equal 0.005 cm convolved over a Gaussian beam with different allowed convolution errors using conv. The result with allowed error of 0.01 has discontinuity around r = 0.15 cm. Using an allowed error of 0.001 eliminates the discontinuity. The Gaussian beams have total energy of 1 J and 1/e^2 radii of 0.1 cm.

Part II. User Manual

8. Installing mcml and conv

This chapter provides the instructions on how to install the software. Since both mcml and conv are written in ANSI Standard C, they in principle should be able to be compiled on any computer systems that support ANSI C. Subject to the computer systems available to this laboratory, we will only provide the executables for Sun workstations, IBM PC compatibles, and Macintoshes. On Sun SPARCstations 2, we have compiled the mcml and conv using the ANSI C (acc). On IBM PC compatibles, we used Microsoft QuickC. And on Macintoshes, we used Symantec THINK C. We will provide the source code, users can feel free to compile them on their computer systems. Consult corresponding manuals for information on how to compile the code.

As Monte Carlo simulations are computationally intensive, we suggest that you use workstations such as Sun SPARCstations on which you can submit background jobs and which provide high speed computation. The convolution program is also more pleasant to use if you have a fast computer, although it is not as computation-intensive as Monte Carlo simulations.

8.1 Installing on Sun workstations

The distribution disk is an IBM format double density 3 1/2" disk, which Sun SPARCstation 2 should be able to read. All the files are packed into one file. Copy the file mcR1_1.tar to a working directory using the command: `mcopy a:mcR1_1.tar .`, where the period means the current directory, and then untar the file using the command: `tar -xvfo mcR1_1.tar`.

The package includes three directories: mcmlcode, convcode, and Sun. The directory mcmlcode includes all the source code of mcml and the makefile used for acc. The directory convcode (not provided this time) includes all the source code of conv and the corresponding makefile. You need to modify the makefiles for other compilers (See Appendix C). The directory Sun includes all the executables, a template file of mcml input (template.mci), a sample mcml output file (sample.mco), and a short manual (mcmlconv.man) which is Chapter 8-10 of this manual.

To install the executables, copy the executables to the sub directory ~/bin under your home directory. Then, put the directory ~/bin under the search path in .cshrc or .login if you are using C Shell. Consult manual if you are using other shells.

Having finished copying, you can eject the disk using the command eject. If your Sun workstation does not have a floppy drive, you can transfer the files through a networked IBM PC or a compatible. If you have an electronic mail address, we can also send the package to you through mail.

8.2 Installing on IBM PC compatibles

For IBM PC's or compatibles, the distribution disk is a double density 3 1/2" disk. An alternative 5 1/4" disk can be sent upon request. All the files are packed into one file. Copy the self-extracting file mcR1_1.exe to your working directory on your hard drive and run the file to extract all packed files using the command: `mcR1_1.exe -d`, where the option "-d" keeps the directory structure.

The package includes three directories: mcmlcode, convcode, and IBMPC. The directory mcmlcode includes all the source code of mcml. The directory convcode (not provided for now) includes all the source code of conv. The directory IBMPC includes all the executables, a template file of mcml input (template.mci), a sample mcml output file (sample.mco), and a short manual (mcmlconv.man) which is Chapter 8-10 of this manual. The executables include mcml.exe and conv.exe. The code was compiled and linked using Microsoft QuickC 2.5. The executables will be able to detect whether your computer has math coprocessor, and take advantage of the math coprocessors if they are present.

If you want to be able to execute the programs under any directory, you should put the directory IBMPC in the search path. The search path can be changed in the file autoexec.bat.

8.3 Installing on Macintoshes

For Macintoshes, the distribution disk is a double density 3 1/2" disk. All the files are packed into one file. Copy the self-extracting file mcR1.1.sea to a working folder on you hard drive, and double click on the icon to extract the files.

The package includes three folders: mcmlcode, convcode, and Mac. The folder mcmlcode includes all the source code of mcml. The folder convcode includes all the source code of conv. The folder Mac includes all the executables, a template file of mcml input (template.mci), a sample mcml output file (sample.mco), and a short manual (mcmlconv.man) which is Chapter 8-10 of this manual. The executables include mcml.fpu, conv.fpu, mcml.020, conv.020, mcml.000, and conv.000 for different types of computers as discussed subsequently.

Before you install the executables, you need to know what kind of Macintosh you are using. You can test the following conditions to decide which executables to use:

A. MC68040

B. MC68020 or MC68030

C. MC68881 or MC68882

If your Macintosh meets condition A, or conditions B and C, you should copy the executables with extensions ".fpu". If your Macintosh meets condition B only, you should keep the executables with extensions ".020". Otherwise, you should use the executables with extensions ".000". We suggest that you remove the extensions of the executables on your hard drive to keep consistency with the manual.

8.4 Installing by Electronic Mail

For these users who have electronic mail access on UNIX machines, we can deliver the software package through electronic mails. The package is archived using the command tar, compressed using the command compress, then encoded using the command uuencode before it is mailed out using the mail utilities. After you receive the mail, you need to do the following.

1. Save the mail as a file, e.g., mc.mail.

2. Decode the file (mc.mail) to get a file named mc.tar.Z using
   ```
   uudecode mc.mail
   ```

3. Uncompress the file mc.tar.Z to get the file mc.tar
   ```
   uncompress mc.tar.Z
   ```

4. Unarchive the file mc.tar to get the package using:

```
tar -xvfo mc.tar
```

At this moment, you should have three directories under the working directory. They are mcmlcode, convcode, and Sun, or IBMPC, or Mac.

If you ordered a Sun version of the package, you only need to put the executables under the proper directory., e.g., ~/bin (see Section 8.1).

If you ordered an IBM PC version or a Mac version of the package, you need to transfer the files to your local computer using FTP or modem. Then refer to Section 8.2 or 8.3 for details.

It is appropriate to describe in more detail how we send the package through electronic mails which is exactly the opposite of the above procedure. We put the package in a working directory which include three subdirectories: mcmlcode, convcode, and Sun, or IBMPC, or Mac. Then:

```
tar -cvf mc.tar

compress mc.tar

uuencode mc.tar.Z mc.tar.Z > mc.mail

mail your_address
```

In the mail utility, you can add in any messages in the beginning of the mail, then you need to use the command r to read in the file mc.mail. Then, you can send the file by typing a period "." and a return in a new line (see the manual page of mail).

9. Instructions for mcml

This chapter describes the actual instructions to use mcml. Macintoshes, IBM PC compatibles and UNIX machines are used as examples of computer systems, although mcml can execute on any computer systems that support ANSI Standard C. The reader is assumed to be familiar with the operating system and comfortable with at least one of the text editors on the computer system to be used to execute mcml. Three steps involved in the Monte Carlo simulation using mcml are included in the following sections: preparing the input data file, executing the program mcml with the input data file, processing the output data in the data files named in the input data file. We will also show some known bugs.

9.1 File of input data

The first step to do the simulation using mcml is to prepare an input data file (e.g., "filename.mci"). Any valid filenames on your system without spaces will be acceptable, but extension ".mci" is recommended. In ANSI C, spaces are used as separators. Therefore, filenames with spaces may not be accepted by mcml, although they are allowed by some operating systems themselves such as the Macintosh System. We will use "filename.mci" as an example in the following discussions.

This input data file may be edited with any text editors such as Apple Edit, MockWrite or Microsoft Word on Macintoshes, Norton editor NE or Microsoft Word on IBM PC compatibles, vi editor or EMACS on UNIX systems. However, if you use word processors like Microsoft Word to edit the file, make sure that you save the file in text format since mcml does not accept binary files as input. If you are using the UNIX system and are uncomfortable with vi or other editors available on UNIX, you can use editors on your personal computer, then transfer the file using Kermit if you use modem or FTP if your personal computer is on a network. Make sure to use ASCII or text mode when you transfer this file.

The best way to write an input data file is to make a copy of the template file called "template.mci" (See Appendix D), then modify the parameters in the file. The input data file is organized line by line. All parameters must be in the right order. The lines with parameters in order must also be in order themselves. However, feel free to insert comment lines or space lines in between to make the file more readable. Comment lines start with the symbol "#". The symbol "#" can also be used after the parameters in a line to mark the start of comments.

The parameters in the input data file are read by mcml line by line. If there are multiple parameters in a line, use tabs or spaces to separate them. A tab is preferred, because it aligns the parameters for better readability. All dimensional quantities are in cm or derived from cm. The thickness of each layer is in cm. The grid line separations are also in cm. Absorption coefficient and scattering coefficient are in 1/cm. Each line of the input file is explained in the order that they appear in the input data file as follows.

1. File version of the input data file. Always use "1.0" for now.

2. Number of runs (integer). Each run is an independent simulation. You can specify any number of runs, which is not subject to memory limit. Make sure you use an integer instead of a floating point number for this parameter, e.g., 5 instead of 5.0.

3. Output filename and file format. Extension ".mco" is recommended for the output filenames, e.g., "output1.mco". The program mcml currently only supports ASCII format, therefore always use "A" as the second parameter in this line. Make sure that you use different output filenames if you have multiple runs in an input data file, although mcml checks for this mistake. What is more important is that the filenames should not be the same as the names of existent ones unless you want to overwrite the existent files on purpose. Since the program mcml does not check this error, you will lose the existent files.

4. Number of photon packets to be traced (integer).

5. Separations (in cm) between grid lines in z and r direction of the cylindrical coordinate system. These are floating point numbers. Both z and r originate from the photon incident point on the surface of first layer, and the z axis points down into the turbid medium. Make sure these parameters are large enough to give you an acceptable variance, and small enough to give you an acceptable resolution. These parameters should be determined coordinately with the number of photons to achieve both accuracy and resolution. Also note that users should try to choose grid size in the z direction so that grid boxes do not cross tissue-tissue interfaces or boundaries (see Section 9.5).

6. Number of grid elements (integers) in the z, r directions of the cylindrical coordinate system and in the alpha direction, where alpha is the angle spanned between the photon exiting direction and the surface normal. Since the angle always covers 0 through 90 degrees, the angular separation is 90 degrees divided by the number of angular grid elements specified in this line. Be careful with this line, if the numbers are too large, the output file will be very big because 2D arrays are written into the output file. If you do not need to resolve one of the directions (z or r) or the angle, use 1 (not 0) for that parameter. Make sure to use integers for these three parameters.

7. Number of layers (integer). This number does not include the ambient media above or below the tissue.

8. Refractive index for the top ambient medium above the first layer (e.g., 1.0 for air).

9. Layer parameter lines. One line for each layer. In each line are the refractive index, the absorption coefficient (1/cm), the scattering coefficient (1/cm), the anisotropy factor, and the thickness (cm). To simulate semi-infinite tissue, use a very large thickness (e.g., 1E8 cm) compared with the mean free path of the tissue.

10. Refractive index for the bottom ambient medium below the last layer (e.g., 1.0 for air).

11. Repeat lines 3 through 10 for each additional run if you have multiple runs.

Note: Two points are worth noting. The only limit to the number of grid elements and layers is the amount of memory allocated to mcml in your system because the arrays are dynamically allocated according to these parameters. Do not use floating point numbers for the integers. Otherwise, the program may interpret them incorrectly. However, you may use integers for floating point numbers, e.g., 100 instead of 100.0.

9.2 Execution

Once the input data file is prepared, the program mcml can be executed using the input data file. During the execution, the program mcml will report an output message which gives the number of photons remaining in the simulation, the number of runs left, and the time of ending the job. The first report is after 10 photon packets are traced, then it is updated when every 1/10 of the total number of photon packets are traced. The methods of execution are slightly different on different operating systems.

Macintosh

To run mcml on Macintosh System 6, you have to copy or move the executable mcml to your working folder where the input data file resides, then double click on the mcml icon to start the program. The program mcml will prompt for the input data filename, which is entered through the keyboard. If the input data file cannot be found, the program will prompt you again until it finds the file or a period "." is typed, where "." is used to abort the program. If you use Macintosh System 7, you may use an alias of mcml instead of a copy of it.

IBM PC compatibles

For IBM PC compatibles, make sure that the directory with mcml is in the search path, which can be checked by typing the command "path" or the file "autoexec.bat". To run mcml with the input data file as a command parameter under DOS command prompt, type:

```
mcml filename.mci
```

If you want to save the output message as a file (e.g., message.out), type:

```
mcml filename.mci > message.out
```

which redirects the output message to the file "message.out". To run mcml in the interactive mode, type the following command without input data filename:

```
mcml
```

Then, the program mcml will prompt for the input data file.

UNIX

On a UNIX system, you should place the executable mcml in a directory that is in the search path. The directory ~/bin is a good choice. The search path can be found and modified in the file ".cshrc" if you are using C Shell or the file ".login". The three ways of invoking mcml under DOS can be used under UNIX operating systems. Moreover, if you wish to discard the messages during the execution, use the command:

```
mcml filename.mci > /dev/null
```

which redirects the output to the "bit bucket" (/dev/null). You can also simply submit a background job using:

```
mcml filename.mci > /dev/null &
```

Refer to your UNIX manual for how to inquire about the status of a background job. If you are still in the same session, the command "jobs" can be used in C Shell. Otherwise, you should use the UNIX command "ps" to check for background processes. You can also directly look for the output files to check if the job is done.

9.3 File of output data

When the job is completed, the results will be written into the output data files as you named in your input data file. A sample output data file is shown in Appendix E. The output data files can be read with any text editors if they are ASCII as a result of using "A" for the file format in the input data file. They may be big if your numbers of grid elements are large.

The contents of output files are self explanatory. The same policy for the input data file is used for the output data file, that is, comment lines starting with a symbol "#" and space lines are written to the file for clarity. The first line is used for file type identification when the file is read by other applications. Then, the user time spent on the simulation is reported in a comment line. Then, a few categories of data are reported sequentially in the following order: pure numbers, 1D arrays and 2D arrays. The definitions of the output data can be found in Chapter 4. The category "InParm" reports all the input parameters specified in the input data file again so that the output file is a complete reference and the input parameters may also be double checked against any errors in the input data file. The category "RAT" reports the specular reflectance, the total diffuse reflectance, the total absorption, and the total transmittance. The category "A_l" is the absorption as a function of layer. The category "A_z" is the absorption as a function of depth z. The categories "Rd_r" and "Rd_a" are the diffuse reflectances as a function of radius r and angle alpha respectively. The categories "Tt_r" and "Tt_a" are the transmittance as a function of radius r and angle alpha respectively. The 2D arrays A_rz, Rd_ra, and Tt_ra are then reported. The category A_rz is the absorption as a function of depth z and radius r. The categories Rd_ra and Tt_ra are correspondingly the diffuse reflectance and transmittance as a function of radius r and angle alpha. The name of each category is written before the data, such that the data can be easily identified. The units for these data were discussed in Chapter 4.

9.4 Subset of output data

Sometimes, only a subset of the output data is needed for presentation or processing. For example, we may need to print a 1D array into a file in XY format, namely two columns of data, or a 2D array in XYZ format. These files can then be read into some commercial applications such as AXUM on IBM PC compatibles and KaleidaGraph on Macintoshes. This subset extraction can be done using another program -- conv. The program conv is intended to read in the output data file of mcml that gives responses of infinitely narrow photon beam, and convolve the output data if the responses of finite size beam are to be computed. The program conv can output the original data or the convolved data in various formats. The convolution part of the program conv has not been finished, although it can be used to extract subsets of the original output data.

The program conv is made to be interactive. After the program is invoked, the menu system will direct the data input, output, or process. On Macintosh, copy or move the program conv to your working folder. Start conv by double clicking on the icon. On IBM PC compatibles or UNIX machines, invoke the program conv by typing:

```
conv
```

Follow the menu to input an mcml output file (e.g., "filename.mco"). Then, output specific data to new files. However, for the sake of efficiency, we wrote a C Shell script file "conv.bat" for UNIX users. For shell programming, refer to Anderson *et al.* (1986) or Arthur (1990). A similar file can be written on MS-DOS operating system. The file "conv.bat" is used for fast batch process. For example, if there are several mcml output files named "outfile1.mco", "outfile2.mco"... "outfilen.mco", and you need to select the diffuse reflectance as a function of radius r of these mcml output files on a UNIX system, then you can use the command:

```
conv.bat "outfile*.mco" Rr
```

This command takes two arguments. The first one gives the mcml output files to be processed. If wild cards, such as * or ?, are used, the argument has to be within quotes to prevent immediate file expansion. The second argument gives the type of subsets to be extracted. In this case, it is the diffuse reflectance as a function of r. The files of the subsets will be named as "outfile*.Rr". In each of these output files, there are two columns, the first one is the radius, and the second one is the reflectance. To check the complete usage of "conv.bat", type "conv.bat" on command line. More examples are:

```
conv.bat "outfile*.mco" Az
```

for 1D absorption as a function of z. In each of the output files of this command, there are two columns representing z and the internal absorption respectively.

```
conv.bat "outfile*.mco" Azr
```

for 2D absorption as a function of z and r. In each of the output files of this command, there are three columns representing z, r, and the internal absorption respectively.

If you use UNIX to do the simulation and want to present the results using Macintosh or IBM PC compatibles, transfer the smaller subset files using KERMIT if you use modem or FTP if you use Ethernet.

9.5 Bugs of mcml

1. Users have to be careful with several known bugs about the program mcml version 1.0. If a grid element crosses a medium interface, e.g., a glass/tissue interface, the photon absorption within this grid element is considered to be the absorption in the medium where the center of the grid element is located. Therefore, if the center is on the side of the glass, mcml may report small absorption in the glass. Sometimes, this problem may be avoided by choosing the z-grid system carefully so that the boundaries of elements align with the layer interfaces.

2. The user time of a simulation can be reported as zero if the simulation is long enough to overflow the timer (See the function `clock()` in the file "mcmlmain.c").

