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Analysis of the inverse problem associated with diffuse correlation tomography

Hari. M. Varma,[1] A. K. Nandakumaran[2⋆], R. M. Vasu[1]

[1] Department of Instrumentation, Indian Institute of Science, Bangalore, 560012, India

[2] Department of Mathematics, Indian Institute of Science, Bangalore, 560012, India

⋆ *Corresponding Author*. E-mail: nands@math.iisc.ernet.in

Abstract. The aim of this article is to study the mathematical analysis for an inverse problem and its numerical implementation associated with diffuse correlation tomography. The coefficients of the diffusion equation governing the propagation of field autocorrelation through a turbid medium (tissue-like) depend on both the optical and mechanical properties of the medium. Assuming the mechanical property is given by a time independent particle diffusion coefficient (D_B), we consider the development of regularized Gauss-Newton algorithm for the recovery of D_B from boundary measurements. We study the existence and uniqueness of the forward problem and also for the Fréchet derivative operator which are essential for convergence study. The nonlinear minimization problem associated with the recovery of D_B is locally linearized and solved through a regularized Gauss-Newton algorithm. The conditions to be satisfied for the convergence of the Gauss-Newton algorithm are established. Finally, the method is proven through numerical recovery of D_B from intensity autocorrelation measured at the boundary. Once D_B is obtained one can also recover other mechanical properties.

1 Introduction

Near infrared (NIR) light has found applications in the recent past for probing soft-tissue organs such as human breast and prostate for detecting pathological changes which accompany certain diseases [1, 2]. The important parameters which are recovered by NIR light probe are absorption and scattering coefficients [3, 4]; in particular absorption spectrum in the NIR range can help us compute functional parameters of interest to physicians, such as partial pressure of oxygen and total haemoglobin content, which are of immense value for early diagnosis of cancer. Along with optical absorption changes brought forth by angiogenesis associated with malignant tumor, there are also changes in elastic properties [5]. Therefore imaging based on elastic property changes was pursued vigorously in the past

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[6, 7, 8], leading to the development of elastography which, through a two step procedure, computes the strain distribution known as the elastogram and also the shear modulus distribution.

When a coherent light is used to probe a turbid medium like tissue, optical properties such as absorption and scattering coefficients affect its complex amplitude. However if one considers the propagation of a correlation function, say mutual coherence function or the amplitude auto-correlation, it is affected both by the optical properties and the dynamics of the scatterers in the body. The scatterers suffer temperature-induced Brownian-motion which also contributes to decrease in the amplitude auto-correlation. Since the mean-square displacement of the scatterers due to temperature-induced fluctuations is an indication of the stiffness of the surrounding medium, the way the auto-correlation decreases has been used in the past to measure the micro-rheological properties of the medium. This is one of the applications of the so-called diffusing wave spectroscopy (DWS)[9].

Tomographic reconstruction from DWS data is also explored, wherein the aim is to reconstruct the movement of particles (say distribution of blood flow in capillaries) from the boundary measurement of a quantity related to amplitude auto-correlation ([10]-[14]). It has also been established using the newly developed diffuse correlation tomography (DCT) that we can recover both optical and mechanical property distributions of tissue from sufficiently large sets of intensity auto-correlation measurements at the boundary of the object [15].

The amplitude correlation function obeys a radiative transfer equation (RTE) [11] which can be simplified to a diffusion equation under certain assumptions [15]. With diffusion equation as the forward model for the correlation propagation, one can set up the inverse problem to recover the coefficients of the partial differential equation (PDE) using a mean-square error minimization approach. This will involve a Gauss-Newton type of algorithm (or one of its variants) wherein one has to repeatedly solve the forward equation and also set up and invert the normal equation connected with the minimization problem. The forward model, which is the diffusion equation derived from the correlation transport equation, is usually solved employing the finite element method [16].

Whereas publications dealing with the numerical/compuational aspects of the above inverse problem are many, those trying to establish a proper and rigorous mathematical framework examining aspects such as existence and Fréchet differentiability of the forward operator, and convergence of the iterative algorithm implementing the Newton procedure for minimization are not available to the best of our knowledge. However, there are some papers which deal with the mathematical aspects of similar inverse problems of diffuse optical tomography (DOT) and electrical impedance tomography [17, 18]. In reference [17], convergence of an iteratively regularized Gauss-Newton approach to solve the DOT problem is studied wherein the usefulness of relative weighting of the regularization term in guiding the iteration is established. The convergence of the Levenberg-Marquardt(LM) method to solve the inverse conductivity problem via regularized least-square minimization is studied in [18]. The inverse problem associated with light propagation through a diffuse object with varying refractive index distribution is analyzed in [19]. Here, using an L^2 source in a diffusion model for light propagation, the existence of the forward solution is first established, followed by the computation of its Fréchet derivative.

In this work, we address the inverse problem of DCT using a regularized least-square approach for the recovery of particle diffusion coefficient. The issues considered are: (1) the existence of the forward solution and its Fréchet derivative when the illumination is from a source which is either an L^2 or a delta function, (2) establishment of the regularity of the forward operator and its derivative, (3) existence of a minimizer for the error functional and (4) the convergence of LM method used to arrive at the above minimum. In particular, we show that the weak solution of the forward equation driven by a delta source is in L^2 using the method of transposition [20]. In [21], the same problem is addressed and the existence of a weak solution for the DOT forward equation is established using Levi function.

Summary of the rest of the paper is as follows. In section 2, we introduce the forward model for the propagation of field autocorrelation. We prove the existence of weak solution for the forward operator for both collimated and diffusive type sources. This is relatively easy. In section 3, we derive the Fr*é*chet derivative and its adjoint operators and prove the existence of weak solution. The inversion of the forward equation, posed as a regularized least square minimization problem, is discussed in section 4, where we introduce the objective functional used for minimization. Regularity estimates of the objective functional needed for proving the existence of the minimizer is also derived in section 4. We state and prove the convergence theorem, in respect of LM procedure used in the minimization, in section 5. In section 6, we verify the established inversion scheme through numerical simulations. For the sake of completeness, we just present one inversion computation, but further details on numerical implementation are available in [22]. Section 7 gives our conclusion drawn from this study.

2 Forward model for the field autocorrelation through a turbid tissue like medium

The basic quantity of interest to be propagated is the specific intensity $I(\mathbf{r},\hat{\mathbf{s}},\tau)$, which obeys the following correlation transport equation [11, 12];

$$\hat{\mathbf{s}}\cdot\nabla I(\mathbf{r},\hat{\mathbf{s}},\tau) = -\mu_t I(\mathbf{r},\hat{\mathbf{s}},\tau) + \mu_s \int I(\mathbf{r},\hat{\mathbf{s}}',\tau) g_1^s(\hat{\mathbf{s}},\hat{\mathbf{s}}',\tau) d\hat{\mathbf{s}}' + S(\mathbf{r},\hat{\mathbf{s}}). \tag{2.1}$$

Here $\mu_t = \mu_a + \mu_s$, where μ_a and μ_s are the absorption and scattering coefficients respectively, and $S(\mathbf{r},\hat{\mathbf{s}})$ is the source at the location $\mathbf{r}$. Also $g_1^s(\hat{\mathbf{s}},\hat{\mathbf{s}}',\tau)$ is the incremental specific intensity added in the direction $\hat{\mathbf{s}}$ owing to a single scattering event from direction $\hat{\mathbf{s}}'$ to $\hat{\mathbf{s}}$. To get the diffusion approximation of the above transport equation, we expand $I(\mathbf{r},\hat{\mathbf{s}},\tau)$ as

$$I(\mathbf{r},\hat{\mathbf{s}},\tau) \approx G(\mathbf{r},\tau) + 3\hat{\mathbf{s}}\cdot J(\mathbf{r},\tau)/4\pi,$$

where $G(\mathbf{r},\tau)$ and $J(\mathbf{r},\tau)$ are defined by

$$G(\mathbf{r},\tau) = \int I(\mathbf{r},\hat{\mathbf{s}},\tau) d\hat{\mathbf{s}} \ \text{ and } \ J(\mathbf{r},\tau) = \int \hat{\mathbf{s}} I(\mathbf{r},\hat{\mathbf{s}},\tau) d\hat{\mathbf{s}}.$$

