

NOTE

The use of the Henyey–Greenstein phase function in Monte Carlo simulations in biomedical optics

T Binzoni^{1,2}, T S Leung³, A H Gandjbakhche⁴, D Rüfenacht²
and D T Delpy³

¹ Département des Neurosciences Fondamentales, Centre Médical Universitaire, University of Geneva, 1 rue Michel-Servet, 1211 Geneva 4, Switzerland

² Département de Radiologie et Informatique Médicale, University Hospital, Geneva, Switzerland

³ Department of Medical Physics and Bioengineering, University College London, UK

⁴ Laboratory of Integrative and Medical Biophysics, National Institute of Child Health and Human Development, National Institutes of Health, Bethesda, MD, USA

E-mail: Tiziano.Binzoni@medecine.unige.ch

Received 10 May 2006, in final form 14 June 2006

Published 15 August 2006

Online at stacks.iop.org/PMB/51/N313

Abstract

Monte Carlo (MC) simulations are often at the heart of the testing procedure in biomedical optics. One of the critical points in MC simulations is to define the new photon direction after each scattering event. One of the most popular solutions is to use the Henyey–Greenstein phase function or some linear combinations of it. In this note, we demonstrate that randomly generating the angle defining the new direction of a photon after a collision, by means of the Henyey–Greenstein phase function, is not equivalent to generating the cosine of this angle, as is classically done. In practice, it is demonstrated that for a nearly isotropic medium (asymmetry parameter $g \sim 0$) this discrepancy is not large, however for an anisotropic medium as is typically found *in vivo* (e.g. $g = 0.98$) the two methods give completely different results.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Assessing the optical properties of human biological tissues is of great interest for clinical diagnostics and fundamental research, since biomedical optics allow the measurement of important physiological parameters such as the tissue haemoglobin concentration, tissue haemoglobin oxygen saturation (Ferrari *et al* 2004), tissue blood speed/flow (Briers 2001), etc. In recent years, it has also become possible to build 2D or 3D maps of these quantities, such as the 3D imaging of the neonatal brain (Gibson *et al* 2005) or human breast (Yates *et al* 2005). The success of these biomedical optics techniques has been made possible thanks

to the development of various algorithms describing the propagation of photons in tissues (Arridge *et al* 1992, Arridge and Hebden 1997, Briers 2001, Dagdug *et al* 2003). Since these algorithms describe only an approximation to the propagation of the light in the investigated medium, their validity needs to be tested.

To test these algorithms, one usually resorts to two methods. The first is based on real measurements made in phantoms with known optical properties close to those found in biological tissue (Firbank *et al* 1995). This method has the advantage of testing simultaneously the hardware utilized for the measurement and the algorithms in a real situation. The disadvantage is that in practice it is difficult to test the algorithms on a large set of different optical parameters or complex heterogeneous geometries because this would require the use of a large number of phantoms. For this reason, a second method based on Monte Carlo (MC) simulations was introduced by Wilson and Adam (1983). This mathematical method numerically describes the propagation of light in tissues with known optical parameters and geometry and generates synthetic experimental data sets. This approach has become one of the 'gold standards' in biomedical optics and it allows in principle the test of any analytical algorithm. Moreover, thanks to increasing computational power, the MC method has also been proposed as a tool to directly 'fit' experimental data and thus obtain the wanted optical parameters (Pifferi *et al* 1998).

The precision of this method is due to the fact that in the MC methods one describes the propagation of each photon one by one. Thus, to have a realistic model, it is necessary to give a series of rules describing with precision the photon propagation inside the tissue (Prahel *et al* 1989, Wang *et al* 1995). In practice, these rules take into account the following physical phenomena: (1) the probability for a photon to be absorbed; (2) the probability for a photon to interact with the tissue (scattering) and change direction of propagation; (3) the probability for a photon to be reflected at a boundary or at an interface between two different tissues; (4) a rule, usually called a phase function, giving the new direction of the photon after a scattering event. It is this latter point that is critical to define and it is also probably the part of the simulation that may require the largest amount of computation time (for one photon run) if a high precision is required.

Biological tissues have a very complex structure and it is not a trivial matter to decide which phase function will be the best choice. Fortunately, in many cases, if the distance between the source of light and the detector is large enough (e.g. 20–30 mm) (Canpolat and Mourant 2000), the problem simplifies and it becomes possible to reasonably describe the photon scattering by a very general phase function. The Henyey–Greenstein (HG) phase function (Henyey and Greenstein 1941) plays this role and takes into account all the scattering bodies of the tissue as a whole 'mean' scattering body (Jacques *et al* 1987). The original HG function described the probability of scattering at a particular angle, i.e. θ . The evaluation of the HG function may take a relatively long computation time during the photon path estimation, but by using a clever mathematical transformation (Witt 1977) it is possible to express the HG function in terms of $\cos(\theta)$ and obtain a very simple analytical solution that can be used to implement a fast numerical algorithm allowing the generation of a specific random distribution of scattering angles.