3. The input parameters in the input data file have to be in the order as specified. Furthermore, you have to use integers for number of photon packets, number of layers, and number of grid elements in the input data file. If floating point numbers

are inadvertently used, mcml can not detect the error and may read in the wrong parameters.

If you find any new bugs, please report to us using the information in Appendix G. It is very important that you provide us enough information about the bug so that we can reproduce it.

10. Instructions for conv

This chapter describes the instructions to use the program conv, which is used to convolve the impulse responses of mcml over incident beams of finite size. This program reads the output of mcml, then convolves the impulse responses according to the user specified incident beams. The program can output the original data from mcml or the convolved data in various ASCII formats as discussed subsequently.

10.1 Start conv

To start conv on IBM PC compatibles or UNIX machines, invoke the program conv by typing:

```
conv
```

To use conv on Macintoshes, copy or move the program conv to your working folder. Then, double click the conv icon to start it. If you are using System 7, you may take advantage of the alias mechanism.

10.2 Main menu of conv

Once conv is started, it is in the main menu of the program after showing some information about the program. In the main menu, the program prompts for a command as:

```
> Main menu (h for help) =>
```

To show all the available command, type "h" and return key. It will show you the following information and prompt for the next command. You only need to show the help information when you forget the commands.

```
i  = Input filename of mcml output
b  = specify laser Beam
r  = convolution Resolution.
e  = convolution Error.
oo = Output Original data
oc = Output Convolved data
co = Contour output of Original data
cc = Contour output of Convolved data
so = Scanning output of Original data
sc = Scanning output of Convolved data
q  = Quit
* Commands in conv are not case-sensitive

> Main menu (h for help) =>
```

Each command will be introduced subsequently.

10.3 Command "i" of conv

You have to provide the filename of the mcml output to conv. This can be done by typing "i" and return key in the main menu prompt, then type in the filename of the mcml output. For example:

```
> Main menu (h for help) => i
Input filename of mcml output(or . to quit): example.mco

> Main menu (h for help) =>
```

The program returns to the main menu automatically. If the file cannot be located or opened, the program will prompt you to type in another filename. You can also type "." and return key to quit inputting the filename. If the file is not the output of mcml, the program will quit to the operating system. You need to start the program again.

10.4 Command "b" of conv

You need to specify the type and parameters of the incident beam. In version 1.0 of conv, only Gaussian beams and circularly flat (rectangular) beams are supported. To enter the incident beam, use command "b". Then you have to choose from "f" for flat beam, "g" for Gaussian beam, or "q" to quit this command. If you choose either flat beam or Gaussian beam., conv asks the total energy and the radius of the beam. For example:

```
> Main menu (h for help) => b
Beam profile:f=flat, g=Gaussian. q=quit: f
Total energy of the flat beam [J]: 1
Radius of the flat beam [cm]: .1
Total power:        1 J, and radius:      0.1 cm.

> Main menu (h for help) =>
```

It returns to the main menu automatically. Although we specify units of energy for the incident beam, you can substitute units of power throughout the program. To get reliable results, the radius should be much larger than the grid separation in the r direction of the original mcml output, and much less than the total covered radius by the grid system in the r direction of the original mcml output. As a rule of thumb, the radius should be in the range between about 3 times the grid separation in the r direction and the total grid coverage in the r direction minus the maximum radius of observation (see Eqs. 7.23 & 7.24 in Section 7.4).

10.5 Command "r" of conv

This command is used to change the grid separation and the number of grid elements in the r direction for the convolution. Since they take the values of the mcml output as the default, you do not have to enter this command if you do not want to change them. The maximum convolution radius should not be larger than that of the original mcml output to get reliable results. For example:

```
> Main menu (h for help) => r
Current resolution:     0.01 cm and number of points: 50
Input resolution in r direction [cm]: .02
Input number of points in r direction: 20
Resolution:     0.02 cm and number of points: 20

> Main menu (h for help) =>
```

Note that if the number of points is chosen too large, the program can exit due to the lack of memory. This is a bug in the current version of conv.

10.6 Command "e" of conv

The integration is computed iteratively. The iteration stops when the difference between the new estimate and the old estimate of the integration is a small part of the new estimate. This small ratio can be controlled by users using command "e". It ranges between 0 to 1. Small values would give better precision but longer computation time and vice versa. Normally, 0.001 to 0.1 is recommended. The default value is 0.1. For example:

```
> Main menu (h for help) => e
Relative convolution error
Current value is  0.05 (0.001-0.1 recommended): .01
```

Special attention has to be paid to this command. The convolution results may have weird discontinuities if the allowed convolution error is too high (see Fig. 7.11), and the convolution process may take too long if the convolution error is too low. The rule of thumb is that you choose the lowest convolution error that does not make the convolution too long to compute. If the convolution results still have any discontinuities which should not be there, you need to decrease the convolution error and redo the convolution.

10.7 Command "oo" of conv

After you input the filename of the mcml output , you can output the original data of the mcml output with various formats. One of the formats can be obtained by the command "oo". For example:

```
> Main menu (h for help) => oo

> Output mcml data (h for help) => h
I   = Input parameters of mcml
3   = reflectance, absorption, and transmittance
AL  = absorption vs layer [-]
Az  = absorption vs z [1/cm]
Arz = absorption vs r & z [1/cm3]
Fz  = fluence vs z [-]
Frz = fluence vs r & z [1/cm2]
Rr  = diffuse reflectance vs radius r [1/cm2]
Ra  = diffuse reflectance vs angle alpha [1/sr]
Rra = diffuse reflectance vs radius and angle [1/(cm2 sr)]
Tr  = transmittance vs radius r [1/cm2]
Ta  = transmittance vs angle alpha [1/sr]
Tra = transmittance vs radius and angle [1/(cm2 sr)]
K   = Keijzer's format
Q   = Quit to main menu
* input filename: example.mco

> Output mcml data (h for help) =>
```

At this point, you can output various physical quantities by inputting the subcommands, which can be listed by command "h" as shown above. After you type the command, the program will ask you for the output filename. The exact physical meanings of these physical quantities can be found in Chapter 4. The command "i" outputs the input parameters of mcml to a file. The command "3" outputs three quantities to a file including specular reflectance, total diffuse reflectance, absorption probability, and total transmittance, which are actually four numbers. The command "Al" outputs the absorption probability as a function layer to a file. The command "Az" outputs the absorption as a function of z coordinate whose dimension is cm^{-1}. The command "Arz" outputs the absorption probability density as a function of r and z whose dimension is cm^{-3}. The commands "Fz" and "Frz" output the results of the commands "Az" and "Arz" divided by the absorption coefficients. The command "Rr" outputs the diffuse reflectance as a function of r whose unit is cm^{-2}. The command "Ra" outputs the diffuse reflectance as a function of the exit angle α, whose dimension is sr^{-1}. The command "Rra" outputs the diffuse reflectance as a function of r and α, whose unit is $cm^{-2}\ sr^{-1}$. Similarly, the commands "Tr", "Ta" and "Tra" are the corresponding commands for the transmittance. The command "K" is used to convert the format of the mcml output to the format of Marleen Keijzer's convolution program (in PASCAL on Macintoshes) which was used by our group before the program conv was written. This command is only useful if you have Marleen Keijzer's program. The command "q" will return the program to the main menu.

For 1D arrays, the outputs are in two columns. The first column gives the independent variable, and the second column gives the physical quantities. For example, the output of the command "Rr" will have two columns. The first column gives the radius in cm, and the second column gives the diffuse reflectance in cm^{-2}.

For 2D arrays, the outputs are in three columns. The first two columns give the first and the second independent variables, and the third column gives the physical quantities. For example, the command "Arz" will give three columns. The first two columns give r and z in cm respectively, and the third column gives the absorption probability density in cm^{-2} sr^{-1} as a function of r and z.

An example is shown as follows:

```
> Output mcml data (h for help) => Rr
Enter output filename with extension .Rr (or . to quit): example.Rr

> Output mcml data (h for help) =>
```

This command will output the diffuse reflectance as a function of r to the file named "example.Rr".

10.8 Command "oc" of conv

After you input the filename of the mcml output and specify the incident photon beam, you can output the convolved data with various formats. One of the formats is writing data in columns, which can be obtained using the command "oc". For example:

```
> Main menu (h for help) => oc

> Output convolved data (h for help) => h
Arz = absorption vs r & z [J/cm3]
Frz = fluence vs r & z [J/cm2]
Rr  = diffuse reflectance vs radius r [J/cm2]
Rra = diffuse reflectance vs radius and angle [J/(cm2 sr)]
Tr  = transmittance vs radius r [J/cm2]
Tra = transmittance vs radius and angle [J/(cm2 sr)]
Q   = Quit to main menu
* input filename: example.mco

> Output convolved data (h for help) =>
```

At this point, you can output various physical quantities by inputting the subcommands, which can be listed by command "h" as shown above. After you type the command, the program will ask you for the output filename. The exact physical meanings of these physical quantities can be found in Chapters 4 and 7. The command "Arz" outputs the absorption energy density as a function of r and z whose dimension is J cm^{-3}. The command "Frz" outputs the results of the command "Arz" divided by the absorption coefficients, which is the fluence in J cm^{-2}. Since we consider steady-state responses only in mcml and conv, you can systematically replace the energy [Joules] with power [Watts] in conv.

The command "Rr" outputs the diffuse reflectance as a function of r whose unit is J cm^{-2}. The command "Rra" outputs the diffuse reflectance as a function of r and α, whose unit is J cm^{-2} sr^{-1}. Similarly, the commands "Tr" and "Tra" are the corresponding commands for the transmittance. The command "q" will return the program to the main menu.

For 1D arrays, the outputs are in two columns. The first column gives the independent variable, and the second column gives the physical quantities. For example, the output of the command "Rr" will have two columns. The first column gives the radius in cm, and the second column gives the diffuse reflectance in J cm^{-2}.

For 2D arrays, the outputs are in three columns. The first two columns give the first and the second independent variables respectively, and the third column gives the physical quantities. For example, the command "Arz" will give three columns. The first two columns give r and z in cm respectively, and the third column gives the absorption energy density in J cm^{-2} sr^{-1} as a function of r and z.

An example is shown as follows:

```
> Output convolved data (h for help) => Rr
Enter output filename with extension .Rrc (or . to quit): example.Rrc

> Output convolved data (h for help) =>
```

This command will output the diffuse reflectance as a function of r to the file named "example.Rrc".

10.9 Command "co" of conv

After you input the filename of the mcml output, you can output the original data of the mcml output with various formats. One of the formats for 2D arrays is writing data in contour lines. Every contour line will be given by two columns. This format can be obtained using the command "co" standing for "contours of the original data". Then, the output file can be imported to some plotting software such as KaleidaGraph on Macintoshes, and the contour lines can be drawn. For example:

```
> Main menu (h for help) => co

> Contour output of mcml data (h for help) => h
```

```
A = absorption vs r & z [1/cm3]
F = fluence vs r & z [1/cm2]
R = diffuse reflectance vs radius and angle [1/(cm2 sr)]
T = transmittance vs radius and angle [1/(cm2 sr)]
Q   = Quit to main menu
* input filename: example.mco

> Contour output of mcml data (h for help) =>
```

Since only the 2D arrays need to be presented in contour lines, there are only four physical quantities. The command "A" outputs the absorption probability density as a function of r and z whose dimension is cm^{-3}. The command "F" outputs the probability fluence as a function of r and z in cm^{-2}. The commands "R" and "T" output diffuse reflectance and transmittance as a function of r and α in cm^{-2} sr^{-1}.

After you input one of the commands, the program will prompt for the output filename and the isovalues for the contour output. The value range of the physical quantity is shown so that valid isovalues can be provided by users. You can enter as many isovalues as you want. System memory is the only thing that limits the number of isovalues. Stop entering isovalues by inputting a period ".". For example:

```
> Contour output of mcml data (h for help) => A
Enter output filename with extension .iso (or . to quit): example.iso
The range of the value is 0.156280 to 3294.800000.
Input an isovalue or . to stop: 1000
Input an isovalue or . to stop: 100
Input an isovalue or . to stop: 10
Input an isovalue or . to stop: 1
Input an isovalue or . to stop: .

> Contour output of mcml data (h for help) =>
```

The output file of this example will have eight columns, each pair of columns describe one contour line. The values of the contour lines are 1000, 100, 10, and 1 respectively.

10.10 Command "cc" of conv

After you input the filename of the mcml output and specify the incident photon beam, you can output the convolved data with various formats. One of the formats for 2D arrays is writing data in contour lines. Every contour line will be given by two columns. This format can be obtained using the command "cc". The output file can be imported to some plotting software such as KaleidaGraph, and the contour lines can be drawn. For example:

```
> Main menu (h for help) => cc

> Contour output of convolved data (h for help) => h
A = absorption vs r & z [J/cm3]
F = fluence vs r & z [J/cm2]
```

```
R = diffuse reflectance vs radius and angle [J/(cm2 sr)]
T = transmittance vs radius and angle [J/(cm2 sr)]
Q   = Quit to main menu
* input filename: example.mco

> Contour output of convolved data (h for help) =>
```

Since only the 2D arrays need to be presented in contour lines, there are only four physical quantities. The command "A" outputs the absorption energy density as a function of r and z whose dimension is J cm^{-3}. The command "F" outputs the fluence as a function of r and z in J cm^{-2}. The commands "R" and "T" output diffuse reflectance and transmittance as a function of r and α in J cm^{-2} sr^{-1} respectively.

After you input one of the commands, the program will prompt for the output filename and the isovalues for the contour output. The value range of the physical quantity is shown so that valid isovalues can be provided by users. You can enter as many isovalues as you want. System memory is the only thing that limits the number of isovalues. Stop entering isovalues by inputting a period ".". For example:

```
> Contour output of convolved data (h for help) => A
Enter output filename with extension .iso (or . to quit): exampleAc.iso
The range of the value is 0.048200 to 95.624939.
Input an isovalue or . to stop: 80
Input an isovalue or . to stop: 8
Input an isovalue or . to stop: 0.8
Input an isovalue or . to stop: .

> Contour output of convolved data (h for help) =>
```

The output file of this example will have six columns, each pair of columns describe one contour line. The values of the contour lines are 80, 8, and 0.8 respectively.

10.11 Command "so" of conv

After you input the filename of the mcml output, you can output the original data of the mcml output with various formats. One of the formats for 2D arrays is writing data in two columns, where the two columns give the physical quantity as a function of one of two independent variables. The other variable is fixed at a certain value which can be chosen by users. This format, we call scanning output, can be obtained using the command "so". The output file can be imported to some plotting software such as KaleidaGraph. For example:

```
> Main menu (h for help) => so

> Scans of mcml data (h for help) => h
Ar = absorption vs r @ fixed z [1/cm3]
Az = absorption vs z @ fixed r [1/cm3]
Fr = fluence vs r @ fixed z [1/cm2]
```

```
Fz = fluence vs z @ fixed r [1/cm2]
Rr = diffuse reflectance vs r @ fixed angle [1/(cm2 sr)]
Ra = diffuse reflectance vs angle @ fixed r [1/(cm2 sr)]
Tr = transmittance vs r @ fixed angle [1/(cm2 sr)]
Ta = transmittance vs angle @ fixed r [1/(cm2 sr)]
Q  = quit
* input filename: example.mco

> Scans of mcml data (h for help) =>
```

The command "Ar" outputs the absorption probability density as a function of r for a fixed z, whose dimension is cm^{-3}. The command "Az" outputs the absorption probability density as a function of z for a fixed r, whose dimension is cm^{-3}. The command "Fr" outputs the probability fluence as a function of r for a fixed z in cm^{-2}. The command "Fz" outputs the probability fluence as a function of z for a fixed r in cm^{-2}. The command "Rr" outputs the diffuse reflectance as a function of r for a fixed α in $cm^{-2}sr^{-1}$. The command "Ra" outputs the diffuse reflectance as a function of α for a fixed r in $cm^{-2}sr^{-1}$. The commands "Tr" and "Ta" output the transmittance in the same format as for the diffuse reflectance. The command "q" returns to the main menu.

After you input one of the commands, the program will prompt for the output filename and the grid index to the value of the fixed variable. If you want to abort this output, you can input a period "." as the filename. For example:

```
> Scans of mcml data (h for help) => Ar
Enter output filename with extension .Ars (or . to quit): example.Ars
z grid separation is 0.01       cm.
Input fixed z index (0 - 39): 0

> Scans of mcml data (h for help) =>
```

This command outputs the absorption as a function of r for a fixed z. The program shows that the z grid separation is 0.01 cm. The number of grid elements in the z direction is 40. The grid index in the z direction is in the range from 0 to 39. The command will generate two columns. The first column is r, and the second is the absorption.

10.12 Command "sc" of conv

After you input the filename of the mcml output and specify the incident photon beam, you can output the convolved data with various formats. One of the formats for 2D arrays is writing data in two columns, where the two columns give the physical quantity as a function of one of two independent variables. The other variable is fixed at a certain value which can be chosen by users. This format, we call scanning output, can be obtained using the command "sc". Then, the output file can be imported to some plotting software such as KaleidaGraph. For example:

```
> Main menu (h for help) => sc

> Scans of convolved data (h for help) => h
Ar = absorption vs r @ fixed z [J/cm3]
Az = absorption vs z @ fixed r [J/cm3]
Fr = fluence vs r @ fixed z [J/cm2]
Fz = fluence vs z @ fixed r [J/cm2]
Rr = diffuse reflectance vs r @ fixed angle [J/(cm2 sr)]
Ra = diffuse reflectance vs angle @ fixed r [J/(cm2 sr)]
Tr = transmittance vs r @ fixed angle [J/(cm2 sr)]
Ta = transmittance vs angle @ fixed r [J/(cm2 sr)]
Q  = quit
* input filename: example.mco

> Scans of convolved data (h for help) =>
```

The command "Ar" outputs the absorption energy density as a function of r for a fixed z, whose dimension is J cm^{-3}. The command "Az" outputs the absorption energy density as a function of z for a fixed r, whose dimension is J cm^{-3}. The command "Fr" outputs the fluence as a function of r for a fixed z in J cm^{-2}. The command "Fz" outputs the fluence as a function of z for a fixed r in J cm^{-2}. The command "Rr" outputs the diffuse reflectance as a function of r for a fixed α in J cm^{-2} sr^{-1}. The command "Ra" outputs the diffuse reflectance as a function of α for a fixed r in J cm^{-2} sr^{-1}. The commands "Tr" and "Ta" output the transmittance in the same format as for the diffuse reflectance. The command "q" returns to the main menu.

