MOCARTS: A LIGHTWEIGHT RADIATION TRANSPORT SIMULATOR FOR EASY HANDLING OF COMPLEX SENSING GEOMETRIES

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ABSTRACT

In applications of Diffuse Optical Imaging (DOI) such as functional neuroimaging (fNIRS), elaborated sensing geometries judiciously pairing multiple irradiation sources and detectors arranged over the tissue surface are needed. A variety of software tools for probing forward models of radiation transport in tissue exist, but their handling of intricate sensing geometries and specification of complex tissue architectures is, most times, cumbersome. In this work, we introduce a lightweight simulator, Monte Carlo Radiation Transport Simulator (MOCARTS) that attends these demands for simplifying specification of tissue architectures and simulation of complex sensing geometries. An object-oriented architecture facilitates such goal. The simulator core is evolved from the Monte Carlo Multi-Layer (*mcml*) tool but extended to support multi-channel simulations. Verification against *mcml* yields negligible error (RMSE~4·10e-9) over a photon trajectory attributable to different rounding approximations in the logarithm function among compilers. Full simulations show concurrent validity of the proposed tool. Finally, the ability of the new software to simulate multi-channel sensing geometries and to define biological tissue models in an intuitive nested-hierarchy way are exemplified. The proposed tool eases research for instance in image reconstruction, where it facilitates investigating the impact of extracerebral scalp blood flow on fNIRS.

Index Terms— Monte Carlo, radiation propagation, sensing geometries, image formation

1. INTRODUCTION

Diffuse Optical Imaging (DOI), also known as functional Near infrared Spectroscopy (fNIRS) when applied to neuroimaging, exploits the optical window to non-invasively monitor function of biological tissues such as brain [1], breast [2] or muscle [3]. DOI measures the optical attenuation ascribable to the cromophores present in the tissue, and capitalizes on the different extinction spectra of those chromophores [4]. The physical process of light-tissue interaction, known as image formation, encodes in the remitted light, information about tissue histology and physiology. Mathematically, DOI involves solving an inverse and ill-posed problem [5]. This requires modeling and resolution of the so called *forward* (formation) and *inverse* (reconstruction) problems. The forward problem should consider both: the physical phenomena of light interaction with matter and the modeling of biological tissue within a computer system to output the spectrum of light exiting the tissue and reaching the photoreceptor. Radiation transport in matter obeys the radiation transport equation (RTE) [6] which has only been solved for specific cases, and thus more tractable approximations such as diffusion theory [7] are popular.

A number of software tools have been developed to simulate radiation transport in biological matter, permitting inference and analysis of otherwise inviable or difficult to acquire observations. Among others; NIRFAST [8], TOAST [9], GEANT4 [10], MCX [11] and Monte Carlo Multi-Layer (*mcml)*[12]. Each one of these uses a different model of light propagation and exhibits varying capabilities. The first two, for instance, are based on diffusion theory as light propagation model and employ a mesh representation for the tissue. The latter three use the Monte Carlo method for approximating light propagation (although GEANT4 is also able to simulate other kinds of particles). In particular, *mcml* has become one of the most popular and widely used despite its interface limitations. For instance, *mcml* is unable to simulate several sources of light at once, tissue specification is not friendly nor flexible as soon as one deviates from flat homogeneous layers, and input and output format and data is rigid.

This paper presents a simulator of radiation transport in biological media. The new simulator, inspired on *mcml*, addresses three main interface shortcomings of its predecessor. First, it provides a flexible way to describe biological tissues in a more intuitive and reusable manner. Second, it provides support to define and simulate multiple light sources and detectors that can be arranged in complex sensing geometries. And third, the formatting and organization of the input and output data is redefined over a more human-readable XML file format.

In the remaining, section 2 presents basic light transport models. Section 3 details the proposed simulator and its

contributions. Section 4 presents the verification and validation of the new software tool. Finally, a discussion and conclusions are given in section 5.

