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TDMS: An open source Time Domain Maxwell Solver for simulating optical coherence tomography image formation

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ABSTRACT

Realistic modelling of image formation in optical coherence tomography, which models light propagation in the sample using Maxwell's equations, is useful for applications such as training researchers and clinicians, image interpretation and technique development. Such models, however, require specialised knowledge of numerical techniques for solving Maxwell's equations, and for modelling optical systems. Here I present a freely available, open source package, aimed at making such simulations accessible to researchers throughout the optical coherence tomography community. Time Domain Maxwell Solver (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 systems. TDMS includes several use case examples aimed at making it easy for users with limited background in simulation to use the package.

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

1. INTRODUCTION

There are a growing number of applications where the ability to predict optical coherence tomography (OCT) image formation, based upon 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, shedding light on image formation for features near or below the resolution of an optical coherence tomography system and also on the impact of phenomena usually described as diffraction, interference and scattering, but which, more generally, are the result of light propagation in in-homogeneous media as governed by Maxwell's equations. A realistic model also allows for inverse scattering methods to be developed, which do not assume the first-order Born approximation. Finally, a realistic model can provide gold standard verification of a variety of quantitative techniques currently being developed throughout the field.

A number of such models, including my own, have been reported.[1–4] However, to the best of my knowledge, the code for such models has not been made available and their use requires specialist knowledge. In this abstract I report on an open source software package, Time Domain Maxwell Solver (TDMS) which is aimed at making realistic modelling of OCT image formation accessible to researchers in the field, who may have only limited simulation experience. Several use case examples are provided with the intention of enabling users to rapidly develop their own simulations.

2. THE MODEL

TDMS is capable of performing both spectral and time domain simulations, and so both flavours of OCT system can be modelled. For brevity, here I described only simulation of image formation for a spectral domain system, as schematised in Fig. 1. The image formation model has broadly principle components: illumination, light propagation in the sample and detection. I now outline by example how each of these components is imeplemented in TDSM.

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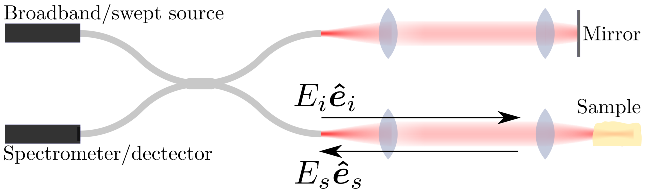

Figure 1. Schematic diagram of an OCT imaging system with incident light $E_i\hat{\boldsymbol{e}}_i$ that exits the fibre, and scattered light $E_s\hat{\boldsymbol{e}}_{\boldsymbol{s}}$ which is incident upon the fibre.

2.1 Illumination

The model uses an open source implementation of the Debye-Wolf integral[5] to calculate the complex amplitude of the field incident upon the sample. This ensures that the calculated field satisfies Maxwell's equations. It also allows for phenomena including finite aperture sizes, aberrations, polarisation control, particular optical fiber mode field diameters, etc., to be modelled. This allows a very broad range of illuminations to be modelled.

2.2 Light propagation in the sample

Light propagation in the sample is calculated using either the FDTD or PSTD methods, depending on the application. Both methods are closely related and differ only by how the spatial derivatives present in Maxwell's equations are discretised. The FDTD method discretises spatial derivatives using central differences, i.e.:

$$f'(x) \approx \frac{f(x+\Delta x/2) - f(x-\Delta x/2)}{\Delta x}. \tag{1}$$

The PSTD method, however, uses Fourier theory to evaluate spatial deriveatives as:

$$f'(x) \approx \mathcal{F}^{-1}\left\{ik\mathcal{F}\left\{f(x)\right\}\right\}, \tag{2}$$

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.

Both methods require material and field quantities to be discretised on a 1, 2, or 3 dimensional grid with sampling period of Δ in each dimension. The FDTD method usually requires $\Delta < \lambda/10$, where λ is the smallest simulated wavelength. However, smaller values of Δ are often required. Since the PSTD method makes use of Fourier theory, spatial sampling can be courser, and approach the Nyquist limit, allowing Δ to approach $\lambda/2$. This allows for much larger sample volumes to be simulated, compared with the FDTD method, when the same number of sample points is employed. This, however, comes at the expense of placing a low limit on the sample feature sizes that can be modelled, which are also limited to Δ.

