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Modeling Nonlinear Transformations Which Reduce The Approximation Error Between Photon Transport Models in Diffuse Optical Tomography

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ABSTRACT

Diffuse Optical Tomography (DOT) is an emerging medical imaging technique. This method of imaging has incredible potential for global impact on access to healthcare due to low cost compared to other imaging modalities (X-Ray, CT, etc.). DOT is safer than the aforementioned modalities, and utilizes near-infrared light (NIRS), which is not harmful for humans. DOT is currently impractical because it produces scans that are not accurate enough for medical diagnoses. One point of inaccuracy is that NIRS is highly scattering while propagating through biomedical tissue (photons take a random variety of paths), so it is extremely difficult to find a model of this propagation that can support accurate image reconstruction. This project compares the Monte Carlo Model and Diffusion Equation Model of photon transport. The Monte Carlo Model (MCM) is well known to be extremely accurate, however is too computationally intensive to put into practice. The Diffusion Equation Model is a partial differential equation approximation of the MCM, so it is less accurate, however more efficient. By using the ValoMC software to simulate the MCM and the Toast++ software to simulate the Diffusion Equation Model, both with a variety of parameters, a pattern of approximation error in solutions of photon fluence can be found and modeled. The main objective is to use these models of approximation error to transform Toast++'s raw solutions to be more similar to the ValoMC solutions, and therefore more accurate.

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1 Introduction

Currently, almost half of the world's population faces difficulty finding and receiving essential healthcare services. This disparity affects billions, especially in third world countries and poverty-stricken areas. A huge contribution to why it is so difficult for people to obtain health services is the cost [1]. Lowering the cost of healthcare proves to be an extremely difficult task, but one aspect involves biomedical imaging. Most are familiar with X-ray, computerized tomography (CT), and magnetic resonance imaging (MRI) since they are extremely common methods of imaging worldwide. While these devices are very accurate in their imaging and save lives every day, they lack safety and accessibility. It is very expensive to buy, install, and run these machines in a hospital; therefore, it is very expensive for a patient to receive these scans,

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especially MRI scans. Doctors need certain information from scans to create diagnoses and treatment plans for their patients, but if a patient cannot afford this technology, they are left with little hope for a proper diagnosis [2]. Along with the cost, another downfall of specifically X-ray and CT scanning is that they are radiation-based. These electromagnetic waves can be very harmful towards people, and increase the risk of cancer in the future [3]. In order to eventually replace these machines, researchers have been exploring diffuse optical tomography (DOT), which utilizes Near-Infrared Spectroscopy, or NIRS (See Fig. 1).

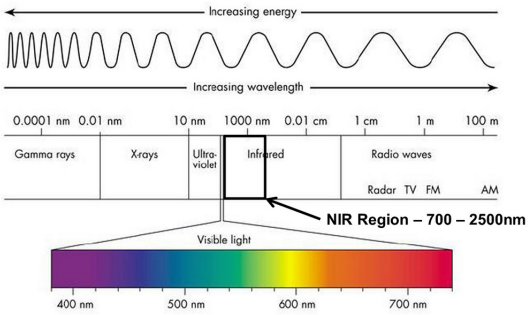


Figure 1.1: NIRS on the electromagnetic spectrum [4].

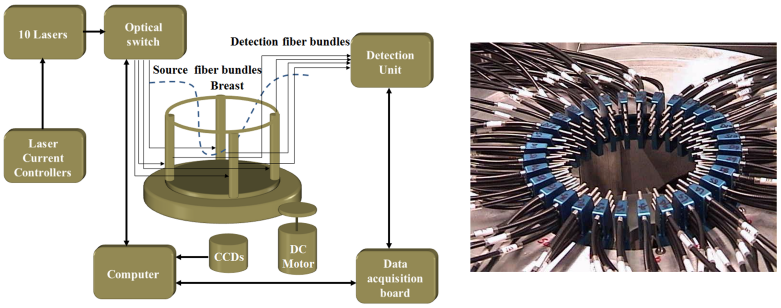


Figure 1.2: (a) Diagram of DOT (b) Image of breast/fiber optic array [6].