After you input one of the commands, the program will prompt for the output filename and the grid index to the value of the fixed variable. If you want to abort this output, you can input a period "." as the filename. For example:

```
> Scans of convolved data (h for help) => Ar
Enter output filename with extension .Arsc (or . to quit): example.Arsc
z grid separation is 0.01       cm.
Input fixed z index (0 - 39): 0

> Scans of convolved data (h for help) =>
```

This command outputs the absorption as a function of r for a fixed z. The program shows that the z grid separation is 0.01 cm. The number of grids in the z direction is 40. The grid index in the z direction is in the range from 0 to 39. The command will generate two columns. The first column is r, and the second is the absorption.

10.13 Command "q" of conv

If you want to quit the program conv, use the command "q" in the main menu. The program will ask you if you really mean to quit. You can answer yes or no. The program will quit if the answer is "y". Otherwise, the program will return to the main menu. For example:

```
> Main menu (h for help) => q
Do you really want to quit conv (y/n): n

> Main menu (h for help) => q
Do you really want to quit conv (y/n): y
```

10.14 Bugs of conv

The convolution results may have weird discontinuities if the allowed convolution error is too high, and the convolution process may take too long if the convolution error is too low. We do not have a good way to predict the best convolution error yet. The rule of thumb is that you choose the lowest convolution error that does not make the convolution too long to compute. If the convolution results still have any discontinuities which should not be there, you need to decrease the convolution error and redo the convolution.

As we discussed in Section 7.5, the radius of the incident beam has to be in the right range to get reliable convolution integration due to the spatial resolution and the range of grid system. As a rule of thumb, the radius should be in the range between about 3 times the grid separation in the r direction and the total grid coverage in the r direction minus the maximum radius of observation (see Eqs. 7.23 & 7.24 in Section 7.4).

If the number of points in the r direction is chosen too large in the command "r", the program can exit due to the lack of memory.

11. How to Modify mcml

The current version of program mcml simulates responses of an infinitely narrow photon beam normally incident on multi-layered turbid media. We intend to make mcml more general in the future. However, if you need to solve a different problem, such as responses of isotropic photon sources instead of infinitely narrow photon beams, responses of buried beams instead of externally incident beams, or time-resolved simulations, then you will need to modify the program slightly. To do so, you need to have prior knowledge of C language and understand Chapter 5. Appendix A and Appendix B are provided to aid you in modifying the program. Appendix A gives you an overall flow of the program, and Appendix B provides line-numbered source codes, which can be used in combination with Appendix A for quick reference of the detail of the program.

As an example, let us modify several places of the program mcml to compute the responses of buried isotropic photon sources. First, we need to allow users to provide the depth of the isotropic photon source inside the tissue, which can be entered in the input data file. For example, we can add the depth of the source as the second parameter in the line for the number of photon packets. Second, we define one more member called `source_z` in the structure InputStruct to store the depth of the source. Third, we read the depth into the member `source_z` of structure InputStruct in function `ReadParm()` which is in the file "mcmlio.c". Fourth, we need to modify the function `LaunchPhoton()` in the file "mcmlgo.c" such that the photons are initialized isotropically at the correct depth according to `source_z`. If you know the program well, you will know that you can make the source isotropic utilizing the function `Spin()` in the file "mcmlgo.c". To do so, we can initialize the photon packet to be unidirectional (e.g., +z direction) temporarily, then pretend that the whole photon packet suffers an isotropic scattering on the same spot as initialized using the function `Spin()`. All you need to do is to provide an anisotropy factor g equal 0 as the real parameter for the function. The propagation simulation functions need no change, and the scoring procedures need no change either because the problem is still cylindrically symmetric. After you modify the source code, you need to recompile and link (refer to the manual with the compiler and linker).

After we modified mcml like this, we simulated the diffuse reflectances of a buried isotropic photon source in two media separately, whose optical properties are equivalent according to the similarity relations (Wyman *et al.*, 1989a and 1989b). The optical properties for the isotropic scattering medium (g = 0) are: absorption coefficient μ_a = 0.1 cm^{-1}, scattering coefficient μ_s = 10 cm^{-1}, anisotropy factor g = 0, relative refractive index n$_{rel}$ = 1. The optical properties for the anisotropic scattering medium (g 0) are: μ_a = 0.1 cm^{-1}, μ_s = 100 cm^{-1}, g = 0.9, n$_{rel}$ = 1. The depth of the isotropic photon source is 1 transport mean free path (mfp'), which is computed by 1 mfp' = 1/(μ_a + μ_s(1–g)) = 1/(0.1 + 10) ≈ 0.1 cm. The grid separations in the z and r directions are both 0.005 cm, and the numbers of grid elements in the z and r directions are both 200. One million photon packets were used in the modified mcml.

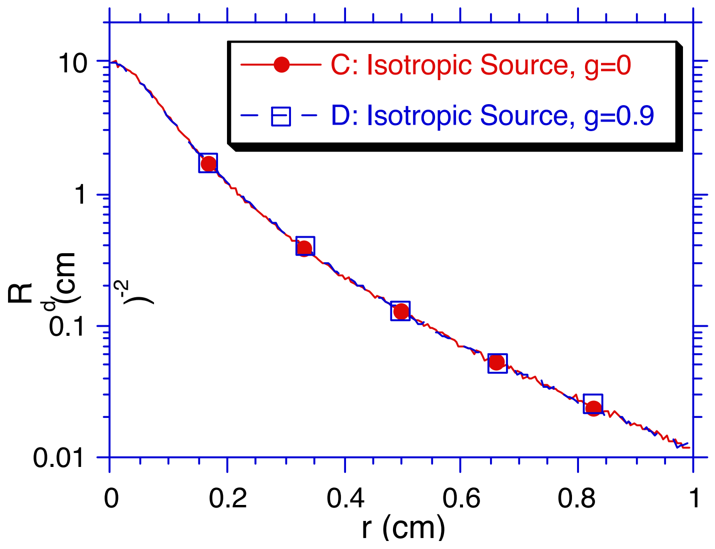

Fig. 11.1. Comparison of diffuse reflectances as a function of radius r for two semi-infinite media whose optical properties are governed by the similarity relations.The diffuse reflectances and the fluences for the two media are compared in Figs. 11.1 and 11.2 respectively. The results of the diffuse reflectances show that the similarity relations work well for photon sources deep inside the tissue, and the results of the fluences show that the similarity relations work well when the observation point is far away from the source. The fluence near the source for the isotropic scattering medium is larger than that for the anisotropic scattering medium. Similar to the discussion in Section 4.2, the fluences presented here are the responses of an isotropic infinitely wide plane source with a difference of a constant factor which is the power density of the source.

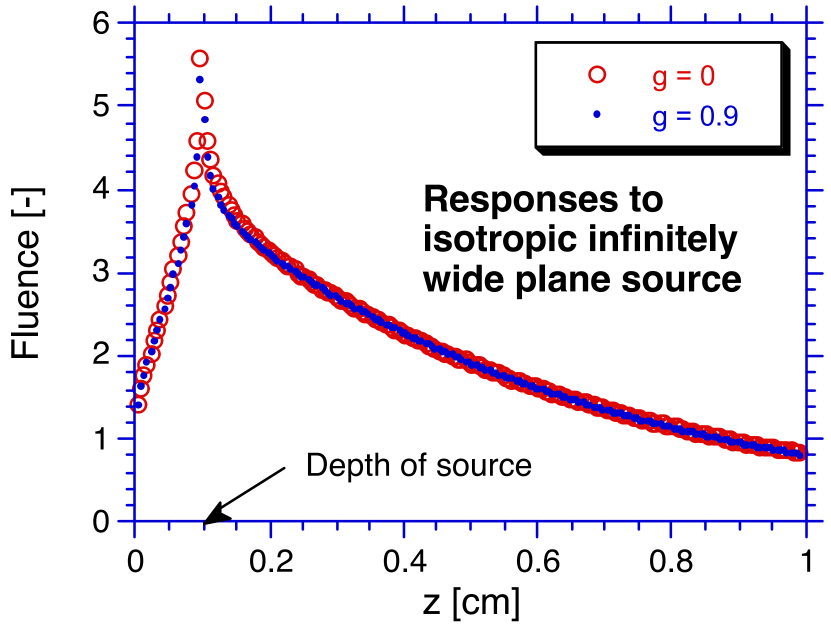

Fig. 11.2. Comparison between fluences as a function of z for two semi-infinite media whose optical properties are governed by the similarity relations (see Section 4.2 for discussion of an infinitely wide incident beam).

Appendices

Appendix A. Cflow Output of the Program mcml

We have listed the short format of the UNIX command cflow output in Section 5.5. To show all depth of the nesting levels, we list here the results of the UNIX command:

```
    cflow  mcmlgo.c
```

```
1    main: char(), <mcmlmain.c 198>
2        ShowVersion: void*(), <mcmlio.c 49>
3            CenterStr: char*(), <mcmlio.c 28>
4                strlen: <>
5                strcpy: <>
6                strcat: <>
7            puts: <>
8        GetFnameFromArgv: void*(), <mcmlmain.c 150>
9            strcpy: 5
10       GetFile: struct*(), <mcmlio.c 94>
11           printf: <>
12           scanf: <>
13           strlen: 4
14           exit: <>
15           fopen: <>
16       CheckParm: void*(), <mcmlio.c 514>
17           ReadNumRuns: short(), <mcmlio.c 205>
18               FindDataLine: char*(), <mcmlio.c 184>
19                   fgets: <>
20                   printf: 11
21                   CheckChar: char(), <mcmlio.c 139>
22                       strlen: 4
23                       nrerror: void*(), <mcmlnr.c 19>
24                           fprintf: <>
25                           exit: 14
26                       KillChar: void*(), <mcmlio.c 123>
27                   CommentLine: char(), <mcmlio.c 165>
28                       strspn: <>
29                       strcspn: <>
30               strcpy: 5
31               nrerror: 23
32               sscanf: <>
33           printf: 11
34           ReadParm: void*(), <mcmlio.c 425>
35               ReadFnameFormat: void*(), <mcmlio.c 225>
36                   FindDataLine: 18
37                   strcpy: 5
38                   nrerror: 23
39                   sscanf: 32
40                   toupper: <>
41               ReadNumPhotons: void*(), <mcmlio.c 243>
42                   FindDataLine: 18
43                   strcpy: 5
44                   nrerror: 23
45                   sscanf: 32
46               ReadDzDr: void*(), <mcmlio.c 260>
47                   FindDataLine: 18
48                   strcpy: 5
49                   nrerror: 23
50                   sscanf: 32
```

```
51              ReadNzNrNa: void*(), <mcmlio.c 276>
52                  FindDataLine: 18
53                  strcpy: 5
54                  nrerror: 23
55                  sscanf: 32
56              ReadNumLayers: void*(), <mcmlio.c 299>
57                  FindDataLine: 18
58                  strcpy: 5
59                  nrerror: 23
60                  sscanf: 32
61              ReadLayerSpecs: void*(), <mcmlio.c 375>
62                  malloc: <>
63                  nrerror: 23
64                  ReadAmbient: void*(), <mcmlio.c 318>
65                      FindDataLine: 18
66                      strcpy: 5
67                      sprintf: <>
68                      nrerror: 23
69                      sscanf: 32
70                  ReadOneLayer: char(), <mcmlio.c 347>
71                      FindDataLine: 18
72                      strcpy: 5
73                      sscanf: 32
74                  sprintf: 67
75              CriticalAngle: void*(), <mcmlio.c 405>
76                  sqrt: <>
77          FnameTaken: char(), <mcmlio.c 487>
78              NameInList: char(), <mcmlio.c 446>
79                  strcmp: <>
80              AddNameToList: void*(), <mcmlio.c 459>
81                  malloc: 62
82                  strcpy: 5
83          sprintf: 67
84          free: <>
85          nrerror: 23
86          FreeFnameList: void*(), <mcmlio.c 500>
87              free: 84
88          rewind: <>
89      ReadNumRuns: 17
90      ReadParm: 34
91      DoOneRun: void*(), <mcmlmain.c 163>
92          InitOutputData: void*(), <mcmlio.c 546>
93              nrerror: 23
94              AllocMatrix: double**(), <mcmlnr.c 52>
95                  malloc: 62
96                  nrerror: 23
97              AllocVector: double*(), <mcmlnr.c 33>
98                  malloc: 62
99                  nrerror: 23
100         Rspecular: double(), <mcmlgo.c 117>
101         PunchTime: long(), <mcmlmain.c 60>
102             clock: <>
103             time: <>
104             sprintf: 67
105             puts: 7
106             strcpy: 5
107             difftime: <>
108         ReportStatus: void*(), <mcmlmain.c 122>
109             printf: 11
110             PredictDoneTime: void*(), <mcmlmain.c 95>
111                 time: 103
112                 localtime: <>
113                 strftime: <>
114                 printf: 11
115                 PunchTime: 101
116         LaunchPhoton: void*(), <mcmlgo.c 143>
117             Rspecular: 100
```

```
118         HopDropSpin: void*(), <mcmlgo.c 726>
119             HopInGlass: void*(), <mcmlgo.c 675>
120                 StepSizeInGlass: void*(), <mcmlgo.c 265>
121                 Hop: void*(), <mcmlgo.c 246>
122                 CrossOrNot: void*(), <mcmlgo.c 660>
123                     CrossUpOrNot: void*(), <mcmlgo.c 547>
124                         RFresnel: double(), <mcmlgo.c 421>
125                             sqrt: 76
126                         RandomNum: double(), <mcmlgo.c 83>
127                             time: 103
128                             ran3: float(), <mcmlgo.c 32>
129                         RecordR: void*(), <mcmlgo.c 480>
130                             sqrt: 76
131                             acos: <>
132                     CrossDnOrNot: void*(), <mcmlgo.c 609>
133                         RFresnel: 124
134                         RandomNum: 126
135                         RecordT: void*(), <mcmlgo.c 508>
136                             sqrt: 76
137                             acos: 131
138             HopDropSpinInTissue: void*(), <mcmlgo.c 706>
139                 StepSizeInTissue: void*(), <mcmlgo.c 295>
140                     RandomNum: 126
141                     log: <>
142                 HitBoundary: char(), <mcmlgo.c 323>
143                 Hop: 121
144                 CrossOrNot: 122
145                 Drop: void*(), <mcmlgo.c 365>
146                     sqrt: 76
147                 Spin: void*(), <mcmlgo.c 204>
148                     SpinTheta: double(), <mcmlgo.c 176>
149                         RandomNum: 126
150                     sqrt: 76
151                     RandomNum: 126
152                     cos: <>
153                     fabs: <>
154             Roulette: void*(), <mcmlgo.c 395>
155                 RandomNum: 126
156         ReportResult: void*(), <mcmlmain.c 133>
157             strcpy: 5
158             PunchTime: 101
159             SumScaleResult: void*(), <mcmlio.c 802>
160                 Sum2DRd: void*(), <mcmlio.c 607>
161                 Sum2DA: void*(), <mcmlio.c 652>
162                     IzToLayer: short(), <mcmlio.c 637>
163                 Sum2DTt: void*(), <mcmlio.c 677>
164                 ScaleRdTt: void*(), <mcmlio.c 720>
165                     sin: <>
166                 ScaleA: void*(), <mcmlio.c 766>
167             WriteResult: void*(), <mcmlio.c 1091>
168                 fopen: 15
169                 nrerror: 23
170                 toupper: 40
171                 WriteVersion: void*(), <mcmlio.c 819>
172                     fprintf: 24
173                 fprintf: 24
174                 WriteInParm: void*(), <mcmlio.c 833>
175                     fprintf: 24
176                 WriteRAT: void*(), <mcmlio.c 872>
177                     fprintf: 24
178                 WriteA_layer: void*(), <mcmlio.c 895>
179                     fprintf: 24
180                 WriteA_z: void*(), <mcmlio.c 1035>
181                     fprintf: 24
182                 WriteRd_r: void*(), <mcmlio.c 941>
183                     fprintf: 24
184                 WriteRd_a: void*(), <mcmlio.c 960>
```

```
185                     fprintf: 24
186                 WriteTt_r: void*(), <mcmlio.c 1054>
187                     fprintf: 24
188                 WriteTt_a: void*(), <mcmlio.c 1073>
189                     fprintf: 24
190                 WriteA_rz: void*(), <mcmlio.c 1008>
191                     fprintf: 24
192                 WriteRd_ra: void*(), <mcmlio.c 914>
193                     fprintf: 24
194                 WriteTt_ra: void*(), <mcmlio.c 980>
195                     fprintf: 24
196                 fclose: <>
197         FreeData: void*(), <mcmlio.c 581>
198             free: 84
199             FreeMatrix: void*(), <mcmlnr.c 86>
200                 free: 84
201             FreeVector: void*(), <mcmlnr.c 77>
202                 free: 84
203     fclose: 196
```

Appendix B. Source Code of the Program mcml

The whole program is divided into several files. The file "mcml.h" is the header file, which defines data structures and some constants. The file "mcmlmain.c" contains the function `main()`. It also deals with the timings and status report. The file "mcmlio.c" reads or writes data from or to data files. The file "mcmlgo.c" does most of the Monte Carlo simulations. The file "mcmlnr.c" (nr stands for numerical recipes) contains several functions for dynamical data allocations and error report.

