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Leveraging LU-Decomposition for Accelerated Tissue Chromophore Quantification in Diffuse Optical Imaging

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Abstract **-** Accurate and fast quantification of the concentration of the main chromophores in tissue is crucial for cancer characterization. Previously, Photo-Magnetic Imaging (PMI) technique has been proposed to undergo this task with high resolution and quantitative accuracy. The standard iterative PMI method for chromophore quantification, while effective, can be computationally intensive, especially when dealing with large and complex geometries. In this paper, a non-iterative method is introduced for the fast and accurate determination of chromophore concentrations. By using linear algebraic methodology, particularly LU decomposition, the computational time is significantly reduced without degrading the accuracy of PMI. This new approach is evaluated on a numerical phantom with a tumor-like inclusion containing a mixture of two different dyes mimicking tissue chromophores. By using only two laser wavelengths, the chromophores concentrations were accurately resolved with an error as low as 7% using both methods. Nevertheless, the computational time was reduced 140-fold using the new approach. This accelerated method has the potential to revolutionize real-time monitoring and diagnostics, enabling faster analysis of tumor characteristics, treatment planning and response.

Keywords**:** Photo-Magnetic imaging, Near-infrared lasers, Diffuse optical imaging, Spectroscopy, Biomedical imaging, Computer simulation

1. Introduction

Diffuse optical imaging is a non-invasive technique that is beneficial for cancer detection and characterization. Tumor tissue exhibits distinct optical properties due to the changes in its composition compared to healthy tissue. By employing multiple wavelengths, optical imaging provides accurate quantification of the tumor composition which consequently provides valuable insights into tumor vascularization and metabolic activity, aiding in early detection, accurate diagnosis, and effective treatment planning [1-3].

Photo-Magnetic Imaging (PMI) is designed to recover chromophore concentrations by illuminating the imaged medium with near-infrared laser to slightly raise the temperature. This temperature change is measured using Magnetic Resonance Thermometry (MRT), and then can accurately converted into optical absorption distributions, using PMI dedicated algorithm [4, 5]. Recovering the absorption distribution at multiple wavelengths allows calculating the chromophore concentrations. Different approaches can be used to obtain the concentration values. In the standard implementation of PMI, iterative methods based on linear least squares minimization are employed to solve the system of equations that arise from the absorption measurements [6]. These methods are flexible and can be applied to a broad range of problems, including overdetermined systems. Additionally, boundary constrains such as the non-negativity or upper limits restrictions can be imposed. While effective, these iterative methods can become computationally expensive, especially because the concentration distribution varies spatially, and needs to be calculated at each point within the medium. Therefore, alternative approaches can be considered to reduce computational time without compromising the accuracy. For example, LU decomposition-based method reduces the calculation time since it eliminates the need for iterative convergence tests. This method is based on decomposing the coefficient matrix into two matrices, lower and upper triangular matrices. This transformation simplifies solving systems of linear equations using forward and backward substitution [7, 8]. This significantly improves the processing performance while the accuracy of chromophore concentration recovery is maintained. In this study, a numerical phantom with one inclusion filled with a mixture of two chromophores is used to evaluate the proposed method. Two laser wavelengths, chosen across the isosbestic point and each corresponding to the peak absorption

wavelength of the respective chromophore, were used to slightly heat the phantom and consequently obtain the absorption distribution at each wavelength. The obtained absorption data are then utilized to construct the system of equations that describes the relation of the recovered absorption coefficient with the chromophore concentrations. The system of equations is then solved using both the standard iterative PMI approach and the proposed non-iterative one to compare their computational time and accuracy. The results show that the iterative method required an average of 7.93 seconds to converge to a solution, whereas the non-iterative method, using LU decomposition, reduced the computational time to just 0.05 seconds.