DOT is much cheaper than the aforementioned imaging modalities and poses little to no risk to the patient [5]. See Figure 2 for a typical setup of the breast/fiber optic array in a Diffuse Optical Tomography System. The main problem with these DOT techniques is that scans are not very clear or accurate. Doctors would have difficulty making conclusions based on the scans produced by this method. This is why many researchers have been working to improve the quality of the image reconstruction in these scans. One important factor in the quality of image reconstruction is the accuracy of models of photon transport throughout the body. This research aims to improve the accuracy of existing photon transport models. In the literature for modeling photon transport, researchers use various models including Diffusion Equation and Monte Carlo [8,10,13,15], however heuristic model to correct for the error between any two particular methods is missing because most papers introduce a new model and demonstrates their efficacy and limiations. In this work, we focus on nonlinear transformation because the difference between the solution using Diffusion Model and Monte Carlo model is expected to be a nonlinear function since Diffusion Model is a simpler approximation of the photon transport model such as Monte Carlo Method which is highly nonlinear. Based on our simulations, the error between the models is approximated using a function at each point on the domain and they don't follow a linear behavior.

2 Modeling Methodology

In this paper, we utilize simulation models of the Monte Carlo Model and Diffusion Equation Models of photon transport to study approximation error. By simulating these models with various parameters, models for the approximation error between each model can be developed. The long-term goal of this field of research is to contribute to better resolution

in DOT, which can make a huge positive impact on the world. In the literature, researchers use various methods to simulate photon transport including Diffusion Equation and Monte Carlo [8, 9, 10, 13, 15], however heuristic methods to correct for the error between any two particular models are not investigated since most papers introduces new model(s) and describes their efficacy and limitations. This paper aims to find a nonlinear transformation that can reduce the approximation error between the Diffusion Equation and the Monte Carlo Simulation for Photon Transport.

2.1 Photon Transport Models

Model One The Monte Carlo Method (MC) is a stochastic method where one simulates many paths for a photon and then averages those paths to determine the most likely path. This approach is too extremely computationally intensive and inefficient for real-world health emergencies [7]. Each layer of the biological tissue has given optical properties. These include mainly refractive index, an absorption coefficient, and a scattering coefficient, which depend on the density and type of tissue such as fat, muscles, or fluid. The optical properties vary based on these factors, as well as the tissue's interaction with photons. For example, an absorption coefficient is the probability of a photon being absorbed after a certain length of travel, and a scattering coefficient is the probability of a photon being scattered at a particular angle after a certain length of travel [8]. We use the ValoMC software to simulate photon transport using the Monte Carlo algorithm [9,10]. The software uses the following logical expressions to create a path for a photon launched at the source. Then many paths are simulated using Monte Carlo simulations to provide an average path which represents the photon density for a given point in a given direction (See Fig.3). Throughout this study, Model One's simulation results are used as truth and control data (Note that this project will consider the simplistic case where refractive index is constant and only absorption and scattering vary).