B.1 mcml.h

```
/***********************************************************
 *  Copyright Univ. of Texas M.D. Anderson Cancer Center
 *  1992.
 *
 *  Monte Carlo simulation of photon distribution in
 *  multi-layered turbid media in ANSI Standard C.
 ****
 *  Starting Date:  10/1991.
 *  Current Date:   6/1992.
 *
 *  Lihong Wang, Ph. D.
 *  Steven L. Jacques, Ph. D.
 *  Laser Biology Research Laboratory - 17
 *  M.D. Anderson Cancer Center
 *  University of Texas
 *  1515 Holcombe Blvd.
 *  Houston, TX 77030
 *  USA
 *
 *  This program was based on:
 *  (1) The Pascal code written by Marleen Keijzer and
 *  Steven L. Jacques in this laboratory in 1989, which
 *  deals with multi-layered turbid media.
 *
 *  (2) Algorithm for semi-infinite turbid medium by
 *  S.A. Prahl, M. Keijzer, S.L. Jacques, A.J. Welch,
 *  SPIE Institute Series Vol. IS 5 (1989), and by
 *  A.N. Witt, The Astrophysical journal Supplement
 *  Series 35, 1-6 (1977).
 *
 *  Major modifications include:
 *      . Conform to ANSI Standard C.
 *      . Removal of limit on number of array elements,
 *        because arrays in this program are dynamically
 *        allocated. This means that the program can accept
 *        any number of layers or gridlines as long as the
 *        memory permits.
 *      . Avoiding global variables whenever possible.  This
 *        program has not used global variables so far.
 *      . Grouping variables logically using structures.
 *      . Top-down design, keep each subroutine clear &
 *        short.
 *      . Reflectance and transmittance are angularly
 *        resolved.
 ****
 *  General Naming Conventions:
```

```
 *  Preprocessor names: all capital letters,
 *      e.g. #define PREPROCESSORS
 *  Globals: first letter of each word is capital, no
 *      underscores,
 *      e.g. short GlobalVar;
 *  Dummy variables:  first letter of each word is capital,
 *      and words are connected by underscores,
 *      e.g. void NiceFunction(char Dummy_Var);
 *  Local variables:  all lower cases, words are connected
 *      by underscores,
 *      e.g. short local_var;
 *  Function names or data types:  same as Globals.
 *
 ****
 *  Dimension of length: cm.
 *
 ****/

#include <math.h>
#include <stdlib.h>
#include <stdio.h>
#include <stddef.h>
#include <time.h>
#include <string.h>
#include <ctype.h>

#define PI 3.1415926
#define WEIGHT 1E-4     /* Critical weight for roulette. */
#define CHANCE 0.1      /* Chance of roulette survival. */
#define STRLEN 256      /* String length. */

#define Boolean char

#define SIGN(x) ((x)>=0 ? 1:-1)

/***************** Stuctures ****************************/

/****
 *  Structure used to describe a photon packet.
 ****/
typedef struct {
  double x, y ,z;   /* Cartesian coordinates.[cm] */
  double ux, uy, uz;/* directional cosines of a photon. */
  double w;         /* weight. */
  Boolean dead;     /* 1 if photon is terminated. */
  short layer;      /* index to layer where the photon */
                    /* packet resides. */
  double s;         /* current step size. [cm]. */
  double sleft;     /* step size left. dimensionless [-]. */
} PhotonStruct;

/****
 *  Structure used to describe the geometry and optical
 *  properties of a layer.
 *  z0 and z1 are the z coordinates for the upper boundary
 *  and lower boundary respectively.
 *
 *  cos_crit0 and cos_crit1 are the cosines of the
 *  critical angle of total internal reflection for the
 *  upper boundary and lower boundary respectively.
 *  They are set to zero if no total internal reflection
 *  exists.
 *  They are used for computation speed.
 ****/
typedef struct {
  double z0, z1;    /* z coordinates of a layer. [cm] */
  double n;         /* refractive index of a layer. */
  double mua;       /* absorption coefficient. [1/cm] */
  double mus;       /* scattering coefficient. [1/cm] */
  double g;         /* anisotropy. */

  double cos_crit0, cos_crit1;
} LayerStruct;

/****
 *  Input parameters for each independent run.
 *
 *  z and r are for the cylindrical coordinate system. [cm]
 *  a is for the angle alpha between the photon exiting
 *  direction and the surface normal. [radian]
 *
 *  The grid line separations in z, r, and alpha
 *  directions are dz, dr, and da respectively.  The numbers
 *  of grid lines in z, r, and alpha directions are
 *  nz, nr, and na respectively.
 *
 *  The member layerspecs will point to an array of
 *  structures which store parameters of each layer.
 *  This array has (number_layers + 2) elements. One
 *  element is for a layer.
 *  The layers 0 and (num_layers + 1) are for top ambient
 *  medium and the bottom ambient medium respectively.
 ****/
typedef struct {
  char   out_fname[STRLEN]; /* output file name. */
  char   out_fformat;       /* output file format. */
                            /* 'A' for ASCII, */
                            /* 'B' for binary. */
  long   num_photons;       /* to be traced. */
  double Wth;               /* play roulette if photon */
                            /* weight < Wth.*/

  double dz;                /* z grid separation.[cm] */
  double dr;                /* r grid separation.[cm] */
  double da;                /* alpha grid separation. */
                            /* [radian] */
  short nz;                 /* array range 0..nz-1. */
  short nr;                 /* array range 0..nr-1. */
  short na;                 /* array range 0..na-1. */

  short num_layers;         /* number of layers. */
  LayerStruct * layerspecs; /* layer parameters. */
} InputStruct;

/****
 *  Structures for scoring physical quantities.
 *  z and r represent z and r coordinates of the
 *  cylindrical coordinate system. [cm]
 *  a is the angle alpha between the photon exiting
 *  direction and the normal to the surfaces. [radian]
 *  See comments of the InputStruct.
 *  See manual for the physcial quantities.
 ****/
typedef struct {
  double    Rsp;    /* specular reflectance. [-] */
  double ** Rd_ra;  /* 2D distribution of diffuse */
                    /* reflectance. [1/(cm2 sr)] */
  double *  Rd_r;   /* 1D radial distribution of diffuse */
                    /* reflectance. [1/cm2] */
  double *  Rd_a;   /* 1D angular distribution of diffuse */
                    /* reflectance. [1/sr] */
  double    Rd;     /* total diffuse reflectance. [-] */

  double ** A_rz;   /* 2D probability density in turbid */
```

```
                       /* media over r & z. [1/cm3] */
  double *  A_z;       /* 1D probability density over z. */
                       /* [1/cm] */
  double *  A_l;       /* each layer's absorption */
                       /* probability. [-] */
  double    A;         /* total absorption probability. [-] */

  double ** Tt_ra;     /* 2D distribution of total */
                       /* transmittance. [1/(cm2 sr)] */
  double *  Tt_r;      /* 1D radial distribution of */
                       /* transmittance. [1/cm2] */
  double *  Tt_a;      /* 1D angular distribution of */
                       /* transmittance. [1/sr] */
  double    Tt;        /* total transmittance. [-] */
} OutStruct;

/**********************************************************
 *  Routine prototypes for dynamic memory allocation and
 *  release of arrays and matrices.
 *  Modified from Numerical Recipes in C.
 ****/
double  *AllocVector(short, short);
double **AllocMatrix(short, short,short, short);
void     FreeVector(double *, short, short);
void     FreeMatrix(double **, short, short, short, short);
void     nrerror(char *);
```

B.2 mcmlmain.c

```
/***********************************************************
 *  Copyright Univ. of Texas M.D. Anderson Cancer Center
 *  1992.
 *
 *  main program for Monte Carlo simulation of photon
 *  distribution in multi-layered turbid media.
 *
 ****/

/****
 *  THINKCPROFILER is defined to generate profiler calls in
 *  Think C. If 1, remember to turn on "Generate profiler
 *  calls" in the options menu.
 ****/
#define THINKCPROFILER 0

/* GNU cc does not support difftime() and CLOCKS_PER_SEC.*/
#define GNUCC 0

#if THINKCPROFILER
#include <profile.h>
#include <console.h>
#endif

#include "mcml.h"

/*  Declare before they are used in main(). */
FILE *GetFile(char *);
short ReadNumRuns(FILE* );
void ReadParm(FILE* , InputStruct * );
void CheckParm(FILE* , InputStruct * );
void InitOutputData(InputStruct, OutStruct *);
void FreeData(InputStruct, OutStruct *);
double Rspecular(LayerStruct * );
void LaunchPhoton(double, LayerStruct *, PhotonStruct *);
void HopDropSpin(InputStruct  *,PhotonStruct *,OutStruct *);
void SumScaleResult(InputStruct, OutStruct *);
void WriteResult(InputStruct, OutStruct, char *);


/***********************************************************
 *  If F = 0, reset the clock and return 0.
 *
 *  If F = 1, pass the user time to Msg and print Msg on
 *  screen, return the real time since F=0.
 *
 *  If F = 2, same as F=1 except no printing.
 *
 *  Note that clock() and time() return user time and real
 *  time respectively.
 *  User time is whatever the system allocates to the
 *  running of the program;
 *  real time is wall-clock time.  In a time-shared system,
 *  they need not be the same.
 *
 *  clock() only hold 16 bit integer, which is about 32768
 *  clock ticks.
 ****/
time_t PunchTime(char F, char *Msg)
{
#if GNUCC
  return(0);
#else
  static clock_t ut0;   /* user time reference. */
  static time_t  rt0;   /* real time reference. */
  double secs;
  char s[STRLEN];

  if(F==0) {
    ut0 = clock();
    rt0 = time(NULL);
    return(0);
  }
  else if(F==1)  {
    secs = (clock() - ut0)/(double)CLOCKS_PER_SEC;
    if (secs<0) secs=0; /* clock() can overflow. */
    sprintf(s, "User time: %8.0lf sec = %8.2lf hr.  %s\n",
        secs, secs/3600.0, Msg);
    puts(s);
    strcpy(Msg, s);
    return(difftime(time(NULL), rt0));
  }
  else if(F==2) return(difftime(time(NULL), rt0));
  else return(0);
#endif
}

/***********************************************************
 *  Print the current time and the estimated finishing time.
 *
 *  P1 is the number of computed photon packets.
 *  Pt is the total number of photon packets.
 ****/
void PredictDoneTime(long P1, long Pt)
{
  time_t now, done_time;
  struct tm *date;
  char s[80];

  now = time(NULL);
  date = localtime(&now);
  strftime(s, 80, "%H:%M %x", date);
  printf("Now %s, ", s);

  done_time = now +
            (time_t) (PunchTime(2,"")*(Pt-P1)/(double)P1);
  date = localtime(&done_time);
  strftime(s, 80, "%H:%M %x", date);
  printf("End %s\n", s);
}

/***********************************************************
 *  Report estimated time, number of photons and runs left
 *  after calculating 10 photons or every 1/10 of total
 *  number of photons.
 *
 *  Num_Runs is the number of runs left.
 *  Pi is the index to the current photon, counting down.
 *  Pt is the total number of photons.
 ****/
void ReportStatus(short Num_Runs,long Pi,long Pt)
{
  if(Pt-Pi == 10 || Pi*10%Pt == 0 && Pi != Pt) {
    printf("%ld photons & %hd runs left, ", Pi, Num_Runs);
    PredictDoneTime(Pt-Pi, Pt);
  }
}

/***********************************************************
```

```
 *  Report time and write results.
 ****/
void ReportResult(InputStruct In_Parm, OutStruct Out_Parm)
{
  char time_report[STRLEN];

  strcpy(time_report, " Simulation time of this run.");
  PunchTime(1, time_report);

  SumScaleResult(In_Parm, &Out_Parm);
  WriteResult(In_Parm, Out_Parm, time_report);
}

/***********************************************************
 *  Get the file name of the input data file from the
 *  argument to the command line.
 ****/
void GetFnameFromArgv(int argc,
                      char * argv[],
                      char * input_filename)
{
  if(argc>=2) {         /* filename in command line */
    strcpy(input_filename, argv[1]);
  }
  else
    input_filename[0] = '\0';
}


/***********************************************************
 *  Execute Monte Carlo simulation for one independent run.
 ****/
void DoOneRun(short NumRuns, InputStruct *In_Ptr)
{
  register long i_photon;
    /* index to photon. register for speed.*/
  OutStruct out_parm;       /* distribution of photons.*/
  PhotonStruct photon;

#if THINKCPROFILER
  InitProfile(200,200); cecho2file("prof.rpt",0, stdout);
#endif

  InitOutputData(*In_Ptr, &out_parm);
  out_parm.Rsp = Rspecular(In_Ptr->layerspecs);
  i_photon = In_Ptr->num_photons;
  PunchTime(0, "");

  do {
    ReportStatus(NumRuns, i_photon, In_Ptr->num_photons);
    LaunchPhoton(out_parm.Rsp, In_Ptr->layerspecs, &photon);
    do  HopDropSpin(In_Ptr, &photon, &out_parm);
    while (!photon.dead);
  } while(--i_photon);

#if THINKCPROFILER
  exit(0);
#endif

  ReportResult(*In_Ptr, out_parm);
  FreeData(*In_Ptr, &out_parm);
}

/***********************************************************
 *  The argument to the command line is filename, if any.
 *  Macintosh does not support command line.
 ****/
```

```
char main(int argc, char *argv[])
{
  char input_filename[STRLEN];
  FILE *input_file_ptr;
  short num_runs;   /* number of independent runs. */
  InputStruct in_parm;

  ShowVersion("Version 1.1, 1992");
  GetFnameFromArgv(argc, argv, input_filename);
  input_file_ptr = GetFile(input_filename);
  CheckParm(input_file_ptr, &in_parm);
  num_runs = ReadNumRuns(input_file_ptr);

  while(num_runs--)  {
    ReadParm(input_file_ptr, &in_parm);
    DoOneRun(num_runs, &in_parm);
  }

  fclose(input_file_ptr);
  return(0);
}
```