2. LIGHT PROPAGATION

Light interaction with matter can be described as a succession of absorption and scattering events. The latter generalizing specific boundary phenomena such as reflection, refraction and diffraction, and for biological media it follows the Mie regime [13]. Several models of radiation transport exist. The more general is the RTE, a balance equation (1) that determines the radiation at a location due to incoming, outgoing, absorbed and emitted photons within an infinitesimal volume in the medium [14].

$$\frac{1}{c}\frac{\partial I}{\partial t}+\nabla I(r,t,\hat{s})+(\mu_a+\mu_s)I(r,t,\hat{s})=\mu_s\int f(\hat{s},\hat{s})I(r,t,\hat{s})d^2\hat{s}+q(r,t,\hat{s}) \quad (1)$$

In the above equation, c is the speed of light in the medium, $I(r,t,\widehat{s})$ is the radiance at point r in time t and direction $\hat{s}$, μ_a and μ_s are the absorption and scattering coefficients respectively, $f(\hat{s},\widehat{s'})$ is the phase function representing photon scattering from direction $\hat{s}$ to $\hat{s}'$ and $q(r,t,\widehat{s})$ is the light source. Analytical solutions to this equation are limited to homogeneous tissues and non complex geometries. A derivation of the RTE, known as Diffusion Equation [7] has been used in complex scenarios through the use of numerical methods [15, 8]. Other numerical approximations include Kubelka-Munk theory [16] and Inverse Adding-Doubling [17].

A probabilistic alternative approximation to the RTE is based on the Monte Carlo (MC) method. MC is a stochastic method which provides approximated solutions to mathematical problems [18]. MC simulations approximate the RTE sampling two probability distributions that jointly model the propagation phenomena [19]. The first distribution determines the length of the photon packet step as it travels through the tissue before it suffers a new extinction event. The second distribution dictates the direction of the photon's propagation after a scattering event, that is the tissue (an-)isotropy function. In *mcml* the Henyey-Greenstein distribution is used to approximate the anisotropy of biological tissues. The propagation of radiation within the tissue is estimated by simulating the wandering of large numbers of photons until they wane or escape the tissue. Figure 1 shows the general flowchart for such procedure.

The main disadvantage of this technique is the high computational cost required to afford a good approximation to the solution. However, in cases where there are non-scattering tissues (e.g. the cerebrospinal fluid in the human head) this technique yields a more accurate solution than that of Diffusion Equation [7].

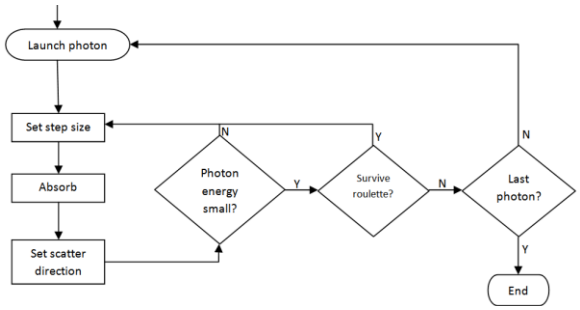

Fig 1. Monte Carlo radiation transport simulation flowchart (Adapted from [12]).

3. MOCARTS: THE NEW RADIATION TRANSPORT SIMULATOR

The core of the simulator developed in this work, MOCARTS, is founded in *mcml*. However, MOCARTS has been coded in Java and redesigned under the object-oriented paradigm (the original *mcml* was developed in C under the structured paradigm) in order to provide a portable and flexible tool and allowing the possibility to grow by independent modules. We only briefly describe the main features here, but a full description of the tool can be found in [20]. The software is available from; http://ccc.inaoep.mx/~f.orihuela-espina/Src/MOCARTS/.

3.1. Software architecture

The software architecture has been organized around 5 packages, namely: Simulation, Tissue model, Sensing geometry, Utilities and User Interface. This design intends to decouple each part of the system, increasing the software modularity and permitting future growing of each part independently. The Simulation package is the cornerstone of the tool and is the physics engine. The Tissue model package contains the classes needed to represent and characterize the *biological tissue* and describing its corresponding optical properties. The Sensing geometry package accommodates those classes describing the emitters, receptors and their pairings. Finally, the latter two provide some basic functionality and encode the input parser and output writer.

3.1. Radiation transport simulation

MOCARTS has been developed under the same basis as *mcml*, i.e., physics governing light-tissue interaction was simulated with the Monte Carlo method considering the same two probabilities distributions: a negative exponential for the length of the photon step and Henyey-Greenstein for the angle of scattering direction. Analogous to *mcml*, photon scattering at the boundaries between layers are treated especially because these consider the differing refractive index between the layers according to Fresnel law. Light propagation is simulated launching one photon at a time.

3.2. Flexibilization of the input parameters and tissue model specification.

In *mcml*, tissue specification is given by defining the optical properties of a set of flat homogeneous piled layers that compose the modeled tissue. In MOCARTS a nested-hierarchy format is proposed to define tissues in a more intuitive, reusable and readable manner (Figure 2). In the top of the hierarchy is the *BiologicalSlab* that may be composed by a set of *BiologicalSlices*. Organs, tissues and tissue layers are all specific kinds of slices. An *Organ* in turn is composed by a set of *Tissue*s and finally each *Tissue* is represented by a collection of *Layer*s each characterized by their *OpticalProperties*. The model is defined by the user through an XML file formatted [21] according to the DTD in Figure 3.