In fact, this procedure is not strictly necessary and in the present note we will show that this procedure may introduce large errors in the MC simulations. By using this fast algorithm, the MC simulation may on one hand reproduce the experimental data quite well but it does not accurately represent the physics for which it was theoretically designed and this might lead to errors in the physical/physiological interpretation of the data, in the testing of the analytical models, or in the derivation of synthetic data with the aim of developing direct MC-based fitting algorithms. To summarize, in the present work we will compare two very well known

methods to generate the HG phase function and show that if utilized in MC simulations they are not exactly equivalent as has previously been assumed.

2. Materials and methods

2.1. Computer cluster for the Monte Carlo simulation

The MC simulations were performed on a cluster of nine computers (DELL™, OptiPlex GX620, USA) having CPUs running at 3.2 GHz (Kirkby and Delpy 1997). One computer was utilized as a client, distributing the jobs to the remaining eight workers. The MC code was developed in MATLAB® 7.2 language (The Mathworks Inc., Natick, MA) and the interaction between the computers was controlled by the MATLAB® Distributed Computing Engine 2. It has been estimated that a gain of a time factor of ~ 7.5 can be obtained with eight machines compared to only one.

2.2. Photon propagation in a semi-infinite isotropic medium

To demonstrate the influence on the MC data of using different algorithms to randomly generate θ , a simple semi-infinite isotropic medium has been chosen. An infinitely narrow light beam source normal to the surface has been utilized. The detector was also placed normal to the surface at a distance r (mm) from the source (interoptode distance). The light source was considered as a continuous-wave source. The intensity of the photons detected at a distance r from the source, $R(r)$, was expressed as a photon probability per unit area (mm^{-2}) and this was one of the measured parameters.

The MC code has been written following the same approaches given in the classical literature (Prahl *et al* 1989, Wang *et al* 1995) and in this work two different approaches were used to generate the scattering angles (see the next section).

The parameters common to all the simulations were $\mu_a = 0.025 \text{ mm}^{-1}$, $\mu'_s = 0.6 \text{ mm}^{-1}$ (representing e.g. a ‘typical’ muscle tissue), the number of photon packets in the simulation $N = 1000\,000$, $r \in [0, 40]$ mm. All the simulations obtained with these parameters were repeated twice, with $n = 1$ and $n = 1.4$, respectively.

2.3. Computation of the Henyey–Greenstein phase function: direct (‘exact’) solution

The HG phase function (Henyey and Greenstein 1941) can be written as

$$P_{\text{HG}}(\theta) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos(\theta))^{3/2}}, \quad (1)$$

where $P_{\text{HG}}(\theta)$ is a probability density function and $\theta \in [0, \pi]$ (rad) is the angle existing between the direction of the photon before a scattering event and the direction after the scattering event. The parameter g is defined as

$$g \equiv \langle \cos(\theta) \rangle = \int_0^\pi \cos(\theta) P_{\text{HG}}(\theta) 2\pi \sin(\theta) d\theta. \quad (2)$$

A value $\theta = 0$ rad means that the photon carries on in the same direction as before the collision. If $g = 0$, then the medium is said to be isotropic, this means that the photon has the same probability of going in any direction. In practice, the angle θ is generated millions of times during an MC simulation and the obtained angles must satisfy the behaviour of the probability density function described by equation (1). As originally proposed by Witt (1977), it is possible

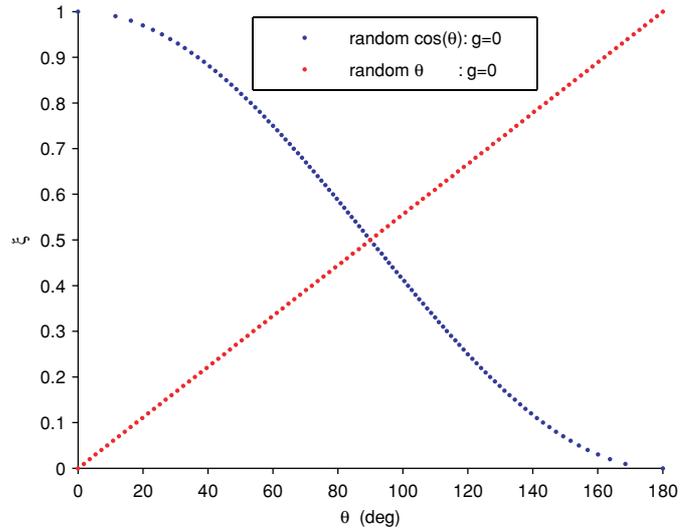


Figure 1. Parameter ξ as a function of the angle θ , for $g = 0$, obtained by using equations (3) (red points) and (6) (blue points). The ξ values are uniformly spaced and vary from 0 to 1 in steps of 0.01 (the same ξ are utilized for the blue and red points).

