The Direct Robin Boundary Value Parabolic System of Time-Resolved Diffuse Optical Tomography with Fluorescence

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Abstract. We consider a system of parabolic PDEs with measure data modelling a problem of the time resolved diffuse optical tomography with a fluorescence term and Robin boundary conditions. We focus on the direct problem where the quantity of interest is the density of photons in the diffusion equations and which constitutes a major step to solve the inverse problem of identifiability and reconstruction of diffusion, absorption and concentration of the fluorescent markers. We study the problem under a variational form and its discretization with finite element method and we give some numerical simulation results for verification purpose as well as simulations with real data from a tomograph.

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1 Introduction

We consider the Time-Resolved Diffuse Optical Tomography (TR-DOT) problem with fluorescence arising in the medical and biological imaging for soft tissues, small animal studies and noninvasive methods of tumor detection [1, 9, 13, 14]. The final goal in this imaging modalities is the reconstruction of physical parameters such as diffusion and absorption coefficients. While IRM and X-Ray tomography are usually of high resolution and deep penetration properties allowing exploring the object in-depth but with poor
contrast, the optical tomography is very sensitive to the contrast but with poor resolution. In addition, the optical tomography is only efficient in thin regions close to the detectors. However, due to its cheap cost and noninvasive features, its recommended for some type of tumor (skin, breasts, neonatal imaging,. . . ). In order to increase its efficiency, it is usually coupled with the use of fluorescent molecules which enhance the contrast in the tissues. The mathematical model of (TR-DOT) is a parabolic system with a memory term and measure data. In simple geometric setting (disk, cylinder) and assuming some regularity of the solutions, the mathematical study of the resulting problem follows from standard methods of the calculus of variations but in the general setting one has to use more technical and involved methods to solve the parabolic systems (e.g. approximation approach [2, 3, 12]). Moreover, there are two different experimental setting leading to two kind of data and measurements: the contact case where the detection and excitation fibers are set directly on the object under consideration and the non-contact case where they are not. This yields two mathematical models for which the governing equations are unchanged while the data and measurement terms are either Dirac masses on isolated points in the first case or Dirac masses on lines in 2D and surfaces in 3D configurations (any all cases sets of small dimension). The main goal in this article is to study such problems and to perform the numerical analysis as well as preliminary numerical simulations on both academic data for verification purpose in different implementation settings (Matlab and Feel++ softwares) as well as real data from an experimental tomograph of Icube Laboratory (university of Strasbourg). The diffusion approximation for the optical tomography called time resolved diffuse optical tomography, DOT-TR, is widely used and documented in medical and biological imaging, we refer the reader to the review of S. Arridge and the references therein [1]. In contrast, only a few references are available for the fluorescent case and to our knowledge almost no mathematical and numerical study have been done yet. We refer to [4] for the physical model and related references on the subject. The paper is organized as follows. The Section 2 proposes a study for the well-posedness of the coupled system of equations for the contact case, Section 2.1 and the non-contact case, Section 2.2. Some mathematical preliminaries are introduced, the weak formulations and some theoretical results are stated. In Section 3, we set the discrete framework with emphasis on the methods to handle the fluorescence source term which can be seen as a memory source term, but can also be treated without explicit integration (Duhamel formulae) by introducing an Ordinary Differential Equations (ODE) to the initial system. Finally, two convergence results are given depending on the chosen source term for the contact and the non-contact mode.

2 Mathematical model-Weak formulations

In this section, we briefly give some mathematical tools and results on the models under consideration. We derive also the associated weak formulations on which our discretization is based. We refer for details to [4]. We call tomograph an experimental device which
consists of \( N_s \in \mathbb{N} \) optical fibers, acting as light sources and detectors, and placed on a ring and surrounding for instance a phantom object or a small animal to be imaged by the tomograph. Let \( \Omega \) be a bounded domain of \( \mathbb{R}^d \) \((d = 2 \text{ or } 3) \) and \( T > 0 \). We denote \( \ell \in \{x, m\} \) the subscript respectively for the diffusion and fluorescence excitation wavelength. The system of equations that describes the tomograph setup as a sequence of diffusion problems within each fiber and through \( \Omega \) is written: \( 1 \leq k \leq N_s \),

\[
\begin{cases}
-\nabla \cdot (\kappa_x \nabla \phi^k_x) + c_x \mu_{a,x} \phi^k_x + \frac{\partial \phi^k_x}{\partial t} = q^k_x & \text{on } \Omega \times (0,T), \\
-\nabla \cdot (\kappa_m \nabla \phi^k_m) + c_m \mu_{a,m} \phi^k_m + \frac{\partial \phi^k_m}{\partial t} = \gamma q^k_m & \text{on } \Omega \times (0,T), \\
\phi^k_x + 2A \kappa_x \frac{\partial \phi^k_x}{\partial n} = 0 & \text{on } \partial \Omega \times (0,T), \\
\phi^k_m + 2A \kappa_m \frac{\partial \phi^k_m}{\partial n} = 0 & \text{on } \partial \Omega \times (0,T), \\
\phi^k_x(0,\cdot) = 0, & \phi^k_m(0,\cdot) = 0,
\end{cases}
\tag{2.1}
\]

where the wavelength dependent quantities denote respectively \( \phi^k_x \) the photon density, \( \mu_{a,\ell} \) the absorption coefficients, and \( \kappa_\ell \) the diffusion coefficients given by

\[
\kappa_\ell = \frac{c_\ell}{3(\mu_{a,\ell} + \mu'_{s,\ell})},
\tag{2.2}
\]

where \( \mu'_{s,\ell} \) is the scattering coefficients. The fluorophore coefficient \( \gamma = \eta \sigma \xi \) depends on the fluorophor concentration \( \xi \), the fluorophore molar extinguishing coefficient \( \sigma \) and the fluorophore yield \( \eta \). Finally, \( \tau \) corresponds to the fluorophore average lifetime and \( A \) is a given constant (see [4]). There are two approaches to handle the source terms \( q^k_x \), the contact mode where \( q^k_x \) is a Dirac mass on a single point in \( \Omega \) or the non contact mode where \( q^k_m \) is a Dirac mass supported on low dimensional set, a line when \( d=2 \) and a surface when \( d=3 \). Our contributions in this modelling part is to consider systematically and rigourously these two models and to compare them both theoretically and numerically. We set

\[
q^k_x = \begin{cases}
\delta_{x_0}(x) \delta(t_0) & \text{(contact case)},
\delta_{\Sigma_0}(x) \delta(t_0) & \text{(non contact case)}.
\end{cases}
\tag{2.3}
\]