The field auto-correlation $G(\mathbf{r},\tau)$ is related to the power spectrum of light through a Fourier transform with respect to τ. Under the assumption that $\mu_s >> \mu_a$, the diffusion approximation to (2.1) is obtained as [23];

$$\nabla\cdot D\nabla G(\mathbf{r},\tau) - (\mu_a + \frac{1}{3} < \Delta r^2(\mathbf{r},\tau) > \alpha k_0^2 \mu_s') G(\mathbf{r},\tau) = -q_0(\mathbf{r}-\mathbf{r}_0), \tag{2.2}$$

where k_0 is the modulus of propagation vector of light, $\mu_s' = (1-g)\mu_s$, α is the percentage of light scattered by the moving scatterers, g is the anisotropic factor of scattering and $D = \dfrac{1}{3(\mu_a + \mu_s')}$ is the optical diffusion coefficient. In the above model, we assume that the scattering is isotropic with a length scale $l^* = \frac{1}{\mu_s'}$. The term $q_0(\mathbf{r}-\mathbf{r}_0)$ is the isotropic source located at $\mathbf{r} = \mathbf{r}_0$. If we assume the medium is purely viscous, then the scattering particles are pictured to diffuse through the medium. Here $< \Delta r^2(\mathbf{r},\tau) >$ represents the *mean square displacement (MSD)* suffered by the particle at $\mathbf{r}$. We assume that MSD has a linear time evolution given by $< \Delta r^2(\mathbf{r},\tau) >= 6 D_B(\mathbf{r})\tau$, where $D_B(\mathbf{r})$ is the time independent particle diffusion coefficient related to the viscosity η of the medium [15]. We use the mixed boundary condition, to solve the propagation equation (2.2) for $G(\mathbf{r},\tau)$:

$$D(\mathbf{r})\frac{\partial G(\mathbf{r},\tau)}{\partial \mathbf{n}} = -G(\mathbf{r},\tau),$$

on the boundary, $\partial\Omega$. This implies that the light input is only from the source at $\mathbf{r}_0$. To simplify notation, we denote $A = 2\alpha\mu_s' k_0^2$ and $f = D_B$. Thus, we have

$$\begin{cases} \nabla \cdot D\nabla G(\mathbf{r},\tau) - (\mu_a + Af\tau)G(\mathbf{r},\tau) = -q_0(\mathbf{r}-\mathbf{r}_0) \\ D(\mathbf{r})\frac{\partial G(\mathbf{r},\tau)}{\partial \mathbf{n}} = -G(\mathbf{r},\tau) \end{cases} \tag{2.3}$$

The inverse problem presented here attempts to find the particle diffusion coefficient f using the boundary measurement of $G(\mathbf{r},\tau)$ and the forward model by posing it as a minimization problem. We employ the Lavenberg Marquardt method for the minimization, which involves the computation of Fréchet derivative and its adjoint. First, we present the existence of solution of forward operator and its regularity. We assume, for simplicity that $G(\mathbf{r},\tau)$ is positive, real and hence we can work with the boundary measurement of $G(\mathbf{r},\tau)$ rather than its modulus.

Remark 2.1. In a practical experiment, $G(\mathbf{r},\tau)$ is not easy (or impossible) to measure. The more realistic experimental measurement is the intensity autocorrelation $|g_1(\mathbf{r},\tau)| = |\frac{G(\mathbf{r},\tau)}{G(\mathbf{r},0)}|$ which is given by

$$< I(\mathbf{r},\tau)I(\mathbf{r},t+\tau) > \equiv g_2(\tau) = 1 + \beta|g_1(\mathbf{r},\tau)|^2.$$

Here β is a constant dependent on the collection optics used in the experiments. This indeed increases the computational difficulty. □

Notations: Let Ω be a open bounded subset of $\mathbb{R}^n$, $n \geq 2$. Let f be the function to be reconstructed starting with a known background value f'. Let Ω' be the region, fully contained in Ω such that f equals the back ground value f' outside Ω'. That is $f = f' + \rho$ with *supp* $\rho \subset \Omega'$, where $\Omega' \subset\subset \Omega$. Thus Ω' is the region of interest for the reconstruction, where f varies from the background value. The notation $\Omega' \subset\subset \Omega$ means that Ω' is open and $\overline{\Omega'} \subset \Omega$ and $supp f$ is the support of f, that is $supp f = \overline{\{x \in \Omega : f(x) \neq 0\}}$.

Let $L^2(\Omega)$ be the space of square integrable measurable functions with the norm defined by $\|u\|^2_{L^2(\Omega)} = \int_\Omega |u|^2$ and $H^1(\Omega)$ be the Sobolev space of $L^2(\Omega)$ functions whose weak(generalized) derivatives are also in $L^2(\Omega)$ with the norm given by $\|u\|^2_{H^1(\Omega)} = \|u\|^2_{L^2(\Omega)} + \|\nabla u\|^2_{L^2(\Omega)}$. The space $H^{-1}(\Omega)$ is the dual of $H^1_0(\Omega)$ with the dual norm, where $H^1_0(\Omega) = \{u \in H^1(\Omega) : u = 0 \,\text{on}\, \partial\Omega\}$ endowed with the H^1 norm itself. One can also define the $H^s(\Omega)$, but we skip the details [24]. Let $C(\bar{\Omega})$ be the space of continuous functions in $\bar{\Omega}$ with the Sup norm and $C(\bar{\Omega})'$ be the dual. By Riesz representation theorem, this dual space can be identified with the space $M(\Omega)$ of Radon measures.

2.1 Delta source Excitation

We use the method of *transposition* to prove the existence of the forward solution when the illumination to the object is from a collimated pencil of light, which means q_0 is a delta source at one transport mean free path inside the object from the boundary point of illumination [16]. The necessity of adopting such a method is due to the presence of the delta source on the right hand side of the forward operator. In order to get a weak solution $G(\mathbf{r},\tau)$ in $H^1(\Omega)$, we need a more regular source $q_0 \in H^{-1}(\Omega)$. A delta source q_0, is in $H^s(\Omega)$ if $s < -n/2$. Thus, $q_0 \in H^{-1}(\Omega)$ only if the dimension $n = 1$, but, in our situation $n \geq 2$, in particular $n = 2$ or 3 and hence $q_0 \notin H^{-1}(\Omega)$. Thus, we cannot apply standard weak formulation to get $G(\mathbf{r},\tau) \in H^1(\Omega)$. This indeed causes difficulty in future analysis and we are not in a position to carry out the entire analysis with delta source. But we show by the method of transposition that $G(\mathbf{r},\tau) \in L^2(\Omega)$ thus losing the smoothness of the forward solution.

Weak formulation with $q_0 \in M(\Omega) = C(\bar{\Omega})'$

Since $q_0 \in M(\Omega) = C(\bar{\Omega})'$, we need test functions in $C(\bar{\Omega})$ to define a weak formulation. We define the test functions via the solution to an adjoint PDE. Let ϕ be in a class to be defined later. Consider

$$\begin{cases} \nabla \cdot D\nabla\psi(\mathbf{r},\tau) - (\mu_a + Af\tau)\psi(\mathbf{r},\tau) = \phi \\ \psi + D\frac{\partial\psi}{\partial n} = 0. \end{cases} \tag{2.4}$$

Multiply (2.3) by ψ and (2.4) by $G(\mathbf{r},\tau)$, integrate by parts on each of the equations and then subtract to get the weak formulation

$$\langle \phi, G\rangle = -\langle q_0, \psi\rangle \tag{2.5}$$

We use the notation $\langle\cdot,\cdot\rangle$ to represent either the inner product or duality bracket which is self explanatory according to the functions involved inside. For example the RHS in (2.5) is a duality bracket and hence the weak formulation given in (2.5) is valid if $\psi \in C(\bar{\Omega})$ because then $\langle q_0, \psi\rangle$ will represent the duality. So we have to choose the test functions ϕ suitably so that the regularity of $\psi \in C(\bar{\Omega})$ is achieved.