B.3 mcmlio.c

```
/***********************************************************
 *  Copyright Univ. of Texas M.D. Anderson Cancer Center
 *  1992.
 *
 *  Input/output of data.
 ****/

#include "mcml.h"

/***********************************************************
 *  Structure used to check against duplicated file names.
 ****/
struct NameList {
  char name[STRLEN];
  struct NameList * next;
};

typedef struct NameList NameNode;
typedef NameNode * NameLink;


/***********************************************************
 *  Center a string according to the column width.
 ****/
char * CenterStr(short  Wid,
                 char * InStr,
                 char * OutStr)
{
  size_t nspaces;   /* number of spaces to be filled */
                    /* before InStr. */

  nspaces = (Wid - strlen(InStr))/2;
  if(nspaces<0) nspaces = 0;

  strcpy(OutStr, "");
  while(nspaces--)  strcat(OutStr, " ");

  strcat(OutStr, InStr);

  return(OutStr);
}

/***********************************************************
 *  Print some messages before starting simulation.
 *  e.g. author, address, program version, year.
 ****/
#define COLWIDTH 80
void ShowVersion(char *version)
{
  char str[STRLEN];

  CenterStr(COLWIDTH,
    "mcml - Monte Carlo Simulation of Multi-layered Turbid Media",
    str);
  puts(str);
  puts("");

  CenterStr(COLWIDTH, "Lihong Wang, Ph. D.", str);
  puts(str);

  CenterStr(COLWIDTH, "Steven L. Jacques, Ph. D.", str);
  puts(str);

  CenterStr(COLWIDTH,
    "Laser Biology Research Laboratory - Box 17",str);
  puts(str);

  CenterStr(COLWIDTH, "M.D. Anderson Cancer Center", str);
  puts(str);

  CenterStr(COLWIDTH, "University of Texas", str);
  puts(str);

  CenterStr(COLWIDTH, "Houston, TX 77030", str);
  puts(str);

  CenterStr(COLWIDTH, "Fax: (713)792-3995", str);
  puts(str);
  puts("");

  CenterStr(COLWIDTH, version, str);
  puts(str);
  puts("\n\n\n\n");
}
#undef COLWIDTH

/**************************************************************
 *  Get a filename and open it for reading, retry until
 *  the file can be opened.  '.' terminates the program.
 *
 *  If Fname != NULL, try Fname first.
 ****/
FILE *GetFile(char *Fname)
{
  FILE * file=NULL;
  Boolean firsttime=1;

  do {
    if(firsttime && Fname[0]!='\0') {
      /* use the filename from command line */
      firsttime = 0;
    }
    else {
      printf("Input filename(or . to exit):");
      scanf("%s", Fname);
      firsttime = 0;
    }

    if(strlen(Fname) == 1 && Fname[0] == '.')
      exit(1);          /* exit if no filename entered. */

    file = fopen(Fname, "r");
  }  while(file == NULL);

  return(file);
}

/**************************************************************
 *  Kill the ith char (counting from 0), push the following
 *  chars forward by one.
 ****/
void KillChar(size_t i, char * Str)
{
  size_t sl = strlen(Str);

  for(;i<sl;i++) Str[i] = Str[i+1];
}

/**************************************************************
```

```
 *  Eliminate the chars in a string which are not printing
 *  chars or spaces.
 *
 *  Spaces include ' ', '\f', '\t' etc.
 *
 *  Return 1 if no nonprinting chars found, otherwise
 *  return 0.
 ****/
Boolean CheckChar(char * Str)
{
  Boolean found = 0;    /* found bad char. */
  size_t sl = strlen(Str);
  size_t i=0;

  while(i<sl)
    if (Str[i]<0 || Str[i]>255)
      nrerror("Non-ASCII file\n");
    else if(isprint(Str[i]) || isspace(Str[i]))
      i++;
    else {
      found = 1;
      KillChar(i, Str);
      sl--;
    }

  return(found);
}

/************************************************************
 *  Return 1 if this line is a comment line in which the
 *  first non-space character is "#".
 *
 *  Also return 1 if this line is space line.
 ****/
Boolean CommentLine(char *Buf)
{
  size_t spn, cspn;

  spn = strspn(Buf, " \t");
  /* length spanned by space or tab chars. */

  cspn = strcspn(Buf, "#\n");
  /* length before the 1st # or return. */

  if(spn == cspn)   /* comment line or space line. */
    return(1);
  else              /* the line has data. */
    return(0);
}

/************************************************************
 *  Skip space or comment lines and return a data line only.
 ****/
char * FindDataLine(FILE *File_Ptr)
{
  char buf[STRLEN];

  buf[0] = '\0';
  do {  /* skip space or comment lines. */
    if(fgets(buf, 255, File_Ptr) == NULL)  {
      printf("Incomplete data\n");
      buf[0]='\0';
      break;
    }
    else
      CheckChar(buf);
  } while(CommentLine(buf));

  return(buf);
}

/***********************************************************
 *  Skip file version, then read number of runs.
 ****/
short ReadNumRuns(FILE* File_Ptr)
{
  char buf[STRLEN];
  short n=0;

  FindDataLine(File_Ptr); /* skip file version. */

  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0') nrerror("Reading number of runs\n");
  sscanf(buf, "%hd",&n);
  return(n);
}


/***********************************************************
 *  Read the file name and the file format.
 *
 *  The file format can be either A for ASCII or B for
 *  binary.
 ****/
void ReadFnameFormat(FILE *File_Ptr, InputStruct *In_Ptr)
{
  char buf[STRLEN];

  /** read in file name and format. **/
  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0')
    nrerror("Reading file name and format.\n");
  sscanf(buf, "%s %c",
    In_Ptr->out_fname, &(In_Ptr->out_fformat) );
  if(toupper(In_Ptr->out_fformat) != 'B')
    In_Ptr->out_fformat = 'A';
}


/***********************************************************
 *  Read the number of photons.
 ****/
void ReadNumPhotons(FILE *File_Ptr, InputStruct *In_Ptr)
{
  char buf[STRLEN];

  /** read in number of photons. **/
  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0')
    nrerror("Reading number of photons.\n");
  sscanf(buf, "%ld", &In_Ptr->num_photons);
  if(In_Ptr->num_photons<=0)
    nrerror("Nonpositive number of photons.\n");
}


/***********************************************************
 *  Read the members dz and dr.
 ****/
void ReadDzDr(FILE *File_Ptr, InputStruct *In_Ptr)
{
  char buf[STRLEN];

  /** read in dz, dr. **/
  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0') nrerror("Reading dz, dr.\n");
  sscanf(buf, "%lf%lf", &In_Ptr->dz, &In_Ptr->dr);
  if(In_Ptr->dz<=0) nrerror("Nonpositive dz.\n");
  if(In_Ptr->dr<=0) nrerror("Nonpositive dr.\n");
}


/**************************************************************
 *  Read the members nz, nr, na.
 ****/
void ReadNzNrNa(FILE *File_Ptr, InputStruct *In_Ptr)
{
  char buf[STRLEN];

  /** read in number of dz, dr, da. **/
  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0')
    nrerror("Reading number of dz, dr, da's.\n");
  sscanf(buf, "%hd%hd%hd",
    &In_Ptr->nz, &In_Ptr->nr, &In_Ptr->na);
  if(In_Ptr->nz<=0)
    nrerror("Nonpositive number of dz's.\n");
  if(In_Ptr->nr<=0)
    nrerror("Nonpositive number of dr's.\n");
  if(In_Ptr->na<=0)
    nrerror("Nonpositive number of da's.\n");
  In_Ptr->da = 0.5*PI/In_Ptr->na;
}


/**************************************************************
 *  Read the number of layers.
 ****/
void ReadNumLayers(FILE *File_Ptr, InputStruct *In_Ptr)
{
  char buf[STRLEN];

  /** read in number of layers. **/
  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0')
    nrerror("Reading number of layers.\n");
  sscanf(buf, "%hd", &In_Ptr->num_layers);
  if(In_Ptr->num_layers<=0)
    nrerror("Nonpositive number of layers.\n");
}


/**************************************************************
 *  Read the refractive index n of the ambient.
 ****/
void ReadAmbient(FILE *File_Ptr,
                 LayerStruct * Layer_Ptr,
                 char *side)
{
  char buf[STRLEN], msg[STRLEN];
  double n;

  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0') {
    sprintf(msg, "Rading n of %s ambient.\n", side);
    nrerror(msg);
  }

  sscanf(buf, "%lf", &n );
  if(n<=0) nrerror("Wrong n.\n");
  Layer_Ptr->n = n;
```

```
}


/**************************************************************
 *  Read the parameters of one layer.
 *
 *  Return 1 if error detected.
 *  Return 0 otherwise.
 *
 *  *Z_Ptr is the z coordinate of the current layer, which
 *  is used to convert thickness of layer to z coordinates
 *  of the two boundaries of the layer.
 ****/
Boolean ReadOneLayer(FILE *File_Ptr,
                     LayerStruct * Layer_Ptr,
                     double *Z_Ptr)
{
  char buf[STRLEN], msg[STRLEN];
  double d, n, mua, mus, g; /* d is thickness. */

  strcpy(buf, FindDataLine(File_Ptr));
  if(buf[0]=='\0') return(1);   /* error. */

  sscanf(buf, "%lf%lf%lf%lf%lf", &n, &mua, &mus, &g, &d);
  if(d<0 || n<=0 || mua<0 || mus<0 || g<0 || g>1)
    return(1);          /* error. */

  Layer_Ptr->n  = n;
  Layer_Ptr->mua = mua;
  Layer_Ptr->mus = mus;
  Layer_Ptr->g   = g;
  Layer_Ptr->z0 = *Z_Ptr;
  *Z_Ptr += d;
  Layer_Ptr->z1 = *Z_Ptr;

  return(0);
}

/**************************************************************
 *  Read the parameters of one layer at a time.
 ****/
void ReadLayerSpecs(FILE *File_Ptr,
                    short Num_Layers,
                    LayerStruct ** Layerspecs_PP)
{
  char msg[STRLEN];
  short i=0;
  double z = 0.0;   /* z coordinate of the current layer. */

  /* Allocate an array for the layer parameters. */
  /* layer 0 and layer Num_Layers + 1 are for ambient. */
  *Layerspecs_PP = (LayerStruct *)
    malloc((unsigned) (Num_Layers+2)*sizeof(LayerStruct));
  if (!(*Layerspecs_PP))
    nrerror("allocation failure in ReadLayerSpecs()");

  ReadAmbient(File_Ptr, &((*Layerspecs_PP)[i]), "top");
  for(i=1; i<=Num_Layers; i++)
    if(ReadOneLayer(File_Ptr, &((*Layerspecs_PP)[i]), &z)) {
      sprintf(msg, "Error reading %hd of %hd layers\n",
              i, Num_Layers);
      nrerror(msg);
    }
  ReadAmbient(File_Ptr, &((*Layerspecs_PP)[i]), "bottom");
}

/**************************************************************
```

```
 *  Compute the critical angles for total internal
 *  reflection according to the relative refractive index
 *  of the layer.
 *  All layers are processed.
 ****/
void CriticalAngle( short Num_Layers,
                    LayerStruct ** Layerspecs_PP)
{
  short i=0;
  double n1, n2;

  for(i=1; i<=Num_Layers; i++)  {
    n1 = (*Layerspecs_PP)[i].n;
    n2 = (*Layerspecs_PP)[i-1].n;
    (*Layerspecs_PP)[i].cos_crit0 = n1>n2 ?
        sqrt(1.0 - n2*n2/(n1*n1)) : 0.0;

    n2 = (*Layerspecs_PP)[i+1].n;
    (*Layerspecs_PP)[i].cos_crit1 = n1>n2 ?
        sqrt(1.0 - n2*n2/(n1*n1)) : 0.0;
  }
}

/**************************************************************
 *  Read in the input parameters for one run.
 ****/
void ReadParm(FILE* File_Ptr, InputStruct * In_Ptr)
{
  char buf[STRLEN];

  In_Ptr->Wth = WEIGHT;

  ReadFnameFormat(File_Ptr, In_Ptr);
  ReadNumPhotons(File_Ptr, In_Ptr);
  ReadDzDr(File_Ptr, In_Ptr);
  ReadNzNrNa(File_Ptr, In_Ptr);
  ReadNumLayers(File_Ptr, In_Ptr);

  ReadLayerSpecs(File_Ptr, In_Ptr->num_layers,
              &In_Ptr->layerspecs);
  CriticalAngle(In_Ptr->num_layers, &In_Ptr->layerspecs);
}

/**************************************************************
 *  Return 1, if the name in the name list.
 *  Return 0, otherwise.
 ****/
Boolean NameInList(char *Name, NameLink List)
{
  while (List != NULL) {
    if(strcmp(Name, List->name) == 0)
      return(1);
    List = List->next;
  };
  return(0);
}

/**************************************************************
 *  Add the name to the name list.
 ****/
void AddNameToList(char *Name, NameLink * List_Ptr)
{
  NameLink list = *List_Ptr;

  if(list == NULL) {    /* first node. */
    *List_Ptr = list = (NameLink)malloc(sizeof(NameNode));
    strcpy(list->name, Name);
    list->next = NULL;
  }
  else {                /* subsequent nodes. */
    /* Move to the last node. */
    while(list->next != NULL)
      list = list->next;

    /* Append a node to the list. */
    list->next = (NameLink)malloc(sizeof(NameNode));
    list = list->next;
    strcpy(list->name, Name);
    list->next = NULL;
  }
}

/**************************************************************
 *  Check against duplicated file names.
 *
 *  A linked list is set up to store the file names used
 *  in this input data file.
 ****/
Boolean FnameTaken(char *fname, NameLink * List_Ptr)
{
  if(NameInList(fname, *List_Ptr))
    return(1);
  else {
    AddNameToList(fname, List_Ptr);
    return(0);
  }
}

/**************************************************************
 *  Free each node in the file name list.
 ****/
void FreeFnameList(NameLink List)
{
  NameLink next;

  while(List != NULL) {
    next = List->next;
    free(List);
    List = next;
  }
}

/**************************************************************
 *  Check the input parameters for each run.
 ****/
void CheckParm(FILE* File_Ptr, InputStruct * In_Ptr)
{
  short i_run;
  short num_runs;   /* number of independent runs. */
  NameLink head = NULL;
  Boolean name_taken;/* output files share the same */
                     /* file name.*/
  char msg[STRLEN];

  num_runs = ReadNumRuns(File_Ptr);
  for(i_run=1; i_run<=num_runs; i_run++)  {
    printf("Checking input data for run %hd\n", i_run);
    ReadParm(File_Ptr, In_Ptr);

    name_taken = FnameTaken(In_Ptr->out_fname, &head);
    if(name_taken)
      sprintf(msg, "file name %s duplicated.\n",
                     In_Ptr->out_fname);

    free(In_Ptr->layerspecs);
    if(name_taken) nrerror(msg);
  }
  FreeFnameList(head);
  rewind(File_Ptr);
}


/***********************************************************
 *  Allocate the arrays in OutStruct for one run, and
 *  array elements are automatically initialized to zeros.
 ****/
void InitOutputData(InputStruct In_Parm,
                    OutStruct * Out_Ptr)
{
  short nz = In_Parm.nz;
  short nr = In_Parm.nr;
  short na = In_Parm.na;
  short nl = In_Parm.num_layers;
  /* remember to use nl+2 because of 2 for ambient. */

  if(nz<=0 || nr<=0 || na<=0 || nl<=0)
    nrerror("Wrong grid parameters.\n");

  /* Init pure numbers. */
  Out_Ptr->Rsp = 0.0;
  Out_Ptr->Rd  = 0.0;
  Out_Ptr->A   = 0.0;
  Out_Ptr->Tt  = 0.0;

  /* Allocate the arrays and the matrices. */
  Out_Ptr->Rd_ra = AllocMatrix(0,nr-1,0,na-1);
  Out_Ptr->Rd_r  = AllocVector(0,nr-1);
  Out_Ptr->Rd_a  = AllocVector(0,na-1);

  Out_Ptr->A_rz  = AllocMatrix(0,nr-1,0,nz-1);
  Out_Ptr->A_z   = AllocVector(0,nz-1);
  Out_Ptr->A_l   = AllocVector(0,nl+1);

  Out_Ptr->Tt_ra = AllocMatrix(0,nr-1,0,na-1);
  Out_Ptr->Tt_r  = AllocVector(0,nr-1);
  Out_Ptr->Tt_a  = AllocVector(0,na-1);
}

/***********************************************************
 *  Undo what InitOutputData did.
 *  i.e. free the data allocations.
 ****/
void FreeData(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nz = In_Parm.nz;
  short nr = In_Parm.nr;
  short na = In_Parm.na;
  short nl = In_Parm.num_layers;
  /* remember to use nl+2 because of 2 for ambient. */

  free(In_Parm.layerspecs);

  FreeMatrix(Out_Ptr->Rd_ra, 0,nr-1,0,na-1);
  FreeVector(Out_Ptr->Rd_r, 0,nr-1);
  FreeVector(Out_Ptr->Rd_a, 0,na-1);

  FreeMatrix(Out_Ptr->A_rz, 0, nr-1, 0,nz-1);
  FreeVector(Out_Ptr->A_z, 0, nz-1);
  FreeVector(Out_Ptr->A_l, 0,nl+1);

  FreeMatrix(Out_Ptr->Tt_ra, 0,nr-1,0,na-1);
  FreeVector(Out_Ptr->Tt_r, 0,nr-1);
  FreeVector(Out_Ptr->Tt_a, 0,na-1);
}

/***********************************************************
 *  Get 1D array elements by summing the 2D array elements.
 ****/
void Sum2DRd(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nr = In_Parm.nr;
  short na = In_Parm.na;
  short ir,ia;
  double sum;

  for(ir=0; ir<nr; ir++)  {
    sum = 0.0;
    for(ia=0; ia<na; ia++) sum += Out_Ptr->Rd_ra[ir][ia];
    Out_Ptr->Rd_r[ir] = sum;
  }

  for(ia=0; ia<na; ia++)  {
    sum = 0.0;
    for(ir=0; ir<nr; ir++) sum += Out_Ptr->Rd_ra[ir][ia];
    Out_Ptr->Rd_a[ia] = sum;
  }

  sum = 0.0;
  for(ir=0; ir<nr; ir++) sum += Out_Ptr->Rd_r[ir];
  Out_Ptr->Rd = sum;
}

/***********************************************************
 *  Return the index to the layer according to the index
 *  to the grid line system in z direction (Iz).
 *
 *  Use the center of box.
 ****/
short IzToLayer(short Iz, InputStruct In_Parm)
{
  short i=1;    /* index to layer. */
  short num_layers = In_Parm.num_layers;
  double dz = In_Parm.dz;

  while( (Iz+0.5)*dz >= In_Parm.layerspecs[i].z1
    && i<num_layers) i++;

  return(i);
}

/***********************************************************
 *  Get 1D array elements by summing the 2D array elements.
 ****/
void Sum2DA(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nz = In_Parm.nz;
  short nr = In_Parm.nr;
  short iz,ir;
  double sum;

  for(iz=0; iz<nz; iz++)  {
    sum = 0.0;
    for(ir=0; ir<nr; ir++) sum += Out_Ptr->A_rz[ir][iz];
    Out_Ptr->A_z[iz] = sum;
  }

  sum = 0.0;
  for(iz=0; iz<nz; iz++) {
    sum += Out_Ptr->A_z[iz];
    Out_Ptr->A_l[IzToLayer(iz, In_Parm)]
      += Out_Ptr->A_z[iz];
  }
  Out_Ptr->A = sum;
}

/***********************************************************
 *  Get 1D array elements by summing the 2D array elements.
 ****/
void Sum2DTt(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nr = In_Parm.nr;
  short na = In_Parm.na;
  short ir,ia;
  double sum;

  for(ir=0; ir<nr; ir++)  {
    sum = 0.0;
    for(ia=0; ia<na; ia++) sum += Out_Ptr->Tt_ra[ir][ia];
    Out_Ptr->Tt_r[ir] = sum;
  }

  for(ia=0; ia<na; ia++)  {
    sum = 0.0;
    for(ir=0; ir<nr; ir++) sum += Out_Ptr->Tt_ra[ir][ia];
    Out_Ptr->Tt_a[ia] = sum;
  }

  sum = 0.0;
  for(ir=0; ir<nr; ir++) sum += Out_Ptr->Tt_r[ir];
  Out_Ptr->Tt = sum;
}

/***********************************************************
 *  Scale Rd and Tt properly.
 *
 *  "a" stands for angle alpha.
 ****
 *  Scale Rd(r,a) and Tt(r,a) by
 *      (area perpendicular to photon direction)
 *      x(solid angle)x(No. of photons).
 *  or
 *      [2*PI*r*dr*cos(a)]x[2*PI*sin(a)*da]x[No. of photons]
 *  or
 *      [2*PI*PI*dr*da*r*sin(2a)]x[No. of photons]
 ****
 *  Scale Rd(r) and Tt(r) by
 *      (area on the surface)x(No. of photons).
 ****
 *  Scale Rd(a) and Tt(a) by
 *      (solid angle)x(No. of photons).
 ****/
void ScaleRdTt(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nr = In_Parm.nr;
  short na = In_Parm.na;
  double dr = In_Parm.dr;
  double da = In_Parm.da;
  short ir,ia;
  double scale1, scale2;

  scale1 = 4.0*PI*PI*dr*sin(da/2)*dr*In_Parm.num_photons;
    /* The factor (ir+0.5)*sin(2a) to be added. */

  for(ir=0; ir<nr; ir++)
    for(ia=0; ia<na; ia++) {
      scale2 = 1.0/((ir+0.5)*sin(2.0*(ia+0.5)*da)*scale1);
      Out_Ptr->Rd_ra[ir][ia] *= scale2;
      Out_Ptr->Tt_ra[ir][ia] *= scale2;
    }

  scale1 = 2.0*PI*dr*dr*In_Parm.num_photons;
    /* area is 2*PI*[(ir+0.5)*dr]*dr.*/
    /* ir+0.5 to be added. */

  for(ir=0; ir<nr; ir++) {
    scale2 = 1.0/((ir+0.5)*scale1);
    Out_Ptr->Rd_r[ir] *= scale2;
    Out_Ptr->Tt_r[ir] *= scale2;
  }

  scale1  = 2.0*PI*da*In_Parm.num_photons;
    /* solid angle is 2*PI*sin(a)*da. sin(a) to be added. */

  for(ia=0; ia<na; ia++) {
    scale2 = 1.0/(sin((ia+0.5)*da)*scale1);
    Out_Ptr->Rd_a[ia] *= scale2;
    Out_Ptr->Tt_a[ia] *= scale2;
  }

  scale2 = 1.0/(double)In_Parm.num_photons;
  Out_Ptr->Rd *= scale2;
  Out_Ptr->Tt *= scale2;
}

/***********************************************************
 *  Scale absorption arrays properly.
 ****/
void ScaleA(InputStruct In_Parm, OutStruct * Out_Ptr)
{
  short nz = In_Parm.nz;
  short nr = In_Parm.nr;
  double dz = In_Parm.dz;
  double dr = In_Parm.dr;
  short nl = In_Parm.num_layers;
  short iz,ir;
  short il;
  double scale1;

  /* Scale A_rz. */
  scale1 = 2.0*PI*dr*dr*dz*In_Parm.num_photons;
    /* volume is 2*pi*(ir+0.5)*dr*dr*dz.*/
    /* ir+0.5 to be added. */
  for(iz=0; iz<nz; iz++)
    for(ir=0; ir<nr; ir++)
      Out_Ptr->A_rz[ir][iz] /= (ir+0.5)*scale1;

  /* Scale A_z. */
  scale1 = 1.0/(dz*In_Parm.num_photons);
  for(iz=0; iz<nz; iz++)
    Out_Ptr->A_z[iz] *= scale1;

  /* Scale A_l. Avoid int/int. */
  scale1 = 1.0/(double)In_Parm.num_photons;
  for(il=0; il<=nl+1; il++)
    Out_Ptr->A_l[il] *= scale1;

  Out_Ptr->A *=scale1;
}

/***********************************************************
 *  Sum and scale results of current run.
 ****/
```

```
void SumScaleResult(InputStruct In_Parm,
                    OutStruct * Out_Ptr)
{
  /* Get 1D & 0D results. */
  Sum2DRd(In_Parm, Out_Ptr);
  Sum2DA(In_Parm,  Out_Ptr);
  Sum2DTt(In_Parm, Out_Ptr);

  ScaleRdTt(In_Parm, Out_Ptr);
  ScaleA(In_Parm, Out_Ptr);
}

/***********************************************************
 *  Write the version number as the first string in the
 *  file.
 *  Use chars only so that they can be read as either
 *  ASCII or binary.
 ****/
void WriteVersion(FILE *file, char *Version)
{
  fprintf(file,
    "%s \t# Version number of the file format.\n\n",
    Version);
  fprintf(file, "####\n# Data categories include: \n");
  fprintf(file, "# InParm, RAT, \n");
  fprintf(file, "# A_l, A_z, Rd_r, Rd_a, Tt_r, Tt_a, \n");
  fprintf(file, "# A_rz, Rd_ra, Tt_ra \n####\n\n");
}

/***********************************************************
 *  Write the input parameters to the file.
 ****/
void WriteInParm(FILE *file, InputStruct In_Parm)
{
  short i;

  fprintf(file,
    "InParm \t\t\t# Input parameters. cm is used.\n");

  fprintf(file,
    "%s \tA\t\t# output file name, ASCII.\n",
    In_Parm.out_fname);
  fprintf(file,
    "%ld \t\t\t# No. of photons\n", In_Parm.num_photons);

  fprintf(file,
    "%G\t%G\t\t# dz, dr [cm]\n", In_Parm.dz,In_Parm.dr);
  fprintf(file, "%hd\t%hd\t%hd\t# No. of dz, dr, da.\n\n",
      In_Parm.nz, In_Parm.nr, In_Parm.na);

  fprintf(file,
    "%hd\t\t\t\t\t\t# Number of layers\n",
    In_Parm.num_layers);
  fprintf(file,
    "#n\tmua\tmus\tg\td\t# One line for each layer\n");
  fprintf(file,
    "%G\t\t\t\t\t# n for medium above\n",
    In_Parm.layerspecs[0].n);
  for(i=1; i<=In_Parm.num_layers; i++)  {
    LayerStruct s;
    s = In_Parm.layerspecs[i];
    fprintf(file, "%G\t%G\t%G\t%G\t%G\t# layer %hd\n",
        s.n, s.mua, s.mus, s.g, s.z1-s.z0, i);
  }
  fprintf(file, "%G\t\t\t\t\t# n for medium below\n\n",
    In_Parm.layerspecs[i].n);
}
```

```

/**************************************************************
 *  Write reflectance, absorption, transmission.
 ****/
void WriteRAT(FILE * file, OutStruct Out_Parm)
{
  fprintf(file,
    "RAT #Reflectance, absorption, transmission. \n");
    /* flag. */

  fprintf(file,
    "%-14.6G \t#Specular reflectance [-]\n", Out_Parm.Rsp);
  fprintf(file,
    "%-14.6G \t#Diffuse reflectance [-]\n", Out_Parm.Rd);
  fprintf(file,
    "%-14.6G \t#Absorbed fraction [-]\n", Out_Parm.A);
  fprintf(file,
    "%-14.6G \t#Transmittance [-]\n", Out_Parm.Tt);

  fprintf(file, "\n");
}

/**************************************************************
 *  Write absorption as a function of layer.
 ****/
void WriteA_layer(FILE * file,
                  short Num_Layers,
                  OutStruct Out_Parm)
{
  short i;

  fprintf(file,
    "A_l #Absorption as a function of layer. [-]\n");
    /* flag. */

  for(i=1; i<=Num_Layers; i++)
    fprintf(file, "%12.4G\n", Out_Parm.A_l[i]);
  fprintf(file, "\n");
}

/**************************************************************
 *  5 numbers each line.
 ****/
void WriteRd_ra(FILE * file,
                short Nr,
                short Na,
                OutStruct Out_Parm)
{
  short ir, ia;

  fprintf(file,
      "%s\n%s\n%s\n%s\n%s\n%s\n",   /* flag. */
      "# Rd[r][angle]. [1/(cm2sr)].",
      "# Rd[0][0], [0][1],..[0][na-1]",
      "# Rd[1][0], [1][1],..[1][na-1]",
      "# ...",
      "# Rd[nr-1][0], [nr-1][1],..[nr-1][na-1]",
      "Rd_ra");

  for(ir=0;ir<Nr;ir++)
    for(ia=0;ia<Na;ia++)  {
      fprintf(file, "%12.4E ", Out_Parm.Rd_ra[ir][ia]);
      if( (ir*Na + ia + 1)%5 == 0) fprintf(file, "\n");
    }

  fprintf(file, "\n");
}
```

```

/**************************************************************
 *  1 number each line.
 ****/
void WriteRd_r(FILE * file,
               short Nr,
               OutStruct Out_Parm)
{
  short ir;

  fprintf(file,
    "Rd_r #Rd[0], [1],..Rd[nr-1]. [1/cm2]\n");  /* flag. */

  for(ir=0;ir<Nr;ir++) {
    fprintf(file, "%12.4E\n", Out_Parm.Rd_r[ir]);
  }

  fprintf(file, "\n");
}

/**************************************************************
 *  1 number each line.
 ****/
void WriteRd_a(FILE * file,
               short Na,
               OutStruct Out_Parm)
{
  short ia;

  fprintf(file,
    "Rd_a #Rd[0], [1],..Rd[na-1]. [sr-1]\n");   /* flag. */

  for(ia=0;ia<Na;ia++) {
    fprintf(file, "%12.4E\n", Out_Parm.Rd_a[ia]);
  }

  fprintf(file, "\n");
}

/**************************************************************
 *  5 numbers each line.
 ****/
void WriteTt_ra(FILE * file,
                short Nr,
                short Na,
                OutStruct Out_Parm)
{
  short ir, ia;

  fprintf(file,
      "%s\n%s\n%s\n%s\n%s\n%s\n",   /* flag. */
      "# Tt[r][angle]. [1/(cm2sr)].",
      "# Tt[0][0], [0][1],..[0][na-1]",
      "# Tt[1][0], [1][1],..[1][na-1]",
      "# ...",
      "# Tt[nr-1][0], [nr-1][1],..[nr-1][na-1]",
      "Tt_ra");

  for(ir=0;ir<Nr;ir++)
    for(ia=0;ia<Na;ia++)  {
      fprintf(file, "%12.4E ", Out_Parm.Tt_ra[ir][ia]);
      if( (ir*Na + ia + 1)%5 == 0) fprintf(file, "\n");
    }

  fprintf(file, "\n");
}