The fluorescence source term \( q^k_m \) in this modelling is a response at the wavelength \( \lambda_m \) and takes the form of convolution (in time) of the photon density at \( \lambda_x \) with an exponential kernel times a fluorophor concentration. This source term modelizes the fluorophore excitation photons generated once the diffusion photons hit the biomarker

\[
q^k_m(x,t) = \frac{1}{\tau} \int_0^t \phi^k_x(x,s) e^{(t-s)/(\tau)} ds.
\tag{2.4}
\]

**Remark 2.1.** We assume null initial conditions which means that we neglect the mean free path otherwise we should have to take into account a direction information for the particles transport.
We denote by $Q = \Omega \times (0, T)$ the time-space domain and by $M(\bar{\Omega}) = C(\bar{\Omega})'$, the usual bounded Radon measures space (i.e. dual of the space of the continuous functions equipped with its usual norm). We consider the coupled system of parabolic equations (2.1) and we will drop the index $k$ equipped with its usual norm). We consider the coupled system of parabolic equations

\begin{align*}
\kappa_t A t, \mu_{a,t} \in L^\infty(\Omega), \\
0 < \kappa_0 \leq \kappa_x, \kappa_m \leq \kappa_1.
\end{align*}

(2.5)

We have to distinguish the two cases: contact model where the datum $q_x$ is only in $H^{-s}(\Omega), s \geq 2$ and the non contact model where it belongs to the dual space $(H^1(\Omega))'$. 

**Remark 2.2.** Note that in the case of smooth coefficients $\kappa_x, \mu_{a,x}$ (e.g. Hölder continuous), and simple geometries, the first equation may be solved with the fundamental solution method and the second one is then uncoupled from the first one and with a regular right-hand side, thus fit under the framework of the standard variational theory [7]. In the general case (2.5), we have to consider a more general setting of parabolic equations with measure data [2,3].

### 2.1 The contact case

Let $\ell = \{x,m\}$, $q_x \in M(\bar{\Omega})$. We recall that in our setting we have $q_x = \delta_{x_0}$, with $x_0 \in \Omega$. The theory of parabolic equations with measure data show that weak solutions or only defined in the spaces $W_q = L^q(0, T; W^{1,q}(\Omega))$ for any $1 \leq q < \frac{d+2}{d-1}$ (e.g. [3]), loosely speaking one wants the tests functions to be in $H^1(\Omega) \cap C(\bar{\Omega})$. In the case of our system the first equation fit under this general framework, whereas the second equation possesses more regularity for the right-hand side term and solutions are searched in classical spaces for second order parabolic equations. More precisely, let $V^c = \bigcup_{q > \frac{d}{d-1}} W^{1,q}(\Omega), d \geq 2$. In order to write the weak formulation of the system (2.1), we consider each equation:

\begin{itemize}
  \item[(i)] Find $\phi_x(t) \in \cap_{p < \frac{d}{d-1}} W^{1,p}(\Omega)$, and $\frac{\partial \phi_{x}}{\partial t} \in \cap_{p < \frac{d}{d-1}} W^{-1,p}(\Omega)$ for a.e $t > 0$

\begin{equation}
\int_\Omega \kappa_x \nabla \phi_x \nabla v + \int_\Omega c^e \mu_{a,d} \phi_x v + \int_\Omega \frac{1}{2A} \phi_x v + \int_\Omega \frac{\partial \phi_{x}}{\partial t} v = (q_x, v) \quad \forall v \in V^c.
\end{equation}

\end{itemize}

Note that $v$ is continuous, and $(q_x, v)$ is $v(x_0)$. The integral $\int_\Omega \frac{\partial \phi_{x}}{\partial t} v$ is to be understood in the dual sense ( $\frac{\partial \phi_{x}}{\partial t} \in W^{-1,p}(\Omega)$ for $p < \frac{d}{d-1}$, and $v \in V^c$ a.e $t > 0$).

\begin{itemize}
  \item[(ii)] the source term $q_m$ depends on $\phi_x$. We look for a solution $\phi_m \in H^1(\Omega)$ more regular than $\phi_x$ such that

\begin{equation}
\int_\Omega \kappa_m \nabla \phi_m \nabla v + \int_\Omega c^e m_{d,m} \phi_m v + \int_\Omega \frac{1}{2A} \phi_m v + \int_\Omega \frac{\partial \phi_{m}}{\partial t} v = (\gamma q_m, v)_{H^{1}(\Omega), H^{1}(\Omega)}.
\end{equation}

\end{itemize}

As a detailed mathematical analysis of the problem is beyond the scope of this article, we only state the well posedness result in the contact case without proof and we refer the interested reader to [4] for details.
Theorem 2.1. Under the hypothesis (2.5) for any \(1 \leq q < \frac{d+2}{d+1}\) there exists a solution \((\phi_x, \phi_m)\) to the system (2.1), such that \(\phi_x \in W_q\), and \(\phi_m\) is such that: \(\phi_m \in L^2(0,T;H^1(\Omega)) \cap C([0,T];L^2(\Omega))\), \(\phi'_m \in L^2(0,T;(H^1(\Omega))')\). If \(d = 2\), and \(\phi_m, \phi'_m \in L^p(0,T,W^{1,p}(\Omega))\) \((p \leq \frac{4}{3})\). If \(d = 3\).

Note that the solutions given by the theorem are such that the initial conditions \(\phi_i(0.\,= 0, \ell = \{x, m\}\) are taken in the classical sense since \(\phi_m(t)\) is continuous and \(\phi_x\) belongs to \(C([0,T];H^{-s}(\Omega))\) for large \(s > 0\) [3].

Remark 2.3. The theorem suggests, due to the different regularity properties for \(\phi_x\) and \(\phi_m\), that the discretization errors will be better for \(\phi_m\), thus it may be advantageous to use different finite elements for each variable [4].

