Hyperspectral Diffuse Optical Tomography Using the Reduced Basis Method and Sparsity Constraints

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HYPERSPECTRAL DIFFUSE OPTICAL TOMOGRAPHY
USING THE REDUCED BASIS METHOD AND SPARSITY
CONSTRAINTS

A Dissertation
Presented to
the Graduate School of
Clemson University

In Partial Fulfillment
of the Requirements for the Degree
Doctor of Philosophy
Mathematical Sciences

by
Rachel Elizabeth Grotheer
May 2016

Accepted by:
Dr. Taufiquar Khan, Committee Chair
Dr. Jeong-Rock Yoon
Dr. Christopher Cox
Dr. Hai Xiao
Abstract

Diffuse Optical Tomography (DOT) has long been investigated as an effective imaging technique for soft tissue imaging, such as breast cancer detection. DOT has many benefits, including its use of non-ionizing light and its ability to produce high contrast images, but it also has low resolution. In recent years hyperspectral DOT (hyDOT) has been proposed, in an effort to improve that resolution by adding more information in the spectral domain. In this imaging modality, hundreds or even thousands of different wavelengths in the visible to near infrared range are used in the imaging process. Since tissue absorbs and scatters light differently at different wavelengths, it has been conjectured that this increase of information should provide images that give a better overall idea of the complete spatial reconstruction of the optical parameters.

Although hyDOT has been investigated experimentally, a formal theoretical investigation into its mathematical foundations has not been thoroughly performed. This dissertation seeks to lay the groundwork for the mathematical formulation of this imaging modality. First, the forward problem for hyDOT is formulated and the spectral regularity of the solution investigated. We demonstrate that the solution to the governing PDE is very smooth with respect to wavelength. This spectral regularity allows for the application of a model reduction technique to the forward problem known as the Reduced Basis Method. Several proofs are given for the hyDOT
forward solution and the spectral regularity term, including existence and uniqueness proofs and proofs showing the continuity of the solution with respect to the diffusion and absorption coefficients and the wavelength. The appropriate function spaces for the optical coefficients with respect to their dependence on the wavelength are explored and a new norm is proposed.

Additionally, the hyDOT inverse problem is formulated. New cost functionals are proposed to solve the inverse problem that incorporate the spatial sparsity of the optical parameters and their spectral regularity. Finally, a gradient-based reconstruction algorithm that enforces the spatial sparsity with respect to wavelength, is shown to be very effective and robust in solving the hyDOT inverse problem when used on simulations with a simple geometry.
Dedication

To the glory of God and to my parents.
Acknowledgments

It’s difficult to summarize my gratitude for all the people who have loved, supported, and encouraged me and helped me to grow throughout my years in graduate school. Of course, one does not even get to graduate school with the love and support of many others along the way and my thanks goes to all who helped me to that point as well.

Academically, there are many that I would like to thank. First and foremost, I am grateful for my advisor, Dr. Taufiquar Khan, who advised me ever since my first year at Clemson. He has always had confidence in my abilities and has encouraged me to pursue my passions and do what was best for me since the beginning. I am also thankful for the many opportunities he opened for me, such as spending a summer in Bremen, Germany and a semester working with the Air Force Research Lab in San Antonio, TX. I special thank you to Peter Maass’ group in Bremen, and Robert Thomas, Ted Early and all of the wonderful people at the AFRL for making my time in both those places enjoyable and rewarding.

Thank you to all the mathematical sciences faculty and staff at Clemson who have been so kind and supportive. I would like to especially thank my committee members Dr. Jeong-Rock Yoon, who gave me an excellent foundation in rigor, and Dr. Chris Cox, who has always been available over the years to listen and offer help whenever I needed it. I would also like to thank Dr. Hai Xiao from the Electrical
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A deep thanks to Jeannie Friedel and Andrew Hill, my first and closest friends in
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generally for being good friends and colleagues.