Theorem 2.2. Let $\phi \in L^q$, $q > n/2$, $\frac{1}{p} + \frac{1}{q} = 1$ and $p < \frac{n}{n-2}$. Then there exists a unique $y \in L^p$ such that

$$\int y\phi = \langle q_0, \psi\rangle,\ \forall \phi \in L^q, \tag{2.6}$$

where ψ solves (2.4).

Proof. Since $\phi \in L^q$, $q > n/2$, the regularity of (2.4) implies that $\psi \in W^{2,q}(\Omega) \subset C^{0,\theta}(\bar{\Omega})$, $0 < \theta \le 1$ which in turn gives $\psi \in C(\bar{\Omega})$ and

$$\|\psi\|_{C(\bar{\Omega})} \le C\,\|\psi\|_{W^{2,q}} \le C\,\|\phi\|_{L^q}.$$

Now define $\Lambda : L^q \longrightarrow C(\bar{\Omega})$ by $\Lambda\phi = \psi$. Then, we have

$$\|\Lambda\phi\|_{C(\bar{\Omega})} = \|\psi\|_{C(\bar{\Omega})} \le C\,\|\phi\|_{L^q}.$$

This implies that Λ is continuous. Define the adjoint operator $\Lambda^* : M(\Omega) \longrightarrow L^p$ by the duality

$$\langle \Lambda^* q_0, \phi\rangle := \langle q_0, \Lambda\phi\rangle = \langle q_0, \psi\rangle$$

for all $q_0 \in M(\Omega)$. Here the first bracket is the duality between L^p and L^q and the second and third are the duality between $M(\Omega)$ and $C(\bar{\Omega})$. This is well defined and

$$|\langle \Lambda^* q_0, \phi\rangle| = |\langle q_0, \Lambda\phi\rangle| \le C\,\|q_0\|_{M(\Omega)}\,\|\psi\|_{C(\bar{\Omega})} \le C\,\|q_0\|_{M(\Omega)}\,\|\phi\|_{L^q}.$$

Hence

$$\|\Lambda^* q_0\|_{L^p} \le C\,\|q_0\|_{M(\Omega)}$$

which proves the continuity of Λ^* . Therefore, for a given $q_0 \in M(\Omega)$, the function $y = \Lambda^* q_0$ is also defined and satisfies (2.6). Uniqueness of y follows directly from (2.6) as $\int y\phi = 0\ \forall\phi \in L^q$, implies $y \equiv 0$ which proves the theorem.

The above theorem motivates the following definition.

Definition 2.3 (Transposition Solution)**.** For $q_0 \in M(\Omega)$, the function $G(.,\tau) \in L^p(\Omega)$ is called a *transposition solution* to the problem (2.3) if

$$\int_\Omega G(.,\tau)\phi = \langle q_0, \psi\rangle$$

for all $\phi \in L^q(\Omega)$ and $\psi \in C(\bar{\Omega})$ is the unique solution to the problem (2.4). □

Remark 2.4. The above theorem establishes the existence of a unique G. We also remark that, since in our case $n = 2$ or 3, we can as well take $q = 2$ and $p = 2$. Indeed $G(.,\tau) \in L^2(\Omega)$ and hence the trace $G(,.\tau)|_{\partial\Omega}$ is not well-defined. For the inversion, we need the boundary data/measurement, namely $G(.,\tau)|_{\partial\Omega}$ to be well defined in $L^2(\partial\Omega)$. For the further convergence analysis, we assume the source $q_0 \in L^2(\Omega)$ and we can use the standard weak formulation instead of the transposition method. □

2.2 Gaussian source

We assume source q_0 to be an isotropic Gaussian source located at a distance of one transport mean free path (typically 1 mm) inside the tissue so that $q_0 \in L^2(\Omega)$. Let V be the space of $H^1(\Omega)$ functions, but with the inner product defined as

$$\langle G, \psi\rangle = \langle \nabla G, \nabla\psi\rangle_{L^2(\Omega)} + \langle G|_{\partial\Omega}, \psi|_{\partial\Omega}\rangle = \int_\Omega \nabla G\cdot\nabla\psi + \int_{\partial\Omega} G\psi. \tag{2.7}$$

with the induced norm

$$\|G\|_V = \left[\|\nabla G\|^2_{L^2(\Omega)} + \|G\|^2_{L^2(\partial\Omega)}\right]^{1/2}.$$

We remark that the $\|.\|_V$ is equivalent to $\|.\|_{H^1(\Omega)}$. Consider the weak formulation of (2.3), as: Find $G \in V$ satisfying

$$\int_\Omega D\nabla G\cdot\nabla\psi + \int_{\partial\Omega} G\psi + \int_\Omega (\mu_a + Af\tau)G\psi = \int_\Omega q_0\psi \tag{2.8}$$

where $G \in V$. Define the bilinear and linear forms in $V \times V$ and V respectively by

$$B(G,\psi) = \int_\Omega D\nabla G\cdot\nabla\psi + \int_{\partial\Omega} G\psi + \int_\Omega (\mu_a + Af\tau)G\psi$$

$$L(\psi) = \int_\Omega q_0\psi.$$

Assume there are positive constants $b_1, a_1, a_2, a_3, a_4, a_5$ such that $0 < b_1 < D \le a_1$, $\|\mu_a\|_{L^\infty(\Omega)} \le a_2$, $\|f\|_{L^\infty(\Omega)} \le a_3$ $\|A\|_{L^\infty(\Omega)} \le a_4$ and then $\|\mu_a + Af\tau\|_{L^\infty(\Omega)} \le a_5$. These are standard assumptions which are realistic. Using Hölders inequality, we have

$$
\begin{aligned}
|B(G,\psi)| &\leq a_1 \left(\int_\Omega |\nabla G|^2\right)^{1/2} \left(\int_\Omega |\nabla \psi|^2\right)^{1/2} + a_5 (\int_\Omega |G|^2)^{1/2} (\int_\Omega |\psi|^2)^{1/2} \\
&\quad + \left(\int_{\partial\Omega} |G|^2\right)^{1/2} \left(\int_{\partial\Omega} |\psi|^2\right)^{1/2} \\
&\leq a_1 \left(\int_\Omega |\nabla G|^2 + \int_{\partial\Omega} |G|^2\right)^{1/2} \left(\int_\Omega |\nabla \psi|^2 + \int_{\partial\Omega} |\psi|^2\right)^{1/2} \\
&\quad + a_5 \left(\int_\Omega |G|^2\right)^{1/2} \left(\int_\Omega |\psi|^2\right)^{1/2} \\
&\quad + \left(\int_\Omega |\nabla G|^2 + \int_{\partial\Omega} |G|^2\right)^{1/2} \left(\int_\Omega |\nabla \psi|^2 + \int_{\partial\Omega} |\psi|^2\right)^{1/2}
\end{aligned}
$$

which gives

$$
\begin{aligned}
|B(G,\psi)| &\leq a_1 \|G\|_V \|\psi\|_V + a_5 \|G\|_{L^2(\Omega)} \|\psi\|_{L^2(\Omega)} + \|G\|_V \|\psi\|_V \\
&\leq (a_6) \|G\|_V \|\psi\|_V
\end{aligned}
$$

for some $a_6 > 0$. In order to prove the coercivity of B we proceed as below. Let $a_7 = min\{b_1, 1\}$, then

$$
\begin{aligned}
|B(G,G)| &\geq a_7 (\int_\Omega |\nabla G|^2 + \int_{\partial\Omega} |G|^2) + \int_\Omega (\mu_a + A f \tau) |G|^2 \\
&= a_7 \|G\|_V^2 + \int_\Omega (\mu_a + A f \tau) |G|^2
\end{aligned}
$$