2.2 The non-contact case

Let us consider the non contact case \(q_{x0} = \delta_{\Sigma_0} \in H^{1'}(\Omega)\) when \(\Sigma_0\) is a closed surface in \(\Omega\), as it may be checked that

\[
<q_{x0}, v>_H^{1'}, H^1 = \int_{\Sigma_0} v d\sigma, \quad \forall v \in H^1(\Omega). \tag{2.8}
\]

Remark 2.4. If \(\Sigma_0\) is an open surface, we have to modify the functional setting but a part from technicalities the study follows the same lines. We focus on the case of a closed surface for brevity.

We set \(V = H^1(\Omega)\). The weak formulation in this case is given by:

(i) Find \(\phi_x(t) \in V\), and \(\frac{\partial \phi_x}{\partial t} \in V'\) for a.e \(t > 0\)

\[
\int_{\Omega} \kappa_x \nabla \phi_x \nabla v + \int_{\Omega} c_x \mu_x v + \int_{\Omega} \frac{1}{2A} \phi_x v + \int_{\Omega} \frac{\partial \phi_x}{\partial t} v = (q_x, v)_{V', V} \quad \forall v \in V. \tag{2.9}
\]

Note that \((q_x, v)\) is the integral \(\int_{\Sigma} v d\sigma\).

(ii) the source term \(q_m\) depends on \(\phi_x\), we therefore search a solution \(\phi_m \in V\), with \(\frac{\partial \phi_m}{\partial t} \in L^2(\Omega)\) such that

\[
\int_{\Omega} \kappa_m \nabla \phi_m \nabla v + \int_{\Omega} c_x \mu_x m v + \int_{\Omega} \frac{1}{2A} \phi_m v + \int_{\Omega} \frac{\partial \phi_m}{\partial t} v = (\gamma q_m, v)_{V', V}. \tag{2.10}
\]

Note that the integral \(\int_{\Omega} \frac{\partial \phi_m}{\partial t} v\) is to be understood in the duality sense \(V', V\).

Remark 2.5. Note that we take \(\mu_{a,x}\) nonnegative which is too stringent. However, if \(\mu_{a,x} \equiv 0\) on \(w \subset \Omega\), then we have to modify the functional setting to ensure the Poincaré-Wirtinger inequality and the results hold.

We refer to [4] for the proof of the following theorem.
Theorem 2.2. Under the hypothesis (2.5) there exists a unique solution \((\phi_n, \phi_m)\) to the system (2.1), such that \(\phi_n \in L^2(0,T;H) \cap C([0,T];V')\) and \(\phi_m \in L^2(0,T;V) \cap C([0,T];H)\), and \(\frac{\partial \phi_m}{\partial t} \in L^2(0,T;V').\)

We note that when the coefficients \(\kappa, \mu, \ell \in \{x,m\}\) are regular, say \(W^{1,\infty}(\Omega)\), the solution \(\phi_m \in L^2(0,T;H^2(\Omega) \cap V) \cap C([0,T];V)\) and \(\frac{\partial \phi_m}{\partial t} \in L^2(0,T;H)\) (see [6,7]). In all cases, the solutions satisfy the initial conditions in the classical sense and the Robin boundary condition in the usual sense of traces.

3 Discrete formulations

3.1 Semi-discrete formulation

In the following section, we drop the index \(k\) for simplicity. We discretize in time such that \(t_n = n\Delta t\). We denote \(\phi^{(n)}(x) = \phi(x, t_n)\) the solution of the system (2.1) and \(q^{(n)} = q(\phi_n; x, t_n)\) the source term. We discretize the time dependent term using a backward Euler scheme in time. Thus, the semi-discrete formulation reads

\[
\int_\Omega \left( \kappa \nabla \phi^{(n+1)} \cdot \nabla v + c_n \mu \phi^{(n+1)} v \right) + \int_{\partial \Omega} \frac{1}{2A} \phi^{(n+1)} v + \int_\Omega \frac{\phi^{(n+1)}}{\Delta t} v = \int_\Omega q^{(n+1)} v + \int_\Omega \frac{\phi^{(n)}}{\Delta t} v. \tag{3.1}
\]

We must yet see how to deal with the source term for the fluorescence \(q_m\). We can use the Chasle relation to rewrite the integral such that

\[
q^{(n+1)}_m = \frac{1}{\tau} \int_{t_n}^{t_{n+1}} \phi_x(x,s) e^{\left(\frac{t_{n+1}-s}{\tau}\right)} ds = f(t_{n+1}) (B_n(x) + R_n(x)) \tag{3.2}
\]

with \(f(t) = \frac{1}{\tau} e^{\frac{t}{\tau}}\) and \(B_n(x)\) a memory term defined such that

\[
B_n(x) = \int_0^{t_n} \phi_x(x,s) e^{-\frac{s}{\tau}} ds, \tag{3.3}
\]

stored and \(R_n(x)\) a remain term to compute such that

\[
R_n(x) = \int_{t_n}^{t_{n+1}} \phi_x(x,s) e^{-\frac{s}{\tau}} ds. \tag{3.4}
\]

Therefore we just have to compute the integral \(R_n(x)\) knowing that \(\phi_x(x,t)\) is first order polynomial of the time on the restricted interval \([t_n, t_{n+1}]\) and also that its boared values are fixed.

\[
\phi_x(x,t) = a(x) t + b(x), \tag{3.5}
\]

where the coefficients \(a\) and \(b\) are respectively,

\[
a(x) = \frac{\phi_x^{(n+1)}(x) - \phi_x^{(n)}(x)}{\Delta t}, \quad b(x) = \phi_x^{(n+1)} - a(x) t_{n+1}. \tag{3.6}
\]
We integrate by parts the integral (3.4),

\[
R_n(x) = \left[ -\tau \phi_x(x,s)e^{-\frac{s}{\tau}} \right]_{t_n}^{t_{n+1}} + \tau \int_{t_n}^{t_{n+1}} \phi'_x(x,s)e^{-\frac{s}{\tau}} ds
\]

\[
= -a(x)\tau \Delta t(n\omega_1 + 1) - \tau (b(x) + a(x)\tau) \omega_1,
\]