to simulate the random event for which the variable θ falls with probability $P_{\text{HG}}(\theta) d\theta$ in the interval $[\theta, \theta + d\theta]$ by using a uniformly distributed random number $\xi = [0, 1]$ such that

$$\int_0^\theta P_{\text{HG}}(\theta') d\theta' = \xi. \quad (3)$$

Thus, the problem is to solve equation (3) and to obtain an analytical solution expressing θ as a function of ξ . Unfortunately, to our knowledge, this can be done only numerically and this certainly increases the duration of the simulation. To solve equation (3), in the present case we have followed the procedure proposed by Toublanc (1996).

In practice, the integral in equation (3) has been numerically evaluated only once at the beginning of the MC simulation (for a given g and different θ varying from 0 to π in steps of $\pi \times 10^{-3}$ rad) by using an adaptive Lobatto quadrature rule (Gander and Gautschi 2000). This gives a monotonically increasing table of values as a function of θ . The obtained values have been normalized from 0 to 1. Thus, for a randomly generated ξ value it is easy to find the corresponding angle θ by linear interpolation. By construction, θ obtained by generating a set of uniformly distributed values ξ follow the distribution law given by equation (1) and can be utilized for the MC simulation. Figure 1 shows ξ as a function of θ using the direct solution, i.e. equation (3).

2.4. Computation of the Henyey–Greenstein phase function: classical solution

Classically, the angle θ is not computed directly because, as it was highlighted in section 2.3, this can demand a lot of computation time. Thus, to increase the computation speed, Witt (1977) has proposed to compute directly $\cos(\theta)$. In fact, it is $\cos(\theta)$ that is utilized in the longest loops of the MC code and not directly θ . The probability density function for $\cos(\theta)$ ($\tilde{P}_{\text{HG}}(\cos(\theta))$) is easily found by slightly modifying equation (1) and is expressed as

$$\tilde{P}_{\text{HG}}(\cos(\theta)) = \frac{1}{2} \frac{1 - g^2}{(1 + g^2 - 2g \cos(\theta))^{3/2}}. \quad (4)$$

To generate the distribution $\tilde{P}_{\text{HG}}(\cos(\theta))$, one can use the same procedure as in section 2.3 by writing

$$\int_{-1}^{\cos(\theta)} \tilde{P}_{\text{HG}}(\cos(\theta')) d(\cos(\theta')) = \xi. \quad (5)$$

The advantage of this formulation is that equation (5) has an exact analytical solution that can be expressed as

$$\cos(\theta) = \begin{cases} \frac{1}{2g} \left[1 + g^2 - \left(\frac{1 - g^2}{1 - g + 2g\xi} \right)^2 \right], & \text{if } g \neq 0, \\ 2\xi - 1, & \text{if } g = 0. \end{cases} \quad (6)$$

The hypothesis often made is that the random $\cos(\theta)$ obtained by generating a set of uniformly distributed values ξ follow the distribution law given by equation (4) (derived from equation (1)) and thus can also be utilized for the MC simulation.

3. The simulations

To highlight the eventual differences existing between the approaches represented by equations (1) and (4), in the present work we have performed two MC simulations. Each of the two simulations was performed for the direct (equation (1)) and for the classical (equation (4)) case. In all the simulations, the measured parameters were $R(r)$ and θ . All the generated θ were used to create a histogram with 420 equally spaced containers covering the $[0, 180]^\circ$ range (each container covers 0.43°). In the classical case, when $\cos(\theta)$ is generated, the angle θ was computed applying the relationship $\theta = \text{acos}(\cos(\theta))$ before counting.

Simulation 1. In this MC simulation, the simplest case has been considered where the medium is perfectly isotropic, i.e. $g = 0$. This means that the distribution of the measured θ should be ‘flat’, i.e. the light is scattered with the same probability in all directions (Bohren and Huffman 1983).

Simulation 2. This is same as simulation 1 but with $g = 0.98$. This is the value often chosen to describe a biological tissue. The photons are in this case strongly forward scattered.