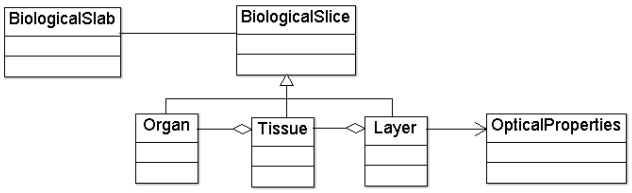

Fig 2. Class diagram for tissue characterization in MOCARTS. This design allows definition of biological tissues following a nested description.

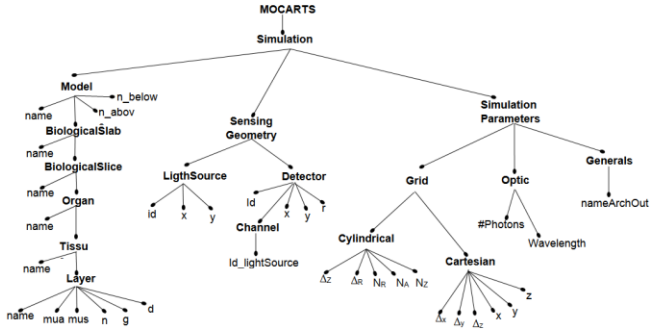

Fig 3. The proposed Document Type Definition (DTD) of MOCARTS' input XML file format.

3.3. Characterization of sensing geometries

In addition to tissue specification, other input parameters regarding simulation have been made flexible. Mainly, sensing geometries are now more detailed capturing the definition of light sources (LS) and detectors (D) at explicit locations. Channels pairs LS-D are defined as an attribute of the detector setting the corresponding light source(s) from which the detector can accept light. The actual setup may involve modulation in different frequency bands.

In *mcml*, information of absorption, reflection and transmittance is stored in a 2D matrix, by collapsing the radial information since only one source is simulated and the receptor is never explicitly modeled. Hence, MOCARTS departs in this aspect using a 3D matrix instead. This is because with multiple irradiation sources, light absorbed, reflected or transmitted must be identifiable for each light source to be analyzed, studied and/or captured by the possible multiple detectors. Figure 4 shows the new flowchart of the simulation process. Simulation of multiple sources are carried out one at a time.

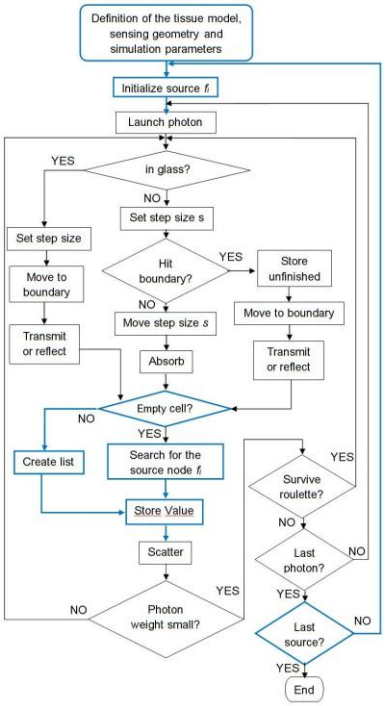

Fig 4. Flowchart of photon simulation with multiple light sources. Black boxes and lines correspond to the original flowchart of *mcml*. Blue boxes are the additional steps performed by MOCARTS.

To provide traceability of the energy deposited by each light source, we use a three dimensional array where a linked list structure in each cell encode where every transport event has occurred. Every node in the list stores the values of the absorption, reflection or transmission at that location for every corresponding light source. Figure 5 schematically depicts the proposed data structure.

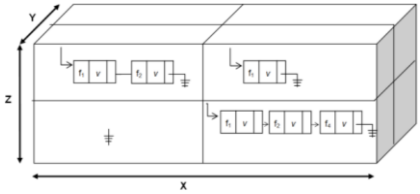

Fig 5. Schematic representation of the data structure used to trace photon deposition for each light source.

4. EXPERIMENTS AND RESULTS

To assert the correctness function of MOCARTS verification and validation was performed. For the following results, a 4 layer tissue model of the human head was defined to serve as a testbed. The optical properties listed in Table 1 were taken from [22].

TABLE 1. Optical properties for the adult human head tissues. n is the refractive index, μ_a is the absorption coefficient, μ_s is the scattering coefficient, g is the anositropy factor and T is the tissue thickness.