(3.7)

where the coefficients \( \omega_1 \) reads

\[
\omega_1 = 1 - e^{\Delta t/\tau}.
\]

(3.8)

Now, if we replace \( a(x) \) and \( b(x) \) with their values (3.6), the remaining term can be expressed such that

\[
R_n(x) = C_1 \phi_x^{(n+1)} + C_2 \phi_x^{(n)},
\]

(3.9)

where the coefficients \( C_1 \) and \( C_2 \) are,

\[
C_1 = \tau \left( -1 - \frac{\tau \omega_1}{\Delta t} \right), \quad C_2 = \tau \left( 1 + \frac{\tau}{\Delta t} \right) \omega_1.
\]

(3.10)

Using Chasle relation again in Section 3.3, the recursive formula for \( B_n(x) \) can be established

\[
B_n(x) = B_{n-1}(x) + R_{n-1}(x).
\]

(3.11)

In particular we have \( B_0 = 0 \) and \( R_0 \) defined such that

\[
R_0(x) = \phi_x^{(0)} \tau (1 - \omega_1) - \tau \phi_x^{(1)}.
\]

(3.12)

Finally, we obtain the semi-discrete formulation

\[
\int_\Omega (\kappa \nabla \phi^{(n+1)} : \nabla v + c_e u \phi^{(n+1)} \cdot v) + \int_\Omega \frac{1}{2\Lambda} \phi^{(n+1)} \cdot v + \int_\Omega \frac{\phi^{(n+1)}}{\Delta t} \cdot v
\]

\[
= \int_\Omega \left( q_x^{(n+1)} \right) \cdot v + \int_\Omega \left( \gamma(x) f^{(n+1)} B_n(x) \right) \cdot v + \int_\Omega \frac{\phi^{(n)}}{\Delta t} \cdot v.
\]

(3.13)

**Remark 3.1.** For \( n > 0 \), the term \( B_n(x) \) is known and has to be updated for each time step.

**Second method** Instead of handling the memory term in the fluorescence equation, a second method consists in introducing the ODE on the fluorescence source term \( q_m \) detailed in Section 2.1 in the original model. Thus, a new degenerated problem is considered consisting of (2.1) with, in addition the following equation

\[
\begin{aligned}
(2.1),
\end{aligned}
\]

(3.14)

Considering equation (3.14), we convert a memory cost for a computational cost, but more efficient by solving the new ODE equation (3.14) explicitly. A possible advantage is for different time grids. As the solution for the fluorescence problem depends on the regularity of \( \phi_x \), we might choose a coarse grid for the fluorescence and adapt the ODE scheme (e.g high order Runge Kutta (RK method) to regularize the solution with the aim to reduce the computational cost of the global system.
3.2 Full Discrete formulation

We now turn to the Galerkin approximation of the semi-discrete problem (3.13). The space discretization may vary depending on the contact or non-contact case follow Section 2 analysis. Let \( Z_h = V_h \times W_h \subset [H^1(\Omega)]^2 \) the discrete spaces of the problem (3.13), \( V_h \) associated the diffusion and \( W_h \) associated to the fluorescence equations respectively. The subscript \( h \) denotes the space discretization step. Let \( T_h \) be a space grid for the domain \( \Omega \). Let \( N_i \) denotes the mesh vertices of \( T_h \) with \( i \in [1,N_h] \). We introduce a vectorial basis \( \{ \varphi_j \} \) for \( Z_h \) defined by

\[
\varphi_j(N_i) = \{ \varphi^x_j(N_i) | k \in \{ x,m \} \},
\]

the basis function of the space \( V_h \) and \( W_h \) for \( k = x \) and \( k = m \) respectively, such that

\[
\varphi^k_j(N_i) = \begin{cases} 0 & i \neq j, \\ 1 & i = j, \end{cases} \quad i,j = 1,...,N_h.
\]

We introduce the Galerkin approximation \( \phi_h^{(n)} = \{ \phi^{(n)}_x, \phi^{(n)}_m \} \in [V_h]^2 \) defined for each \( t \approx t_n \) with \( n > 0 \) of (3.13).

\[
\phi^{(n)}_h(x) = \sum_{j=1}^{N_h} \phi^m_j \varphi_j(x),
\]

and we denote \( \phi^{(n)}_h = \phi^{(n)}_h(x) \) for brevity. The semi-discrete formulation (3.13) reads

\[
\int_{\Omega} (K \nabla \phi^{(n+1)}_h : \nabla v_h + c_e m_a \phi^{(n+1)}_h \cdot v_h) + \int_{\partial \Omega} \frac{1}{2A} \phi^{(n+1)}_h \cdot v_h + \int_{\Omega} \frac{\phi^{(n+1)}_h}{\Delta t} \cdot v_h
\]

\[
= \int_{\Omega} (q(x) B_h(x)) \cdot v_h + \int_{\Omega} (\gamma(x) f^{(n+1)} R_h(x)) \cdot v_h + \int_{\Omega} \frac{\phi^{(n)}_h}{\Delta t} \cdot v_h.
\]

We introduce the Galerkin approximation \( q^{(n)}_{x,h} \) for the diffusion source term such that for the contact case (i), we have

\[
q^{(n)}_{x,h} = \begin{cases} \sum_{j=1}^{N_h} \delta_{h,j} \varphi_j(x) & n = 0, \\ 0 & n > 0, \end{cases}
\]

such that

\[
\delta_{h,j} = \begin{cases} 1 & j = j_0 (x = x_0), \\ 0 & \text{else}, \end{cases}
\]

and for the non contact case, we have

\[
q^{(n)}_{x,h} = \begin{cases} \sum_{i=1}^{N_h} \delta_{h,i} \varphi_i(x_{\Sigma_0}) & n = 0, \\ 0 & n > 0. \end{cases}
\]
The remainder term written in the finite element basis is
\[ R_n = C_1 \sum_{j=1}^{N_h} \phi_j^{(n+1)} \phi_j + C_2 \sum_{j=1}^{N_h} \phi_j^{(n)} \phi_j, \] (3.22)
then we may write
\[ a_{ij} = \int_{\Omega} \kappa \nabla \phi_j : \nabla \phi_i, \quad b_{ij} = \int_{\Omega} \mu \phi_j \phi_i, \] (3.23a)
\[ m_{ij} = \int_{\Omega} \phi_j \phi_i, \quad f_{ij} = \int_{\Omega} \gamma(x) \left( \phi_j \right) \phi_i. \] (3.23b)
We obtain the algebraic form
\[ A \Phi^{(n+1)} + c_1 B \Phi^{(n+1)} + M \left( \frac{1}{2A} + \frac{1}{\Delta t} \right) \Phi^{(n+1)} - C_1 F \Phi^{(n+1)} = Q^n. \] (3.24)