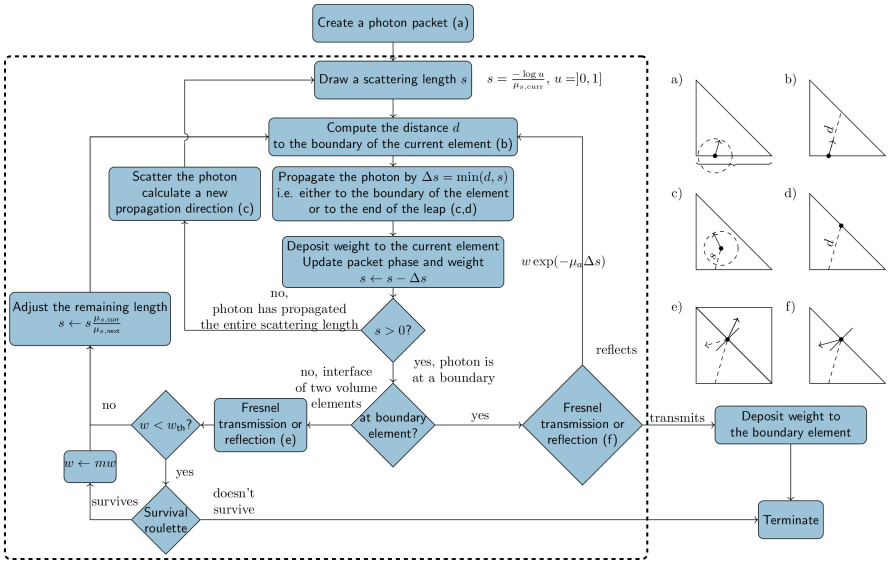


Figure 2.1: MCM algorithm in the ValoMC software [10].

Model Two The Diffusion Equation (DE) model is a partial differential equation whose solution yields the approximate photon density at any point in the domain (does not provide the direction of photon density). This is essentially the model for heat diffusion, but the photon transport takes the role of the heat diffusing through the body [11]. The DE is an approximation of the MC, so we will study the approximation error between DE solutions and MC solutions. Model Two is simulated with the Toast++ Software, which utilizes the following equations [12, 13]:

$$-\nabla \cdot \kappa(r)\nabla\phi(r,\omega) + \left[\mu_a(r) + \frac{i\omega}{c}\right]\phi(r,\omega) \quad = \quad 0, r \in \Omega \tag{2.1}$$

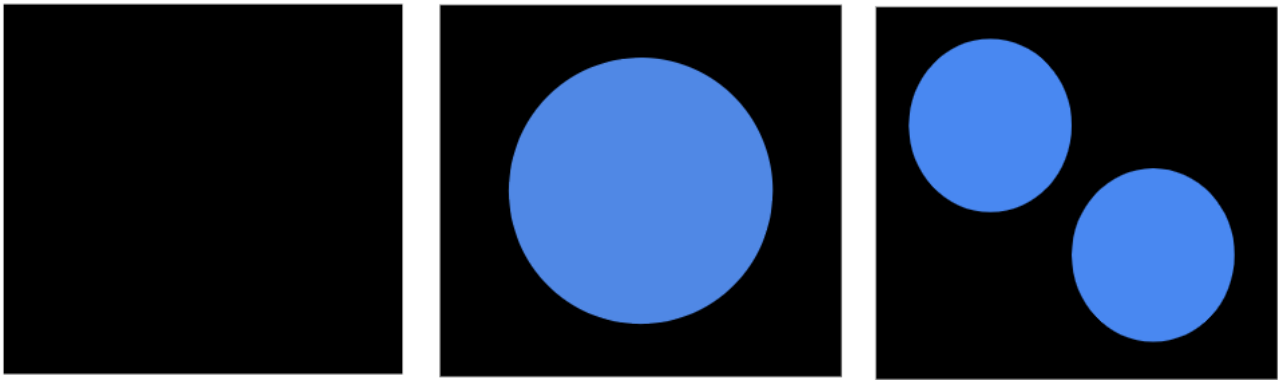
with the boundary condition

$$\phi(m,\omega) + 2\zeta(c)\kappa(m)\frac{\partial\phi(m,\omega)}{\partial\nu} \quad = \quad q(m,\omega), m \in \partial\Omega \tag{2.2}$$

where κ is the diffusion coefficient which is $[3(\mu_a + \mu_s)]^{-1}$, μ_s is the scattering coefficient, μ_a is the absorption coefficient, ϕ is the photon fluence, q is the light source, m is a point on the boundary of the domain, ω is the modulation frequency, and r is a point in the domain [13].

2.2 Simulation Setup

For each software and error approximation, we have run three simulations: background with no inhomogeneity, one disk inhomogeneity, and two disk inhomogeneities (See Fig. 4).



