Optimizing deep tissue monitoring with diffuse optics: virtual tools for TD-NIRS and TD-SCOS development

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Abstract: We present an instrument simulator framework for optimizing a simultaneous TD-NIRS and TD-SCOS system featuring a multi-pixel SNSPD. Monte Carlo simulations generate realistic data to improve detector performance and enhance depth sensitivity in both modalities.

1. Introduction

Deep tissue monitoring is a critical challenge in biomedical optics, particularly for non-invasive imaging of physiological parameters such as oxygenation, blood flow, and metabolism. Time-Domain Near-Infrared Spectroscopy (TD-NIRS) and Time-Domain Speckle Contrast Optical Spectroscopy (TD-SCOS) are powerful techniques that leverage diffuse optics to probe brain tissues non-invasively [1,2]. However, optimizing these systems for maximum depth sensitivity and accuracy requires precise control over key instrument parameters, such as source-detector geometry, time-gating strategies, and signal processing methodologies.

In the recent years, Superconducting Nanowire Single-Photon Detector (SNSPDs) have been explored to be introduced in Time-Domain Diffuse Optics (TD-DO) systems [3]. Indeed, these detectors offer an unprecedent detection capabilities in terms of quantum efficiency, time resolution, and low noise levels [4]. Thus, they offer a great possibility of refinement for TD-DO. A particularly interesting development is the emergence of multi-pixel SNSPDs, which introduce imaging capabilities to these detectors [5]. This advancement paves the way for simultaneous measurements of multiple TD-DO modalities, such as TD-SCOS and TD-NIRS.

However, the integration of these two modalities present specific challenges in terms of photon counts, time resolution and noise. Indeed, optimizing a detector able to cope with these two techniques simultaneously will require trade-offs between many parameters, such as the pixel size and filling factor of the detector array, as these factors will influence the overall detection efficiency and speckle imaging capabilities. In order to address these issues, we propose to develop an instrument simulator that would incorporate all the key parameters of the instruments, both from the sources and the detector point of view, together with accurate photon propagation in tissue modelling. Indeed, by integrating Monte Carlo-based photon transport simulations with realistic noise models and system constraints, this framework enables the optimization of real-world instrument parameters to enhance depth sensitivity and quantitative accuracy. In this work, we present the basic framework of this instrument simulator and present an example of its use.

2. Instrument Simulator Framework

The instrument simulator framework (ISF) follows a standard approach where we first simulate light propagation in tissue using a multilayer Monte Carlo (MC) simulation of light diffusion. For each detected photon, the MC simulation provides the essential outputs needed for further analysis: its weight, angular momentum (used for SCOS calculations), and the pathlength in each tissue layer. Note that the MC code is flexible in its implementation, as long as it supplies these key parameters. In this work, we used the code implemented in Wojtkiewicz and Liebert [6]. Firstly, to generate the TD-NIRS data, the information from the photon weight and pathlength of each detected photons are used to generate the probability of detection of photons in each time bin [6]. Then, this probability distribution is scaled in order to generate realistic Distribution of Time Of Flights (DTOF). The scaling is based on the parameters of (i) the source, i.e. the source power, wavelength, and the repetition rate of the laser, (ii) the coupling efficiency of the light between the tissue and the detector, which depends on the detection geometry, typically an optical fibre with parameters: core diameter and Numerical Aperture (NA), and (iii) the detector. The detector is modelled by its Dark Count Rates (DCR), Quantum Efficiency (QE), and detector area. In our case, to simulate a multi-pixel SNSPD, the detector area is function of the pixel matrices which depends on the number of pixels, the size of the pixels, and the Filling Factor (FF). Finally, we set the system Integration Time (IT). Once all these parameters are set, the probability distribution is scaled by multiplying it with each of these factors to produce a realistic ideal DTOF. Once it is done, the simulated ideal DTOF is convolved with the IRF profile to produce the final simulated DTOF profile. The last step is to take into account the Poisson noise inherent to optical detection and the dark noise of the detector. To do so,

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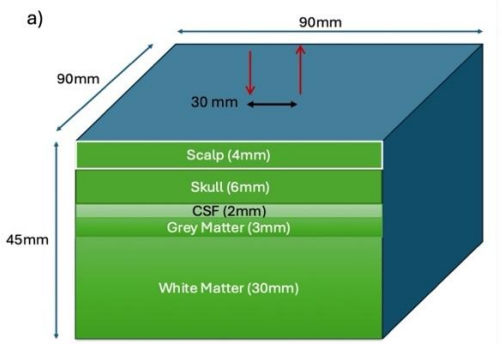
the DTOF and the dark signals are generated from the simulated distributions using a Poisson process. For the SCOS part, we use the pipeline detailed in reference [7], by taking as an input the MC data.

3. Example of generated data

We present below an example of the use of this instrument simulator. We simulated the brain as a slab model, presented in figure 1.a, with typical thicknesses taken from the literature [8]. We used 1e9 photons for the simulation and placed the detector 30mm (5mm diameter) from the source. The simulation was run at 785nm, with the optical properties taken from the literature [9], listed in figure1. b. For the system parameters, we fixed a collection fibre diameter of 500µm, a quantum efficiency of the detector to 74%, the efficiency of one of the systems that we currently use, and an IRF profile with a FWHM of 70ps (also typical from the system). We then varied the other parameters used to test their effects on the signal generated by the ISF.



b)

Structure	$\mu_s'[mm^{-1}]$	$\mu_a[mm^{-1}]$
Scalp	0.85613	0.01333
Skull	0.89146	0.00848
CSF	0.01	0.00213
Grey matter	0.91090	0.01396
White matter	1.03114	0.00989

Figure 1. MC simulation parameters. a) Geometry of the simulation. b) Table of the optical properties used (at 785nm).