Tissue	n [-]	μ_a[cm^{-1}]	μ_s[cm^{-1}]	g	T [cm]
Scalp	1.42	0.127	190.376	0.900	0.3
Skull	1.555	0.147	161.245	0.900	0.5
Gray matter	1.360	0.270	75.157	0.899	0.4
White matter	1.380	0.931	372.501	0.870	0.2

4.1. Verification

During the verification, we confirm that MOCARTS behaves exactly as its predecessor *mcml* for strictly controlled input where the stochastic seed of the random number generator is fixed. Simulations were carried out with 10^4, 10^5 and 10^6 photons. The compared endpoints, according to the Root Mean Square Error in Eq. 2, were the individual photon trajectory as well as the total absorption, reflectance and transmittance. Verification results are summarized in Table 2 and different rounding made by the logarithm functions in the C and Java compilers was found to be responsible for the discrepancy.

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(\hat{Y}_i - Y_i)^2} \qquad (2)$$

TABLE 2. Root Mean Square Error during the verification process.

Output	Root Mean Square Error		
	10^3 photons	10^4 photons	10^6 photons
Photon trajectory	-	4.0335e-009	-
Absorption	0.0136	0.0026	0.0011
Reflectance	0.2731	0.0728	0.0293
Transmitance	4.7207e-004	1.1360e-004	7.3175e-005

4.2. Concurrent Validity

We hypothesized that both tools should lead to probabilistically similar results (concurrent validity). Thus, to validate the tool we carried out an experiment where the factor is the tool with two treatments; MOCARTS (intervention) and *mcml* (used as gold standard control). The experimental unit is the head model from where the observations are retrieved. As the control only allows simulations of one source of radiation, the number of sources was set to one. Unlike during verification, here the random number generator seed is not fixed, and hence replication was used to assert no significant difference exists in the results. Figure 6 shows the measured absorption, reflectance and transmittance for simulations with 10, 10^2, 10^3, 10^4, 10^5 and 10^6 photons.

4.3. Simulation of multichannel sensing geometries

Finally, to show the extra functionality of MOCARTS to deal with complex sensing geometries simulations, an example is shown in Figure 7 for a configuration of 5 light sources (blue) and 4 detectors (red) as well as a simulation in a model of the human head based on a MRI image.

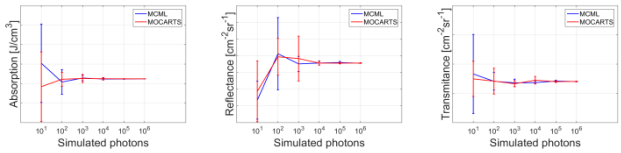

Fig 6. Absorption (left), Reflectance (center) and Transmittance (right) observed from the human head model for both *mcml* and MOCARTS for simulations with increasing number of photons. The similar trend and converging behavior with larger number of photons can be appreciated.

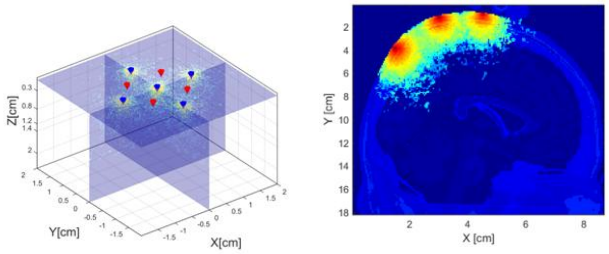

Fig 7. Exemplification of multiple channels simulations in MOCARTS. Blue planes in the left figure correspond to slices of a flat modeled tissue. It can be seen, through the slices, the absorbed light in the tissue for every irradiation source. Right figure shows the absorption of three sources over a head model based on the structure segmented from a MRI image.

5. DISCUSSION AND CONCLUSIONS

Analytical solutions to radiation transport are difficult and thus computational simulations are now a popular tool for addressing questions of image formation. The probabilistic Monte Carlo model, despite being computationally expensive can produce excellent approximations when the tissue optical properties are accurately described. A number of simulators with varying degree of complexity are available. Here, we have verified and validated a novel lightweight alternative, MOCARTS, which inherits from *mcml* its physics engine but additionally offers three interface advantages; easy complex sensing geometries simulation, nested tissue characterization and XML based input/output formatting. Our next step for improving the tool shall be the parallelization of the individual photon simulation. Our research continues to characterize the impact of extracerebral scalp blood flow on fNIRS.

6. ACKNOWLEDGMENT

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