pyxopto: An Open-Source Python Library with Utilities for Fast Light Propagation Modeling in Turbid Media

Peter Naglič[1], Yevhen Zelinskyi[1], Franjo Pernuš[1], Boštjan Likar[1], Miran Bürmen[1]
[1]*Faculty of Electrical Engineering, University of Ljubljana, Tržaška cesta 25, 1000 Ljubljana, Slovenia*
Author e-mail address peter.naglic@fe.uni-lj.si

Abstract: We present a multi-layered and voxel-based Monte Carlo methods with auxiliary utilities implemented in Python for user-friendly, open-source and multi-purpose modeling of light propagation in turbid media based on PyOpenCL computational platform.

1. Introduction

Light propagation in turbid media such as biological tissue is one of the central topics in biomedical optics and pertains to various fields including diffuse optical tomography, spatial frequency domain imaging, opto-acoustic imaging, hyperspectral imaging, tissue and sample characterization with integrating spheres, light treatment planning, and many more.

Light propagation in highly turbid media such as biological tissue is mathematically well-described by the radiative transfer equation. However, accurate analytical or closed-form solutions to the radiative transfer equation are rare or highly specific to constrained and impractical geometries. While various approximations can be utilized to solve the radiative transfer equation in the interest of simplicity and time effectiveness, these approximations exhibit limitations even in most common experimental settings. For example, the popular diffusion approximation is inaccurate near light-sources and in regions with high-absorption [1]. Since its inception [2], the stochastic Monte Carlo (MC) method has become a widely utilized alternative in providing numerical solutions to the radiative transfer equation in biomedical optics. Nowadays, it is regarded as a reference standard method and has seen an immense advancement in various aspects. The most notable milestones are graphics processing unit (GPU) parallelization [3] and implementation of mesh-based approaches [4] for modeling light propagation in complex shapes and configurations of biological tissues such as a human head. Thanks to immense development in hardware, especially GPUs, and deep learning approaches, the MC method is becoming more time efficient and a serious contender to the approximate solutions of the radiative transfer equation for inverse problems where light propagation modeling is utilized for estimation of optical properties of turbid media [5].

While the MC methods have been significantly advanced in recent years, adaptation by the general biomedical optics community is still hindered by the lack of completely free and open-source availability of the MC method. In this regard, significant effort has been made by various groups. Most notably, the group of Fang has a track of successful publications that established and developed the well-known mesh-based MC method for accurate simulations of light propagation in complex tissue structures [6]. Recently, Leino *et al*. have proposed a mesh-based MC software ValoMC interfaced with MATLAB® for easier utilization [7]. In the interest of user-friendliness and use in educational environment, Marti *et al*. have developed a MCmatlab light transport solver with heat-diffusion and tissue-damage simulator [8]. While all the proposed implementations have undoubtedly contributed to wider acceptance and utilization of the MC method, the implementations still lack the required modularity and being independent of licensed software such as MATLAB®.

On the other hand, Python programming language is becoming more and more popular in the scientific community, offering seamless interface to visualization and highly optimized numerical tools for scientific computations. Therefore, Python is an ideal candidate for establishing a collection of computational tools offering cross-platform, freely available and user-friendly software that can be shared and distributed through platforms such as PyPI, Conda package manager systems, etc.

In this summary, we present a user-friendly open-source Python library *pyxopto* for light propagation in turbid media based on the stochastic MC method. We briefly describe the most notable components that represent novel utilities in comparison to the other existing MC methods. Firstly, we describe the core of the light propagation model in the proposed Python library *pyxopto*, which can be run on a CPU or GPU using the PyOpenCL platform. Subsequently, we focus on source and detection schemes, that can be adapted to various experimental configurations and offer acquisition of measurable quantities. Finally, we describe other auxiliary utilities that are offered by the Python library *pyxopto*, which are commonly required in the field of biomedical optics.

Diffuse Optical Spectroscopy and Imaging VIII, edited by Davide Contini, Yoko Hoshi,
Thomas D. O'Sullivan, Proc. of SPIE-OSA Vol. 11920, 1192012 · © 2021 OSA-SPIE
CCC code: 1605-7422/21/$21 · doi: 10.1117/12.2615340

2. Overview of the Python library *pyxopto*

Figure 1 briefly highlights different simulation utilities offered by our Python library *pyxopto*. The central part is the PyOpenCL-based light propagation core, which can be executed on CPU or GPU computational devices irrespective of the vendor, offering cross-platform and cross-device deployment. The light propagation is based on either multi-layered or voxel-based configurations, which are appropriate for simple and more complex tissue structures. The optical properties are described by the standard absorption and scattering coefficients, scattering phase function for sampling the scattering angles and refractive indices, as well as necessary materials for describing boundary conditions such as metallic surfaces of optical fiber probes.