2. Material and Method

2.1. PMI concentration recovery algorithm

The PMI image recovery algorithm is a multi-step process. First, synthetic heat maps (T) are generated at various wavelengths using the PMI forward problem which uses the finite element method (FEM) to simulate light propagation $\Phi(r)$ and heat transfer $T(r,t)$ within the tissue, using the following equation [9]:

$$\rho c \frac{\partial T(r,t)}{\partial t} - \nabla \left[k \nabla T(r,t) \right] = \mu_a \Phi(r) \tag{1}$$

where ρ, c and k are the thermal properties of the imaged medium. On the other hand, the inverse problem seeks to recover the unknown absorption distribution μ_a from these temperature maps. This is achieved by minimizing the difference between the measured and predicted heat distributions using the Levenberg–Marquardt optimization technique [6]. Once the absorption coefficient is recovered, the concentration distribution (C) is then determined by applying the modified Beer-Lambert Law, as follows:

$$\boldsymbol{\mu_{a_{[\Lambda \times N]}} = \varepsilon_{[\Lambda \times P]} C_{[P \times N]}} \tag{2}$$

where μ_a represents the vector of total recovered absorptions at each wavelength, ε is the wavelength-dependent extinction coefficient, and C represents the unknown chromophore concentration. While Λ, P and N represent the number of the utilized wavelengths, chromophores, and FEM mesh nodes, respectively. The PMI standard method applies an iterative minimization method to recover the concentration C at each node of the FEM mesh using Equation 2. This technique has been extensively validated, demonstrating its ability to achieve high resolution and quantitative accuracy.

In this study, a non-iterative approach based on linear algebraic techniques, specifically LU decomposition, was employed to solve the system of equations obtained from the absorption measurements at multiple wavelengths.

By performing LU decomposition, the extinction coefficient ε matrix is decomposed into lower (L) and upper (U) triangular matrices. Therefore, Equation 2 can be written as:

$$\boldsymbol{\mu_{a_{tot}} = LUC} \tag{3}$$

The concentration is calculated by solving two successive triangular systems. First, the lower triangular system which can be solved by forward substitution $\boldsymbol{\mu_{a_{tot}} = Ly}$. Then, the result is used in the upper triangular system $\mathbf{y} = \boldsymbol{UC}$, which is solved using the backward substitution to obtain the unknown concentration [8]. By solving the system using these matrices, the concentration values of each chromophore can be efficiently recovered non-iteratively. This method is applicable to any square matrix system, where the number of lasers Λ equals the number of chromophores P to be determined.

2.2. Simulation study

A cylindrical numerical phantom with a diameter of 25 mm was used in this study, containing a single 4 mm inclusion at its center to mimic a tumor. This inclusion was modelled to contain two combined chromophores, one with a peak absorption at 780 nm and the other one at 860 nm. This design presents a challenging case, as previous studies employed separate inclusions, each containing a single chromophore. The chromophores were mixed within the inclusion at concentrations of 2 a.u. and 0.5 a.u., respectively, resulting in absorption contrasts of 7 and 5, respectively, compared to the background that has 0.01 mm^{-1} absorption coefficient. To accurately separate the concentration of each chromophore, two laser wavelengths across the isosbestic point of the two chromophores and matching the absorption peak of each chromophore were employed.

Four illumination windows were positioned around the phantom to ensure that light adequately reached the centrally located inclusion. Fig. 1 illustrates the geometry of the phantom and the distribution of the illumination sources.

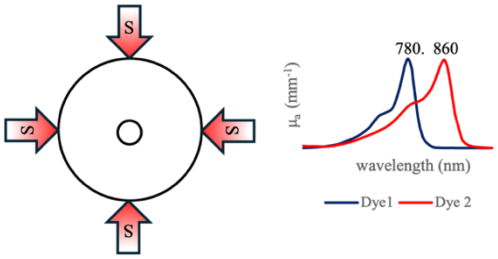

Fig. 1: A cross-sectional view of the 25 mm numerical phantom with the centrally located 4 mm inclusion. The positioning of the illumination sources is indicated by arrows (S). The absorption spectra of the two NIR chromophores used in the study are also present.