### 3.3 Convergence results

We now give a convergence result depending on the type of source \( q_s \) considered. The contact case result is based on the proof of [11] whereas the non-contact one is based on [5] results. For the non-contact case, we are taking into account that the surface for the \( \delta \)-Dirac source can be taken on a different mesh from the domain \( \Omega \) introducing an interpolation error for the worst scenario.

**Contact case** We give the error bound for general finite elements approximation of degree \( m \), since we implemented various type conforming finite elements. We place ourselves under the same hypothesis as [11]. Let us denote \( \Omega \) the whole domain and \( T_h \) a triangulation on \( \Omega \in \mathbb{R}^d \) with \( d > 0 \) the dimension. We denote \( V \) the Sobolev completion of \( H^m(\Omega) \). We recall the result of [11]. Let \( V \) be a Hilbert space associated to the variational formulation of an elliptic problem with right-hand side a Dirac measure \( \delta_{x_0}, \ x_0 \in \Omega \), for an operator of order \( 2m, \ m \geq 1 \) (\( V \) is the completion of smooth functions in the Sobolev space \( H^m(\Omega) \)). Let \( S^h \) be a finite element subspace of \( V \). We say that \( S^h \) approximates to degree \( k \) in \( V \) if for each smooth \( u \) in \( V \):

\[ \inf_{v \in S^h} \| u - v \|_{H^s(\Omega)} \leq C(x_0) h^{k-s} \| u \|_k, \quad \text{for } 0 \leq s \leq m. \] (3.25)

Typically, for \( m = 1 \) the degree \( k = \ell + 1 \), where \( \ell \) is the polynomial degree in \( S^h = V_h \). Then we have the theorem (see [11]).

**Theorem 3.1.** If \( \phi_s \) solves (2.1) in the sense of distributions for \( q_s = \delta_{x_0} \) and \( \phi_{s,h} \) is the solution to the associated variational problem, then

\[ \| \phi_s - \phi_{s,h} \|_{H^s} \leq C(x_0) h^{2m - \frac{d}{2} - s} \quad \text{for } 2m - k < s < 2m - \frac{d}{2}, \] (3.26)

if \( k \geq 2m \) then \( C(x_0) \) goes to infinity as \( x_0 \) approaches \( \partial \Omega \).
In particular, according to (3.25), we have for \( d = 2, m = 1 \) and \( \ell = 1 \) the convergence rate \( O(h^{1-s}) \) for \( 0 \leq s \leq 1 \). With \( d = 3 \), we obtain \( O(h^{\frac{1}{2}-s}) \) for \( 0 \leq s \leq \frac{1}{2} \).

**Remark 3.2.** In our case, the distance \( d(x_0, \partial \Omega) \) corresponds to the mean free path which is the medium length of a path covered by a photon (or particle) between subsequent impacts. In practice, this distance is taken equal to the inverse of the reduced scattering coefficient \( d(x_0, \partial \Omega) = \frac{1}{\mu_s} \). Note that as \( x_0 \) goes to \( \partial \Omega \) the constant \( C(x_0) \) goes \( +\infty \) [11].

**Non contact case** In the following section, an error estimate is proposed for our special source term of Dirac type.

In [5] consider a Laplace equation in 2D for which they derive an error estimate. We follow the same approach that we extend to the 3D case. To cover the cases that we have implemented and for sake of completeness we give the results even for \( \Sigma \) an open curve and with different meshes on \( \Omega \) and \( \Sigma \) (not compatible in general).

The method consists in approximating the source term by a sum of Dirac masses for \( \Sigma_0 \). To handle the right hand side \( q_x(x,t) \), we denote \( q(x) = \delta_{\Sigma_0} \) and \( \Sigma_0 \). Then for any \( v \in V \subset H^1(\Omega) \), we have

\[
<q_x, v>_H^{-1, H^1} = <\delta_{\Sigma_0}, v>_H^{-1, H^1} = \int_{\Sigma_0} v. (3.27)
\]

Given a triangulation \( T_h \) of \( \Omega \) we introduce \( T_{\tilde{h}} \) a discretization of \( \Sigma_0 \) of \( d-1 \) dimension. One denotes \( E_h \) the interior edges of the mesh \( T_h \). We assume that \( T_{\tilde{h}} \) is not a submesh of \( E_h \) (Note that if \( T_{\tilde{h}} \) is a submesh of \( E_h \), then following calculations are simpler since it is not necessary to interpolate between meshes). Recall that \( V_h \) is the \( P_1 \) conforming finite element space defined by

\[
V_h = \left\{ v_h \in C^0(\Omega), v_h|_K \text{ affine, } \forall K \in T_{\tilde{h}} \right\}. (3.28)
\]

**Lemma 3.1.** Let \( D \in \mathbb{R}^d \) with \( d = 1,2 \) be a smooth domain. Let \( \Sigma_0 \) an open curve, \( \Sigma_e \) a smooth curve such that \( \Sigma_0 \cap \Sigma_e = \emptyset \) and \( \partial D = \Sigma_0 \cup \Sigma_e \). Let denote \( h > 0 \) and \( T_{\tilde{h}} \) a family of quasi-uniform \( d \)-dimensional triangulations of \( \Sigma_0 \) with \( \Sigma_i, 1 < i < N \) the subintervals. The quasi-uniformity expresses

\[
ch^d \leq |\Sigma_i| \leq Ch^d, \quad \text{with } 0 < c < C. (3.29)
\]