A special thank you to my roommates over the years: Kate Ritchey, Lauren
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cried, had fun, had serious and thought-provoking discussions, and shared meals,
and we learned to survive grad school together. To my dear friends Ashley Hornsby,
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the years have helped me more than you can know. I can not thank you enough and
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spending time with you every Friday night was one of the highlights of my week.
Finally, I would like to thank my church family at Clemson Presbyterian Church and
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death a false theology of striving to be “good enough”, and silence the menacing whispers of imposter syndrome. Surviving grad school would not have been possible without those things. I love you all and I am grateful that no earthly distance can keep us apart.

And last, but certainly not least, I would like to thank my dear family. Back when I was a little girl I always said I would get a Masters’ in math just like my dad. I forgot about that dream over the years and certainly never thought I’d be here at the end with my PhD. This would not have been possible if I did not have parents who believed I could do anything, who encouraged me to follow my desires, who comforted me when things got hard, and gave me the words I needed to hear when I felt like giving up (which happened many times). I know they would have been just as proud of me if I hadn’t made it all the way through, and that knowledge is invaluable. I love you both so much. I also am thankful to my dear brothers, John and Joseph, and to my sister-in-law Anne, for their encouragement over the years, patience when I lost my temper, and understanding and kindness when I had to miss family boat trips to study. And thank you to my dear Aunt Bep, who never stopped believing in me and has been a firm supporter of mine all these years.

I know there are many I forgot to thank or thanked inadequately. When I look back at all the people who have touched my life in just these few years, I am overwhelmed. But the biggest praise goes to my loving God, who gave me the ability to learn math and get a PhD. I literally would not be here without Him. I only pray that I would use this gift as He intends it to be used: for His kingdom and His glory.
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Chapter 1

Introduction

In recent years optical imaging, imaging using a low-energy light source in the visible to near infrared range, has become a popular alternative in medical imaging to traditional imaging techniques such as x-ray or computed tomography (CT). The advantages of optical imaging are that the low-energy light is non-ionizing and thus, not harmful to tissue, the devices cost less than existing medical imaging devices, and they are helpful in providing functional, rather than anatomical, information [4]. The functional information that optical imaging provides pertains to potential physiological changes in the tissue since chromophores such as haemoglobin and cytochrome can be identified by their individual absorption coefficients [97]. Further, optical imaging has the benefit of being able to distinguish between different kinds of soft tissues, whereas this distinction cannot be detected by other imaging modalities. This is due to tissues having different absorption and scattering properties within the wavelengths used in optical imaging.

Since optical imaging is especially effective in reconstructing images of soft tissue where light penetrates more easily, one of the most desired applications of this imaging technique is in breast cancer detection. Currently, the most common imaging
modality for breast cancer detection is mammography. However, mammography has many drawbacks such as the harmful radiation of the X-ray and the reliance on painful manipulation of the breast due to the coaxial nature of the imaging (that is, everything must be on the same plane) [97]. Optical tomography is a desirable alternative not only because the light source is non-ionizing, but also because the tomographic, or “slicing” nature of the imaging means that no manipulation of the tissue is required. Additionally, X-ray mammography is not effective at imaging dense breast tissue and cannot distinguish between malignant and benign tumors. Additionally, it has up to a 22% false negative rate for women over 50 (the women most likely to be screened) [18]. Optical tomography also has applications in other sorts of non-invasive procedures involving soft tissue, such as testing the oxygenation of blood in the brains of newborns (for this and other applications, see [4, 5, 37, 45] and the references therein). Overcoming the ill-posedness of the the inverse problem in the image reconstruction for optical imaging has been crucial in the process of making this type of imaging more accessible in practice rather than just attractive in theory.

1.1 Diffuse Optical Tomography

Diffuse optical tomography, a type of optical imaging, is the process of imaging an object through sectioning by use of an optical wave, that is, a wave from a light source. Typically, this source is laser light in the visible (about 400 to 700nm) or near infrared range (about 700 to 1600 nm). Tissue is a highly scattering medium and so, as the collimated laser beam passes through the tissue some of the light is absorbed by chromophores (such as hemoglobin, lipid and water), but most is scattered. In fact, in the near-infrared range (specifically about 650 to 950 nm), it has been shown
that absorption of light by biological tissue is minimized, and so it can penetrate up to about 6 cm in breast tissue and about 2 to 3 cm in the brain and joints [52].