(a) Simulation 1 (b) Simulation 2 (c) Simulation 3

Figure 2.2: A sketch of the simulation setup; black areas have an absorption coefficient of 0.05 and a scattering coefficient 1.5, while blue areas have an absorption coefficient of 0.1 and a scattering coefficient of 0.75 (to represent a tumor in the body).

2.3 Error Model Formulation

We began our error model formulation by running three simulations with different background setups (See Fig. 4) using both ValoMC and Toast++. After performing each simulation, the Toast++ approximation error was calculated by subtracting the Toast++ solutions from the ValoMC Solutions.

Symbol	Description
x	Element number
$T(x)$	Toast++ solution for photon fluence at element x
$V(x)$	ValoMC solution for photon fluence at element x
$E(x)$	Approximation error of Toast++ at element x
$F(x)$	Eight-coefficient Fourier model of $E(x)$
$C(x)$	Cubic spline model of $E(x)$

Table 2.1: Notation utilized throughout study.

Using the notation provided in Table 1, the approximation error is denoted by the following equation:

$$E(x) = V(x) - T(x). \tag{2.3}$$

Then, $E(x)$ is fitted using an eight-term Fourier series, $F(x)$, which when applied to Toast++ solutions $T(x)$, yields:

$$T_F(x) = T(x) + F(x). \tag{2.4}$$

Similarly, $E(x)$ is fitted using a cubic spline piecewise polynomial, $C(x)$, which when applied to Toast++ solutions $T(x)$, yields:

$$T_C(x) = T(x) + C(x). \tag{2.5}$$

Therefore, if our fitted approximation with Fourier series approximation is effective then we expect $E_F(x) = V(x) - T_F(x)$ to be significantly smaller than $E(x)$ and similarly if cubic spline approximation is effective then we expect $E_C(x) = V(x) - T_C(x)$ to be significantly smaller than $E(x)$. For the purposes of this study, we use the Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{N}\sum_{x}(V(x) - \hat{T}(x))^2} \tag{2.6}$$

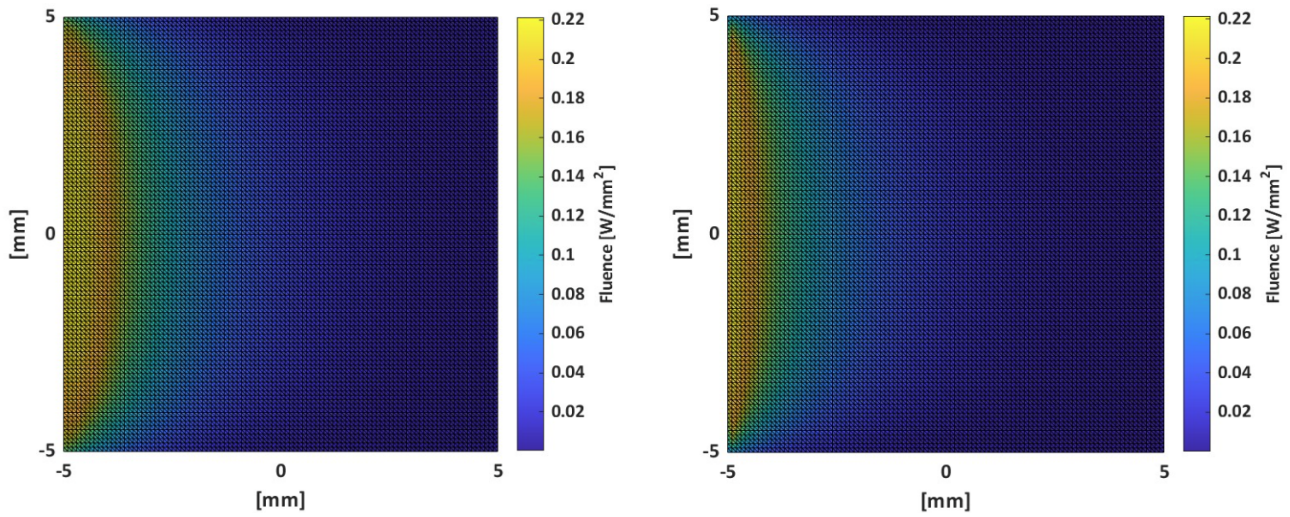
where N represents the total number of elements, as a measure to compare the performance of each approximation error model.