We consider a set of points in the subsurfaces \( x_i \in \Sigma_i \). For \( v \in H^1(\Sigma_i) \), the piecewise constant interpolant reads

\[
v_{\tilde{h}} = \sum_{i=1}^{N} v(x_i) \mathbb{I}_{\Sigma_i}. (3.30)
\]

Then for \( 0 \leq s < 1/2 \), we have

\[
\|v - v_{\tilde{h}}\|_{H^s} \leq C h^{1-s} |v|_{1}, (3.31)
\]
with $|v|_1$ the $H^1$ seminorm and the associated usual Sobolev norm

$$
\|w\|_{H^s} = \left( \int_{\Sigma_0} |w|^2 \right)^{1/2} + \left( \int_{\Sigma_0} \int_{\Sigma_0} \frac{|w(y) - w(x)|^2}{\|y - x\|^{2(s + \frac{d}{2})}} \right)^{1/2}, \quad 0 \leq s < 1/2. \quad (3.32)
$$

**Proof.** For $d=1$ the proof follows [5]. For $d=2$, we have to find a majoration of (3.32). We first split the second term in the Sobolev norm (3.32) to treat, for the case $y - x = 0$, the diagonal (i) and the non-diagonal terms (ii), then find a majoration for the first $L_2$ norm term (iii). We denote $w_h = v - v_h$ now and hereafter.

(i) For the diagonal terms, using the Taylor formula then applying the Cauchy-Schwarz inequality, we find

$$
\sum_{i=1}^N \int_{\Sigma_i} \int_{\Sigma_i} |v(y) - v(x)|^2 \leq \sum_{i=1}^N \int_{\Sigma_i} \int_{\Sigma_i} \left( \int_0^1 |Dv(x + tv)|^2 dt \right) \frac{|v|^2}{\|v\|^{2(s + \frac{d}{2})}} \\
\leq \sum_{i=1}^N \left( \int_{\Sigma_i} |Dv(z)|^2 dz \right) \int_{\Sigma_i} |v|^{-2(s + \frac{d}{2}) + 2}. \quad (3.33)
$$

For the last double integral, we perform a majoration on $\Sigma_i = I_1 \times I_2$. For $d=1$ the majoration is given in [5]. For $d=2$, let $(x_j, y_j)$ for $1 \leq j \leq 2$ be a couple of points in $\Sigma_i,

$$
\int_{\Sigma_i} \int_{\Sigma_i} |v|^{-2s} = \int_{\Sigma_i} \left( \int_{I_1} \int_{I_2} |(y_1 - x_1)^2 + (y_2 - x_2)^2|^{-s} \right), \quad (3.34)
$$

we note that $|w|^a$ is convex for $a < 0$. Thus for $\theta \in [0,1]$ convexity writes as

$$
|\theta a + (1 - \theta)b|^a \leq \theta |a|^a + (1 - \theta) |b|^a \quad (3.35)
$$

and choosing coefficients

$$
\alpha = \left( \frac{y_1 - x_1}{\theta} \right), \quad \beta = \left( \frac{y_2 - x_2}{1 - \theta} \right), \quad (3.36)
$$

there exists $C_\theta > 0$

$$
|(y_1 - x_1)^2 + (y_2 - x_2)^2|^a \leq C_\theta |y_1 - x_1|^{2\alpha} + C_\theta |y_2 - x_2|^{2\beta}. \quad (3.37)
$$

For $\theta = \frac{1}{2}$, the constant is $C_0 = \frac{1}{2^{1-\alpha}}$. For $\alpha = -s$ and going back to (3.34) one has the following majoration

$$
\int_{\Sigma_i} \int_{\Sigma_i} |v|^{-2s} \leq C_0 \tilde{h}^2 \int_{I_1} \int_{I_1} |y_1 - x_1|^{-2s} + C_0 \tilde{h}^2 \int_{I_2} \int_{I_2} |y_2 - x_2|^{-2s}. \quad (3.38)
$$
For the last integral of (3.38) denoted $I$, let consider the following mapping

$$
\varphi_i: \Sigma_i = I_1 \times I_2 \rightarrow [0, \tilde{h}] \times [0, \tilde{h}],
$$

$$(x, y) \rightarrow \varphi_i(x, y)$$

and $J_{\varphi}$ the associated jacobian such that $\det(J_{\varphi}) \leq \tilde{h}^2$. Then the last integral of (3.38) can be calculated,

$$
I = \int_{0}^{\tilde{h}} \int_{0}^{\tilde{h}} |y-x|^{-2s} |\det(J_{\varphi})|^{-1} dxdy = \frac{2\tilde{h}^{-2s}}{(1-2s)(2-2s)}.
$$

Thus, a majoration of (3.38) reads

$$
\sum_{i=1}^{N} \int_{\Sigma_i} \int_{\Sigma_i} |v|^{-2s} \leq \frac{\tilde{h}^{2-2s}}{2^{s-1}(1-2s)(2-2s)}.
$$

Then back to (3.33), we obtain the majoration

$$
\sum_{i=1}^{N} \int_{\Sigma_i} \int_{\Sigma_i} \frac{|v(y) - v(x)|^2}{\|y-x\|^{2s+\frac{3}{2}}} \leq C_1 \tilde{h}^{2-2s} \left( \int_{\Sigma_0} |Dv(z)|^2 dz \right)
$$

with a constant $C_1 = \frac{2^{1-s}}{(1-2s)(2-2s)}$.

(ii) Similarly, a majoration can be determined for the non diagonal term in the second term of (3.32). Relying on the Cauchy-Schwartz inequality and (3.41), we have

$$
\sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \int_{\Sigma_i} \int_{\Sigma_j} \frac{|w_i(y) - w_i(x)|^2}{\|y-x\|^{2s+\frac{3}{2}}} \leq 4 \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \int_{\Sigma_i} \int_{\Sigma_j} \frac{|w_i(x)|^2}{w^{2s+\frac{3}{2}}}
$$

$$
\leq 4 \sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} \int_{\Sigma_i} \int_{\Sigma_j} \left( \int_{0}^{1} |Dv(z)|^2 dz \right) |v|^{-2s}
$$

$$
\leq C_2 \tilde{h}^{2-2s} \left( \int_{\Sigma_0} |Dv(z)|^2 dz \right)
$$

with a constant $C_2 = \frac{2^{3-s}}{(1-2s)(2-2s)}$.