Detectors placed on the boundary of the tissue collect the scattered beams, and from this data a 2-D image (slice) of the tissue is reconstructed in the form of a spatial map of the tissue’s absorption and scattering coefficients [52]. This is demonstrated in Figure (1.1). The reduced scattering coefficient is the reciprocal of the photon transport mean-free path which is the average distance traveled by a photon before its direction is randomized by interaction with another object. The absorption coefficient is the reciprocal of the average distance traveled by a photon before it is absorbed. Both of these coefficients are dependent on the wavelength, \( \lambda \), of the light source [31]. Since cells in tumors have higher absorption coefficients than normal cells due to an increased water or ionic concentration, and they also scatter photons differently, the absorption and scattering coefficients of the cells being imaged are the most important parameters to be determined in most medical applications [52, 99]. In fact, it has been shown experimentally that breast tissue with malignant tumors has more than 50% higher water, deoxy- and oxy-hemoglobin content than healthy breast tissue [18, 50, 51].

The forward problem in OT is to determine the measurements, \( g \), on the boundary \( \partial \Omega \) of the medium \( \Omega \) given a light source, \( f \), on the boundary and the absorption and scattering coefficients, \( \mu_a \) and \( \mu_s \), respectively, for all locations \( x \in \Omega \). The relationships between these variables is most often described using the radiative transport equation (RTE):

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \hat{s} \cdot \nabla I + (\mu_a + \mu_s)I = \mu_s \int p(\hat{s}', \hat{s})I(x, \hat{s}')d\hat{s}'
\]  

(1.1)

where \( I(x, \hat{s}, t) \), the variable of interest, is the specific intensity, also known as the
Figure 1.1: Diagram representing the placement of detectors along the boundary of a 3-D medium in a typical Optical Tomography set-up, with a 2-D slice of the scattering and absorption parameters as the output (from [22, 45]).

spectral radiance (number of photons per unit volume), at position \( x \), in the direction \( \hat{s} \) at time \( t \) [7, 56].

Since the RTE is computationally expensive, an approximation is usually used. The most common approximation is the diffusion approximation, which results in a modality known as diffuse optical tomography (DOT). In the time domain mode of DOT, where the laser source is a high-power pulsed laser, the forward problem is expressed using the photon diffusion model

\[
- \frac{n \partial \Phi(x,t)}{c} + \nabla \cdot D \nabla \Phi(x,t) - \mu_a \Phi(x,t) = -S(x,t) \tag{1.2}
\]

where \( n \) is the refractive index of the medium, \( c \) is the speed of light in a vacuum, \( \Phi \) is the photon density, \( S \) is the strength of the source, and \( D \) is the diffusion coefficient, expressed as \( D = 1/3(\mu_a + \mu'_s) \) where \( \mu_a \) is the absorption coefficient and \( \mu'_s \) is the reduced scattering coefficient [4, 7, 52]. The diffusion model is a first-order approximation to the radiative transport equation, assuming \( \mu'_s \gg \mu_a \) and the detector and source are not too close together [7, 52]. It is obtained from the RTE through the \( P_N \) approximation where the angular dependence of the intensity
is expanded in spherical harmonics and only the first order terms are kept \[7, 56\]. The derivation of this approximation is given in Appendix A. The approximation in (1.2) is a parabolic differential equation in the time-dependent case and an elliptic differential equation in the frequency domain \[4, 7\]. The inverse problem of DOT is a nonlinear, ill-posed problem of estimating the optical parameters, \(D, \mu_a\) given a known source, \(f\), and the boundary measurements, \(g\) \[52, 49\]. The 2-D spatial maps of the optical parameters for each slice are assembled to get a three-dimensional image of the object.