4. Results

In figure 2 (simulation 1), the photon probability per unit area $R(r)$ is reported as a function of the interoptode distance r for different n values and $g = 0$ (isotropic medium). The distance r is reported in steps of 0.3 mm. There is no large difference between the data generated using equation (1) (random generation of θ) or equation (4) (random generation of $\cos(\theta)$). The influence of n on $R(r)$ is also small.

Figure 3 (simulation 1) shows the histogram of the scattering angles θ (in degrees) for the four distinct runs reported in figure 2. It is clear that for the data generated using equation (1) the θ distribution is perfectly ‘flat’, and this is exactly what one must find with an isotropic medium (i.e. the same probability of diffusing in all directions). However, if one investigates the data generated using equation (4), one realizes that the distribution does not represent an isotropic medium and that very small (0°) or very large (180°) angles have practically zero probability of appearing. The curves with $n = 1.4$ have in general higher values when compared to the companion $n = 1$ curves because the photons are reflected at the air/medium boundary and remain for more steps inside the medium.

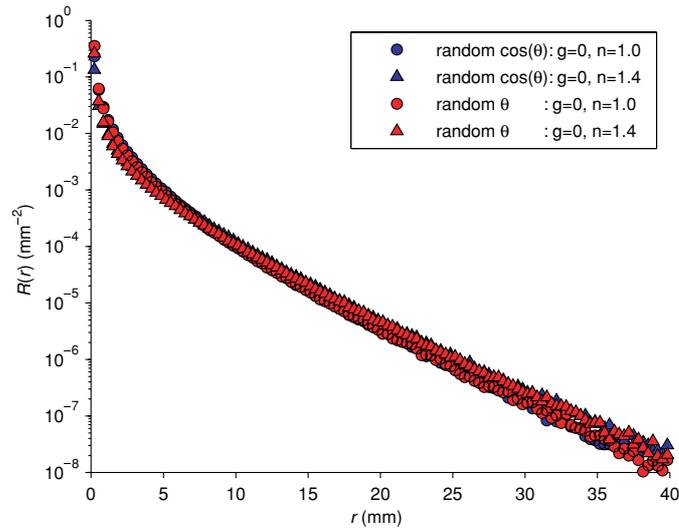


Figure 2. Photon probability per unit area $R(r)$ reported as a function of the interoptode distance r . Random $\cos(\theta)$ means that the cosine of θ has been generated during the Monte Carlo simulation. Random θ means that θ has been directly generated during the Monte Carlo simulation.

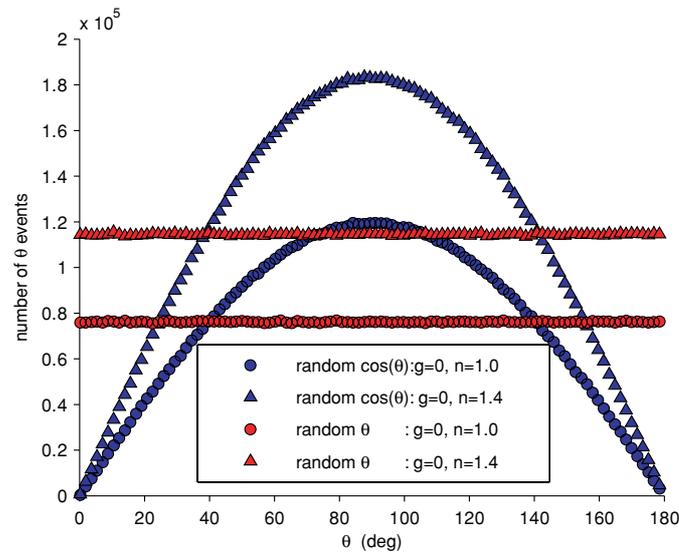


Figure 3. Histograms of the scattering angles θ in degrees during the four distinct MC simulations. Random $\cos(\theta)$ means that the cosine of θ has been generated during the Monte Carlo simulation. Random θ means that θ has been directly generated during the Monte Carlo simulation.

Figure 4 (simulation 2) is the same as figure 2 but with the difference that $g = 0.98$. This means that the photons are very strongly forward scattered. In this case, the choice of the phase function becomes critical and the results are completely different depending on whether one chooses the approach represented by equation (1) or (4).

The histograms of the scattering angles θ for $g = 0.98$ using equations (1) and (4) are shown in figure 5 (simulation 2). For better visibility, only θ in the range $[0, 10]^\circ$ are shown.