As a consequence, the majoration for the double integral term in the Sobolev norm (3.32) reads

$$
\left( \int_{\Sigma_0} \int_{\Sigma_0} \frac{|w(y) - w(x)|^2}{\|y-x\|^{2s+\frac{3}{2}}} \right)^{1/2} \leq C_3 \tilde{h}^{2-2s} |v|_{1, \Sigma_0}^2
$$

with a constant $C_3 = C_1 + C_2 = \frac{5.2^{1-s}}{(1-s)(2-s)}$. 
(iii) For the $L_2$ norm, using again Cauchy-Schwartz inequality, we deduce

$$
\int_{\Sigma_0} |w_\tilde{h}|^2 = \sum_{i=1}^N \int_{\Sigma_i} |w_i|^2 \\
\leq \sum_{i=1}^N \left( \int_{\Sigma_i} |Dv(z)|^2 dz \right) \int_{\Sigma_i} |v|^2 \leq C_4 \tilde{h}^2 |v|_{1,\Sigma_0}^2
$$

(3.45)

with $C_4 = \frac{1}{6}$. Finally, we deduce the Lemma 3.1 norm with an order $1-s$. \hfill \Box

We recall the trace without proof (see [4] and in 2D [5]), the trace theorem lemma.

**Lemma 3.2.** Let $\Omega \in \mathbb{R}^d$ with $d = 2,3$ and $D$ be a smooth subdomain of $\Omega$. Let $\Sigma_0$ an open curve, $\Sigma_e$ a smooth curve such that $\Sigma_0 \cap \Sigma_e = \emptyset$, $\Sigma_0 \cup \Sigma_e = \partial D$ the boundary. Let $(T_h)_h$ be a regular family of triangulations, and $V_h$ the associated $P_1$ finite element space. Then the trace operator $\gamma_0$ maps $V_h$ into $H^{1/2}_{\Sigma_0}$ and one has

$$
|\gamma_0(v_h)|_{1,\Sigma_0} \leq \frac{C}{h^{1/2}} |v_h|_{1,\Omega}.
$$

(3.46)

Then the approximation error is given in the following propositions.

**Proposition 3.1.** Let $\Omega$ be a domain of $\mathbb{R}^d$ with $d = 3$ and $D \subset \subset \Omega$ a smooth subdomain with boundary $\partial D$. Let define $\Sigma_0$ an open curve, $\Sigma_e$ a smooth curve such that $\Sigma_0 \cap \Sigma_e = \emptyset$ and $\Sigma_0 \cup \Sigma_e = \partial D$. Let $(T_h)_h$ be regular family of triangulations with $V_h$ the associated $P_1$ finite element space. Let $\varphi \in H^{-1/2+s}(\Sigma_0)$. Let $S_h$ be a family of quasi-uniform triangulation of $\partial D = \bigcup \Sigma_i$ and one denotes $\Sigma_0,i = \{ \Sigma_i | \Sigma_i \in \Sigma_0 \}$. Let $x_i \in \Sigma_i$, one defines

$$
\varphi_h^\tilde{h} = \sum_{i=1}^{N_h} \lambda_i \delta_{x_i}
$$

(3.47)

with the real coefficients $\lambda_i$ define such that

$$
\lambda_i = \langle \varphi, \delta_{\Sigma_i} \rangle
$$

(3.48)

the approximation. Then there exists a constant $C > 0$ such that for all $v_h \in V_h$ :

$$
|\langle \varphi, v_h \rangle - \langle \varphi_h^\tilde{h}, v_h \rangle| \leq C \sqrt{\frac{h}{h}} \tilde{h}^{s} |\varphi|_{-1/2+s,\Sigma_0} |v|_{1,\Omega},
$$

(3.49)

where $\langle \cdot, \cdot \rangle$ denotes the dual pairing for $H^{-1/2+s}(\Sigma_0)$ and $H^{1/2-s}(\Sigma_0)$. 

Proof. From the Dirac source term definition, the interpolant is positive on \( \Sigma_0 \), then

\[
\langle \varphi \tilde{h}_h, v_h \rangle = \left( \sum_{i=1}^{N_h} \langle \varphi, \mathbb{I}_{\Sigma_0} \delta_{x_i}, v_h \rangle \right) = \left( \sum_{i=1}^{N_h} \langle \varphi, \mathbb{I}_{\Sigma_0} \rangle, v_h(x_i) \right).
\]

(3.50)

If we consider the approximation error, one has

\[
\langle \varphi, v_h \rangle - \langle \varphi \tilde{h}_h, v_h \rangle = \langle \varphi, v_h \rangle - \langle \varphi, \mathbb{I}_{\Sigma_0} \rangle v_h(x_i) \leq \| \varphi \|_{H^{1/2}} + s(\Sigma_0) \| v_h - v_h \|_{H^{1/2}}(\Sigma_0)
\]

(3.51)

with the piecewise interpolant of \( v_h \) on \( \Sigma_0 \) such that

\[
v_h = \sum_{i=1}^{N_h} \mathbb{I}_{\Sigma_0} v_h(x_i).
\]

(3.52)

Let denote \( w_h = v_h - v_h \), then (3.31) gives the following majoration

\[
\| w_h \|_{H^{1/2}}(\Sigma_0) \leq C \tilde{h}^{s+1/2} |v|_{1, \Sigma_0}
\]

(3.53)

for \( C > 0 \) adapted. Finally, using Lemma 3.2

\[
\| w_h \|_{H^{1/2}}(\Sigma_0) \leq C \sqrt{\tilde{h} \tilde{h}^{s} |v|_{1, \Omega}},
\]

(3.54)

which ends the proof.