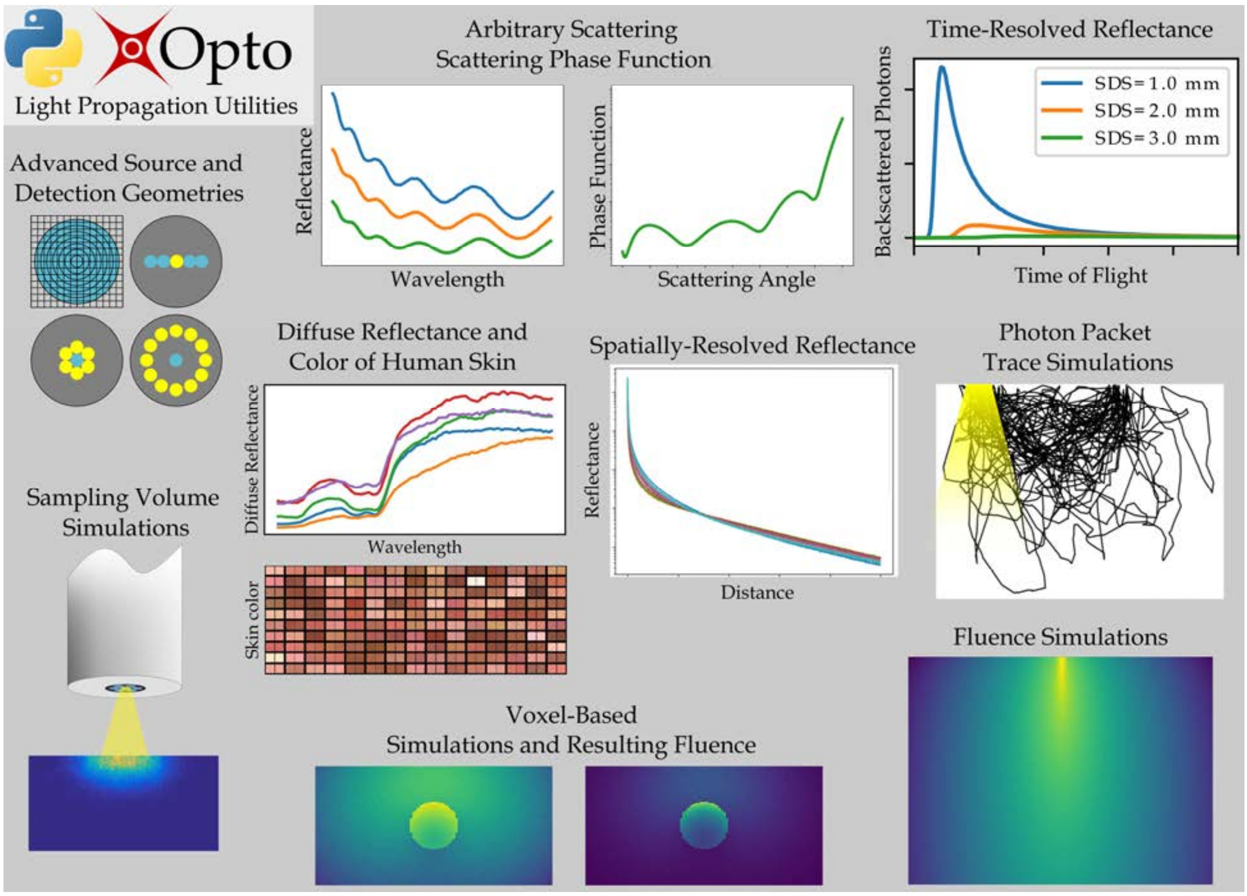

Fig. 1. A collection of simulation utilities offered by the Python library *pyxopto*.

One of the stronger suits of the proposed light propagation model is that we do not strictly implement the generic Henyey-Greenstein scattering phase function. Having a single scattering phase function significantly limits the applicability of the light propagation model for tissues exhibiting microscopic refractive index variations that cannot be accounted for by a single-parameter Henyey-Greenstein scattering phase function. Therefore, we have implemented a general sampling scheme for scattering phase function probability distributions based on lookup tables [9]. Such a scheme supports utilization of various scattering phase functions such as the modified versions of the Henyey-Greenstein, Gegenbauer kernel and Power of Cosines, and more complex scattering phase functions based on the Mie theory and the T-matrix method. The latter can be used to simulate light propagation through water-based suspension of spherical microparticles such as polystyrene microspheres and is therefore ideally suited for fabrication of optical phantoms. Fig. 1 (top) shows an example of a diffuse reflectance spectrum as recorded by an optical fiber probe submerged in a suspension polystyrene microsphere with different concentrations of spherical particles. Such reflectance spectra can then be used for absolute calibration of the MC method [10].

Our proposed Python library *pyxopto* exhibits high modularity in terms of light-source implementations that include standard collimated pencil beams, spatially extended beams, and Gaussian beams. Moreover, custom photon packet launching schemes can be implemented through a lookup table description of a spatially and angularly inhomogeneous light source. Likewise, detection schemes are based on commonly used radial and rectangular accumulators with available extensions to more realistic geometries involving optical fiber probes with precise description of the boundary conditions (Fig. 1, top-left), camera systems with custom acceptance angles and even lookup table acceptance characteristics, which we have proposed and investigated through the years [11,12].

