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Time evolution of photon-pulse propagation in scattering and absorbing media: The dynamic radiative transfer system

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ABSTRACT

A new dynamic-system approach to the problem of radiative transfer inside scattering and absorbing media is presented, directly based on first-hand physical principles. This method, the Dynamic Radiative Transfer System (DRTS), employs a dynamical system formality using a global sparse matrix, which characterizes the physical, optical and geometrical properties of the material-volume of interest. The new system state is generated by the above time-independent matrix, using simple matrix-vector multiplication for each subsequent time step. DRTS is capable of calculating accurately the time evolution of photon propagation in media of complex structure and shape. The flexibility of DRTS allows the integration of time-dependent sources, boundary conditions, different media and several optical phenomena like reflection and refraction in a unified and consistent way. Various examples of DRTS simulation results are presented for ultra-fast light pulse 3-D propagation, demonstrating greatly reduced computational cost and resource requirements compared to other methods.

1. Introduction

Radiative transfer models attempt to describe the temporal and spatial behavior of photon propagation through scattering and absorbing media, which is important in many scientific areas such as astrophysics [1–3], oceanography, high energy physics (neutrino transport) [4], thermal transfer [5–7,39], image processing and, in recent years, bio-sciences [8–11]. Starting from a conceptual framework for a simple description of the physical phenomenon, the well-known “Radiative Transfer Equation” (RTE) was developed:

$$\frac{1}{c}\frac{\partial I(\boldsymbol{X},\boldsymbol{S},t)}{\partial t}+\frac{\partial I(\boldsymbol{X},\boldsymbol{S},t)}{\partial s}+(\mu_a+\mu_s)I(\boldsymbol{X},\boldsymbol{S},t) - \mu_s\iint I\big(\boldsymbol{X},\boldsymbol{S}',t\big)g\big(\mathbf{S},\boldsymbol{S}'\big)d\boldsymbol{S}'=0 \quad (1)$$

Many different solutions or approximations for RTE have been proposed [12], such as Monte Carlo [13,14], Diffusion Approximation, calculations using different basis functions [4,6,15–17], Finite-Element-like methods (FEM) [1,5,7] and combinations of the above [5,8,10,18,19]. In a very simple case a solution has been found based on a “moving” unity partition of normal distribution, decreasing over time by an exponential factor according to the absorption parameter. Diffusion approximation connects the directed flow with undirected flow by a constant that simplifies the mathematical problem and turns it to an elliptical partial differential equation. However, this is not physically true near sources or boundaries. Another approach, use spherical harmonics [4,6,20,21], does not lead to an applicable solution because of the symmetry of base functions that makes almost impossible to represent a directional flow. Mathematical approximations based on finite element methods (FEM) have been proposed by many authors [1,5,7,22], treating complicated structures such as the human body with partitioning of Euclidean space and creation of mesh structures. These methods however do not preserve the positivity of intensity and produce potential instabilities because of the mathematical type of the RTE model. A combination of FEM with Diffusion approximation reduces the instability but does not fully resolve the problem [8,18,19].

Because of mathematical difficulties [20,21,23,24], procedures based on Mode Carlo (MC) methods are believed to be the best practice, since calculations are going down to physical processes. Parallel array processors have been used [25,26] to handle the huge amount of calculations required by this type of methods. Usually in standard MC techniques only space partition is implemented, so there is a lack of time and direction information and these are not suitable to describe transient phenomena. Specifically, since only spatial information is given, there is no practical way to convolve the results with any specific pulsed-shaped source. In time-dependent MC [27,28] the computational

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requirements explode, especially in systems with dense partitioning in space and time, as this method generally requires computational effort proportional to the dynamic range of the expected values – here on the order of 10^{20}. These MC shortcomings are particularly evident in cases involving ultra-short light pulses.

A solution of the time-dependent photon transport has been attempted by Fourier transform [8,23], "Time-dependent Monte-Carlo" [29,30] or other time-domain methods [31–33,40–42]. These can lead to a meaningful approximate solution only when source power changes are slow enough compared to the fast rates of scattering effects. Under these circumstances, intensity will represent the mean-time value under the effect of power-source changes. But when source changes are fast, frequencies of the source will be convolved with those of the system, a fact that makes computations impractical for very short time-scale phenomena, due to the range of frequencies involved, which tend to infinity. Recent developments in medical diagnostics, however, using *fs* laser pulses, e.g. for internal tumor imaging, will require accurate solutions of the radiation propagation problem in absorptive-diffusive media in very short time scales.

There are many difficulties regarding numerical solution of the RTE, or its physical incompleteness or inconsistencies [24,34,35]. To overcome these problems, a new method is described in this paper, based on the physical photon-matter interaction in a consistent treatment. This method, the Dynamic Radiative Transfer System (DRTS), computes the time evolution of photon distribution of inside scattering absorbing media by the construction of a probabilistic dynamic system. This is especially useful in bio-engineering for e.g. solving the Optical Tomography "forward problem" [36] using pulsed excitation. . In such cases DRTS is quite capable to deliver accurate results, where other methods might be questionable. DRTS is also capable of calculating accurately the time evolution of photon propagation in media of complex structure and shape. Additionally, DRTS allows the integration of time-dependent sources, boundary conditions, different media and several optical phenomena (like reflection and refraction) in a unified and consistent way. Especially for the purpose of instrument design, the new DRTS method provides a tool that allows an accurate measurement-system implementation. Therefore DRTS can be viewed as an improved and generalized solution method, accurately treating time effects in both short and long time scale, which avoids the inconsistencies and drawbacks of the RTE model.