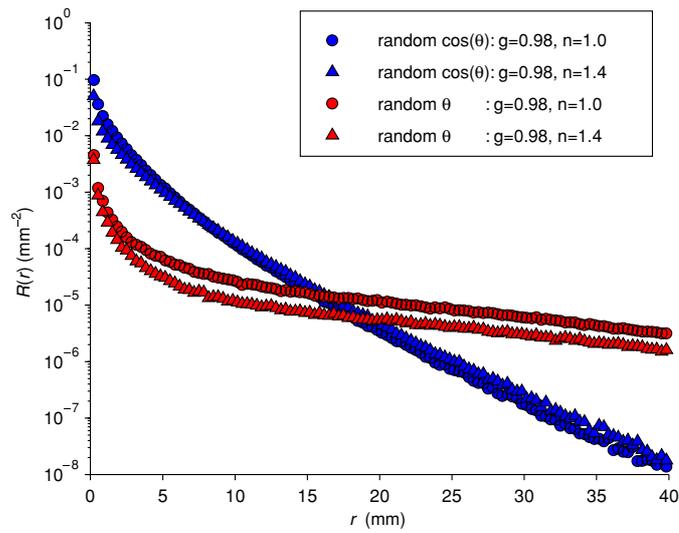


Figure 4. Photon probability per unit area $R(r)$ reported as a function of the interoptode distance r for the same simulations as in figure 2, but where $g = 0.98$. Random $\cos(\theta)$ means that the cosine of θ has been generated during the Monte Carlo simulation. Random θ means that θ has been directly generated during the Monte Carlo simulation.

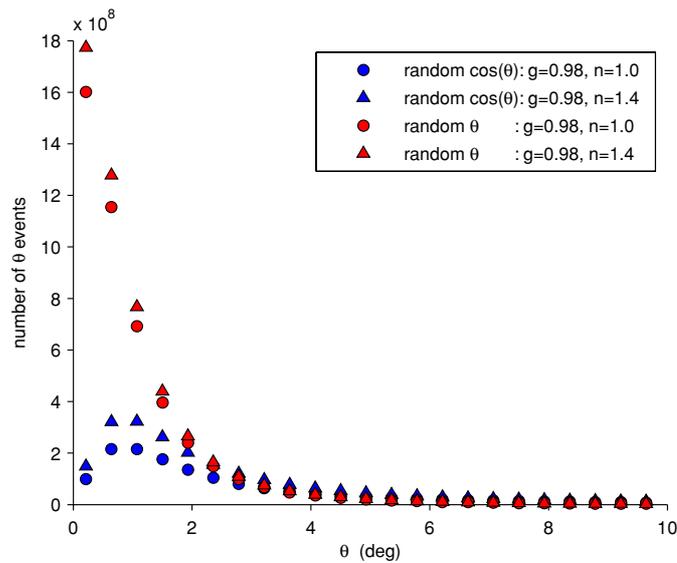


Figure 5. Histograms of the scattering angles θ in degrees during the four distinct MC simulations as in figure 3 but with $g = 0.98$. Random $\cos(\theta)$ means that the cosine of θ has been generated during the Monte Carlo simulation. Random θ means that has θ been directly generated during the Monte Carlo simulation.

It is interesting to note that the classical algorithm generating $\cos(\theta)$ flattens the θ distribution by decreasing the probability of the small angles.

To illustrate the practical consequences of these findings, figure 6 shows the same data as figure 4 for $n = 1.4$ (corresponds e.g. to a skeletal muscle tissue) together with four very well

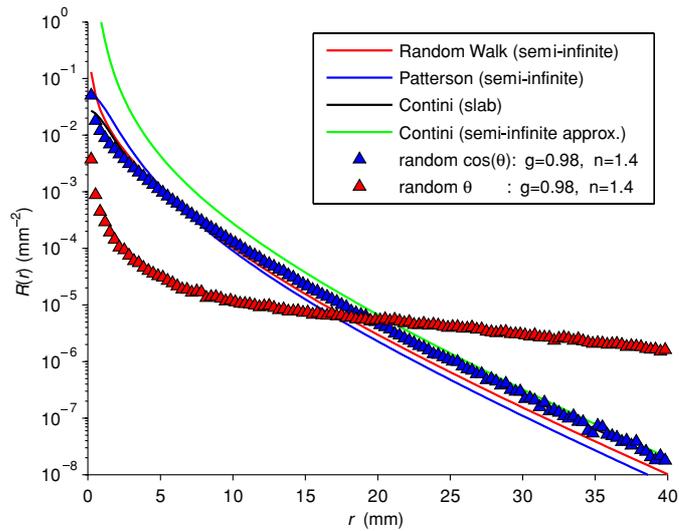


Figure 6. Photon probability per unit area $R(r)$ reported as a function of the interoptode distance r . Comparison of MC simulated data and four analytical models (see the text).