3 Results

For each simulation, the absorption coefficient = 0.05, scattering coefficient = 1.5, refractive index = 1.3, and scattering anisotropy = 0.0. Each was performed on a triangular mesh with 20,000 Elements (Triangles) and 10,201 Nodes (Vertices). A direct light source was used in the ValoMC simulation, which is equivalent to the isotropic point light source used in Toast++.

3.1 Simulation One

In this simulation, we used a homogeneous background (constant scattering and absorption coefficient across the mesh) was used utilized (See Fig. 4). Results are shown below in Figures 5 and 6.



(a) ValoMC Results

(b) Toast++ Results

Figure 3.1: Comparison of the MC and DE results for Simulation One.

The RMSE for the Simulation One Fourier Model was 0.0029, while the RMSE for the Simulation One Cubic Spline Model was 4.9083e-20. The average approximation error with no transformation was 0.0112, with a Fourier transformation was 6.6350e-18, and with a Cubic Spline transformation was 3.5779e-22.

3.2 Simulation Two

In this simulation, we used an inhomogeneous background consisting of a centered disk area (radius = 2.5) in which the absorption coefficient = 0.1 and the scattering coefficient = 0.75 to represent the characteristics of a tumor (See Fig. 4). Results are shown below in Figures 7 and 8.

The RMSE for the Simulation Two Fourier Model was 0.0033, while the RMSE for the Simulation Two Cubic Spline Model was 1.9260e-21. The average approximation error with no transformation was 0.0103, with a Fourier transformation was 1.5296e-17, and with a Cubic Spline transformation was 2.4666e-22.

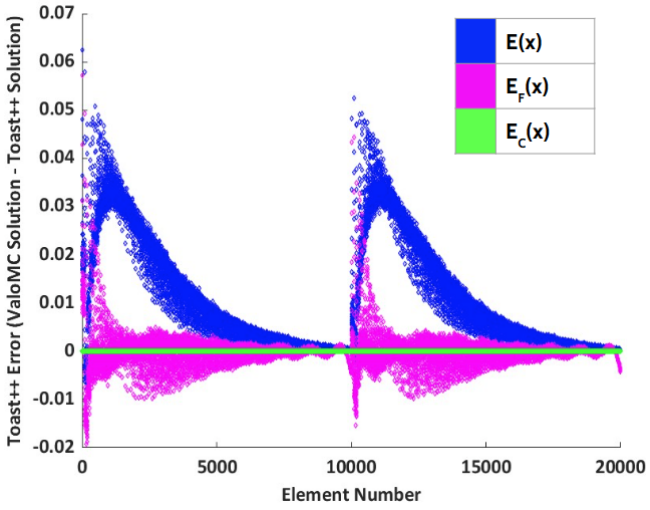
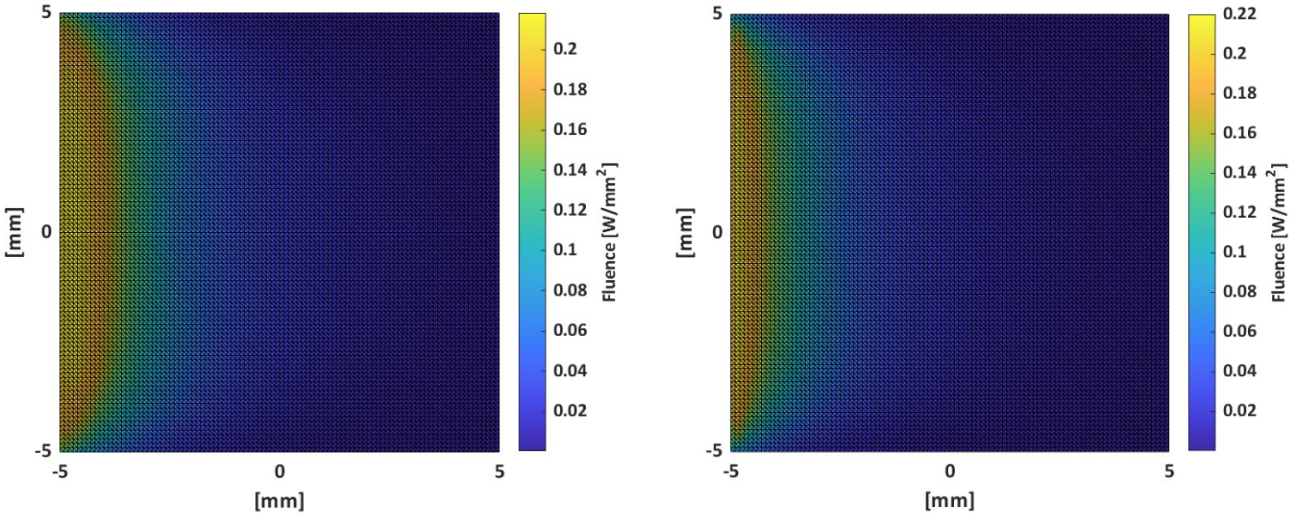


