TDMS: An open source Time Domain Maxwell Solver for simulations in biomedical optics

Peter R.T. Munro

Department of Medical Physics and Biomedical Engineering, University College London, UK

ABSTRACT

Realistic simulation of light propagation in biological tissue is of great use in many biomedical optical imaging applications. For example, simulation of image formation in optical coherence tomography is useful for applications such as training researchers and clinicians, image interpretation and technique development. Simulation of image formation in multi-photon microscopy is powerful for understanding the limitations of such techniques, and understanding novel approaches such as spatiotemporal focusing. Such models usually require specialised knowledge of numerical techniques for solving Maxwell's equations, and for modelling optical systems. The Time Domain Maxwell Solver (TDMS) is a freely available, open source package, aimed at making such simulations accessible to researchers throughout the biomedical optics community. TDMS is based on the finite difference time domain (FDTD) and pseudo spectral time domain (PSTD) methods, and includes functionallity required to model optical systems typically found in OCT and microscopy systems. TDMS includes several simulation examples aimed at making the software more accessible.

Keywords: Optical Coherence Tomography, Simulation, Maxwell's Equations, Numerical Modelling, Optical Microscopy

1. INTRODUCTION

Simulation provides a viable alternative to experiment when particular experiments are unfeasible or perhaps impossible. For example, predicting optical coherence tomography (OCT) image formation, for deterministic refractive index distributions is of great interest. Such a realistic model of image formation, based upon three-dimensional solutions of Maxwell's equations offers a number of tantalising opportunities. For example, investigating image formation for features near or below the resolution of an OCT system, solving inverse scattering problems without assuming the first-order Born approximation and providing gold standard verification of a variety of quantitative techniques are very useful.

Alternative models, including TDMS, have been developed.[1–4] However, to the best of my knowledge, no other models are freely available and most require specialist knowledge. Here I report on TDMS, an open source software package hat aims at making realistic modelling of biomedical optical image formation accessible to researchers in the field, who may have only limited simulation experience. Several examples are provided to help rapidly develop their own simulations.

2. THE MODEL

TDMS can perform simulations in the time and spectral domains, thus allowing both types of OCT system to be modelled. For clarity, here I describe simulation of spectral domain OCT. The image formation model has three primary components: illumination, light propagation in the sample and detection. Below is an explanation through example of how each of component is implemented in TDSM.

The comple amplitude of the illumination uses open source software to compute the Debye-Wolf integral,[5] which means that the illumination satisfies Maxwell's equations. Using this formulation also allows for realistic parameters such as aperture sizes, aberrations, arbitrary polarisation, bespoke optical fiber modes, etc., to be included in the model. The illumination model is thus highly arbitrary and flexible.

Further author information: Send correspondence to p.munro@ucl.ac.uk

Either the FDTD or PSTD method can be used to calculate how light propagates in the sample. The PSTD method is derived from the FDTD method. The FDTD method calculates field spatial derivatives using central differences as $f'(x) \approx \frac{f(x+\Delta x/2)-f(x-\Delta x/2)}{\Delta x}$, whereas the PSTD method uses discrete Fourier-transform based spatial derivatives as: $f'(x) \approx \mathcal{F}^{-1}\left\{ik\mathcal{F}\left\{f(x)\right\}\right\}$, where $\mathcal{F}$ and $\mathcal{F}^{-1}$ are Fourier and inverse fast Fourier transforms, respectively, k is the reciprocal Fourier variable associated with x and i is the imaginary unit. The use of Fourier-based spatial derivatives means that the PSTD method can employ a much coarser spatial sampling, approaching the Nyquist limit of $\lambda/2$. The PSTD and FDTD methods have the advantage of being broadband, meaning that all frequencies of interest can be calculated in a single simulation, significantly reducing the computational burden.

Scattered light detected by an optical fiber is calculated in the sample space as $\alpha_{sc} = \int_{\mathbb{S}} E_s(\mathbf{r}_{sam})E_i(\mathbf{r}_{sam})\mathrm{d}\mathbf{r}_{sam}$, where $\mathbf{r}_{sam}$ is a vector that spans an observation plane $\mathbb{S}$ normal to the optical axis, E_s is the scattered field and E_i is the incident field. A similar calculation where the sample is a mirror gives α_{ref}. The spectrometer current can then be calculated as: $I(k) = S(k)|\alpha_{sc}(k) + \alpha_{ref}(k)|^2$, where S is the source spectrum and k is the wavenumber. The A-scan can then calculated as: $A(z) = \int_0^\infty I(k)\exp(ik2z)\mathrm{d}(1/\lambda)$.

3. EXAMPLE

Figure 1 shows an example of a simulated OCT image, including the sample (Fig 1a)), the free-space incident beam (Fig 1b)), the incident beam scattered by the sample (Fig 1c)), the scattered field, as a function of space an wavenumber (Fig 1d)) and the resulting OCT image (Fig. 1e)).

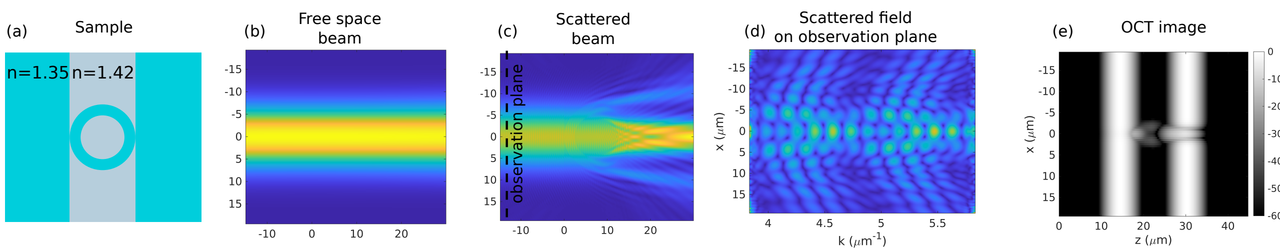

Figure 1. Refractive index of the sample structure (a), the magnitude of the x-component of the incident beam at the central wavelength (b), magnitude of the scattered beam (c), magnitude of the scattered field on an observation plane as a function of k (d) and OCT image (e).

4. CONCLUSIONS

I have outlined the basis for an open source software package which is capable of performing simulations of OCT image formation. The package can be downloaded from https://github.com/UCL/TDMS.

REFERENCES

[1] Brenner, T., Munro, P. R. T., Krüger, B., and Kienle, A., "Two-dimensional simulation of optical coherence tomography images," *Scientific Reports* **9**, 12189 (dec 2019).

[2] Brenner, T., Reitzle, D., and Kienle, A., "Optical coherence tomography images simulated with an analytical solution of Maxwell's equations for cylinder scattering.," *Journal of biomedical optics* **21**, 45001 (apr 2016).

[3] Munro, P. R., Curatolo, A., and Sampson, D. D., "Full wave model of image formation in optical coherence tomography applicable to general samples," *Optics Express* **23**, 2541–2556 (feb 2015).

[4] Munro, P. R. T., "Three-dimensional full wave model of image formation in optical coherence tomography," *Opt. Express* **24**, 27016–27031 (nov 2016).

[5] Munro, P. R. T., "Tool for simulating the focusing of arbitrary vector beams in free-space and stratified media," *Journal of Biomedical Optics* **23**, 1 (sep 2018).