known and tested analytical models describing these data. The models are (1) the random walk model for a semi-infinite medium but for n always equal to 1 (Bonner *et al* 1987), (2) the classical Patterson diffusion equation (Patterson *et al* 1989), (3) the Contini model for a slab where the slab thickness has been set to 1×10^6 mm to simulate a semi-infinite medium (Contini *et al* 1997) and (4) an analytical approximation of the latter model, given by the same authors, for a semi-infinite medium. As expected, the Contini model for the slab is the best fitting model. However, it must be noted that the results of these analytical models only agree well with the MC results using the classical HG (equation (5)), i.e. the phase function for which $\cos(\theta)$ has been generated randomly. The MC results using the direct HG function, i.e. equation (1), however, are different from the analytical results for $g = 0.98$.

5. Discussion and conclusions

In this note, it has been demonstrated that the MC results obtained by randomly generating $\cos(\theta)$ are not equivalent to those by directly generating θ (i.e. the ‘exact’ direct method). In fact, the function ‘cos’ introduces a distortion in the probability density function for θ and thus produces a biased phase function. The results can be explained by the fact that a uniform distribution of $\cos(\theta)$ values does not give by definition a uniform distribution after the operation $\arccos(\cos(\theta))$ (physically, an isotropic medium implies a uniform distribution of θ but not of $\cos(\theta)$). Intuitively, this can be seen in figure 1 where two sets of θ have been generated using the algorithms represented by equations (3) (red points) and (6) (blue points). In this case, the ξ values vary from 0 to 1 and are equally spaced (step of 0.01). However, it is clear that the corresponding θ values are not equally spaced in the case of equation (6) and that the values around 90° are more ‘dense’ (this is not the case for the red curve, equation (3)). Thus, in practice, when sampling with the blue curve, the probability of obtaining 90° angles is higher for instance than that of obtaining e.g. 0° or 180° (considering that ξ or $1 - \xi$ lead to the same distribution, the increasing or decreasing behaviour for the red and blue curves has no consequences on the results).

In practice, even with this distortion the MC results using the classical $\cos(\theta)$ method seem to reproduce the experimental data (e.g. on phantoms) well. Moreover, the MC data also seem to be compatible with a series of known analytical models derived from approximations of the transport equation for the light. This can be explained by the fact that the classical method generates a higher number of θ close to 90° than it should do in the original HG function. This facilitates the randomization (isotropization) of the photons and thus it gives results that by definition are more suitable for comparison with descriptions using the diffusion equation with a transport corrected scattering coefficient.

The present results provide evidence to support the use of more realistic phase functions derived directly from Mie theory, as already proposed by Canpolat and Mourant (2000). This is certainly very important if one would like to study situations where the interoptode spacing is very small (Canpolat and Mourant 2000) and where the photon does not cover enough distance to randomize θ . When the classical $\cos(\theta)$ method is used to perform MC simulations, one must be aware that the scattering angles thus generated are very different from those generated using the original HG function when θ is randomized.

Acknowledgment

We thank the ‘Faculté de Médecine’ of Geneva for the Mimosa grant that has allowed the setting up of the computer cluster.