Figure 3.2: Plot of the different approximation error models for Simulation One.



(a) ValoMC Results

(b) Toast++ Results

Figure 3.3: Comparison of the MC and DE results for Simulation Two.

3.3 Simulation Three

In this simulation, we used an inhomogeneous background consisting two disks on the mesh (radius = 2.5) in which the absorption coefficient = 0.1 and the scattering coefficient = 0.75 to represent the characteristics of two tumors (See Fig. 4). Results are shown below in Figures 9 and 10.
The RMSE for the Simulation One Fourier Model was 0.0027, while the RMSE for the Simulation One Cubic Spline Model was 2.7522e-20. The average approximation error with no transformation was 0.0096, with a Fourier transformation was 8.6861e-18, and with a Cubic Spline transformation was 1.3553e-24.

4 Conclusions

Based on the results, the approximation error between Toast++, or the Diffusion Equation, and ValoMC, or the Monte Carlo Simulation, is greatly reduced with the use of a transformation in the form of a model of approximation error. The mean and the variance of the approximation error with no transformation got lower as more inhomogeneity was introduced to the background of the simulation, which was expected since the Diffusion Equation is known to be more accurate in

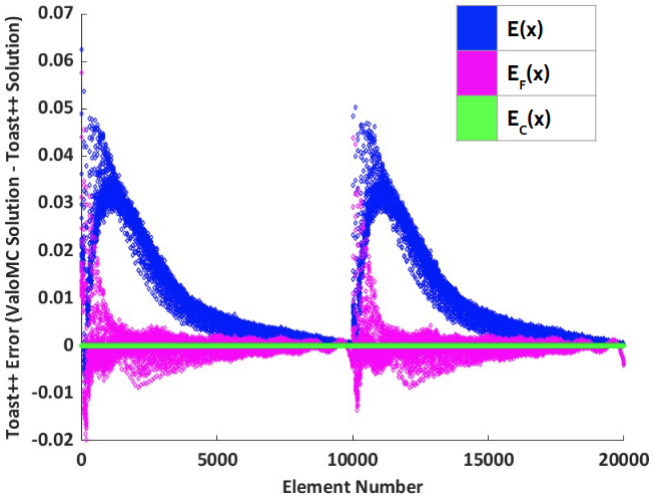
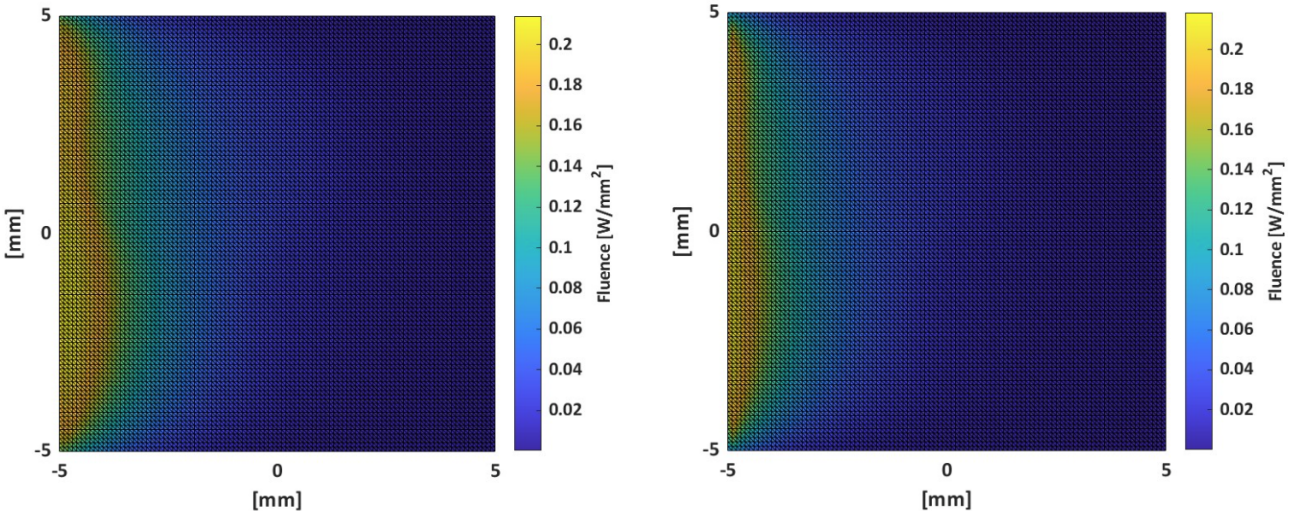


Figure 3.4: Plot of the approximation error between ValoMC and Toast++ for Simulation Two.



(a) ValoMC Results

(b) Toast++ Results

Figure 3.5: Comparison of the MC and DE results for Simulation Three.

