Comparison of wave-optical and Monte Carlo light propagation simulations in scattering media

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This work compares simulations of light propagation in scattering media using solutions to Maxwell's equations (ME), to the radiative transfer equation (RTE), and the Wave Propagation Method (WPM) as a potential alternative in terms of simulation time and agreement.

1 Introduction

The different measurement techniques in diffuse optics are based on the optical properties of materials and the proper modeling of light-matter interaction [1]. Understanding the scattering and absorption properties of complex media often requires computationally expensive and time-consuming Monte Carlo (MC) simulations to solve the RTE or numerical solutions to ME when accounting for wave-optical phenomena. In this study, the light propagation in scattering media based on ME, the WPM, and MC simulations are compared to each other in terms of computational speed and agreement.

2 Methods

Three different software packages were used for the simulations: MEEP to solve ME [2], a custom built WPM tool [3], and the PyXOpto package to solve the RTE using the MC method [4]. Quasi-3D wave-optical simulations were performed in this study as an approximation for timely and stable convergence rather than full 3D as described for example by Ott *et al.* [5], with 63 2D slices throughout the simulation body, each slice 1 µm apart from the other in the y direction. The simulation body is a laterally infinite slab with a thickness of 32 µm and scattering spheres with a diameter of 1 µm placed randomly inside the slab at different volume concentrations f_V (see Fig. 1). The complex refractive indices of the background medium and the scatterers were set to 1 and 1.45 respectively and the illumination to a plane wave with a wavelength of 1 µm propagating in the z direction. The MC simulations were performed in full 3d using a homogeneous scattering medium. The scattering and absorption coefficients, and the anisotropy factor where derived from Mie theory [6]. To mimick a quasi-3D behavior, the anistropy of the medium was formulated as an anisotropy tensor, not allowing for scattering angles into the y direction [7]. The energy densities of all simulations as well as their simulation times were used for comparison [5]. The fluence of the non-absorbing medium in the MC simulation, needed for the energy density, was calculated using the pathlengths of all 10^6 photons at every point [8].

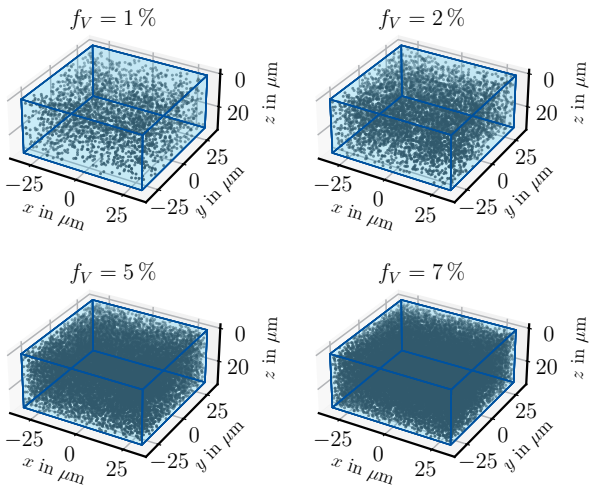

Fig. 1 *Simulation bodies used for wave-optical simulations with increasing volume concentration of scatterers f_V.*

3 Results

Tab. 1 lists the accumulated simulation times required for all slices within the simulation body. The rigorous solutions to ME using MEEP require the longest to compute. These times also increase with increasing f_V. The simulation times for the WPM and PyXOpto are significantly shorter. A comparison of the normalized energy density averaged over the y direction for low and high f_V is shown in Fig. 2. The MEEP and PyXOpto simulations show great correspondence to each other, while the WPM suffers a rapid decrease in energy density. It is apparent that the WPM is only able to qualitatively predict the speckle patterns caused by the scatterers, especially for low f_V but still fails at higher concentrations, mostly due to the missing backscattering in its implementation. This is further highlighted by additionally averaging the energy densities in the x direction to display the average energy density for all f_V as a

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function of depth in Fig. 3. The wave-optical simulations using MEEP and MC simulations with PyXOpto are in agreement with each other within a few percent of relative difference for all f_V and the energy density, again, rapidly decreases for the WPM.

	MEEP	**WPM**	**PyXOpto**
f_V	*Simulation time in seconds*		
1 %	727275	192	13
2 %	782973	199	20
5 %	1250373	204	31
7 %	1554482	201	42
Degree of parallelization	189 MPI processes	4 threads	$\leq$1539 threads

Tab. 1 *Total simulation times needed for the scattering simulations. The simulations were performed on a CPU server with Intel® Xeon® E7-8890 v4 @2.20 GHz CPUs with 96 Cores and 896 GB RAM.*

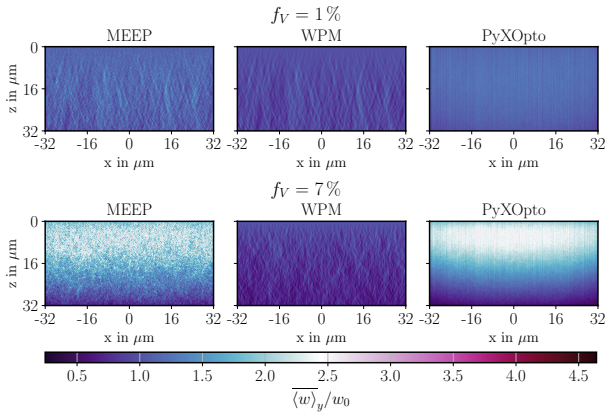

Fig. 2 *Normalized energy densities averaged over all slices.*

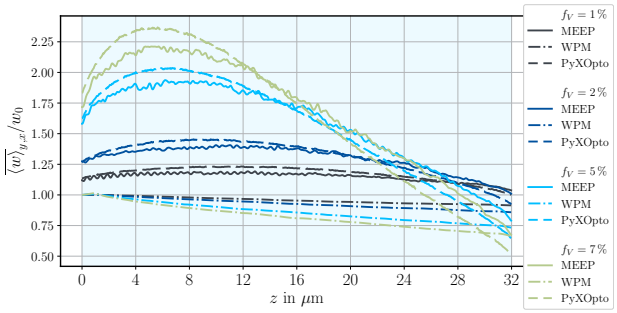

Fig. 3 *Averaged and normalized energy densities as a function of depth.*

4 Discussion and Outlook

The study shows that the WPM is qualitatively able to predict speckle patterns for weak scattering. Quantitative differences between the two wave-optical simulations are mostly due to the strictly forward-directed propagation of the WPM and missing conservation of energy. The small differences between the MEEP and PyXOpto simulations can be explained by the quasi-3D approximations performed in this study. The WPM is the preferred wave-optical simulation tool for weakly scattering media due to its shorter computation time. Future work should incorporate the bidirectional WPM for a higher degree of accuracy regarding the energy density and for applications with reflectance measurements. A hybrid method combining the WPM and the RTE might also be a viable option.

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