References

- Arridge S R, Cope M and Delpy D T 1992 The theoretical basis for the determination of optical pathlengths in tissue: temporal and frequency analysis *Phys. Med. Biol.* **37** 1531–60
- Arridge S R and Hebden J C 1997 Optical imaging in medicine: II. Modelling and reconstruction *Phys. Med. Biol.* **42** 841–53
- Bohren C G and Huffman D R 1983 *Absorption and Scattering of Light by Small Particles* (New York: Wiley)
- Bonner R F, Nossal R, Havlin S and Weiss G H 1987 Model for photon migration in turbid biological media *J. Opt. Soc. Am. A* **4** 423–32
- Briers J D 2001 Laser Doppler, speckle and related techniques for blood perfusion mapping and imaging *Physiol. Meas.* **22** R35–66
- Canpolat M and Mourant J R 2000 High-angle scattering events strongly affect light collection in clinically relevant measurement geometries for light transport through tissue *Phys. Med. Biol.* **45** 1127–40
- Contini D, Martelli F and Zaccanti G 1997 Photon migration through a turbid slab described by a model based on diffusion approximation: I. Theory *Appl. Opt.* **36** 4587–99
- Dagdug L, Weiss G H and Gandjbakhche A H 2003 Effects of anisotropic optical properties on photon migration in structured tissues *Phys. Med. Biol.* **48** 1361–70
- Ferrari M, Mottola L and Quaresima V 2004 Principles, techniques, and limitations of near infrared spectroscopy *Can. J. Appl. Physiol.* **29** 463–87
- Firbank M, Oda M and Delpy D T 1995 An improved design for a stable and reproducible phantom material for use in near-infrared spectroscopy and imaging *Phys. Med. Biol.* **40** 955–61
- Gander W and Gautschi W 2000 Adaptive quadrature—revisited *BIT* **40** 84–101 (<http://www.inf.ethz.ch/personal/gande>)
- Gibson A P, Hebden J C and Arridge S R 2005 Recent advances in diffuse optical imaging *Phys. Med. Biol.* **50** R1–43
- Henyey L G and Greenstein J L 1941 Diffuse radiation in the galaxy *Astrophys. J.* **93** 70–83
- Jacques S L, Alter C A and Prahl S A 1987 Angular dependence of HeNe laser light scattering by human dermis *Lasers Life Sci.* **1** 309–33
- Kirkby D R and Delpy D T 1997 Parallel operation of Monte Carlo simulations on a diverse network of computers *Phys. Med. Biol.* **42** 1203–8
- Patterson M S, Chance B and Wilson B C 1989 Time resolved reflectance and transmittance for the non-invasive measurement of tissue optical properties *Appl. Opt.* **28** 2331–6
- Pifferi A, Taroni P, Valentini G and Andersson-Engels S 1998 Real-time method for fitting time-resolved reflectance and transmittance measurements with a Monte Carlo model *Appl. Opt.* **37** 2774–80

- Prahl S A, Keijzer M, Jacques S L and Welch A J 1989 A Monte Carlo code of light propagation in tissue *Proc. SPIE* **5** 102–11
- Schweiger M, Gibson A P and Arridge S R 2003 Computational aspects of diffuse optical tomography *IEEE Comput. Sci. Eng.* **1** 33–41
- Toublanc D 1996 Henyey–Greenstein and Mie phase functions in Monte Carlo radiative transfer computations *Appl. Opt.* **35** 3270–4
- Wang L, Jacques S L and Zheng L 1995 MCML—Monte Carlo modeling of light transport in multi-layered tissues *Comput. Methods Programs Biomed.* **47** 131–46
- Wilson B C and Adam G 1983 A Monte Carlo model for the absorption and flux distributions of light in tissue *Med. Phys.* **10** 824–30
- Witt A N 1977 Multiple scattering in reflection nebulae: I. A Monte Carlo approach *Astrophys. J.* **35** S1–6
- Yates T, Hebden J C, Gibson A, Everdell N, Arridge S R and Douek M 2005 Optical tomography of the breast using a multi-channel time-resolved imager *Phys. Med. Biol.* **50** 2503–17

LETTER TO THE EDITOR

Comment on ‘The use of the Henyey–Greenstein phase function in Monte Carlo simulations in biomedical optics’

T Binzoni^{1,2}, T S Leung³, A H Gandjbakhche⁴, D Rüfenacht²
and D T Delpy³

¹ Département des Neurosciences Fondamentales, Centre Medical Universitaire, University of Geneva, 1 r. Michel-Servet, Switzerland

² Département de Radiologie et Informatique Médicale, University Hospital, Geneva, Switzerland

³ Department of Medical Physics and Bioengineering, University College London, UK

⁴ Laboratory of Integrative and Medical Biophysics, National Institute of Child Health and Human Development, National Institute of Health, Bethesda, MD, USA

E-mail: Tiziano.Binzoni@medecine.unige.ch

Received 14 September 2006, in final form 3 October 2006

Published 24 October 2006

Online at stacks.iop.org/PMB/51/L39

Abstract

In this letter the authors highlight the presence of an error appearing in the discussion of the note ‘The use of the Henyey–Greenstein phase function in Monte Carlo simulations in biomedical optics’ previously published by them (Binzoni *et al* 2006 *Phys. Med. Biol.* **51** N313). In the light of this error, the discussion and conclusions in the original paper are revised in this letter and the role of the use of the phase functions in MC simulations, interpreted in probabilistic terms, is better clarified. The exact definition for the probability density function for the deflection angle, in the case of the Henyey–Greenstein model, is also given.

In this letter the authors highlight the presence of an unnoticed error appearing in the discussion of the note ‘The use of the Henyey–Greenstein phase function in Monte Carlo simulations in biomedical optics’ previously published by them (Binzoni *et al* 2006). For this reason, we have revised the discussion of the data and the role of the use of the phase functions in Monte Carlo (MC) simulations, interpreted in probabilistic terms, is better clarified.