Since by assumption $\mu_a + A f \tau \geq 0$, we have the coercivity condition

$$
|B(G,G)| \geq a_7 \|G\|_V^2.
$$

Now, L is a bounded linear operator defined on V. Thus for $q_0 \in L^2(\Omega)$ by Lax-Milgram lemma, there exists a unique $G \in V$ which satisfies the weak formulation (2.8). Further we have,

$$
\|G\|_V \leq C \|q_0\|_{L^2(\Omega)}. \tag{2.9}
$$

We also have the interior regularity; given $\Omega' \subset\subset \Omega$, there exists a constant $C > 0$ such that $G \in H^2(\Omega')$ and

$$
\|G\|_{H^2(\Omega')} \leq C \|q_0\|_{L^2(\Omega)}. \tag{2.10}
$$

Using the imbedding $H^2(\Omega') \hookrightarrow C(\overline{\Omega'})$, for $n = 2, 3$, we have $G \in C(\Omega')$ and

$$
\|G\|_{C(\Omega')} \leq C \|q_0\|_{L^2(\Omega)}. \tag{2.11}
$$

3 Fréchet Derivative operator

In order to solve the inverse problem, namely to determine f from the boundary values, first we need to understand the variations in G for small perturbations in f. We introduce, the corresponding Fréchet derivative operators in this direction both for the delta source and Gaussian source. In the forward propagation equation (2.3) for the basic quantity $G(\mathbf{r},\tau)$, we perturb $f(\mathbf{r})$ to $f(\mathbf{r}) + f^\delta(\mathbf{r})$ and obtain a perturbation in $G(\mathbf{r},\tau)$ by $G^\delta(\mathbf{r},\tau)$. That is we represent $G + G^\delta$ as the solution corresponding to $f + f^\delta$. Substituting these in (2.3), after simplification, we get the equation connecting $G^\delta(\mathbf{r},\tau)$ to $f^\delta(\mathbf{r})$, which we call the Fréchet derivative of the forward propagation equation;

$$\begin{cases} \nabla \cdot D\nabla G^{\delta}(\mathbf{r},\tau) - (\mu_a + Af\tau)G^{\delta}(\mathbf{r},\tau) = Af^{\delta}\tau G \\ G^{\delta}(\mathbf{r},\tau) + D\frac{\partial G^{\delta}(\mathbf{r},\tau)}{\partial n} = 0 \end{cases} \tag{3.1}$$

The existence of solution of the Fréchet derivative operator also depends on the nature of excitation, i.e., whether it is a Delta source or Gaussian. If it is a delta source, then the method of transposition can be employed to prove the existence of solution. For the Gaussian source, the usual weak formulation will give a unique solution. In this case, even for the Gaussian source excitation, there is another difficulty due the appearance of the product $f^{\delta}G$.

3.1 Delta source excitation

The presence of delta source will only give the solution $G(\mathbf{r},\tau)$ of the forward operator to be in $L^2(\Omega)$, thus lacking enough smoothness to give a meaning to the restriction of G to the boundary. Further the function on the right hand side of the equation (3.1) is only a L^1 function (as it is a product of two L^2 functions) which can be viewed as a radon measure. Again the solution G^{δ} can be interpreted as a transposition solution. For $\phi \in L^2(\Omega)$, let ψ solves the equation

$$\begin{cases} \nabla \cdot D\nabla \psi - ((\mu_a + Af\tau))\psi = \phi \\ \psi + D\frac{\partial \psi}{\partial n} = 0 \end{cases} \tag{3.2}$$

Thus, as previously, $\psi \in C(\bar{\Omega})$ and now define $G^{\delta} \in L^2(\Omega)$ as the transposition solution to (3.1). That is, G^{δ} satisfies the weak formulation

$$\langle G^{\delta}, \phi \rangle = \langle \mu, \psi \rangle$$

for all $\phi \in L^2(\Omega)$, and the duality pairings are in appropriate spaces. Here $\mu = A\tau f^{\delta}G$. Now

$$\int_{\Omega} \phi G^{\delta} = \langle \mu, \psi \rangle \leq \|\mu\|_{M(\Omega)} \|\psi\|_{C(\bar{\Omega})}$$

Using the regularity result, we have

$$\|\psi\|_{C(\bar{\Omega})} \leq C\|\phi\|_{L^2(\Omega)}$$

Taking $\phi = G^{\delta}$, we have

$$\|G^{\delta}\|^2_{L^2(\Omega)} \leq C\|\mu\|_{M(\Omega)} \|G^{\delta}\|_{L^2(\Omega)}$$

which gives

$$\begin{aligned} \|G^{\delta}\|_{L^2(\Omega')} \leq C\|\mu\|_{M(\Omega)} &\leq C\|f^{\delta}G\|_{L^1(\Omega)} \\ &\leq C\|f^{\delta}\|_{L^2(\Omega)} \|G\|_{L^2(\Omega)} \end{aligned}$$

3.2 Gaussian source excitation

For Gaussian source excitation, the right hand side of (3.1) is in $L^2(\Omega)$ if we assume $f^{\delta} \in L^2(\Omega)$ and the $Suppf^{\delta} \subset \Omega'$. Indeed, this is the region of reconstruction. In this case, we use the interior regularity (see (2.11)) for $G \in C(\Omega')$ to prove that $G^{\delta} \in H^1(\Omega)$, via the standard variational formulation for $n = 2,3$. This gives $A\tau f^{\delta}G \in L^2(\Omega)$ since $Suppf^{\delta} \subset \Omega'$ and we have

$$\|G^{\delta}\|_{H^1(\Omega)} \leq C\|f^{\delta}G\|_{L^2(\Omega)} = C\|f^{\delta}G\|_{L^2(\Omega')} \leq C\|G\|_{C(\Omega')} \|f^{\delta}\|_{L^2(\Omega')}. \tag{3.3}$$

Thus, we have

Theorem 3.1. For $n = 2,3,\ f, f^{\delta} \in L^2(\Omega)$ with $Supp f^{\delta} \subset \Omega'$, $\Omega' \subset\subset \Omega$, the problem (3.1) has a unique solution $G^{\delta} \in H^1(\Omega)$ and satisfies

$$\|G^{\delta}\|_{H^1(\Omega)} \leq C\|G\|_{C(\Omega')}\|f^{\delta}\|_{L^2(\Omega)}. \tag{3.4}$$

Here G is the solution of (2.3) corresponding to f. □

3.3 Adjoint of the Fréchet derivative

Let $G^* \in H^1(\Omega)$ solves the adjoint of the Fréchet derivative operator given by

$$\begin{cases} \nabla \cdot D\nabla G^* - (\mu_a + Af\tau)G^* = 0 \\ G^* + D\frac{\partial G^*}{\partial n} = \phi, \end{cases} \tag{3.5}$$

where $\phi \in L^2(\partial\Omega)$ is given. Using the weak formulation applied to the adjoint equation we get

$$\|G^*\|_{H^1(\Omega)} \leq C\|\phi\|_{L^2(\partial\Omega)}. \tag{3.6}$$

Using the interior regularity of the equation, we have

$$\|G^*\|_{H^2(\Omega')} \leq C\|\phi\|_{L^2(\partial\Omega)} \tag{3.7}$$

Now using the imbedding $H^2(\Omega') \hookrightarrow C(\Omega')$, for $n = 2,3$, we get

$$\|G^*\|_{L^\infty(\Omega')} = \|G^*\|_{C(\Omega')} \leq C\|\phi\|_{L^2(\partial\Omega)} \tag{3.8}$$

We use the same notation C to represent the constant, but it may vary from one equation to another and this will not cause any confusion. Assume a Gaussian source excitation and hence $G^{\delta} \in H^1(\Omega)$ and thus $G|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$. With this, we define the *forward Fréchet derivative map* $DF(f)$ given by

$$DF(f)(f^{\delta}) = G^{\delta}(\mathbf{r},\tau)|_{\partial\Omega} \tag{3.9}$$

Thus $DF(f)(f^{\delta})$ indicates the changes in the boundary values of the field for a change f^{δ} from the background value f. Using the standard definition of the adjoint, we get the *forward Fréchet derivative adjoint map* $DF^*(f)$ given by

$$DF^*(f)(\phi) = A\tau GG^*|_{\Omega'} \tag{3.10}$$

for all $\phi \in L^2(\partial\Omega)$. We remark that, we treat functions in $L^2(\Omega')$ as functions of $L^2(\Omega)$ by extending them to zero outside Ω'.