```

```
/***********************************************************
 *  5 numbers each line.
 ****/
void WriteA_rz(FILE * file,
               short Nr,
               short Nz,
               OutStruct Out_Parm)
{
  short iz, ir;

  fprintf(file,
      "%s\n%s\n%s\n%s\n%s\n%s\n", /* flag. */
      "# A[r][z]. [1/cm3]",
      "# A[0][0], [0][1],..[0][nz-1]",
      "# A[1][0], [1][1],..[1][nz-1]",
      "# ...",
      "# A[nr-1][0], [nr-1][1],..[nr-1][nz-1]",
      "A_rz");

  for(ir=0;ir<Nr;ir++)
    for(iz=0;iz<Nz;iz++)  {
      fprintf(file, "%12.4E ", Out_Parm.A_rz[ir][iz]);
      if( (ir*Nz + iz + 1)%5 == 0) fprintf(file, "\n");
    }

  fprintf(file, "\n");
}

/***********************************************************
 *  1 number each line.
 ****/
void WriteA_z(FILE * file,
              short Nz,
              OutStruct Out_Parm)
{
  short iz;

  fprintf(file,
    "A_z #A[0], [1],..A[nz-1]. [1/cm]\n");  /* flag. */

  for(iz=0;iz<Nz;iz++) {
    fprintf(file, "%12.4E\n", Out_Parm.A_z[iz]);
  }

  fprintf(file, "\n");
}

/***********************************************************
 *  1 number each line.
 ****/
void WriteTt_r(FILE * file,
               short Nr,
               OutStruct Out_Parm)
{
  short ir;

  fprintf(file,
    "Tt_r #Tt[0], [1],..Tt[nr-1]. [1/cm2]\n"); /* flag. */

  for(ir=0;ir<Nr;ir++) {
    fprintf(file, "%12.4E\n", Out_Parm.Tt_r[ir]);
  }

  fprintf(file, "\n");
}

/***********************************************************
```

```
 *  1 number each line.
 ****/
void WriteTt_a(FILE * file,
               short Na,
               OutStruct Out_Parm)
{
  short ia;

  fprintf(file,
    "Tt_a #Tt[0], [1],..Tt[na-1]. [sr-1]\n"); /* flag. */

  for(ia=0;ia<Na;ia++) {
    fprintf(file, "%12.4E\n", Out_Parm.Tt_a[ia]);
  }

  fprintf(file, "\n");
}

/************************************************************
 ****/
void WriteResult(InputStruct In_Parm,
                 OutStruct Out_Parm,
                 char * TimeReport)
{
  FILE *file;

  file = fopen(In_Parm.out_fname, "w");
  if(file == NULL) nrerror("Cannot open file to write.\n");

  if(toupper(In_Parm.out_fformat) == 'A')
    WriteVersion(file, "A1");
  else
    WriteVersion(file, "B1");

  fprintf(file, "# %s", TimeReport);
  fprintf(file, "\n");

  WriteInParm(file, In_Parm);
  WriteRAT(file, Out_Parm);
    /* reflectance, absorption, transmittance. */

  /* 1D arrays. */
  WriteA_layer(file, In_Parm.num_layers, Out_Parm);
  WriteA_z(file, In_Parm.nz, Out_Parm);
  WriteRd_r(file, In_Parm.nr, Out_Parm);
  WriteRd_a(file, In_Parm.na, Out_Parm);
  WriteTt_r(file, In_Parm.nr, Out_Parm);
  WriteTt_a(file, In_Parm.na, Out_Parm);

  /* 2D arrays. */
  WriteA_rz(file, In_Parm.nr, In_Parm.nz, Out_Parm);
  WriteRd_ra(file, In_Parm.nr, In_Parm.na, Out_Parm);
  WriteTt_ra(file, In_Parm.nr, In_Parm.na, Out_Parm);

  fclose(file);
}
```