In the next section the physical phenomenon will be expressed as a dynamical system and the computation of the system matrix elements will be detailed. Time evolution of the photon propagation can afterwards be computed by the simplest linear algebra operations (matrix-vector multiplication and vector additions). Then, the algorithm based on the theoretical analysis is constructed and simulation results are initially demonstrated for several cases of isotropic media with different optical properties. In the last section, a thorough comparative analysis of DRTS vs. the other methods will be detailed.

2. Theoretical foundation of photon propagation

The Dynamic Radiative Transfer System (DRTS) is a new method that models photon propagation through scattering and absorbing media, applicable to time intervals down to the order of femtosecond.

Absorption and scattering processes are considered independent. There are three measures that characterize absorption and scattering probabilities, the absorption parameter μ_a the scattering parameter μ_s and the probability kernel g(***S, S'***) expressing the directional change. The first two are measures over the path of photons that travel inside the medium. The third one expresses the conditional possibility that a photon changes direction from ***S*** to ***S'*** if it has been scattered.

By definition $1/\mu_s$ expresses the mean value of the exponential probability for the photons to be subjected to scattering inside the medium. The expected population of photons that are scattered (N^S) during a time step Δt can be derived by the cumulative distribution function (CDF) of the exponential distribution:

$$\begin{aligned} &\mathrm{N^S(t+\Delta t)} = N(t)P(\text{photon scattering during time interval } \Delta t) \\ &\Rightarrow \mathrm{N^S(t+\Delta t)} = N(t)(1-e^{-\mu_s c\Delta t}) \end{aligned} \tag{2}$$

Correspondingly the photon population that is not subjected to any scattering event (N^0), during the time interval Δt, will be:

$$\mathrm{N^{S^0}(t+\Delta t) = N(t) - N^S}(t+\Delta t) = N(t)e^{-\mu_s c\Delta t} \tag{3}$$

The probability that a photon is subjected to k scattering events in Δt can be derived by the Poisson distribution with expected value $\mu_s c\Delta t$. The population of scattered photons can be grouped in different populations N^{S0},N^{S1},N^{S2},... according to the number of the scattering events encountered, so:

$$N^{S^i}(t+\Delta t) = N(t)P(i = \text{scatter events}) = N(t)\frac{e^{-\mu_s c\Delta t}(\mu_s c\Delta t)^i}{i!} \tag{4}$$

From the above equation, it can be proved that for very small time intervals the probability of the photon population to be subjected to more than one scattering event is negligibly small. This can be proved by calculating the following limit, for $i > 1$:

$$\lim_{\Delta t\to 0}\frac{N^{S^i}}{N^{S^1}} = \lim_{\Delta t\to 0}\left(\frac{\frac{e^{-\mu_s c\Delta t}(\mu_s c\Delta t)^i}{i!}}{e^{-\mu_s c\Delta t}}\right) = \lim_{\Delta t\to 0}\frac{(\mu_s c\Delta t)^i}{i!} = 0, \quad \textit{when } \mu_s c\Delta t \ll 1 \tag{5}$$

At this point it might appear that only single-scattering events are considered. According to Eq. (5) as Δt gets smaller, the probability of multiple scattering is exponentially reduced. However, our method has the capability of including higher-order scattering events during this interval Δt, if so desired, as it will be detailed later in Section 3, after the construction of the system matrix A. Essentially multiple scattering events are produced as a combinatorial sequence of single-scatterings.

To conserve probability and therefore energy, while ignoring multiple scattering events, we approximate the probability of one scattering event $P(i=1)$ as $1-P(i=0)$. Thus, regarding the scattering process we can split the photon population in two groups N^0 and N^1:

$$N^{S^0}(t+\Delta t) = N(t)e^{-\mu_s c\Delta t} \tag{6}$$

$$N^{S^1}(t+\Delta t) = N(t)(1-e^{-\mu_s c\Delta t}), \quad \textit{when } \mu_s c\Delta t \ll 1 \tag{7}$$

For the absorption process, by definition $1/\mu_\alpha$ expresses the mean value of the exponential probability for the decay of photons that travel inside the medium. The expected population (N) of photons surviving after a small time step Δt can be derived by the CDF of the exponential distribution:

$$\begin{aligned} &N(t+\Delta t) = N(t)(1-P(\text{absorption during } \Delta t)) \\ &\quad\Rightarrow N(t+\Delta t) = \mathrm{N}(t)e^{-\mu_a c\Delta t} \end{aligned} \tag{8}$$

By combining both scattering and absorption processes, the expected population group of photons surviving after a small time