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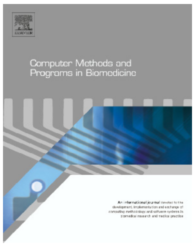

Monte Carlo method for photon heating using temperature-dependent optical properties

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ABSTRACT

The Monte Carlo method for photon transport is often used to predict the volumetric heating that an optical source will induce inside a tissue or material. This method relies on constant (with respect to temperature) optical properties, specifically the coefficients of scattering and absorption. In reality, optical coefficients are typically temperature-dependent, leading to error in simulation results. The purpose of this study is to develop a method that can incorporate variable properties and accurately simulate systems where the temperature will greatly vary, such as in the case of laser-thawing of frozen tissues.

A numerical simulation was developed that utilizes the Monte Carlo method for photon transport to simulate the thermal response of a system that allows temperature-dependent optical and thermal properties. This was done by combining traditional Monte Carlo photon transport with a heat transfer simulation to provide a feedback loop that selects local properties based on current temperatures, for each moment in time. Additionally, photon steps are segmented to accurately obtain path lengths within a homogenous (but not isothermal) material. Validation of the simulation was done using comparisons to established Monte Carlo simulations using constant properties, and a comparison to the Beer–Lambert law for temperature-variable properties.

The simulation is able to accurately predict the thermal response of a system whose properties can vary with temperature. The difference in results between variable-property and constant property methods for the representative system of laser-heated silicon can become larger than 100 K. This simulation will return more accurate results of optical irradiation absorption in a material which undergoes a large change in temperature. This increased accuracy in simulated results leads to better thermal predictions in living tissues and can provide enhanced planning and improved experimental and procedural outcomes.

1. Introduction

Heating a medium using electromagnetic irradiation is a common technique in a variety of disciplines, ranging from electronics to medicine to welding. There exist numerous applications where electromagnetic heating is intended to induce some thermal damage or structural change in a medium. For example, in medicine, lasers are often used in ablative techniques, where the temperature of the

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surrounding tissue needs to stay within a certain threshold [1]. Other techniques use laser heating to prevent thermal damage inherent in cryosurgery [2]. While lasers are often used in medicine due to their precision, other irradiative techniques are gaining prominence, such as microwave irradiation [3].

Myriad tools currently exist to simulate the optical distribution within a material, principally using the Beer–Lambert equation to directly determine optical distribution, or Monte-Carlo simulations to determine photon scattering and distribution [4,5]. No matter the method used, the optical distribution is then used to determine the thermal response of the material to the optical irradiation. These approaches to simulating the optical distribution critically neglect the temperature dependent nature of a material's optical properties.

Current simulation techniques use constant optical properties, often at room temperature, to determine the optical distribution within the material. While this may in practice be a reasonable approximation for materials that do not experience a large change in temperature, this limitation becomes important as thermal gradients become large. This is especially true in the case of a material which undergoes phase change.

Variable Optical Irradiation Distribution Simulation software (VOIDSim) was developed to simulate irradiative heating while using temperature-dependent optical and thermal properties. The software not only will determine the optical distribution within the material, but also will simulate the thermal response of the material to the irradiation. Furthermore, the software is robust enough to allow a variety of irradiative source geometries, temporal irradiative profiles, and an arbitrary system geometry.

2. Description of method

2.1. *Terminology*

The program is called Variable Optical Irradiation Distribution Simulation (VOIDSim). VOIDSim requires the user to define a simulation geometry using a series of CAD files (STL file format), with a single file corresponding to a single material in the simulation. The terminology represented in Fig. 1 will be referenced in this paper.

The "system" refers to all modeled solid bodies in the simulation, or rather, all physical domains wherein energy propagation is considered. The system is divided into domains, which share all properties (constant or variable), and at the outset are homogeneous. Each domain is defined as a collection of triangles which form its surface. Each domain is divided into a regular grid of cells (not shown in Fig. 1) with nodes at the center of each cell. Each cell has uniform homogeneous properties at each moment in time.

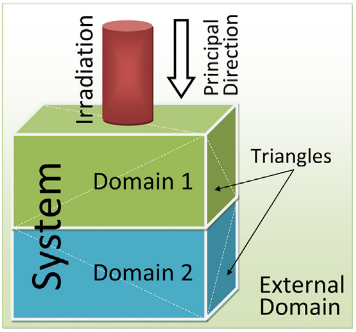

Fig. 1 – Simulation terminology.

2.2. *Program overview*

The program includes Monte Carlo photon tracing algorithms developed by Prahl et al. [4] and refined by Wang et al. [5]. As VOIDSim allows for arbitrary geometries (not limited to a single domain, or horizontal layers) it utilizes ray-tracing techniques to determine angles of incidence, specifically using the ray-triangle intersection algorithm developed by Moller and Trumbore [6]. The flow diagram for VOIDSim is shown below, in Fig. 2.

Before the program can start, the user must provide the appropriate inputs into the program. VOIDSim provides a form-based user interface based on .NET Winforms. The user specifies all pertinent thermal and optical properties for each domain in the GUI. Variable properties are defined as look-up tables, with each data point requiring the temperature and property value. VOIDSim utilizes linear interpolation/extrapolation to retrieve properties based on current system temperatures. In the case of extrapolation, if a physically impossible property is derived (e.g. negative thermal conductivity) that property is set to its logical boundary (e.g. thermal conductivity equals zero). Once all required inputs are satisfied, the user may start the simulation.

In preprocessing, the program converts all user inputs to SI units (kilograms, meters, seconds, and Kelvin) to avoid any conversion errors. Memory is allocated for each node in the system, all constants are computed, and the initial system condition is recorded. For *n* photons "Photon Deposition" occurs, which determines the spatial distribution of a photon packet. Before the distribution can be calculated the photons must be initialized in their starting locations ("Photon Initialization"). Once Photon Deposition has concluded for n photons, "Heat Transfer" in the system is calculated for an incremented moment in time. The simulation time is updated, and the program returns to Photon Deposition if the update condition requires it, otherwise it proceeds with the next time step of Heat Transfer. Once the user-defined simulation time elapses, the simulation is complete.

The majority of the subroutines in Photon Deposition are similar to those found in MCML [5], for example. Where Photon Deposition majorly differs is its treatment of geometries (to allow for arbitrarily-shaped geometries) and how it incorporates variable optical properties.

2.3. *Movement energies*

Rather than immediately determining the distance a photon will move in a medium, based on the medium's total optical attenuation coefficient, a photon is first given Movement Energy, which is defined as the negative natural log of a random number, between zero and one. This is done to reduce