4 Approximate solution of inverse problem using method of regularized least square minimization

The field autocorrelation $G(\mathbf{r},\tau)$ will depend on the particle diffusion coefficient f and therefore denote $G(\mathbf{r},\tau) = G(\mathbf{r},\tau,f)$ to show the dependence. The inverse problem can be stated as follows: Given the measurements $G(\mathbf{r},\tau,f)$ on the boundary $\partial\Omega$, find f over Ω. Clearly, this problem is nonlinear and ill-posed which is usually solved by stating it as an optimization problem. We seek a minimizer

f^* that minimizes an objective functional J over an admissible class of f in which $G(\mathbf{r},\tau,f)$ satisfies the forward problem given in (2.3). Define the forward map $F(f)$ over $Dom(F) \subset L^\infty(\Omega)$ as

$$F(f) = G(\mathbf{r},\tau)|_{\partial\Omega} \tag{4.1}$$

With $f \in L^\infty(\Omega)$ and $q_0 \in L^2(\Omega)$, we have $G \in H^1(\Omega)$ which implies $G|_{\partial\Omega} \in H^{1/2}(\partial\Omega)$. Let M be the measurement $G|_{\partial\Omega}$ corresponding to a particular particle diffusion coefficient f to be reconstructed. Then, we define the objective functional $J(\rho)$ for $\rho \in L^2(\Omega')$ given by

$$J(\rho) = \frac{1}{2}\|F(\tilde{\rho}+f') - M\|^2_{L^2(\partial\Omega)} + \frac{\beta}{2}\|\rho\|^2_{L^2(\Omega')} \tag{4.2}$$

Here $\tilde{\rho} = \rho$ in Ω', $\tilde{\rho} = 0$ in $\Omega \setminus \Omega'$. Starting with an initial background value f' for the particle diffusion coefficient, we need to update f' to $f' + \rho$ to get a better approximation to the particle diffusion coefficient. This is done via the well-known *Tikhonov regularized minimization*, where we minimize $J(\rho)$ over admissible ρ. That is, find ρ which solves $\min\limits_{\rho \in L^2(\Omega')} J(\rho)$, where β is the Tikhonov regularization parameter.

Since we try to minimize the objective function $J(\rho)$, expand it in terms of Taylors series about ρ up to second order differential:

$$J(\rho + \delta\rho) = J(\rho) + DJ(\rho)(\delta\rho) + \frac{1}{2}D^2J(\rho)(\delta\rho, \delta\rho). \tag{4.3}$$

Here $DJ(\rho)(\delta\rho)$ is the differential of $J(\rho)$ in the direction $\delta\rho$. As explained earlier f can be expressed as $f = \rho + f'$, where f' defined on $\Omega \setminus \Omega'$ is known to us. Perturbation in f denoted by f^δ is carried out through ρ as $\delta\rho$ in Ω' only. The differential $DJ(\rho)(\delta\rho)$ can be derived by first principles from the expression of $J(\rho)$ as follows:

$$J(\rho) = \frac{1}{2}\langle F(\tilde{\rho}+f') - M, F(\tilde{\rho}+f') - M\rangle + \frac{\beta}{2}\langle\tilde{\rho},\tilde{\rho}\rangle$$

Differentiating the above expression in the direction $\delta\rho$ we have

$$DJ(\rho)(\delta\rho) = \langle\phi, DF(\tilde{\rho}+f')(\delta\rho)\rangle + \beta\langle\rho,\delta\rho\rangle, \tag{4.4}$$

where $\phi = F(\tilde{\rho}+f') - M$. The above expression can be replaced with an equivalent one by using the definition of the adjoint map $DF^*(f)(\phi)$ given as

$$\langle\phi, DF(\tilde{\rho}+f')(\delta\rho)\rangle = A\tau\langle\delta\rho\,, DF^*(\rho+f')(\phi))\rangle$$

Substituting the above expression in (4.4), we have the first order derivative of $J(\rho)$

$$DJ(\rho)(\delta\rho) = \langle A\tau DF^*(\tilde{\rho}+f')(\phi) + \beta\tilde{\rho}\,, \delta\rho\rangle$$

Define the gradient Gr of the cost function as

$$Gr(\rho) = DF^*(\tilde{\rho}+f')[F(\tilde{\rho}+f') - M] + \beta\tilde{\rho} \tag{4.5}$$

In a similar manner, we can derive the second order differential of $J(\rho)$. Neglecting the second order differential term of the adjoint map, $D^2F^*(f)(\phi)$, we have

$$D^2J(\rho)(\delta\rho,\delta\rho) = \langle DF^*(\tilde{\rho}+f')DF(\tilde{\rho}+f')(\delta\rho)+\beta\delta\rho,\delta\rho\rangle$$

Define the Hessian as

$$H(\rho)(\delta\rho) = DF^*(\tilde{\rho}+f')DF(\tilde{\rho}+f')(\delta\rho) \tag{4.6}$$

The gradient $Gr(\rho)$ and the Hessian $H(\rho)(\delta\rho)$ are connected through the linear system of equations

$$H(\rho)(\delta\rho) = -Gr(\rho) \tag{4.7}$$

This can be solved iteratively for ρ using the Gauss-Newton method given by

$$\rho_{i+1} = \rho_i - H(\rho_i)^{-1}Gr(\rho_i). \tag{4.8}$$

In the next section, we derive the necessary continuity (error) estimates for above scheme which is a crucial section of our paper.

4.1 Regularity estimates for the existence of minimizer

The Fréchet derivative operator defined in section 3 was derived by explicit perturbation in f and expressing the change G^δ in an operator form. We proceed to prove the existence of Fréchet derivative for the case in which the source is a Gaussian source. We also prove the continuity of the forward map $F(f)$ with respect to the parameter to be reconstructed i.e, f. We further prove the continuity of the adjoint map $DF^*(f)(\phi)$ with respect to the parameter f which is very crucial in proving the existence of minimizer.

Lemma 4.1. Assume $n = 2,3$. Let $f,\ f^\delta \in L^\infty(\bar{\Omega})$ with supp $f^\delta \subset \Omega'$, $f,\ f+f^\delta \geq \mathrm{a} > 0$ for some $a > 0$ in Ω. Consider the operators F, DF, DF^*, respectively given by the equations (4.1), (3.9), (3.10). Then, there exists a positive constant C such that

$$\|DF(f)\|_{\mathcal{L}(L^2(\Omega'),L^2(\partial\Omega))} \leq C, \tag{4.9}$$

$$\left\|F(f+f^\delta)-F(f)-DF(f)(f^\delta)\right\|_{L^2(\partial\Omega)} \leq C\left\|f^\delta\right\|^2_{L^2(\Omega')}, \tag{4.10}$$

$$\left\|F(f+f^\delta)-F(f)\right\|_{L^2(\partial\Omega)} \leq C\left\|f^\delta\right\|_{L^2(\Omega')}, \tag{4.11}$$

$$\left\|(DF^*(f+f^\delta)-DF^*(f))(\phi)\right\|_{L^2(\Omega')} \leq C\,\|\phi\|_{L^2(\partial\Omega)}\left\|f^\delta\right\|_{L^2(\Omega')}\left(1+\left\|f^\delta\right\|_{L^2(\Omega')}\right). \tag{4.12}$$