### 1.2 Hypersectral Imaging

Hyperspectral imaging (HSI) is an imaging modality involving the use of hundreds of optical wavelengths that has been generating a lot of research in recent years, specifically regarding its application to remote sensing, and geospatial and military imaging \[92, 95\]. Recently, researchers have been looking at HSI’s applications in the medical field as a tool for non-invasive disease diagnosis and surgical guidance \[65\]. HSI has been suggested for diverse medical applications such as to determine depth of burn damage \[27\], to monitor blood oxygenation levels in the extremities of diabetes patients to look for signs of peripheral arterial disease (PAD) \[80, 81\], to aid diagnosis of oral carcinoma biopsies \[77\], and to detect prostate tumors \[36\]. HSI is a hybrid modality, combining imaging with spectroscopy by collecting spectral information at each pixel of an array while scanning through different wavelengths to generate a three-dimensional hypercube of spatial and spectral data \[65\]. A comparison between a hyperspectral hypercube and a traditional RGB image is given in Figure (1.2). Naturally, the reconstruction for HSI results in an image with high spectral resolution, but generally low spatial resolution which degrades the detection and recognition of
important features [102]. Hyperspectral imaging can be applied to any optical imaging modality, such as DOT, to increase the spectral resolution of the image while maintaining the high spatial resolution given by the optical imaging modality. Some disadvantages have been shown for imaging at just one wavelength. For example, it has been shown that for a continuous wave optical imaging system, a system where the laser light is emitted at a constant intensity or modulated at a low frequency, measuring only intensity at a single wavelength was not enough to distinguish between the effects of scattering and absorption, the two main quantities of interest in the image reconstruction problem [6]. Another benefit of adding hyperspectral imaging to medical optical tomography is that the imaging process can be accelerated so that near real-time screening may be possible. Hyperspectral DOT is just starting to be explored experimentally and has not yet been rigorously mathematically formulated. An example of a current application of hyperspectral DOT is to monitor and map human brain activity as a function of depth in the brain [59]. Cho et al. [21] have also introduced a wavelength-swept laser that is cost effective and eliminates light from the unhelpful ends of the spectrum (that is, the ultraviolet and mid-infrared light) in order to have a more effective multi-wavelength implementation of DOT than current methods.

One of the main topics this dissertation seeks to explore is if and how hyperspectral DOT improves image reconstruction in comparison with DOT. It has been demonstrated that data sets obtained by hundreds or thousands, compared to just one or dozens of wavelengths, improves the quality of the DOT image reconstruction by providing more information about the chromophores [18, 60, 61, 62]. For example, two of the primary indicators of cancer, angiogenesis and hypermetabolism, can be detected by observing the concentration and oxygen saturation of hemoglobin in blood. Since hemoglobin, like other chromophores, absorbs photons when the photons’ en-
ergy matches a level between its internal energy states, the absorption levels vary by wavelength. Thus, the concentration and oxygen saturation of the hemoglobin will be most clearly seen when absorption levels at several wavelengths are examined [65]. In fact, all the absorption chromophores (oxy-Hb, deoxy-Hb, H$_2$O, and lipid) have unique spectral signatures and thus can be derived from the absorption coefficient when multiple wavelengths are used in the imaging [52, 101]. An illustration of the chromophores dependence on wavelength (from [101]) is given in Figure 1.3.

Imaging at several wavelengths has been shown to improve the reconstruction for hybrid modalities as well. Bal and Ren [8] have shown that only two of the three optical parameters in Quantitative Photoacoustic Tomography (QPAT), a hybrid optical and acoustic modality, can be reconstructed uniquely, regardless of the number of radiation illuminations. However, Bal and Ren also showed that in a multispectral setting, that is, when data from several optical wavelengths is available, all three coefficients can be reconstructed simultaneously and stably assuming that the dependence of $D$ and $\mu_a$ is different for at least two wavelengths and the three
Figure 1.3: The spectral dependence of the absorption chromophores in biological tissue (from [101]).

optical parameters are sufficiently smooth with respect to $\lambda$ [9]. These are encouraging results that this dissertation extends to purely optical modalities, demonstrating that the optical parameters $D, \mu_a$ have a great deal of smoothness with respect to $\lambda$.