3. Results

The absorption coefficient values at the selected wavelengths (780 nm and 860 nm) were input in the PMI forward solver to generate the temperature maps, as shown in Fig. 2 ((a) and (b) left). This figure highlights multiple regions within the temperature maps where the temperature rises above the background, reaching around 3 °C. These elevated temperature regions correspond to the inclusion at the center and the laser irradiation site at the boundary of the phantom. The maximum temperature increase at the source area was at 3.16 °C at both wavelength maps. However, due to the differences in the absorption coefficients at the inclusion area, the maximum temperature rise within the inclusion was 3.19 °C for 780 nm wavelength and 2.74 °C for 860 nm wavelength.

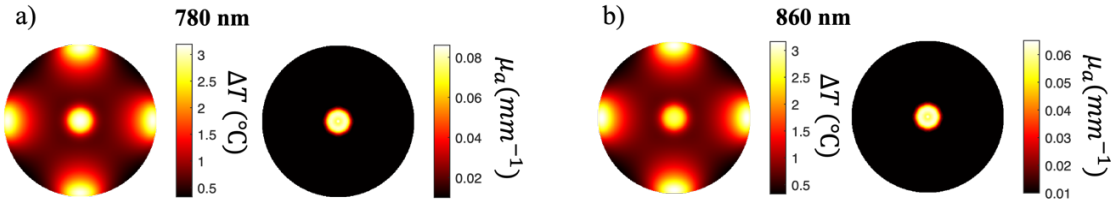

Fig. 2: a) The temperature map (left) and recovered absorption map (right) at 780 nm, b) The temperature map (left) and recovered absorption map (right) at 860 nm

The absorption coefficient distributions were then resolved from the temperature maps at the employed wavelengths with high resolution and quantitative accuracy using PMI inverse problem, resulting in mean coefficients of 0.072 mm^{-1}at 780 nm and 0.057 mm^{-1} at 860 nm, shown in Fig. 2 ((a) and (b) right). Using the accurately resolved absorption coefficient distributions, the concentrations of the two chromophores within the inclusion were successfully separated using the proposed approach. The concentration of the two chromophores using the non-iterative approach were recovered with a percentage error of 7% and 10%, respectively, Fig. 3. The solution was obtained in an average time of only 0.05 seconds.

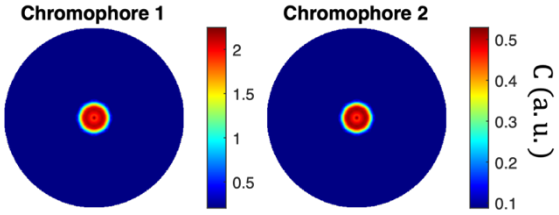

Fig. 3: The calculated concentration map for the two chromophores which successfully separated using the non-iterative approach.

To validate the performance of this method, the resulted concentrations were compared with those obtained using the extensively validated standard PMI method, which took 7.93 seconds to obtain similar accuracy. Table 1 summarizes the recovered mean concentrations of the two chromophores using both methods, along with the computational time required to obtain these results.

Table 1: Comparison of the two methods in terms of processing time and accuracy.

Method	Recovered chromophore 1	Recovered chromophore 2	Computational time (second)
The standard method	1.86 ± 0.29	0.45 ± 0.06	7.93
The non-iterative method	1.86 ± 0.29	0.45 ± 0.06	0.05

4. Conclusion

This study demonstrated the efficacy of a non-iterative approach for the fast and accurate quantification of chromophore concentrations when present in the same region. Using linear algebraic techniques, like LU decomposition, computational time was significantly reduced without compromising the imaging accuracy. The proposed method was tested on a numerical phantom with a tumor-like inclusion at the center containing a mixture of two different chromophores. The results highlight that the non-iterative approach successfully discriminated the concentrations of the two chromophores with minimal errors (7% and 10%) in just 0.05 seconds, as compared to 7.93 seconds when applying the standard iterative PMI method. This approach holds promising potential for real-time tumor characterization and clinical applications. In the future, this method will be extended to more complicated cases, including experimental phantoms and in vivo data.

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