B.4 mcmlgo.c

```
/***********************************************************
 *  Copyright Univ. of Texas M.D. Anderson Cancer Center
 *  1992.
 *
 *  Launch, move, and record photon weight.
 ****/

#include "mcml.h"

#define STANDARDTEST 0
  /* testing program using fixed rnd seed. */

#define PARTIALREFLECTION 0
  /* 1=split photon, 0=statistical reflection. */

#define COSZERO (1.0-1.0E-12)
  /* cosine of about 1e-6 rad. */

#define COS90D  1.0E-6
  /* cosine of about 1.57 - 1e-6 rad. */


/***********************************************************
 *  A random number generator from Numerical Recipes in C.
 ****/
#define MBIG 1000000000
#define MSEED 161803398
#define MZ 0
#define FAC 1.0E-9

float ran3(int *idum)
{
  static int inext,inextp;
  static long ma[56];
  static int iff=0;
  long mj,mk;
  int i,ii,k;

  if (*idum < 0 || iff == 0) {
    iff=1;
    mj=MSEED-(*idum < 0 ? -*idum : *idum);
    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 (k=1;k<=4;k++)
      for (i=1;i<=55;i++) {
    ma[i] -= ma[1+(i+30) % 55];
    if (ma[i] < MZ) ma[i] += MBIG;
      }
    inext=0;
    inextp=31;
    *idum=1;
  }
  if (++inext == 56) inext=1;
  if (++inextp == 56) inextp=1;
  mj=ma[inext]-ma[inextp];
  if (mj < MZ) mj += MBIG;
  ma[inext]=mj;
  return mj*FAC;
}

#undef MBIG
#undef MSEED
#undef MZ
#undef FAC


/***********************************************************
 *  Generate a random number between 0 and 1.  Take a
 *  number as seed the first time entering the function.
 *  The seed is limited to 1<<15.
 *  We found that when idum is too large, ran3 may return
 *  numbers beyond 0 and 1.
 ****/
double RandomNum(void)
{
  static Boolean first_time=1;
  static int idum;  /* seed for ran3. */

  if(first_time) {
#if STANDARDTEST /* Use fixed seed to test the program. */
    idum = - 1;
#else
    idum = -(int)time(NULL)%(1<<15);
      /* use 16-bit integer as the seed. */
#endif
    ran3(&idum);
    first_time = 0;
    idum = 1;
  }

  return( (double)ran3(&idum) );
}

/***********************************************************
 *  Compute the specular reflection.
 *
 *  If the first layer is a turbid medium, use the Fresnel
 *  reflection from the boundary of the first layer as the
 *  specular reflectance.
 *
 *  If the first layer is glass, multiple reflections in
 *  the first layer is considered to get the specular
 *  reflectance.
 *
 *  The subroutine assumes the Layerspecs array is correctly
 *  initialized.
 ****/
double Rspecular(LayerStruct * Layerspecs_Ptr)
{
  double r1, r2;
    /* direct reflections from the 1st and 2nd layers. */
  double temp;

  temp =(Layerspecs_Ptr[0].n - Layerspecs_Ptr[1].n)
       /(Layerspecs_Ptr[0].n + Layerspecs_Ptr[1].n);
  r1 = temp*temp;

  if((Layerspecs_Ptr[1].mua == 0.0)
  && (Layerspecs_Ptr[1].mus == 0.0))  { /* glass layer. */
    temp = (Layerspecs_Ptr[1].n - Layerspecs_Ptr[2].n)
          /(Layerspecs_Ptr[1].n + Layerspecs_Ptr[2].n);
    r2 = temp*temp;
    r1 = r1 + (1-r1)*(1-r1)*r2/(1-r1*r2);
  }

  return (r1);
}

/***********************************************************
 *  Initialize a photon packet.
 ****/
void LaunchPhoton(double Rspecular,
                  LayerStruct  * Layerspecs_Ptr,
                  PhotonStruct * Photon_Ptr)
{
  Photon_Ptr->w     = 1.0 - Rspecular;
  Photon_Ptr->dead  = 0;
  Photon_Ptr->layer = 1;
  Photon_Ptr->s = 0;
  Photon_Ptr->sleft= 0;

  Photon_Ptr->x     = 0.0;
  Photon_Ptr->y     = 0.0;
  Photon_Ptr->z     = 0.0;
  Photon_Ptr->ux    = 0.0;
  Photon_Ptr->uy    = 0.0;
  Photon_Ptr->uz    = 1.0;

  if((Layerspecs_Ptr[1].mua == 0.0)
  && (Layerspecs_Ptr[1].mus == 0.0))  { /* glass layer. */
    Photon_Ptr->layer   = 2;
    Photon_Ptr->z   = Layerspecs_Ptr[2].z0;
  }
}

/***********************************************************
 *  Choose (sample) a new theta angle for photon propagation
 *  according to the anisotropy.
 *
 *  If anisotropy g is 0, then
 *      cos(theta) = 2*rand-1.
 *  otherwise
 *      sample according to the Henyey-Greenstein function.
 *
 *  Returns the cosine of the polar deflection angle theta.
 ****/
double SpinTheta(double g)
{
  double cost;

  if(g == 0.0)
    cost = 2*RandomNum() -1;
  else {
    double temp = (1-g*g)/(1-g+2*g*RandomNum());
    cost = (1+g*g - temp*temp)/(2*g);
  }
  return(cost);
}


/***********************************************************
 *  Choose a new direction for photon propagation by
 *  sampling the polar deflection angle theta and the
 *  azimuthal angle psi.
 *
 *  Note:
 *      theta: 0 - pi so sin(theta) is always positive
 *      feel free to use sqrt() for cos(theta).
 *
 *      psi:   0 - 2pi
 *      for 0-pi  sin(psi) is +
 *      for pi-2pi sin(psi) is -
 ****/
void Spin(double g,
          PhotonStruct * Photon_Ptr)
{
  double cost, sint;    /* cosine and sine of the */
                        /* polar deflection angle theta. */
  double cosp, sinp;    /* cosine and sine of the */
                        /* azimuthal angle psi. */
  double ux = Photon_Ptr->ux;
  double uy = Photon_Ptr->uy;
  double uz = Photon_Ptr->uz;
  double psi;

  cost = SpinTheta(g);
  sint = sqrt(1.0 - cost*cost);
    /* sqrt() is faster than sin(). */

  psi = 2.0*PI*RandomNum(); /* spin psi 0-2pi. */
  cosp = cos(psi);
  if(psi<PI)
    sinp = sqrt(1.0 - cosp*cosp);
      /* sqrt() is faster than sin(). */
  else
    sinp = - sqrt(1.0 - cosp*cosp);

  if(fabs(uz) > COSZERO)  {     /* normal incident. */
    Photon_Ptr->ux = sint*cosp;
    Photon_Ptr->uy = sint*sinp;
    Photon_Ptr->uz = cost*SIGN(uz);
      /* SIGN() is faster than division. */
  }
  else  {       /* regular incident. */
    double temp = sqrt(1.0 - uz*uz);
    Photon_Ptr->ux = sint*(ux*uz*cosp - uy*sinp)
                     /temp + ux*cost;
    Photon_Ptr->uy = sint*(uy*uz*cosp + ux*sinp)
                     /temp + uy*cost;
    Photon_Ptr->uz = -sint*cosp*temp + uz*cost;
  }
}

/***********************************************************
 *  Move the photon s away in the current layer of medium.
 ****/
void Hop(PhotonStruct * Photon_Ptr)
{
  double s = Photon_Ptr->s;

  Photon_Ptr->x += s*Photon_Ptr->ux;
  Photon_Ptr->y += s*Photon_Ptr->uy;
  Photon_Ptr->z += s*Photon_Ptr->uz;
}

/***********************************************************
 *  If uz != 0, return the photon step size in glass,
 *  Otherwise, return 0.
 *
 *  The step size is the distance between the current
 *  position and the boundary in the photon direction.
 *
 *  Make sure uz !=0 before calling this function.
 ****/
void StepSizeInGlass(PhotonStruct *  Photon_Ptr,
                      InputStruct  *  In_Ptr)
{
  double dl_b;  /* step size to boundary. */
  short  layer = Photon_Ptr->layer;
  double uz = Photon_Ptr->uz;

  /* Stepsize to the boundary. */
  if(uz>0.0)
    dl_b = (In_Ptr->layerspecs[layer].z1 - Photon_Ptr->z)
           /uz;
  else if(uz<0.0)
    dl_b = (In_Ptr->layerspecs[layer].z0 - Photon_Ptr->z)
           /uz;
  else
    dl_b = 0.0;

  Photon_Ptr->s = dl_b;
}

/***********************************************************
 *  Pick a step size for a photon packet when it is in
 *  tissue.
 *  If the member sleft is zero, make a new step size
 *  with: -log(rnd)/(mua+mus).
 *  Otherwise, pick up the leftover in sleft.
 *
 *  Layer is the index to layer.
 *  In_Ptr is the input parameters.
 ****/
void StepSizeInTissue(PhotonStruct * Photon_Ptr,
                      InputStruct  * In_Ptr)
{
  short  layer = Photon_Ptr->layer;
  double mua = In_Ptr->layerspecs[layer].mua;
  double mus = In_Ptr->layerspecs[layer].mus;

  if(Photon_Ptr->sleft == 0.0) {  /* make a new step. */
    double rnd;

    do rnd = RandomNum();
      while( rnd <= 0.0 );    /* avoid zero. */
    Photon_Ptr->s = -log(rnd)/(mua+mus);
  }
  else {    /* take the leftover. */
    Photon_Ptr->s = Photon_Ptr->sleft/(mua+mus);
    Photon_Ptr->sleft = 0.0;
  }
}

/***********************************************************
 *  Check if the step will hit the boundary.
 *  Return 1 if hit boundary.
 *  Return 0 otherwise.
 *
 *  If the projected step hits the boundary, the members
 *  s and sleft of Photon_Ptr are updated.
 ****/
Boolean HitBoundary(PhotonStruct *  Photon_Ptr,
                    InputStruct  *  In_Ptr)
{
  double dl_b;  /* length to boundary. */
  short  layer = Photon_Ptr->layer;
  double uz = Photon_Ptr->uz;
  Boolean hit;

  /* Distance to the boundary. */
  if(uz>0.0)
```

```
    dl_b = (In_Ptr->layerspecs[layer].z1
            - Photon_Ptr->z)/uz;    /* dl_b>0. */
  else if(uz<0.0)
    dl_b = (In_Ptr->layerspecs[layer].z0
            - Photon_Ptr->z)/uz;    /* dl_b>0. */

  if(uz != 0.0 && Photon_Ptr->s > dl_b) {
      /* not horizontal & crossing. */
    double mut = In_Ptr->layerspecs[layer].mua
                + In_Ptr->layerspecs[layer].mus;

    Photon_Ptr->sleft = (Photon_Ptr->s - dl_b)*mut;
    Photon_Ptr->s    = dl_b;
    hit = 1;
  }
  else
    hit = 0;

  return(hit);
}

/***********************************************************
 *  Drop photon weight inside the tissue (not glass).
 *
 *  The photon is assumed not dead.
 *
 *  The weight drop is dw = w*mua/(mua+mus).
 *
 *  The dropped weight is assigned to the absorption array
 *  elements.
 ****/
void Drop(InputStruct  *    In_Ptr,
          PhotonStruct *    Photon_Ptr,
          OutStruct *       Out_Ptr)
{
  double dwa;       /* absorbed weight.*/
  double x = Photon_Ptr->x;
  double y = Photon_Ptr->y;
  short  iz, ir;    /* index to z & r. */
  short  layer = Photon_Ptr->layer;
  double mua, mus;

  /* compute array indices. */
  iz = (short)(Photon_Ptr->z/In_Ptr->dz);
  if(iz>In_Ptr->nz-1) iz=In_Ptr->nz-1;

  ir = (short)(sqrt(x*x+y*y)/In_Ptr->dr);
  if(ir>In_Ptr->nr-1) ir=In_Ptr->nr-1;

  /* update photon weight. */
  mua = In_Ptr->layerspecs[layer].mua;
  mus = In_Ptr->layerspecs[layer].mus;
  dwa = Photon_Ptr->w * mua/(mua+mus);
  Photon_Ptr->w -= dwa;

  /* assign dwa to the absorption array element. */
  Out_Ptr->A_rz[ir][iz] += dwa;
}

/***********************************************************
 *  The photon weight is small, and the photon packet tries
 *  to survive a roulette.
 ****/
void Roulette(PhotonStruct * Photon_Ptr)
{
  if(Photon_Ptr->w == 0.0)
    Photon_Ptr->dead = 1;
  else if(RandomNum() < CHANCE) /* survived the roulette.*/
    Photon_Ptr->w /= CHANCE;
  else
    Photon_Ptr->dead = 1;
}

/***********************************************************
 *  Compute the Fresnel reflectance.
 *
 *  Make sure that the cosine of the incident angle a1
 *  is positive, and the case when the angle is greater
 *  than the critical angle is ruled out.
 *
 *  Avoid trigonometric function operations as much as
 *  possible, because they are computation-intensive.
 ****/
double RFresnel(double n1,  /* incident refractive index.*/
                double n2,  /* transmit refractive index.*/
                double ca1, /* cosine of the incident */
                            /* angle. 0<a1<90 degrees. */
                double * ca2_Ptr)  /* pointer to the */
                            /* cosine of the transmission */
                            /* angle. a2>0. */
{
  double r;

  if(n1==n2) {              /** matched boundary. **/
    *ca2_Ptr = ca1;
    r = 0.0;
  }
  else if(ca1>COSZERO) {    /** normal incident. **/
    *ca2_Ptr = ca1;
    r = (n2-n1)/(n2+n1);
    r *= r;
  }
  else if(ca1<COS90D)  {    /** very slant. **/
    *ca2_Ptr = 0.0;
    r = 1.0;
  }
  else  {                   /** general. **/
    double sa1, sa2;
      /* sine of the incident and transmission angles. */
    double ca2;

    sa1 = sqrt(1-ca1*ca1);
    sa2 = n1*sa1/n2;
    if(sa2>=1.0) {
      /* double check for total internal reflection. */
      *ca2_Ptr = 0.0;
      r = 1.0;
    }
    else  {
      double cap, cam;  /* cosines of the sum ap or */
                        /* difference am of the two */
                        /* angles. ap = a1+a2 */
                        /* am = a1 - a2. */
      double sap, sam;  /* sines. */

      *ca2_Ptr = ca2 = sqrt(1-sa2*sa2);

      cap = ca1*ca2 - sa1*sa2; /* c+ = cc - ss. */
      cam = ca1*ca2 + sa1*sa2; /* c- = cc + ss. */
      sap = sa1*ca2 + ca1*sa2; /* s+ = sc + cs. */
      sam = sa1*ca2 - ca1*sa2; /* s- = sc - cs. */
      r = 0.5*sam*sam*(cam*cam+cap*cap)/(sap*sap*cam*cam);
        /* rearranged for speed. */
    }
  }
  return(r);
}

/***********************************************************
 *  Record the photon weight exiting the first layer(uz<0),
 *  no matter whether the layer is glass or not, to the
 *  reflection array.
 *
 *  Update the photon weight as well.
 ****/
void RecordR(double         Refl,   /* reflectance. */
             InputStruct  * In_Ptr,
             PhotonStruct * Photon_Ptr,
             OutStruct *    Out_Ptr)
{
  double x = Photon_Ptr->x;
  double y = Photon_Ptr->y;
  short  ir, ia;    /* index to r & angle. */

  ir = (short)(sqrt(x*x+y*y)/In_Ptr->dr);
  if(ir>In_Ptr->nr-1) ir=In_Ptr->nr-1;

  ia = (short)(acos(-Photon_Ptr->uz)/In_Ptr->da);
  if(ia>In_Ptr->na-1) ia=In_Ptr->na-1;

  /* assign photon to the reflection array element. */
  Out_Ptr->Rd_ra[ir][ia] += Photon_Ptr->w*(1.0-Refl);

  Photon_Ptr->w *= Refl;
}

/***********************************************************
 *  Record the photon weight exiting the last layer(uz>0),
 *  no matter whether the layer is glass or not, to the
 *  transmittance array.
 *
 *  Update the photon weight as well.
 ****/
void RecordT(double         Refl,
             InputStruct  * In_Ptr,
             PhotonStruct * Photon_Ptr,
             OutStruct *    Out_Ptr)
{
  double x = Photon_Ptr->x;
  double y = Photon_Ptr->y;
  short  ir, ia;    /* index to r & angle. */

  ir = (short)(sqrt(x*x+y*y)/In_Ptr->dr);
  if(ir>In_Ptr->nr-1) ir=In_Ptr->nr-1;

  ia = (short)(acos(Photon_Ptr->uz)/In_Ptr->da);
  if(ia>In_Ptr->na-1) ia=In_Ptr->na-1;

  /* assign photon to the transmittance array element. */
  Out_Ptr->Tt_ra[ir][ia] += Photon_Ptr->w*(1.0-Refl);

  Photon_Ptr->w *= Refl;
}

/***********************************************************
 *  Decide whether the photon will be transmitted or
 *  reflected on the upper boundary (uz<0) of the current
 *  layer.
 *
 *  If "layer" is the first layer, the photon packet will
 *  be partially transmitted and partially reflected if
 *  PARTIALREFLECTION is set to 1,
 *  or the photon packet will be either transmitted or
 *  reflected determined statistically if PARTIALREFLECTION
 *  is set to 0.
 *
 *  Record the transmitted photon weight as reflection.
 *
 *  If the "layer" is not the first layer and the photon
 *  packet is transmitted, move the photon to "layer-1".
 *
 *  Update the photon parmameters.
 ****/
void CrossUpOrNot(InputStruct  *    In_Ptr,
                  PhotonStruct *    Photon_Ptr,
                  OutStruct *       Out_Ptr)
{
  double uz = Photon_Ptr->uz; /* z directional cosine. */
  double uz1;   /* cosines of transmission alpha. always */
                /* positive. */
  double r=0.0; /* reflectance */
  short  layer = Photon_Ptr->layer;
  double ni = In_Ptr->layerspecs[layer].n;
  double nt = In_Ptr->layerspecs[layer-1].n;

  /* Get r. */
  if( - uz <= In_Ptr->layerspecs[layer].cos_crit0)
    r=1.0;            /* total internal reflection. */
  else r = RFresnel(ni, nt, -uz, &uz1);

#if PARTIALREFLECTION
  if(layer == 1 && r<1.0) { /* partially transmitted. */
    Photon_Ptr->uz = -uz1;  /* transmitted photon. */
    RecordR(r, In_Ptr, Photon_Ptr, Out_Ptr);
    Photon_Ptr->uz = -uz;   /* reflected photon. */
  }
  else if(RandomNum() > r) {/* transmitted to layer-1. */
    Photon_Ptr->layer--;
    Photon_Ptr->ux *= ni/nt;
    Photon_Ptr->uy *= ni/nt;
    Photon_Ptr->uz = -uz1;
  }
  else                      /* reflected. */
    Photon_Ptr->uz = -uz;
#else
  if(RandomNum() > r) {     /* transmitted to layer-1. */
    if(layer==1)  {
      Photon_Ptr->uz = -uz1;
      RecordR(0.0, In_Ptr, Photon_Ptr, Out_Ptr);
      Photon_Ptr->dead = 1;
    }
    else {
      Photon_Ptr->layer--;
      Photon_Ptr->ux *= ni/nt;
      Photon_Ptr->uy *= ni/nt;
      Photon_Ptr->uz = -uz1;
    }
  }
  else                      /* reflected. */
    Photon_Ptr->uz = -uz;
#endif
}

/**********************************************************
 *  Decide whether the photon will be transmitted  or be
 *  reflected on the bottom boundary (uz>0) of the current
 *  layer.
 *
 *  If the photon is transmitted, move the photon to
 *  "layer+1". If "layer" is the last layer, record the
 *  transmitted weight as transmittance. See comments for
 *  CrossUpOrNot.
 *
 *  Update the photon parmameters.
 ****/
void CrossDnOrNot(InputStruct  *    In_Ptr,
                  PhotonStruct *    Photon_Ptr,
                  OutStruct *       Out_Ptr)
{
  double uz = Photon_Ptr->uz; /* z directional cosine. */
  double uz1;   /* cosines of transmission alpha. */
  double r=0.0; /* reflectance */
  short  layer = Photon_Ptr->layer;
  double ni = In_Ptr->layerspecs[layer].n;
  double nt = In_Ptr->layerspecs[layer+1].n;

  /* Get r. */
  if( uz <= In_Ptr->layerspecs[layer].cos_crit1)
    r=1.0;      /* total internal reflection. */
  else r = RFresnel(ni, nt, uz, &uz1);

#if PARTIALREFLECTION
  if(layer == In_Ptr->num_layers && r<1.0) {
    Photon_Ptr->uz = uz1;
    RecordT(r, In_Ptr, Photon_Ptr, Out_Ptr);
    Photon_Ptr->uz = -uz;
  }
  else if(RandomNum() > r) {/* transmitted to layer+1. */
    Photon_Ptr->layer++;
    Photon_Ptr->ux *= ni/nt;
    Photon_Ptr->uy *= ni/nt;
    Photon_Ptr->uz = uz1;
  }
  else                      /* reflected. */
    Photon_Ptr->uz = -uz;
#else
  if(RandomNum() > r) {     /* transmitted to layer+1. */
    if(layer == In_Ptr->num_layers) {
      Photon_Ptr->uz = uz1;
      RecordT(0.0, In_Ptr, Photon_Ptr, Out_Ptr);
      Photon_Ptr->dead = 1;
    }
    else {
      Photon_Ptr->layer++;
      Photon_Ptr->ux *= ni/nt;
      Photon_Ptr->uy *= ni/nt;
      Photon_Ptr->uz = uz1;
    }
  }
  else                      /* reflected. */
    Photon_Ptr->uz = -uz;
#endif
}

/***********************************************************
 ****/
void CrossOrNot(InputStruct  *  In_Ptr,
                PhotonStruct *  Photon_Ptr,
                OutStruct    *  Out_Ptr)
{
  if(Photon_Ptr->uz < 0.0)
    CrossUpOrNot(In_Ptr, Photon_Ptr, Out_Ptr);
  else
    CrossDnOrNot(In_Ptr, Photon_Ptr, Out_Ptr);
}
```

```

/**********************************************************
 *  Move the photon packet in glass layer.
 *  Horizontal photons are killed because they will
 *  never interact with tissue again.
 ****/
void HopInGlass(InputStruct  * In_Ptr,
                PhotonStruct * Photon_Ptr,
                OutStruct    * Out_Ptr)
{
  double dl;     /* step size. 1/cm */

  if(Photon_Ptr->uz == 0.0) {
    /* horizontal photon in glass is killed. */
    Photon_Ptr->dead = 1;
  }
  else {
    StepSizeInGlass(Photon_Ptr, In_Ptr);
    Hop(Photon_Ptr);
    CrossOrNot(In_Ptr, Photon_Ptr, Out_Ptr);
  }
}

/**********************************************************
 *  Set a step size, move the photon, drop some weight,
 *  choose a new photon direction for propagation.
 *
 *  When a step size is long enough for the photon to
 *  hit an interface, this step is divided into two steps.
 *  First, move the photon to the boundary free of
 *  absorption or scattering, then decide whether the
 *  photon is reflected or transmitted.
 *  Then move the photon in the current or transmission
 *  medium with the unfinished stepsize to interaction
 *  site.  If the unfinished stepsize is still too long,
 *  repeat the above process.
 ****/
void HopDropSpinInTissue(InputStruct  *  In_Ptr,
                         PhotonStruct *  Photon_Ptr,
                         OutStruct    *  Out_Ptr)
{
  StepSizeInTissue(Photon_Ptr, In_Ptr);

  if(HitBoundary(Photon_Ptr, In_Ptr)) {
    Hop(Photon_Ptr);    /* move to boundary plane. */
    CrossOrNot(In_Ptr, Photon_Ptr, Out_Ptr);
  }
  else {
    Hop(Photon_Ptr);
    Drop(In_Ptr, Photon_Ptr, Out_Ptr);
    Spin(In_Ptr->layerspecs[Photon_Ptr->layer].g,
        Photon_Ptr);
  }
}

/**********************************************************
 ****/
void HopDropSpin(InputStruct  *  In_Ptr,
                 PhotonStruct *  Photon_Ptr,
                 OutStruct    *  Out_Ptr)
{
  short layer = Photon_Ptr->layer;

  if((In_Ptr->layerspecs[layer].mua == 0.0)
  && (In_Ptr->layerspecs[layer].mus == 0.0))
    /* glass layer. */
    HopInGlass(In_Ptr, Photon_Ptr, Out_Ptr);
  else
    HopDropSpinInTissue(In_Ptr, Photon_Ptr, Out_Ptr);

  if( Photon_Ptr->w < In_Ptr->Wth && !Photon_Ptr->dead)
    Roulette(Photon_Ptr);
}
```