An example of the effect of various parameters can be seen on figure2.a where we report simulated DTOFs with an IT of 1s and a power of 100mW. We can see the effect of the low DCR of 5cps (typical of our instrument), on the noise of the signal, especially at long arrival time of photons. The big effect of the NA and FF on the photon counts can also be seen. Figure 2.b reports an example of a SCOS image generated with the simulator for a gated signal between 2.2 and 3.2 ns. Here, a matrix of 100 x 100 pixels of pixel size was simulated. We assumed an imaging system which allowed approximate 1:1 imaging of the speckles and therefore fixed the pixel size to equal 1µm.

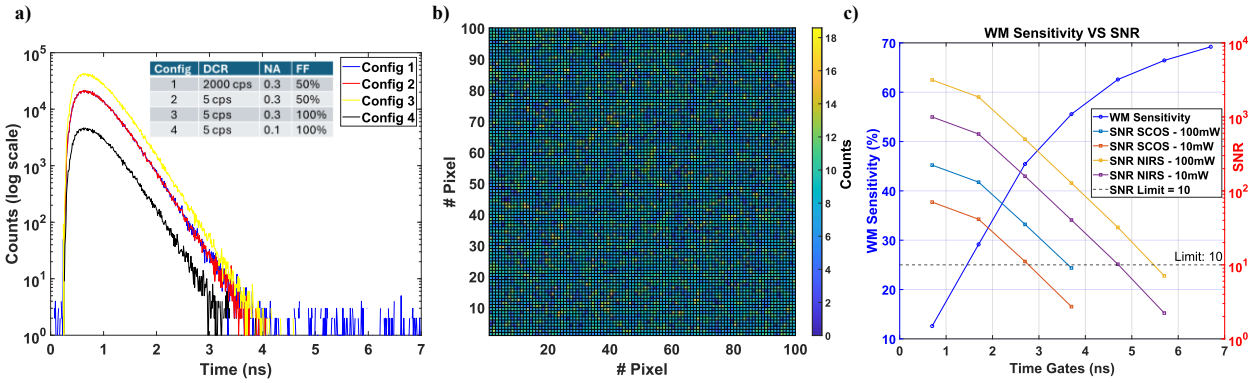


Figure 2. Example of simulated Data. a) The effect of various detector configurations (DCR/NA/FF) on the simulated DTOFs with laser power fixed at 100mW. b) SCOS image generated from a simulation with configuration 2 (see Fig2(a) table), for a time gate between 2.2 and 3.2 ns. The IT was 5 ms, the coherence factor Beta was fixed to 0.5, and a diffusion coefficient db = 1e-8 cm^2/s. Here a matrix of 100x100 pixel is presented, with a pixel size equivalent to the speckle size of 1µm. c) White Matter (WM) sensitivity versus SNR of the signal as function of time gates (1ns width) for two source power (10 and 100mW) for the TD-SCOS (IT: 5ms) and TD-NIRS (IT:1s). The other parameters used for this dataset are the ones of configuration 2.

Finally, figure 2.c reports the effect of the laser power on the detected signal at different gates (with a width of 1ns) for the TD-SCOS and TD-NIRS at 2 different power (10 and 100mW). Here we distinguish the TD-SCOS and TD-NIRS by the IT used by each technique. Indeed, the SCOS technique is limited to a few ms of IT, whereas the TD-NIRS use typically an IT of 1s. By fixing all the other parameters, we can observe the effect of the laser power for the two techniques, and get an idea of the SNR achievable for all time gates. This is especially usefull in order to assess the depth sensitivity of the measurment. Indeed, by using the pathlength information recorded by the MC

simulation, we can estimate the sensitivity of the deep tissue of each time gate (taken as White Matter (WM) sensitivity = 100 % * Pathlength WM / Total Pathlenght). We can see that for the TD-NIRS, gate 4 which has a WM sensitivity >50% is able to achieve an SNR>100, with a 100mW laser, which would be useable for actual measurments. It is worth noting that the spot size of the source would have to be expendend to comply with safety requirement at that power. In the same conditions, the TD-SCOS suffers from its lower IT which shift the gate used to achieve comparable SNR for a single frame to earlier photons, decreasing the WM sensitivity. However, these simulations provide a plateform to help the development of analysis methods to enhance the measured SNR in SCOS, such as frame averaging to improve signal quality.

4. Conclusions and perspectives

We have introduced a virtual instrument simulator for optimizing TD-NIRS and TD-SCOS systems, enabling systematic evaluation and refinement of key parameters. By leveraging Monte Carlo simulations, this approach provides valuable insights into depth sensitivity and signal quality. Here we have shown examples of the data generated by this simulator, and how we can use the results of the MC simulation to get information about the depth sensitivity of the signals. Future work will focus on experimental validation, where the insights gained from simulations will be applied to refine real system prototypes, ensuring their practical feasibility. Indeed, the specific requirements of TD-NIRS and TD-SCOS in terms of SNR and image resolution impose trade-offs in chip design, particularly regarding pixel size and arrangement. Thus, this simulator enables to test various configurations in silico in order to optimize the chip design before production. Concurrently, this simulator will be used to optimize system acquisition parameters like time gate positioning and width, in order to maximise the depth sensitivity of our measurements. Additionally, advanced tissue models will be incorporated to simulate dynamic physiological changes, improving the accuracy of predictions in realistic scenarios. By combining virtual modelling with experimental validation, this approach will drive the development of next-generation deep tissue monitoring systems, improving the accuracy and applicability of TD-NIRS and TD-SCOS in biomedical research and clinical practice.

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