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First principle simulation package for arbitrary acousto-optic interaction in scattering materials

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Abstract: We present and validate a simulation package for simulating the signal generated from arbitrary acousto-optical interaction in scattering media. We further present an example on how the package can be used as a virtual lab.

1. Ultrasound Optical tomography

Ultrasound optical tomography (UOT) could enable non-invasive optical absorption imaging deep inside tissue by circumventing the strong scattering of tissue by encoding, or "tagging", spatial information in the frequency of light with ultrasound pulses. But what ultrasound pulse gives the best trade off in tagged signal strength and spatial resolution? What ultrasound pulses should be used at what depths? What are the effects of inhomogeneities in tissue? How should an image be constructed? The design and development questions remaining for UOT are many and the need for an accurate simulation tool is evident if we are to avoid endless experimental trial and error. In this regard, we at Lund University and Spectracure have, based on the work by Huang et al. [1], built a simulation package for the interaction between arbitrary optical and ultrasonic fields in scattering media [2,3]. This model has been further validated with measurements of tagging efficiencies in intralipid phantoms using fully characterized ultrasound pulses [2]. We will describe this work here and we will conclude by giving an example of how this simulation package can be used as a virtual lab to simulate an UOT scan at a fixed depth.

2. Method

Using a hydrophone, we characterized ultrasonic pulses from a commercial ultrasound system (EPIQ-7, Philips Medical Systems, Bothell, WA, USA) of different focal sizes and with two different center frequencies: 1.6 MHz and 3.5 MHz. These pulses were then used in intralipid tissue phantoms ($\mu_s' = 6.4\,\text{cm}^{-1}$, $g = 0.7$ and $\mu_a = 0.008\,\text{cm}^{-1}$) to generate acousto-optic sidebands in 1 µs optical pulses, which in turn were differentiated from the carrier frequency using slow light filters in Pr:YSO ($\lambda = 606\,\text{nm}$) [2]. By measuring the carrier intensity when no ultrasound is present in the phantom, we acquired the reference signal I_{ref}. The first order acousto-optical tagging efficiency is then calculated as $\eta_1 = I_1/I_{\text{ref}}$ where I_1 is the measured first order intensity.

Using the measured acoustic pulses, we fitted an analytical expression for the pressure P and acoustic amplitude $\mathbf{A}$. From this we defined the refractive index in the medium as $\mathfrak{n} = \mathfrak{n}_0[1 + (d\mathfrak{n}/dP) \cdot P]$, $\mathfrak{n}_0$ normal refractive index and $(d\mathfrak{n}/dP)$ is the piezo-optic coefficient. We then performed a first principle simulation of the experiment in the intralipid phantom following the steps outlined in Fig. 1. I_1 and I_{ref} were calculated as the transmission of the obtained $\mathbb{E}(I_{\text{det}})$ through a notch filter with the same width and frequency separation from the carrier as the slow light filter in our experiments. In the case of I_{ref}, it is the transmission through this notch filter centered on the carrier frequency where $\mathbb{E}(I_{\text{det}})$ is calculated using $P = \mathbf{A} = 0$.

We implemented this simulation scheme in an open source code package which can be used to simulate the interaction between arbitrary optical and acoustical fields [3]. The software further allows for seamless transition into simulation of a inhomogenously absorptive medium. By dividing the medium up into V voxels, the absorption can be vectorized as $\mu_a \to \vec{\mu}_a = [\mu_{a,1}, \mu_{a,2}, ..., \mu_{a,V}]$ and similarly the total path distance can be vectorized into distance travelled in every voxel $\mathscr{D}_m \to \vec{\mathscr{D}}_m = [\mathscr{D}_{m,1}, \mathscr{D}_{m,2}, ..., \mathscr{D}_{m,V}]$. The only change this brings to the simulation outlined in Fig. 1 is the replacement of "$\exp(-\mu_a \mathscr{D}_m)$" in step *ix* by "$\exp(-\vec{\mu}_a \cdot \vec{\mathscr{D}}_m)$," which is computationally cheap in comparison to the Monte Carlo path generation in step *i* and the phase calculation in step *viii*.