highly scattering media. Another finding was that the Cubic Spline Model has a better model fit than the Fourier Model, which was demonstrated in the Cubic Spline's consistently lower root mean squared error. Though, the Cubic Spline Model has over 15,000 pieces (it is a piecewise function), so is less efficient than the Fourier Model, which only has eight coefficients. The main limitation of the proposed method is that for each of the setup for the inhomogeneity, the error correction will need to be updated as the error depends on the geometry of the inhomogeneity. However, given the power of machine learning, one can learn each of these nonlinear functions and use them to predict for any new geometry which is something, we plan to investigate in the future.

In future research, we will focus on modeling the approximation error with machine/deep learning to create a transformation that can almost completely mitigate approximation error, and is much less computationally intensive than a Cubic Spline transformation. This concept can greatly benefit Diffuse Optical Tomography research, since accurate models of photon transport are imperative to the accuracy of image reconstruction. Accuracy in image reconstruction means that DOT can be developed for use in the real world, allowing it to bring the incredible positive impacts on access to healthcare around the world that it offers.

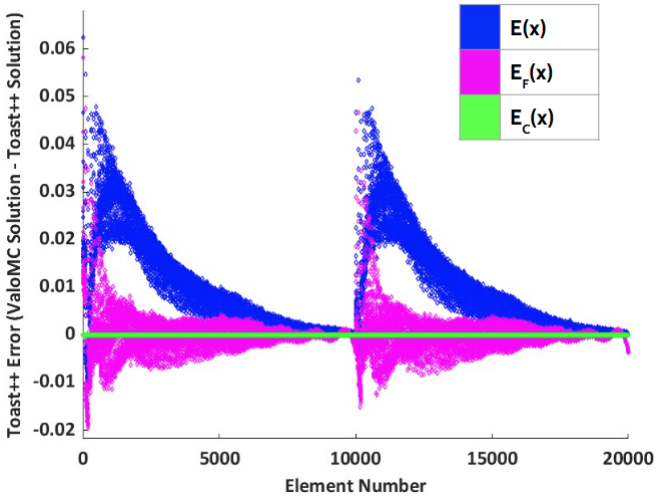


Figure 3.6: Plot of the approximation error between ValoMC and Toast++ for Simulation Three

Conflict of Interests

The author declares the absence of any conflicts of interest.