Proof. Multiplying (3.1) by G^* and (3.5) by G^δ, integrating by parts, we get

$$-\int_{\partial\Omega}\phi G^\delta = \int_{\Omega'} Af^\delta\tau GG^* = \int_{\Omega} Af^\delta\tau GG^*,$$

since $supp\, f^\delta \subset \Omega'$. Now onwards, we take $\phi = G^\delta$ in $\partial\Omega$, then we have

$$\left|\int_{\partial\Omega} G^\delta G^\delta\right| = \left|\int_{\Omega'} Af^\delta\tau GG^*\right|,$$

where G^* corresponds to $\phi = G^\delta|_{\partial\Omega}$. We, thus have

$$\left\|DF(f)(f^{\delta})\right\|^2_{L^2(\partial\Omega)} = \left\|G^{\delta}\right\|^2_{L^2(\partial\Omega)} = \left|\int_{\Omega'} A\tau f^{\delta} G G^*\right| \\ \leq C\left\|f^{\delta}\right\|_{L^2(\Omega')} \|G\|_{L^2(\Omega)} \|G^*\|_{L^{\infty}(\Omega')}.$$

Using (2.9) and (3.8), since $\phi = G^{\delta}$, we get

$$\left\|DF(f)(f^{\delta})\right\|^2_{L^2(\partial\Omega)} \leq C\left\|f^{\delta}\right\|_{L^2(\Omega')} \|q_0\|_{L^2(\Omega)} \left\|G^{\delta}\right\|_{L^2(\partial\Omega)}$$

which gives

$$\left\|DF(f)(f^{\delta})\right\|_{L^2(\partial\Omega)} \leq C\left\|f^{\delta}\right\|_{L^2(\Omega')} \|q_0\|_{L^2(\Omega)}.$$

This proves (4.9). Now, let f be perturbed by f^{δ} which induces a perturbation in G by G^{δ}. Substituting it in (2.3), we get an equation which solves for $G + G^{\delta}$ for the particle diffusion coefficient $f + f^{\delta}$. Introduce $p \in H^1(\Omega)$ which solves

$$\begin{cases} \nabla \cdot D\nabla p - (\mu_a + Af\tau)p = Af^{\delta}\tau G^{\delta} \\ p + D\frac{\partial p}{\partial n} = 0. \end{cases} \tag{4.13}$$

Then, using (2.3) and (3.1), it is easy to see that the trace of p restricted to boundary is given by

$$p|_{\partial\Omega} = F(f + f^{\delta}) - F(f) - DF(f)(f^{\delta}). \tag{4.14}$$

Now introduce $w' \in H^1(\Omega)$ which solves the adjoint of the above equation given by

$$\begin{cases} \nabla \cdot D\nabla w' - (\mu_a + Af\tau)w' = 0 \\ w' + D\frac{\partial w'}{\partial n} = \phi', \end{cases} \tag{4.15}$$

where $\phi' \in L^2(\partial\Omega)$. Then, we have the adjoint form

$$-\int_{\partial\Omega} \phi' p = \int_{\Omega} Af^{\delta}\tau G^{\delta} w'$$

Taking $\phi' = p$ on $\partial\Omega$ in (4.15), we get

$$\left\|F(f + f^{\delta}) - F(f) - DF(f)(f^{\delta})\right\|^2_{L^2(\partial\Omega)} = \left|\int_{\Omega'} A\tau f^{\delta} G^{\delta} w'\right|. \tag{4.16}$$

Using the similar interior regularity results used above, we do get

$$\|w'\|_{L^{\infty}(\Omega')} \leq C\|w'\|_{H^2(\Omega')} \leq C\|\phi'\|_{L^2(\partial\Omega)} = C\|p\|_{L^2(\partial\Omega)}$$

Now applying Hölders inequality to (4.16), we have

$$\left\|F(f + f^{\delta}) - F(f) - DF(f)(f^{\delta})\right\|^2_{L^(\partial\Omega)} \leq C\left\|f^{\delta}\right\|_{L^{\infty}(\Omega')} \left\|G^{\delta}\right\|_{L^2(\Omega')} \|w'\|_{L^{\infty}(\Omega')}$$

Using the estimate (3.3) and (2.11), we have

$$\left\|F(f + f^{\delta}) - F(f) - DF(f)(f^{\delta})\right\|^2_{L^2(\partial\Omega)} \leq C\left\|f^{\delta}\right\|^2_{L^{\infty}(\Omega)} \|p\|_{L^2(\partial\Omega)} \|q_0\|_{L^2(\Omega)}.$$

From (4.14), it follows that

$$\left\|F(f+f^\delta)-F(f)-DF(f)(f^\delta)\right\|_{L^2(\partial\Omega)} \le C_2 \left\|f^\delta\right\|^2_{L^\infty(\Omega)} \|q_0\|_{L^2(\Omega)}$$

which is (4.10). To prove (4.11), as done earlier, subtract (2.3) from the operator which solves for $G+G^\delta$ for a perturbed particle diffusion coefficient $f+f^\delta$ resulting in an equation which solves for v whose value restricted to the boundary is $F(f+f^\delta)-F(f)$. Hence v solves the equation

$$\begin{cases} \nabla\cdot D\nabla v-(\mu_a+Af\tau)v = Af^\delta\tau G \\ v+D\frac{\partial v}{\partial n}=0. \end{cases}$$

Let $v'\in H^1(\Omega)$, solves the adjoint problem given by

$$\begin{cases} \nabla\cdot D\nabla v'-(\mu_a+Af\tau)v' = 0 \\ v'+D\frac{\partial v'}{\partial n}=\psi. \end{cases}$$

where $\psi\in L^2(\partial\Omega)$. In the adjoint (weak) form of the above two system, substitute $\psi=v$ on $\partial\Omega$ and since $v|_{\partial\Omega}=F(f+f^\delta)-F(f)$, we get

$$\left\|F(f+f^\delta)-F(f)\right\|^2_{L^2(\partial\Omega)} = \left|\int_{\Omega'} Af^\delta G v'\right|$$

Applying the Hölders inequality

$$\left\|F(f+f^\delta)-F(f)\right\|^2_{L^2(\partial\Omega')} \le C\left\|f^\delta\right\|_{L^\infty(\Omega')}\|v'\|_{L^\infty(\Omega')}\|G\|_{L^2(\Omega')}.$$

Using the previous results, we obtain

$$\left\|v'\right\|_{L^\infty(\Omega')} \le C\left\|v'\right\|_{H^2(\Omega')} \le C\|\psi\|_{L^2(\partial\Omega)}$$

Then, we have

$$\left\|F(f+f^\delta)-F(f)\right\|_{L^2(\partial\Omega)} \le C_3\|q_0\|_{L^2(\Omega)}\left\|f^\delta\right\|_{L^\infty(\Omega')}.$$

To prove the last inequality, we proceed as follows: When the Fréchet derivative operator was derived in Section 3, we neglected the small term $A\tau f^\delta G^\delta$ from (3.1). We now need to consider the equation without neglecting this small term. Let G' solves the equation similar to that in (3.1) but without neglecting the term $A\tau f^\delta G^\delta$ as

$$\begin{cases} \nabla\cdot D\nabla G'-(\mu_a+A(f+f^\delta)\tau)G' = Af^\delta\tau G \\ G'+D\frac{\partial G'}{\partial n}=0. \end{cases}$$

In the same manner as done above, we derive the Fréchet derivative of the adjoint operator in (3.5) without neglecting the higher order perturbation terms as given below:

$$\begin{cases} \nabla\cdot D\nabla G'^{*}-(\mu_a+A(f+f^\delta)\tau)G'^{*} = Af^\delta\tau G^{*} \\ G'^{*}+D\frac{\partial G'^{*}}{\partial n}=0. \end{cases}$$

Then, we have the identification

$$DF^*(f+f^\delta)\phi = A\tau(G+G')(G^*+G^{'*})$$

and

$$DF^*(f)(f^\delta) = A\tau GG^*$$

Thus, we have the expression

$$-\left((DF^*(f+f^\delta)-DF^*(f))\phi\right) = A\tau[GG^{'*}+G'G^*+G'G^{'*}]$$

which gives

$$\|(DF^*(f+f^\delta)-DF^*(f))\phi\|_{L^2(\Omega')} \le C\Big(\|GG^{'*}\|_{L^2(\Omega')} + \|G'G^*\|_{L^2(\Omega')} + \|G'G^{'*}\|_{L^2(\Omega')}\Big)$$