To demonstrate how this can be used, we investigated a fixed depth UOT scan. We simulated a large medium with $\mu_s' = 5\,\text{cm}^{-1}$, $g = 0.7$. A 1 µs long optical pulse was emitted from a point source on the boundary, coordinates $(x, y, z) = (-1.5, 0, 0)$ cm, and collected by a 1 cm diameter detector at the coordinates $(x, y, z) = (1.5, 0, 0)$ cm. We used a 1.5 mm full width half max, 6 MHz center frequency acoustic pulse propagating along the z-axis. We timed the interaction such the acoustic pulse was located at $x = 0$, $z = 2\,\text{cm}$ and at different y-positions during

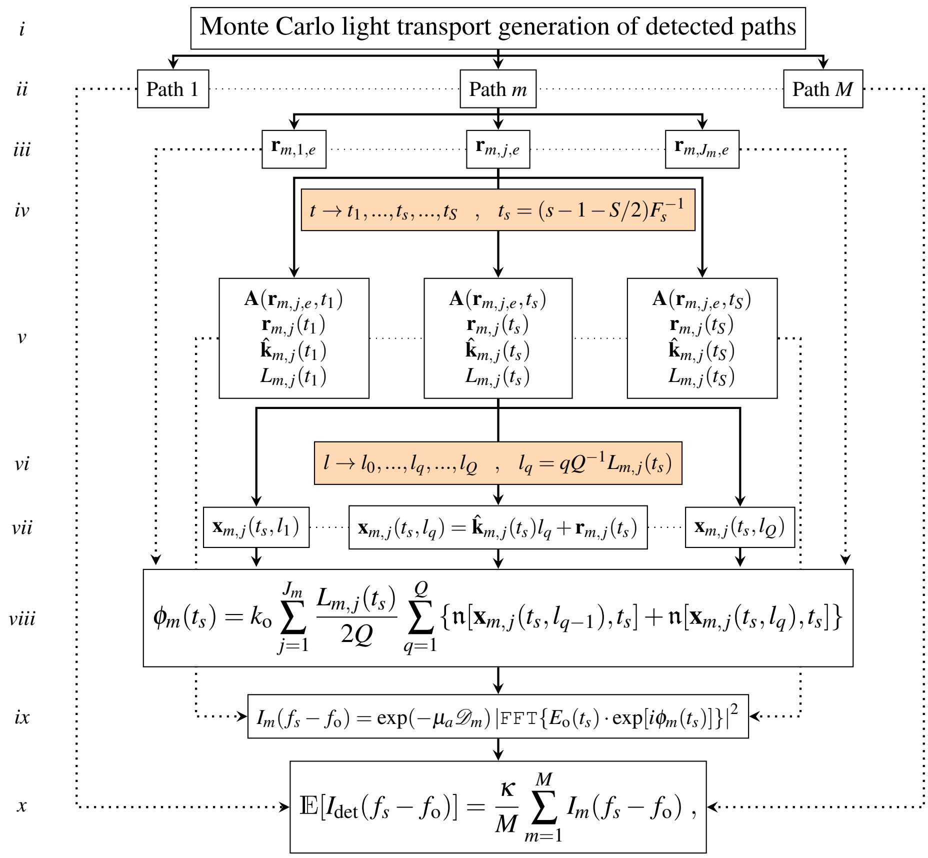

Fig. 1. Simulation outline. We start in step *i* by simulating M paths using the Monte Carlo method for light transport in scattering media [4]. In step *ii* we select one path m, which is broken up into J_m scattering points in step *iii*. In step *iv* time is discretised into S points with a virtual sampling frequency F_s. In step *v*, the movement of each scattering point $\mathbf{r}$ is calculated from the acoustic amplitude $\mathbf{A}$. From the moved scattering positions, the optical wave vector $\hat{\mathbf{k}}$ between successive scattering positions and length L is calculated for each free path length and time step. In step *vi* each these free path lengths L are discretized into Q segments and used in step *vii* to construct $Q+1$ points (denoted $\mathbf{x}$) between scattering points $\mathbf{r}$. In step *viii*, the refractive index $\mathfrak{n}$ is evaluated in all these points. A spatial integral of the refractive index times the optical wave number k_o yields the phase of the individual free paths, and summing for all free paths yields the total phase ϕ for a given time point. This phase is thus an amalgamation of the phase accrued by the change in the refractive index induced by the pressure wave and the change in path lengths due to the movement of the scattering points. In step *ix* the spectrum of path m is calculated as the absolute value squared of the fast Fourier transform of the phase times the optical time envelope E_o. This spectra is weighted with the Beer-Lambert's law absorption experienced by this m-th path with total path distance $\mathscr{D}_m$. The expected spectrum $\mathbb{E}(I_{\text{det}})$ at the detector is then the mean of all M spectra, scaled by some proportionality factor κ.

peak optical intensity. We then ran step *ix* in Fig. 1 multiple times with the previously discussed change in the absorption term $\exp(-\mu_a \mathscr{D}_m)$. We there introduced a 5x5x5 mm^3 voxel centered at $(x,y,z) = (0,0,2)$ cm, which had its absorption changed from 0.2 to 0.6 cm^{-1}. All other voxels had their absorption set to $\mu_a = 0.2\,\text{cm}^{-1}$.