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References

[1] WHO. (2017, December 13). World Bank and WHO: Half the world lacks access to essential health services, 100 million still pushed into extreme poverty because of health expenses. World Health Organization. Retrieved January 11, 2023, from https://www.who.int/news/item/13-12-2017-world-bank-and-who-half-the-world-lacks-access-to-essential-health-services-100-million-still-pushed-into-extreme-poverty-because-of-health-expenses

[2] Graziani, F. R. (2005, January 14). Radiation Diffusion: An Overview of Physical and Numerical Concepts (Conference) — OSTI.GOV. Retrieved January 11, 2023, from https://www.osti.gov/servlets/purl/917504

[3] Watson, K. (2019, December 19). Does Medicare cover MRI scans? Healthline. Retrieved January 11, 2023, from https://www.healthline.com/health/medicare/does-medicare-cover-mri-scans

[4] Lin, E. C. (2010). Radiation risk from medical imaging. Mayo Clinic proceedings. Retrieved January 11, 2023, from https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2996147/

[5] KPM. (n.d.). Near infrared measurements – how do they work? KPM Analytics. Retrieved January 8, 2023, from https://www.kpmanalytics.com/articles-insights/near-infrared-measurements-how-do-they-work

[6] Hielscher, A. H., Bluestone, A. Y., Abdoulaev, G. S., Klose, A. D., Lasker, J., Stewart, M., Netz, U., & Beuthan, J. (2002). Near-infrared diffuse optical tomography. Disease markers, 18(5-6), 313–337.https://doi.org/10.1155/2002/164252

[7] Hajihashemi, M. R., Grobmyer, S. R., Al-Quran, S. Z., & Jiang, H. (2012). Noninvasive evaluation of nuclear morphometry in breast lesions using multispectral diffuse optical tomography. PLoS ONE, 7(9). https://doi.org/10.1371/journal.pone.0045714

[8] Wang, L., Jacques, S. L., & Zheng, L. (1995). MCML—Monte Carlo Modeling of light transport in multi-layered tissues. Computer Methods and Programs in Biomedicine, 47(2), 131–146. https://doi.org/10.1016/0169-2607(95)01640-f

[9] Wang, L., & Jacques, S. L. (1992). Monte Carlo Modeling of light transport in multi-layered tissues in Standard C. University of Texas M. D. Anderson Cancer Center. Retrieved January 11, 2023, from https://omlc.org/software/mc/mcml/MCman.pdf

[10] Leino, A. A., Pulkkinen, A.,& Tarvainen, T. (2017). ValoMC (2017a) [Computer software]. https://inverselight.github.io/ValoMC/

[11] Leino, A. A., Pulkkinen, A., & Tarvainen, T. (2019). VALOMC: A Monte Carlo Software and MATLAB toolbox for simulating light transport in biological tissue. OSA Continuum, 2(3), 957. https://doi.org/10.1364/osac.2.000957

[12] Graziani, F. R. (2005, January 14). Radiation Diffusion: An Overview of Physical and Numerical Concepts (Conference) — OSTI.GOV. Retrieved January 11, 2023, from https://www.osti.gov/servlets/purl/917504

[13] Schweiger, M., & Arridge, S. (2016) Toast++ (2.0.2) [Computer software]. http://web4.cs.ucl.ac.uk/research/vis/toast/download_src.html

[14] Schweiger, M., & Arridge, S. (2014). The toast++ software suite for forward and inverse modeling in optical tomography. Journal of Biomedical Optics, 19(4), 040801. https://doi.org/10.1117/1.jbo.19.4.040801

[15] Jiang, H. (2010) Diffuse Optical Tomography: Principles and Applications, https://doi.org/10.1201/b10482