Using the Hölders inequality

$$\|(DF^*(f+f^\delta)-DF^*(f))\phi\|_{L^2(\Omega')} \le C\Big(\|G\|_{L^2(\Omega')}\|G^{'*}\|_{L^\infty(\Omega')} + \|G'\|_{L^2(\Omega')}\|G^*\|_{L^\infty(\Omega')} + \|G'\|_{L^2(\Omega')}\|G^{'*}\|_{L^\infty(\Omega')}\Big)$$

Assuming $f^\delta \in L^\infty(\Omega')$, we get the existence of $G'^* \in H^1(\Omega)$ and then the regularity of G^* will give the regularity of G'^* as well. Combining, we have

$$\|G'^*\|_{L^\infty(\Omega')} \le C\|\phi\|_{L^2(\partial\Omega)}\|f^\delta\|_{L^2(\Omega')}$$

Substituting all the regularity results, we finally, get

$$\begin{aligned}\left\|(DF^*(f+f^\delta)-DF^*(f))\phi\right\|_{L^2(\Omega')} &\le C\bigg(\|\phi\|_{L^2(\partial\Omega)}\left\|f^\delta\right\|_{L^2(\Omega')}\|q_0\|_{L^2(\Omega')} \\ &\quad + \|\phi\|_{L^2(\partial\Omega)}\|f^\delta\|^2_{L^2(\Omega')}\|q_0\|_{L^2(\Omega')}\bigg) \\ &\le C\|\phi\|_{L^2(\partial\Omega)}\|f^\delta\|_{L^2(\Omega')}\left(1+\|f^\delta\|_{L^2(\Omega')}\right).\end{aligned}$$

This proves (4.12) and hence all inequalities in the lemma.

5 Convergence Analysis

The objective functional $J(\rho)$ defined on $dom(J) \subset L^2(\Omega')$ has a minimizer if certain conditions are imposed on J and $Dom(J)$. Specifically, we look for a weakly closed domain over which J is defined thus ensuring the weak limits to be in $Dom(J)$. In order to prove that J attains a minimum we need either convexity or weak lower semicontinuity of J. Since the functional J is nonlinear with respect to the parameter f, the convexity assumption is unrealistic. We assume that the functional is weakly lower semi continuous in order to prove the existence of minimizer.

Theorem 5.1. Let a be a positive real number and $A = \{\rho \in L^2(\Omega') : \rho + f' \ge a > 0\}$ and assume that the functional J is weakly lower semi continuous. Then J has a minimizer ρ_β in A.

Proof. Let $\{\rho_i\} \subset A$ with $J(\rho_i) \to M_\beta = inf\{J(\rho) : \rho \in A\}$. Then by definition of M_β, for $n \in \mathbb{N}$, there is a subsequence ρ_{i_n} such that

$$J(\rho_{i_n}) \leq M_\beta + \frac{1}{n} \leq M_\beta + 1 \tag{5.1}$$

Thus, we have

$$\frac{\beta}{2} \|\rho_{i_n}\|_{L^2(\Omega')} \leq J(\rho_{i_n}) \leq M_\beta + 1$$

Let $M = \frac{2}{\beta}(M_\beta + 1)$ and consider the set $B = A \cap \{\|\rho\|_{L^2(\Omega')} \leq M\}$. Then B is a closed and bounded set in $L^2(\Omega)$ and hence weakly compact in $L^2(\Omega)$. So the sequence ρ_{i_n} has a convergent subsequence again denoted by ρ_{i_n} which converges weakly to some $\rho_\beta \in B$. That is $\left\|\rho_\beta\right\|_{L^2(\Omega')} \leq M$ and $\rho_\beta \in A$.

Further, if the function J is weakly lower semi continuous, then

$$J(\rho_\beta) \leq \underline{\lim}_n J(\rho_{i_n}) \leq \lim_n (M_\beta + \frac{1}{n})$$

which proves $J(\rho_\beta) \leq M_\beta$. Since $\rho_\beta \in A$, we get $J(\rho_\beta) = M_\beta$ proves the theorem.

The iterative equation given in (4.8) will solve for a ρ which minimizes the RHS of the truncated Taylors expansion of objective functional J given in (4.3). The regularity estimates derived in section 4 can be used to prove that the iterative scheme will converge to a ρ^* which minimizes the functional J in the least square sense as given in (4.2).

Theorem 5.2. Assume $J(\rho)$ has a minimizer ρ_β. Let ρ_0 be the initial iterate which is close to ρ_β. Let the sequence $\{\rho_i\}$ generated by the minimization scheme $\rho_{i+1} = \rho_i - H(\rho_i)^{-1}G(\rho_i)$ lies in a bounded set. Then, for β large enough, we have $\rho_i \to \rho_\beta$.

Proof. Let ρ_1 be the next iterate obtained from iterative equation (4.8). We estimate $\rho_\beta - \rho_1$ in terms $\rho_\beta - \rho_0$ which will set up a strict contraction. Consider the following notations $F_0 = F(\rho_0 + f')$ and $F_\beta = F(\rho_\beta + f')$ and the relations $\rho_\beta - \rho_0 = f^\delta$, $f = \rho_0 + f'$, $\rho_\beta + f' = f + f^\delta$. We assume β is large enough so that the relation $\|H(\rho)^{-1}\| \leq \frac{1}{\beta}$ holds.

Denote $W = DF_0^*(F_\beta - M) - DF_0^*(F_\beta - F_0 - DF_0(\rho_\beta - \rho_0))$. We, now compute using (4.5) and (4.6);

$$\begin{aligned} W &= DF_0^*(F_0 - M) + DF_0^* DF_0(\rho_\beta - \rho_0) \\ &= Gr(\rho_0) - \beta\rho_0 + H(\rho_0)(\rho_\beta - \rho_0)\}. \end{aligned}$$

Therefore

$$\begin{aligned} H(\rho_0)^{-1}(W + \beta\rho_0) &= H(\rho_0)^{-1} Gr(\rho_0) + (\rho_\beta - \rho_0) \\ &= (\rho_0 - \rho_1) + (\rho_\beta - \rho_0) = \rho_\beta - \rho_1, \end{aligned}$$

by (4.8). That is

$$\rho_\beta - \rho_1 = H(\rho_0)^{-1}\left(W + \beta\rho_\beta + \beta(\rho_0 - \rho_\beta)\right).$$

Using the first two regularity estimates in Lemma 4.1, we get

$$\begin{aligned} \left\|DF_0^*(F_\beta - F_0 - DF_0(\rho_\beta - \rho_0))\right\| &\leq C\left\|F_\beta - M) - DF_0^*(F_\beta - F_0 - DF_0(\rho_\beta - \rho_0)\right\| \\ &\leq C\left\|\rho_\beta - \rho_0\right\|^2. \end{aligned}$$

Thus we have

$$\|\rho_\beta - \rho_1\| \le \frac{1}{\beta}\left(\|DF_0^*(F_\beta - M) + \beta\rho_\beta\| + C\,\|\rho_\beta - \rho_0\|^2 + \beta\|\rho_\beta - \rho_0\|\right).$$

But, for minimization of the functional J, we have $G_r(\rho_\beta) = DF_\beta^*(F_\beta - M) + \beta\rho_\beta = 0$ which gives

$$\|\rho_\beta - \rho_1\| \le \frac{C}{\beta}\left(\left\|\left(DF_0^* - DF_\beta^*\right)(F_\beta - M)\right\| + \|\rho_\beta - \rho_0\|^2 + \|\rho_\beta - \rho_0\|\right)$$

Again by Lemma 4.1, the first term on RHS can be estimated by $\|\rho_\beta - \rho_0\|$ and hence we get

$$\|\rho_\beta - \rho_1\| \le \frac{C}{\beta}\|\rho_\beta - \rho_0\|$$

So, β sufficiently large, we see that the above inequality is a strict contraction for the iterative procedure. Hence we have the convergence.