Both methods simulate in the time domain, yet they allow broadband beams to be modelled in the spectral domain. In particular, broadband simulations can be performed by using a pulsed beam as an input to the simulation. The bandwidth of the pulse often has no physical significance, other than it should have a spectrum encompassing all wavelengths of interest. The pulsed illumination is then introduced to the time domain simulation and a Fourier transform, in time, is performed to extract complex amplitudes at the wavelengths of interest. In some applications, the spectrum of the illumination used in the simulation does have physical significance, and in such cases an illumination with a bespoke spectrum can be modelled.

Detection of scattered light Detection by both free space and fiber based OCT systems can be modelled. Detection by a fiber based system is the most numerically efficient approach, and also most frequently encountered, and so I focus on this method. Considering Fig. 1, the coupling coefficient of the scattered field in the sample arm is given by: $\alpha_{sc} = \int_{fiber} E_s(\mathbf{r}_{det})\phi(\mathbf{r}_{det})\mathrm{d}\mathbf{r}_{det}$, where, for simplicity, we are using a scalar description, ϕ is the mode of the fiber, $\mathbf{r}_{det}$ is a vector on the surface of the fiber and integration is performed over the tip of the fiber. However, in order to reduce computation, this integral is performed in the sample space and becomes: $\alpha_{sc} = \int_{\mathbb{S}} E_s(\mathbf{r}_{sam})E_i(\mathbf{r}_{sam})\mathrm{d}\mathbf{r}_{sam}$, where $\mathbf{r}_{sam}$ is a vector that spans a plane $\mathbb{S}$ normal to the optical axis. A similar calculation (i.e., a separate FDTD/PSTD simulation where the sample is a mirror) can then be performed for reflection by the reference mirror resulting in α_{ref}. This then allows calculation of the spectrometer currents 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 is then calculated as: $A(z) = \int_0^\infty I(k)\exp(ik2z)\mathrm{d}(1/\lambda)$.

3. EXAMPLE

Here I give a simple example to demonstrate the model for the simple sample structure shown in Fig. 2a). An OCT image is obtained by performing several such simulations as is shown in Fig. 2 for different lateral positions of the circle depicted in Fig. 2a), rather than scanning the illumination beam.

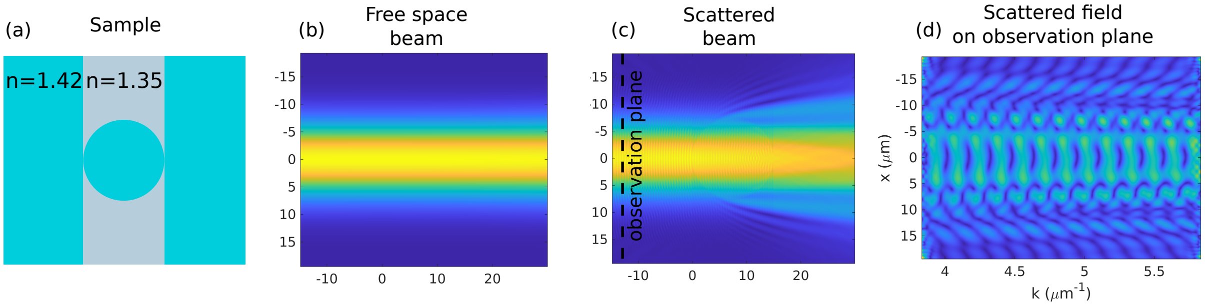

Figure 2. Refractive index of the sample structure (a), the magnitude of the x-component of the incident beam at the central wavelength (b), magnitude of the scattered beam (c) and magnitude of the scattered field on an observation plane as a function of k (d).

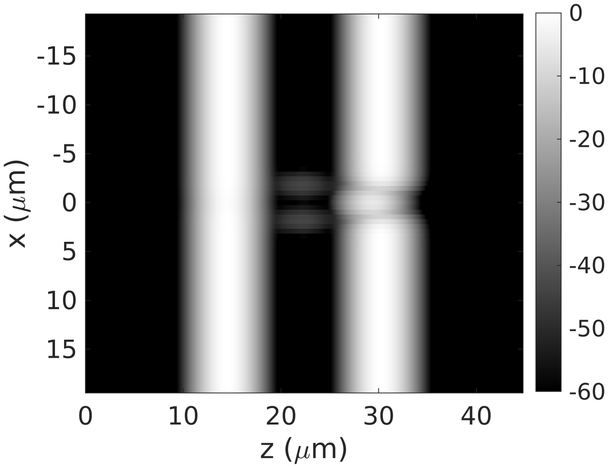

Figure 3. Image of the simulated OCT image on a decibel scale.

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).