There are many ways to computationally solve the inverse problem that arises from hyperspectral DOT, though the addition of a spectral dimension to the already large spatial dimension makes the computational burden large. Dimension reduction is thus key. Efforts have been taken to find computationally efficient algorithms for the already computationally expensive inverse problem for DOT at one wavelength [100] but the dimension reduction for hyperspectral DOT has not been thoroughly studied. There are two approaches in the discretization of the model, specifically with respect to the parameter $\lambda$. Most of the literature involves discretizing by looking at data from only a finite number of key optical wavelengths, and solving the PDE individually for each wavelength. For example, Corlu et al. have shown that in a
multispectral approach where the unknown parameters $\mu_a$ and $\mu_s$ are replaced with the unknown chromophore concentrations, if the measurement wavelengths are optimized so that the problem is spectrally constrained, the chromophore reconstruction problem has a unique solution [23]. This approach, however, becomes computationally expensive very quickly. Additionally, Saibaba et al. have developed algorithms to reduce the computational burden of hyperspectral DOT, using the Born approximation to linearize the forward model, but again, they only look at one wavelength at a time [89].

The second method is to parameterize the problem with respect to $\lambda$ and discretize by basis functions from a function space defined with respect to $\lambda$. The function space formulation needed for a rigorous approach is absent in the literature. Specifically, the regularity of the solution map, $\Phi$, and of the unknown optical parameters $D, \mu_a$ with respect to the wavelength $\lambda$ is not well documented.

It is for this reason that a substantial portion of this dissertation is dedicated to giving a rigorous analysis of the hyDOT forward and inverse problems, including looking at existence of solutions and the appropriate function spaces for the solutions and parameters. This analysis is given in Chapter 2 for the forward problem of both DOT and hyDOT, and in Chapter 3 for the inverse problem. Outlining the appropriate function spaces is essential to defining the appropriate norm and inner products to use for the cost functional in the inverse problem, as well as in the existence and uniqueness proofs. A DOT experiment without wavelength dependence
was modeled in [22] as

\[- \nabla \cdot (D \nabla u) + (\mu + i k) u = 0 \quad \text{in } \Omega \quad (1.3)\]

\[u + 2D \frac{\partial u}{\partial \nu} = f \quad \text{on } \partial \Omega \quad (1.4)\]

\[-D \frac{\partial u}{\partial \nu} = g \quad \text{on } \partial \Omega \quad (1.5)\]

where the source is incorporated as a Robin boundary condition, the forward problem (1.2) is solved, and the measurements are read out of the Neumann type boundary. Here, the solution, $u$, is the photon density and $k$ is the wave number that describes the modulation of the laser. The inverse problem of DOT assumes this map is complete in order to reconstruct the optical parameters $D, \mu_a, \mu_s$, where the latter two are referenced simply by $\mu$ in (1.3). However, in practice there are only a finite number of sources, $M$, so the inverse problem is formulated as an optimization problem with a cost functional [22]. By applying a Tikhonov type regularization with sparsity constraints, this minimization problem is given in [22] by

\[
\min_{q \in \bar{Q}} \frac{1}{2} \sum_{i=1}^{M} \left| \gamma_n F_r^{(k,q)}(0, f_i) - g_i \right|_{H^{-1/2}(\partial \Omega)}^2 + \alpha_D \sum_{i \in \mathbb{N}} |\langle \delta D, \phi_i \rangle_{H^1(\Omega)}| + \alpha_{\mu} \sum_{i \in \mathbb{N}} |\langle \delta \mu, \phi_i \rangle_{L^2(\Omega)}| 
\]

(1.6)

where $\gamma_n F_r^{(k,q)}(0, f)$ is the Robin to Neumann map given by (1.3) - (1.5) where $\gamma_n$ is the Neumann trace, $F_r^{(k,q)}(0, f)$ is the forward operator for the PDE with Robin boundary condition, $\alpha_D$ and $\alpha_{\mu}$ are the regularization parameters for $D$ and $\mu$, respectively, denoted by $q = (D, \mu)$, $\phi_i$ are the basis functions of the spatial variable and $q$ in the space $\bar{Q} = \{H^1(\Omega) \times L^2(\Omega) : 0 < D_0 \leq D \leq D_1, 0 < \mu_0 \leq \mu \leq \mu_1\}$, $f$ is a fixed source, and $g$ are the true Neumann measurements.