In MC simulations one describes the random direction chosen at each step by a photon by means of a so-called phase function. In the MC context, the ‘phase function’ means the ‘probability density’ for the random variables describing the deflection and azimuthal angle of the photon direction changes occurring after each collision inside the medium. In the scientific literature, the difference between the term ‘phase function’ used for instance in the context

of the electromagnetic wave theory of the light scattering process, and the term ‘probability density function’ utilized in a stochastic sense as for MC simulations is often unclear. In the previously published note the authors wished to highlight this fact and, for explanatory purposes, they considered the particular case of the Henyey–Greenstein phase function (HGF).

It is well known that there are two equivalent ways to represent the phase function and/or the probability density for the HGF: one giving directly the probability density for the deflection angle θ and the other the cosine of the angle, $\cos(\theta)$ (appearing in the note as $P_{\text{HG}}(\theta)$ and $\tilde{P}_{\text{HG}}(\cos(\theta))$, respectively). The function $P_{\text{HG}}(\theta)$ is the historical representation of the HGF reported in the majority of the published paper and interpreted as a probability density for the MC simulations. For the purpose of the present letter, it is important to note again that the random variable in this latter case is θ , and thus, from the probabilistic point of view defined by the MC model, $P_{\text{HG}}(\theta)$ must be integrated over θ to obtain a probability and not over any other variable such as the solid angle! The aim of the note was to show that in the Monte Carlo (probabilistic) context $P_{\text{HG}}(\theta)$ and $\tilde{P}_{\text{HG}}(\cos(\theta))$, as presented in the literature, are not equivalent. The problem comes from the fact that it is incorrect to interpret $P_{\text{HG}}(\theta)$ as a probability density function for θ . In so doing, the MC results will be inaccurate. In fact, the authors of the original 1941 paper have utilized a simplified notation that cannot be directly interpreted as a probability density function for θ , and this is the source of the confusion. The advantage of the HGF is that it allows us to demonstrate this problem in a simple manner, i.e. by considering the isotropic case where the solution can be easily foreseen.

The error introduced in the note was the incorrect definition of ‘isotropic scattering’ (representing an isotropic medium). In fact, it was stated that for an isotropic medium the probability density for θ must be a ‘flat’ function in order to have a uniform distribution of the scattering angles. This definition is wrong because it is the number of photons per unit solid angle that must be constant. It is in this way that the projections of all the randomly generated photon directions (for a given input direction) on the surface of a sphere, centred on the scattering site, will be truly uniformly distributed (and thus isotropic).

The consequence of this is that the exact function to be used in MC simulations is $\tilde{P}_{\text{HG}}(\cos(\theta))$ (and not $P_{\text{HG}}(\theta)$ as concluded in the note). Thus, $P_{\text{HG}}(\theta)$ is not an equivalent formulation of the Henyey–Greenstein probability density function because it does not give the correct result. In practice, the exact Henyey–Greenstein probability density for θ should be

$$P_{\text{HG}}(\theta) = \frac{1}{2} \frac{(1 - g^2) \sin(\theta)}{(1 + g^2 - 2g \cos(\theta))^{3/2}}$$

and not the expression so often reproduced in the literature (i.e. equation (1) in the previously published note).

This result seems to be trivial; however, if one considers more sophisticated probability density functions holding for arbitrarily shaped scattering particles (e.g. spheres, cylinders, etc), where there may also be a simultaneous dependence on both the deflection and on the azimuthal angle, an exact definition is necessary. Indeed, in these complex cases, it will not be possible for the reader to check the validity by using for example the particular isotropic case. In such cases, the confusion between ‘phase function’ coming from the wave theory and ‘probability density functions’ utilized in the MC context may lead to the wrong results or interpretation as shown in the note. Of course, if one uses the exact formulations for $\tilde{P}_{\text{HG}}(\cos(\theta))$ and $P_{\text{HG}}(\theta)$ (shown above in this letter) one obtains exactly the same results for both computation strategies.

We hope that this letter has now clarified this point. We would also like to sincerely thank Dr T J Farrell and Dr M S Patterson from the Juravinski Cancer Centre and McMaster

University (Canada) for having notified us of the existence of the error in the original definition of isotropy.

References

- Binzoni T, Leung T S, Gandjbakhche A H, Rufenacht D and Delpy D T 2006 The use of the Henyey–Greenstein phase function in Monte Carlo simulations in biomedical optics *Phys. Med. Biol.* **51** N313–22