Detection schemes enable acquisition of standard quantities such as reflectance and transmittance, as well as fluence and photon packet traces. Reflectance can be stored and represented as spatially resolved reflectance or point-measurements of diffuse reflectance spectra acquired by a single optical fiber or integrating sphere (Fig. 1, center). Fluence offers representation of energy deposition and is useful for laser-treatment planning (Fig. 1, bottom-right). Photon tracing supports acquisition and recording of weights and scattering events, through which sampling volumes can be calculated. Sampling volumes are important for planning appropriate optical fiber probes for, e.g., tissue biopsy.

To provide support for mainstream utilization of the MC method, we have also implemented standard source-detector configurations such as six-around one optical fiber probes, linear optical fiber arrays and even health monitoring modules based on diodes and photodiodes that are used in wearable gadgets. In these terms, Fig. 1 shows an output of a submodule that is available in *pyxopto* for estimation of human skin color based on diffuse reflectance spectra acquired through an optical fiber probe.

In addition to the core that pertains to light propagation, *pyxopto* offers various auxiliary utilities that can be of great use in the biomedical optics community and are not shown on Fig. 1. Especially important is the estimation of optical properties. In *pyxopto*, we have implemented an interface to the TensorFlow open-source machine learning platform, which can be utilized as a regression based inverse model for efficient, fast and accurate estimation of optical properties [5].

Finally, *pyxopto* offers a library of standard materials and components that can be used to fabricate optical phantoms. For example, the included utilities involve computation tools for calculating the absorption and scattering coefficients and scattering phase functions of various regularly shaped particles. Subsequently, the required volume or mass of phantom components can be calculated to yield the desired optical properties.

To summarize, we briefly presented modular and versatile Python library *pyxopto*, which offers MC simulations of light propagation in turbid media through efficient computation within the PyOpenCL framework, that can be executed on various computational devices. The proposed library contains various auxiliary utilities that we believe will be highly useful to the biomedical community.

3. References

1. P. Naglič, L. Vidovič, M. Milanič, L. L. Randeberg, and B. Majaron, "Suitability of diffusion approximation for an inverse analysis of diffuse reflectance spectra from human skin in vivo," OSA Continuum **2**(3), 905 (2019).
2. L. Wang, S. L. Jacques, and L. Zheng, "MCML—Monte Carlo modeling of light transport in multi-layered tissues," Comput. Meth. Prog. Bio. **47**(2), 131–146 (1995).
3. E. Alerstam, T. Svensson, and S. Andersson-Engels, "Parallel computing with graphics processing units for high-speed Monte Carlo simulation of photon migration," J. Biomed. Opt. **13**(6), 060504 (2008).
4. Q. Fang, "Mesh-based Monte Carlo method using fast ray-tracing in Plücker coordinates," Biomed. Opt. Express **1**(1), 165 (2010).
5. M. Ivančič, P. Naglič, F. Pernuš, B. Likar, and M. Bürmen, "Efficient estimation of subdiffusive optical parameters in real time from spatially resolved reflectance by artificial neural networks," Opt. Lett. **43**(12), 2901 (2018).
6. Y. Yuan, S. Yan, and Q. Fang, "Light transport modeling in highly complex tissues using the implicit mesh-based Monte Carlo algorithm," Biomed. Opt. Express **12**(1), 147 (2021).
7. A. A. Leino, A. Pulkkinen, and T. Tarvainen, "ValoMC: a Monte Carlo software and MATLAB toolbox for simulating light transport in biological tissue," OSA Continuum **2**(3), 957 (2019).
8. D. Marti, R. N. Aasbjerg, P. E. Andersen, and A. K. Hansen, "MCmatlab: an open-source, user-friendly, MATLAB-integrated three-dimensional Monte Carlo light transport solver with heat diffusion and tissue damage," J. Biomed. Opt. **23**(12), 1 (2018).
9. P. Naglič, F. Pernuš, B. Likar, and M. Bürmen, "Lookup table-based sampling of the phase function for Monte Carlo simulations of light propagation in turbid media," Biomed. Opt. Express **8**(3), 1895 (2017).
10. P. Naglič, Y. Zelinskyi, L. Rogelj, J. Stergar, M. Milanič, J. Novak, B. Kumperščak, and M. Bürmen, "Optical properties of PlatSil SiliGlass tissue-mimicking phantoms," Biomed. Opt. Express **11**(7), 3753 (2020).
11. Y. Zelinskyi, P. Naglič, F. Pernuš, B. Likar, and M. Bürmen, "Fast and accurate Monte Carlo simulations of subdiffusive spatially resolved reflectance for a realistic optical fiber probe tip model aided by a deep neural network," Biomed. Opt. Express **11**(7), 3875 (2020).
12. P. Naglič, B. Likar, F. Pemuš, and M. Bürmen, "Robust calibration of reflectance acquired with optical fiber probes," in *Clinical and Preclinical Optical Diagnostics II (2019), Paper 11074_80* (Optical Society of America, 2019), p. 11074_80.