This work proposes several cost functionals similar to (1.6) for solving the inverse problem of hyDOT. These cost functionals seek to exploit the smoothness in
the spectral domain and sparsity in the spatial domain of the optical parameters. While several cost functionals for the hyDOT problem are proposed in Chapter 3, the main one, which is used for the simulations in Chapter 5 is

$$J_\alpha(q(\lambda)) = \int_{\lambda_0}^{\lambda_f} \omega(\lambda) \| \gamma_0 u - g \|_2^2 d\lambda + \int_{\lambda_0}^{\lambda_f} \sum_{k=1}^{\infty} \alpha_k(\lambda) |c_{k,\lambda} - \hat{c}_{k,\lambda}| d\lambda \quad (1.7)$$

The well-posedness of the forward problem for both DOT and hyDOT, and the existence of the gradients necessary for the inversion algorithm depend on the determination of the appropriate function spaces for the optical parameters. A complete description of these function spaces with their corresponding norms and inner products is given in Chapter 2. The analytical determination of the appropriate function spaces for hyDOT is unique to this work. Bal and Ren [9] have assumed that, for a similar imaging modality known as multispectral photoacoustic tomography (PAT), the unknown coefficients $D(\lambda)$ and $\mu(\lambda)$ lie in $C^1(\Omega)$. However, there has been no work to show that this assumption is valid, nor what the parameter space would be for a purely optical modality such as DOT. In this work we determine the topology of these coefficients with dependence on wavelength to give a more rigorous theoretical foundation. In fact, we show that the coefficients lie in a smooth topology, as Bal and Ren assumed, when only their dependence on wavelength is considered. Saibaba et al. [89] have provided a graph showing the spectral dependence of the absorption coefficient, $\mu_a$, shown here in Figure (1.4). The graph gives experimental evidence that $\mu(\lambda)$ is indeed very smooth. Since this is the case, we suggest that if the norm that includes this wavelength dependence is used in the image reconstruction this would lead to a more well-posed inverse problem.
Under the Born approximation, the scattered field is assumed to be much smaller than the incident field, i.e., \( s \ll i \). The size of the scatterers, and a scattering exponent \( b \), depends on the size of scatterers in the medium [17].

The reference wavelength is the concentration of species \( l \) for wavelengths in the near infrared range (from [89]). Further details support for the perturbation we wish to image. For the purpose of this paper, we will consider that the chromophore concentrations are co-located. This choice was also considered in [27].

For the diffusion approximation that governs DOT and hyDOT, the perturbation \( r \) corresponds to the detector location. To relate the scattered fluence to the concentrations of \( d \), \( s \), and \( a \), the differential equations can be obtained from the following references [25, 42, 78, 79, 82, 87].

Equations (2.2)-(2.3) can be replaced by

\[
D(\mu_a + \Delta \mu_a) \frac{\partial \Phi}{\partial r} + \mu_a \Phi = 0
\]

where

\[
\Phi = \sum_{l=1}^{L} \sum_{s} \sum_{a=l}^{A} \chi_{ls} \chi_{al} c_l s_a
\]

and therefore, the total fluence \( \Phi(d, r) \) can be derived using the reciprocity property of the adjoint field, which we call the adjoint field, can be derived using the reciprocity property of the Green's function and satisfies the system of equations along with the same boundary conditions in the equations (2.2)-(2.3). Furthermore, if additional information such as spatial variability is known about the background properties of diagnostically important scatterers, the perturbation \( r \) can be incorporated into this model [8].

The solution to the photon fluence rate equation (2.5) can be replaced by

\[
\frac{\partial \Phi}{\partial r} + \mu_a \Phi = 0
\]

where

\[
\Phi = \sum_{l=1}^{L} \sum_{s} \sum_{a=l}^{A} \chi_{ls} \chi_{al} c_l s_a
\]

It should also be noted that both the scattered field and the detection field is the concentration of species \( l \) as a function of the wavelength \( \lambda \) for wavelengths in the range [600, 1000] [nm]. The scattering pre-factor \( s \) is computed at the measurement location.