3. Results and Discussion

Using our simulation we are able to accurately predict the power ratio of the first order sideband for all five types of pulses and at different pressure amplitudes, as seen in Fig. 2. We further found, in contrast to the findings of Huang et al. [1], that $\mathbf{A}$ and thus the acoustic movement of scatterers can be neglected without any loss in accuracy. We attribute this difference to $\mathbf{A}$ being calculated as having a uniform envelope shape in Huang et al.'s source code, while we set it to have the same envelope shape as the pressure wave. Neglecting the movement of the scatterers allows a speed up of the simulation as step *v* to *vii* in Fig. 1 only has to be performed once, not every time step.

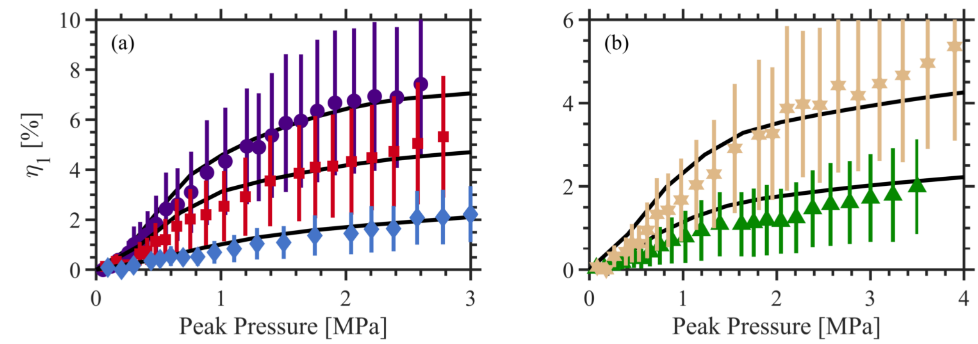

Fig. 2. First order acousto optical efficiency η_1 for (a) differently sized 1.6 MHz ultrasound pulses (purple circle: largest pulse type, blue diamonds: smallest pulse type) and (b) 3.5 MHz ultrasound pulses (green triangle: smallest pulse type). The solid black lines are simulation results and symbols are the mean value of the experiments and the bars the experimental standard deviations.

These results clearly indicate that the model is valid for pulsed optical and acoustic interaction. Following this we hypothesize that it can be used to virtually assess arbitrary optical and ultrasound interactions in scattering media. In line with this hypothesis we examine the example in Section 2, which simulation results can be seen in Fig. 3. The tagged intensity alone in Fig. 3(a) tells little of what has occurred. By normalizing with the homogeneous absorption simulation (i.e. also the voxel centered at $(0,0,2)$ cm has $\mu_a = 0.2\,\text{cm}^{-1}$) as seen in Fig. 3(b), the effects of the variation in fluence along the y-coordinate is cancelled out and it becomes apparent that the scan is sweeping across an inclusion. This example illustrates the usefulness of having a ”virtual lab” to test UOT imaging schemes in. This model also has the benefit of being modular in the generation of detected paths, each path's spectrum and application of absorption to this spectrum. This allows for computationally cheap editing of the absorption in the simulation, which is of special interest for any forward modelling applications.

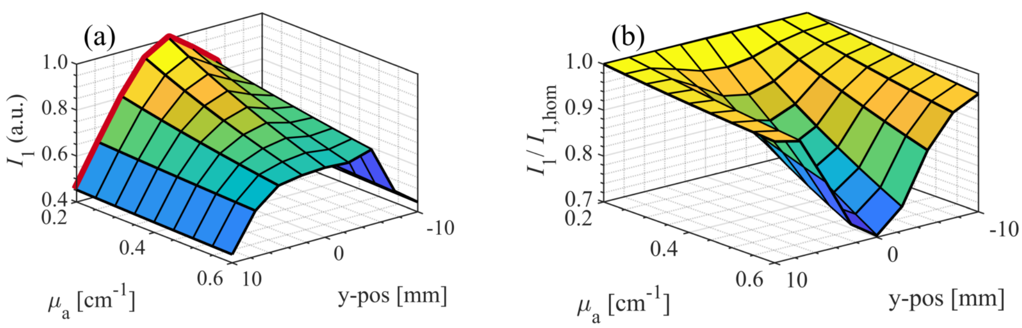

Fig. 3. Signal from the UOT scan example for different inclusion absorptions μ_a and pulse y positions. In (a) the simulated 1st sideband intensity I_1 is depicted, with the homogeneous absorption simulation 1st sideband intensity $I_{1,\mathrm{hom}}$ accentuated in red. (b) is the same as (a) but normalized using the homogeneous absorption sideband intensity.

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