To get the error for \( \phi_x \), we start with the Strang lemma

\[
\| \phi_x - \phi_{x,h} \|_{H^r} \leq C \left( \inf_{v_h \in V_h} \| \phi_x - v_h \| + \sup_{w_h \in V_h} \left( \frac{|\langle \varphi, w_h \rangle - \langle \varphi, w_h \rangle|}{\| w_h \|} \right) \right).
\]

(3.55)

We recall the Lemma 3.2 (Scott), the estimate (with \( m = 1 \)),

\[
\| \phi_x - \phi_{x,h} \|_{H^r} \leq C \tilde{h}^{s+1/2} \| \phi_x - \phi_{x,h} \|_{H^r}, \quad 0 \leq r \leq 1.
\]

(3.56)

We obtain from Proposition 3.1

\[
\| \phi_x - \phi_{x,h} \|_{H^r} \leq C \tilde{h}^{s+1/2} \left( \inf_{v_h \in V_h} \| \phi_x - v_h \| + \sqrt{\frac{\tilde{h}}{h}} |\varphi|_{-1/2+s, \Sigma_0} \right).
\]

(3.57)

If \( h \) and \( \tilde{h} \) are of the same order, then we get
Proposition 3.2. We have the estimate, for $0 \leq r \leq 1$ and $0 \leq s \leq \frac{1}{2}$ and with $P^1$ finite element,
\[
\| \phi_x - \phi_{x,h} \|_{H^r} \leq C h^{1-r} \left( \inf_{\phi_{x,h} \in V_h} \| \phi_{x,h} \|_{H^2} + h^s | \varphi |_{-1/2+s, \Sigma_0} \right).
\] (3.58)

In particular for $d = 2$ and in the extreme case $r = 1$, if we assume $\phi_x \in H^2$, we obtain
\[
\| \phi_x - \phi_{x,h} \|_{H^1} \leq C \left( \sqrt{h} \| \phi_x \|_{H^2} + h^s | \varphi |_{-1/2+s, \Sigma_0} \right),
\] (3.59)
we retrieve the result of [5]. However such regularity on $\phi_x$ seems too strong (Theorem 3.1). Moreover, for the case $d = 3$, even with such regularity assumption a similar estimates
\[
\inf_{v_h \in V_h} \| \phi_x - v_h \|_{H^1} \leq C \sqrt{h} \| \phi_x \|_2
\] (3.60)
to the best of our knowledge, is not known.

In the case $0 \leq r \leq \frac{1}{2}$ and without further assumption on $\phi_x$ than the Theorem 3.1,
\[
\| \phi_x - \phi_{x,h} \|_{H^r} = O(h^{1-r})
\] (3.61)
and the approximation of the source term is of higher order.

4 Numerical results

We implemented the forward problem (2.1) using a Finite Element Embedded Library in C++ www.feelpp.org (FEEL++) developed in our laboratory [10]. This library implements a framework for finite element methods based on the variational formulation with a language very close to the mathematical formulation. The implementation is parallel in a seamless manner for arbitrary dimensions and polynomial order thanks to the underlying features of the library. We highlight hereafter preliminary results for the diffusion problem with contact measurements. We propose a cross-verification with a former Matlab code and a validation by comparison with real measurements. An experimental instrument for small animal imaging was available [8] for performing time acquisitions on different test cases. We have at our disposal a set of measurements that has been acquired on homogeneous cylindrical objects made of plastic materials. The Impulse Response of the instrument is necessary to deconvolve the signal and to obtain the real measurement as a response to a Dirac pulse. However due to the detector sensitivity, the Impulse Response is difficult to obtain directly. Thus China Ink is used by instrumentalists as a medium in order to retrieve a signal which approximates the real Impulse Response. In practice, to perform comparison with physical measurements, our numerical solutions are convolved by the Impulse Response signal. The tests are performed on a cylindrical object with a radius of 20mm. The dataset contains for each source 7 measurements corresponding to the $d \in [0,6]$ detectors dispatched regularly at the opposite location from the
source. We have a total of 16 light sources taken from different angles. The built phantom has optical properties estimated $\mu_a = 0.006$ for the absorption and $\mu'_s = 0.6$ for the reduced scattering coefficient.

The Figure 1 shows cross-validated results with the former matlab code and compared with real measurements. Only 2 detectors for one source are presented in this paper, one located in the direct opposite position from the source $d = 3$. The second detector is located closer to the source $d = 0$. For comparison, numerical 1D results presented in the figure are readjusted with the exact signal time’s grid by interpolation, then centred on the peak and finally normalized. We observe that the solution between the measurements $\Phi_{k,obs}^d(t)$ and the diffusion solutions $\Phi_{x,d}^k(x_d,t)$ for the source $k = 0$ and the $d^{th}$ detector obtained with FEEL++ and the MathWorks Software (Matlab) match perfectly. These numerical solutions are convolved by the Impulse Response Tissue Temporal Point Spread Function (TPSF) in order to compare with real data. The FEEL++ solution without convolution is displayed to highlight the effect of the Impulse Response on the peak slopes. Looking closely, the rising edge of our numerical solutions seems to match measurements, but it does not match for the falling edge. This difference can be interpreted in different ways. The most likely reason is that phantom optical properties $\mu_a, \mu'_s$ are not well estimated, for instance due to the complexity of creating perfectly homogeneous objects. In Figure 2, we have slightly modified the reduced scattering coefficient to reach $\mu'_s = 0.8$. By increasing this parameter, we can see that the curves match less at the beginning of the rising edge, but more on the falling one. The next natural step would consist in an optimization process to find the best suited input parameters $\mu_a, \mu'_s$, thus consider the inverse problem.
5 Conclusion

This paper presented a numerical analysis of the Diffuse Optical Tomography and Fluorescence (DOTF) problem. An analysis for both contact and non-contact measurements mode has been detailed for sources of Dirac’s type. We proposed two strategies to handle the fluorescence coupling model equation (2.1) modeled by two diffusion equations. A first method consists in treating the convolution source term as a memory term, a second one consists to introduce a new ODE that can be solved explicitly. A finite element approach has been considered to handle the numerical aspects. Convergence results have been proposed to distinguish the two measurement modes presented in first sections. Finally, preliminary numerical results have been proposed to verify the mathematical model and the implementation based on a C++ parallel framework for FEM. The comparison with real measurements presented in this paper highlights the difficulty to find proper optical parameters in order to fit the data. Thus, as a perspective and future work, the inverse problem shall be considered in order to identify both fluorescence and diffusion parameters.

References