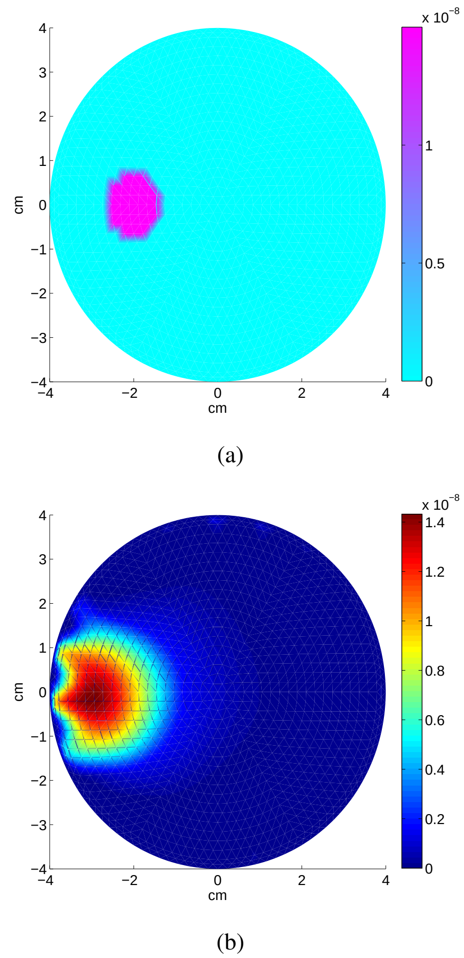

Fig. 1 (a)The grey level plot of the original particle diffusion coefficient distribution (cm^2/sec) used in simulation (b) The grey level plot of the reconstructed particle diffusion coefficient distribution (cm^2/sec)

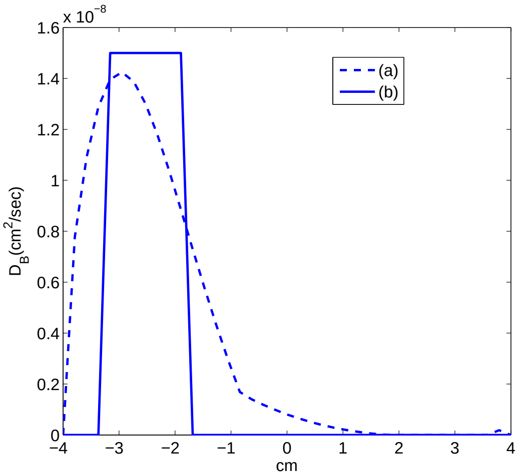

Fig. 2 Cross-sectional plots of reconstructed particle diffusion coefficient distribution through the center of the inhomogeneity (dashed curve (a)) as well as the original inhomogeneous object (solid curve (b)).

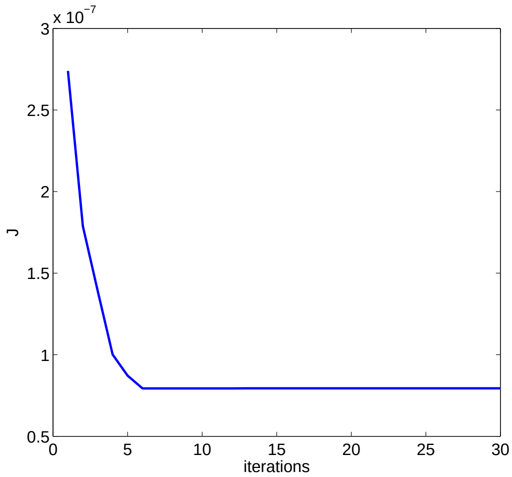

Fig. 3 Decay of the objective functional J with the iteration number

6 Numerical Simulations

The object used in our numerical simulations is circular, taken as the cross-section of a cylinder of diameter 8 cm. The background optical and mechanical properties are kept as $\mu_a^b = 0.001\ cm^{-1}$, $\mu_s'^b = 8cm^{-1}$ and $D_B^b = 0\ cm^2/sec$. There is a circular inhomogeneous inclusion in this object of diameter 1.4 cm which is a D_B-inhomogeneity of $1.5\times 10^{-8}\ cm^2/sec$ at $(-2.5cm, 0cm)$ (The object is assumed to be centered at the origin of the coordinate axes). Therefore the inclusion in the background is

$$D_B(x,y) = 1.5\times 10^{-8} cm^2/sec \quad if \quad \sqrt{(x+2.5)^2+(y)^2} \leq 0.7$$

To generate numerically the experimental data, (2.3) is discretized using the FEM with 1933 nodes and 3723 triangular linear elements. For a collimated source on the boundary, forty detectors are placed equi-angularly on either sides of the diametrically opposite point to the source location, to cover an overall angle of 320 degrees. The discretized forward equation is solved for $G(\mathbf{r},\tau)$ for $\tau = 10^{-6} sec$. The experimental data sets is generated by adding 1% Gaussian noise to $G(\mathbf{r},\tau)$. The above procedure is repeated by rotating the source-detector combination by steps of ten degrees to gather 36 sets of forty readings each.

For inversion of data, we use a coarser mesh, discretizing the domain with 1243 nodal points and 2376 triangular elements. We start the reconstruction algorithm with an initial guess of the property D_B^b which is the background value. Then we calculate the Gradient and Hessian for the measurement $G(\mathbf{r},\tau)$ using the (4.5) and (4.7) described in section 4. The new update is obtained using (4.8), where we use an appropriate regularization parameter β set through trial and error.

Once the updated D_B is obtained, the gradient and Hessian terms are recomputed at the new parameter distribution and (4.8) is itself updated. Inversion of the updated (4.8) gives us the current update for D_B to continue the iteration. The algorithm gave stabilized reconstruction of $D_B(\mathbf{r})$ in about $8-10$ iterations as indicated by the low plateau region reached in the plot of the objective functional vs. iteration number (figure 3).

The grey level plots of the original and the reconstructed D_B distribution are shown in figures 1(a) and (1)(b) respectively. The cross-sections through the centre of the inhomogeneity of the reconstructed and the original D_B distributions are shown in figures 2(a) and 2(b) respectively. From the reconstructed images it is clear that the quantitative recovery of the particle diffusion coefficient D_B from the boundary measurement of $G(\mathbf{r},\tau)$ is reasonably good. The *a priori* convergence analysis done for the Levenberg-Marquardt algorithm is supported by the numerical convergence of the algorithm as indicated by the decay of the error functional J as the number of iteration advances. It is also seen that the rate of convergence of the cost function with the number of iteration decreases as iteration becomes larger. The rate of convergence can be modified by selecting suitable regularization operators instead of the identity operator used for analysis.

7 Conclusion

In this work, we have addressed the mathematical analysis of the inverse problem associated with the propagation of field autocorrelation through a turbid medium. Of the coefficients of the PDE which govern the propagation, which are the optical properties (absorption and scattering coefficients) and the mechanical properties (the MSD approximated through a particle diffusion coefficient) of the medium we have considered the problem of recovering only the particle diffusion coefficient. However the same analysis can easily be extended to the recovery of optical properties as well, particularly the absorption coefficient. Of major concern in the reconstruction is the forward operator which connects the unknown property distributions to the boundary measurement, and its Fréchet derivative. We have established the existence of an L^2 solution of the forward operator when the illumination is from a delta source (a problem that cannot be handled through the usual variational weak formulation of PDE's) by using the method of transposition, which enables us to handle very weak data sets. The parameter recovery is achieved through solving a nonlinear minimization problem, for which the *LM* method is used. We have also proven the existence of the minimizer for the error functional and the convergence of the algorithm to reach this minimum. *En route* to proving this convergence we have proven (i) the existence and Fréchet differentiability of the forward operator and (ii) the continuity of the Fréchet derivative and its adjoint. We have proven the working of the algorithm by numerical reconstruction of particle diffusion coefficient from simulated boundary field correlation data. A complete application of the numerical procedure to reconstruct both mechanical and optical properties will appear in another publication.

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