B.5 mcmlnr.c

```
/***********************************************************
 *  Copyright Univ. of Texas M.D. Anderson Cancer Center
 *  1992.
 *
 *  Some routines modified from Numerical Recipes in C,
 *  including error report, array or matrix declaration
 *  and releasing.
 ****/
#include <stdlib.h>
#include <stdio.h>
#include <math.h>

/***********************************************************
 *  Report error message to stderr, then exit the program
 *  with signal 1.
 ****/
void nrerror(char error_text[])

{
  fprintf(stderr,"%s\n",error_text);
  fprintf(stderr,"...now exiting to system...\n");
  exit(1);
}

/***********************************************************
 *  Allocate an array with index from nl to nh inclusive.
 *
 *  Original matrix and vector from Numerical Recipes in C
 *  don't initialize the elements to zero. This will
 *  be accomplished by the following functions.
 ****/
double *AllocVector(short nl, short nh)
{
  double *v;
  short i;

  v=(double *)malloc((unsigned) (nh-nl+1)*sizeof(double));
  if (!v) nrerror("allocation failure in vector()");

  v -= nl;
  for(i=nl;i<=nh;i++) v[i] = 0.0;   /* init. */
  return v;
}

/***********************************************************
 *  Allocate a matrix with row index from nrl to nrh
 *  inclusive, and column index from ncl to nch
 *  inclusive.
 ****/
double **AllocMatrix(short nrl,short nrh,
                     short ncl,short nch)
{
  short i,j;
  double **m;

  m=(double **) malloc((unsigned) (nrh-nrl+1)
                        *sizeof(double*));
  if (!m) nrerror("allocation failure 1 in matrix()");
  m -= nrl;

  for(i=nrl;i<=nrh;i++) {
    m[i]=(double *) malloc((unsigned) (nch-ncl+1)
                        *sizeof(double));
    if (!m[i]) nrerror("allocation failure 2 in matrix()");
    m[i] -= ncl;
  }

  for(i=nrl;i<=nrh;i++)
    for(j=ncl;j<=nch;j++) m[i][j] = 0.0;
  return m;
}

/************************************************************
 *  Release the memory.
 ****/
void FreeVector(double *v,short nl,short nh)
{
  free((char*) (v+nl));
}

/************************************************************
 *  Release the memory.
 ****/
void FreeMatrix(double **m,short nrl,short nrh,
                short ncl,short nch)
{
  short i;

  for(i=nrh;i>=nrl;i--) free((char*) (m[i]+ncl));
  free((char*) (m+nrl));
}
```

Appendix C. Makefile for the Program mcml

We present the make file used for compiling and linking the code for UNIX users. This make file (named makefile) can be placed under the same directory as the source code, and used by the UNIX command make.

```
CFLAGS =
CC=cc
RM=/bin/rm -rf
LOCAL_LIBRARIES= -lm
OBJS = mcmlmain.o mcmlgo.o mcmlio.o mcmlnr.o

.c.o:
         $(RM) $@
         $(CC) -c $(CFLAGS) $*.c
#####


all : mcml


mcml: $(OBJS)
         $(RM) $@
         $(CC)  -o  $@ $(OBJS) $(LOCAL_LIBRARIES)


clean::
         $(RM) mcml
         $(RM) mcmlmain.o
```

If you use ANSI Standard C compiler (acc) on SPARCstation 2, you need to change cc to acc in the second line. Similarly, if you want to use GNU C compiler, you need to use gcc instead of cc. If you need to use a debugger (e.g., dbx), you need to add the option -g to CFLAGS in the first line, and recompile the source codes using the new make file. Then, you can call the debugger (e.g., dbx mcml). To compile and link use the makefile, use:

```
make
```

Appendix D. A Template of mcml Input Data File

This is a template for the input data file. The template file is named as "template.mci" if nobody has changed its name. You can copy this file to a new file whose extension is preferably ".mci", and modify the parameters in the new file to solve your specific problem. Any valid filenames without spaces are acceptable (see Section 9.1 for detail).

```
####
# Template of input files for Monte Carlo simulation (mcml).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                                 # file version
2                                   # number of runs

### Specify data for run 1
temp1.mco   A                       # output filename, ASCII/Binary
10                                  # No. of photons
20E-4 20E-4                         # dz, dr
10    20    30                      # No. of dz, dr & da.

2                                   # No. of layers
# n   mua   mus   g     d           # One line for each layer
1.0                                 # n for medium above.
1.3   20    200   0.70  0.01        # layer 1
1.4   10    200   0.90  1.0E+8      # layer 2
1.0                                 # n for medium below.

### Specify data for run 2
temp2.mco   A                       # output filename, ASCII/Binary
20                                  # No. of photons
20E-4 20E-4                         # dz, dr
80    80    30                      # No. of dz, dr & da.

1                                   # No. of layers
# n   mua   mus   g     d           # One line for each layer
1.0                                 # n for medium above.
1.4   10    200   0.70  1.0E+8      # layer 1
1.0                                 # n for medium below.
```

Appendix E. A Sample Output Data File of mcml

This is a sample output data file. To limit the length of the file, we used very small numbers of grid elements as can be seen in the section of the input parameter in the file.

```
A1      # Version number of the file format.

####
# Data categories include:
# InParm, RAT,
# A_l, A_z, Rd_r, Rd_a, Tt_r, Tt_a,
# A_rz, Rd_ra, Tt_ra
####

# User time:     0.42 sec =     0.00 hr.   Simulation time of this run.

InParm                  # Input parameters. cm is used.
sample.mco      A               # output file name, ASCII.
100                     # No. of photons
0.1     0.1             # dz, dr [cm]
3       3       4       # No. of dz, dr, da.

2                                       # Number of layers
#n      mua     mus     g       d       # One line for each layer
1                                       # n for medium above
1.3     5       100     0.7     0.1     # layer 1
1.4     2       10      0       0.2     # layer 2
1                                       # n for medium below

RAT #Reflectance, absorption, transmission.
0.0170132       #Specular reflectance [-]
0.259251        #Diffuse reflectance [-]
0.708072        #Absorbed fraction [-]
0.0156549       #Transmittance [-]

A_l #Absorption as a function of layer. [-]
      0.6418
     0.06624

A_z #A[0], [1],..A[nz-1]. [1/cm]
  6.4184E+00
  4.2203E-01
  2.4034E-01

Rd_r #Rd[0], [1],..Rd[nr-1]. [1/cm2]
  7.1961E+00
  3.1968E-01
  1.9419E-02

Rd_a #Rd[0], [1],..Rd[na-1]. [sr-1]
  5.5689E-02
  6.2845E-02
  3.6396E-02
  2.9598E-02

Tt_r #Tt[0], [1],..Tt[nr-1]. [1/cm2]
  1.5008E-01
  4.8650E-02
  4.0457E-02

Tt_a #Tt[0], [1],..Tt[na-1]. [sr-1]
  1.0965E-03
  3.5961E-03
  3.1196E-03
  1.5692E-03

# A[r][z]. [1/cm3]
# A[0][0], [0][1],..[0][nz-1]
# A[1][0], [1][1],..[1][nz-1]
# ...
# A[nr-1][0], [nr-1][1],..[nr-1][nz-1]
A_rz
  1.7934E+02   5.9590E+00   2.9838E+00   7.4003E+00   1.3974E+00
  7.6865E-01   5.5296E-01   6.5647E-01   4.7210E-01

# Rd[r][angle]. [1/(cm2sr)].
# Rd[0][0], [0][1],..[0][na-1]
# Rd[1][0], [1][1],..[1][na-1]
# ...
# Rd[nr-1][0], [nr-1][1],..[nr-1][na-1]
Rd_ra
  1.7856E+00   2.0312E+00   1.8606E+00   4.0608E+00   0.0000E+00
  1.0438E-01   7.3502E-02   2.4768E-01   4.3564E-03   1.2307E-02
  8.2665E-04   5.0690E-03

# Tt[r][angle]. [1/(cm2sr)].
# Tt[0][0], [0][1],..[0][na-1]
# Tt[1][0], [1][1],..[1][na-1]
# ...
# Tt[nr-1][0], [nr-1][1],..[nr-1][na-1]
Tt_ra
  0.0000E+00   2.6871E-02   0.0000E+00   2.5301E-01   0.0000E+00
  9.0115E-05   4.2593E-02   0.0000E+00   7.1173E-03   2.2105E-02
  1.0191E-02   6.0383E-04
```

Appendix F. Several C Shell Scripts

F.1 conv.bat for batch processing conv

The C Shell script "conv.bat" is used to batch process the program conv (see Section 9.4 for description of use of conv.bat).

```
# Shell script for the convolution program "conv"
# Feb. 2, 1992
#
# Format: conv.bat filename(s) output_type
# output_type includes: Rr, Ra, Az ...

# Check parm, echo the help if something is wrong.
if ($#argv == 0 || $#argv >= 3) then
  echo 'Usage: conv.bat "input_filename(s)" output_type'
  echo "output_type includes: "
  echo "I,  3,  K"
  echo "Al, Az, Arz"
  echo "Rr, Ra, Rra"
  echo "Tr, Ta, Tra"
  exit
endif

# Check the second parameter.
if (! ($2 =~ [Ii3Kk] || \
    $2 =~ [Aa][LlZz] || \
    $2 =~ [Aa][Rr][Zz] || \
    $2 =~ [RrTt][RrAa] || \
    $2 =~ [RrTt][Rr][Aa])) then
  echo "Wrong parm -- $2"
  echo "output_type includes: "
  echo "I,  3,  K"
  echo "Al, Az, Arz"
  echo "Rr, Ra, Rra"
  echo "Tr, Ta, Tra"
  exit(3)
endif

foreach infile ($1)
  # make sure the file is existent and readable.
  if (! -e $infile) then
    echo "File $infile not exist"
    exit(2);
  else if (! -r $infile) then
    echo "File $infile not readable"
    exit(2)
  endif

  # remove the existent output files, if any.
  if ( -e $infile:r.$2) then
    rm $infile:r.$2
  endif

  # echo the command sequence to conv.
  (echo i;echo $infile;\
    echo oo;echo $2;echo $infile:r.$2;echo q;echo q;echo y)\
    |conv>/dev/null

end # of foreach
```

F.2 p1 for pasting files of 1D arrays

The C Shell script p1 is used to paste side by side multiple files of 1D arrays, which are in 2 columns. If the files of 1D arrays share the same first column, p1 will not duplicate the first column in the pasted file. If the output file is existent, then it is backed up as the original filename appended with ".bak". The original output file is still kept as part of the new output file. This script is particularly useful to prepare the data for processing and presentation by some commercial plotting softwares such as KaleidaGraph. For example, if you have three mcml output files file1.Rr, file2.Rr, and file3.Rr saved in 2 columns representing the diffuse reflectance as a function of radius r. You can combine these three files into one file by:

```
p1 "file?.Rr" filex.Rrs
```

where filex.Rrs is the filename of the output.

```
#  Paste 1D files (in 2 columns) together side by side.
#  February 7, 1992.

#  Check number of arguments.
if ($#argv != 2) then
  echo 'Usage: p1 "input_file(s)" output_fname'
  exit(1)
endif

onintr catch        # Prepare to catch interrpts.

set com = $0
set infiles = $1:q
set outfile = $2

#  Check validity of arguments for outfile.
if ( -e $outfile) then
  if (! -w $outfile) then
    echo $outfile not writable
    exit(2)
  endif

  cp $outfile $outfile.bak # Backup existent files.
endif

#  Setup temp files with the PID number.
set outbuf = /tmp/$com:t.$$.outbuf
set buf1 = /tmp/$com:t.$$.buf1
set buf2 = /tmp/$com:t.$$.buf2
set cmp1 = /tmp/$com:t.$$.cmp1
set cmp2 = /tmp/$com:t.$$.cmp2

#  Run through each file, keep the results in $outbuf.
foreach infile ($infiles)
  if (! -r $infile) then
    echo $infile not readable
    exit(3)
  endif
  #  Delimit by tab.
  awk -F" " '{print $1 "\t" $2}' $infile >! $buf1

  if (! -e $outbuf) then
    cut -f1 $buf1 >! $cmp1
    cp $buf1 $outbuf
  else
    cut -f1 $buf1 >! $cmp2
    diff $cmp1 $cmp2 > /dev/null

    if ($status) then
      # 1st rows are not the same. Paste both columns.
      paste $outbuf $buf1 >! $buf2; cp $buf2 $outbuf
      cut -f1 $buf1 >! $cmp1
    else
      # 1st rows are the same.  Paste only the 2nd column.
      cut -f2 $buf1 >! $buf2
      paste $outbuf $buf2 >! $buf1; cp $buf1 $outbuf
    endif
  endif

end

#  Copy $outbuf to $outfile
if (! -e $outfile) then
  cp $outbuf $outfile
else
  paste $outfile $outbuf >! $buf1; cp $buf1 $outfile
endif

catch:       # jump to here if interrupted
  rm -f $outbuf  $buf1 $buf2 $cmp1  $cmp2
  exit(1)
```

Appendix G. Where to Get the Programs mcml and conv

We will eventually set up a bulletin board of our own so that you can download the software over the network. For now, you can contact Lihong Wang, or Steven L. Jacques using the following information to get the software.

Lihong Wang, Ph. D.
Laser Biology Research Laboratory – Box 17
University of Texas M. D. Anderson Cancer Center
1515 Holcombe Blvd.
Houston, Texas 77030
Phone: (713)745-1742
Fax: (713)792-3995
email: lihong@laser.mda.uth.tmc.edu

or

Steven L. Jacques, Ph. D.
Laser Biology Research Laboratory – Box 17
University of Texas M. D. Anderson Cancer Center
1515 Holcombe Blvd.
Houston, Texas 77030
Phone: (713)792-3662
Fax: (713)792-3995
email: slj@laser.mda.uth.tmc.edu

Make sure that you tell us the specific machines (including brand and model) you will use for the simulation, so that we can compile the code correctly for you. If you use IBM PC compatibles, please also tell us whether you use a math co-processor or not.

Appendix H. Future Developments of the Package

The release is by no means the end of the package. We plan to make at least the following improvements. As we gather comments from users, we may consider even more improvements.

Collimated responses in mcml

In this version (version 1.0) of mcml, the first photon interactions in the media are scored into the first grid elements in the r direction together with the later interactions. The first interactions are all on the z-axis, and should yield a delta function of r (Gardner *et al.*, 1992b) to be exact. Therefore, they should be scored separately as demonstrated by Gardner *et al.*

The specular reflectance is computed analytically using Fresnel's formulas. However, the reflected photons that are uninteracted inside the tissue are scored into the first grid elements in the r direction of the diffuse reflectance. To be strict, these photons should contribute to the specular reflectance rather than the diffuse reflectance although this is small in thick tissues.

The transmittance in version 1.0 of mcml does not differentiate between diffuse transmittance and unscattered transmittance. This problem and the problem with the reflectance can be solved by keeping track of the number of interactions.

Best points for each grid element

As we have discussed in Section 4.3, we should use:

$$r_b = [(n + 0.5) + \frac{1}{12\,(n + 0.5)}\ ]\,\Delta r$$

instead of the center of the grid element as the coordinate of the simulated data in the nth grid element in the r direction. In the case when the radius of a Gaussian beam is comparable with the grid separation Δr, this may make a considerably large difference in the convolution program conv.

<u>Flexible photon sources</u>

In version 1.0 of mcml, only collimated photon beams incident on the tissue surface are supported. Several other cylindrically symmetric sources should be able to be incorporated without substantially modifying the program.

The convolution program conv 1.0 only supports Gaussian beams and circularly flat beams, it can be easily adopted to convolve over arbitrary beam profiles that are cylindrically symmetric. For beams that are not cylindrically symmetric, the convolution still can be done but with longer integration time.

<u>Faster sampling procedures</u>

The sampling of the step size involves an exponential computation which is computation intensive. Faster approaches can be used as discussed in Section 3.2.

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