1.3 The Reduced Basis Method

Due to the added dimensionality from imaging at hundreds of wavelengths, reduction of the hyDOT problem is necessary for an accurate image reconstruction. In this work, we apply a dimensionality reduction technique known as the Reduced Basis Method (RBM). The RBM was originally applied to the structural analysis of beams and arches [2, 70, 75] but has recently been applied to solve PDEs of many types, including elliptic PDEs such as the diffusion approximation that governs DOT and hyDOT.

The RBM is most successful when it is applied to parameterized PDEs [25, 42, 78, 79, 82, 87]. This is due to the structure of the method. The RBM gives an approximate solution of a given PDE at any parameter value by using a linear combination of the exact (or finite element) solution of the PDE at a relatively small number of parameter values with respect to the number of basis elements in the finite element.
element solution. That is, if \( u \) is the solution to (1.3), (1.4), then

\[
u(\lambda) \approx \sum_{i=1}^{N} \hat{c}_i(\lambda) u(\lambda_i)
\]

where \( u(\lambda_i) \) is the finite element solution at \( \lambda_i \) and \( N \) is the number of elements in the reduced basis. We note that if the number of basis elements for the finite element solution is \( N \), then \( N \ll N \). Since hyDOT is parameterized by wavelength, it is an ideal candidate for use of the RBM.

Successful application of the RBM to the hyDOT forward problem demonstrated that only the “exact” solution at a small number of wavelengths was necessary to get a good approximation of the solution at any wavelength. The simulations in Chapter 5 also indicate that the reduced basis itself does not vary much with respect to the geometry of the problem. Thus, we conjectured that we would be able to use the same reduced basis to solve the forward problem in each iteration of the inversion algorithm for hyDOT to reduce the complexity. A complete analytical formulation for application of the RBM to the forward problem in hyDOT is given in Chapter 4. This chapter includes a discussion and comparison of different methods used to find a reduced basis. This work, given in [41], has been submitted for publication. A discussion of the difficulties of applying the RBM to the inverse problem of hyDOT and suggestions for how to implement it is given in the last section of Chapter 4.

1.4 Sparsity Regularization in Hyperspectral DOT

Once the analytical formulation for the hyperspectral case has been completed in Chapter 3, we extend the theory and application of sparsity regularization to broadband (hyperspectral) signals in DOT in an effort to improve the ill-posedness
of the problem. Sparsity is a natural consideration in medical DOT because the
goal is to find relatively small areas of high contrast with regards to the absorption
and scattering parameters which represent tumors against the healthy background
tissue. These isolated areas of high contrast against a dominant relatively homogenous
background allow for a sparse spatial basis and, hence, a sparse solution.

Hyperspectral imaging has been shown to be intrinsically sparse in the spa-
tial domain and smooth in the spectral domain, as the details of an image can be
represented by a small number of general structural shapes in the form of basis func-
tions [19, 102]. Zhao et al., for example, used basis elements taken from a dictionary
learned from panchromatic images along with $\ell_1$ regularization in the spectral do-
main to obtain a hyperspectral image in a geospatial imaging application with super-
resolution [102]. We show how sparsity can be exploited in hyDOT in the spatial
domain while incorporating the spectral dependence of the parameters in Chapter 3.
Specifically, in the cost functional given in (1.7) the sparsity regularization parameter
$\alpha$ is dependent on the wavelength $\lambda$. Some of the other cost functionals listed in
Chapter 3 include a sparsity term that enforces sparsity on terms that include the
spectral dependence more explicitly. Additionally, we have shown analytical results
for the solution $\frac{\partial u}{\partial \lambda}$ to the derivative of the PDE governing hyDOT with respect to
$\lambda$ in Chapters 2 and 3 to prove the validity of these functionals that they may be
implemented in the future.

The significant contribution of this dissertation is that it lays the mathematical
framework for exploring hyperspectral DOT that was not previously present in the
literature. Notably, we demonstrate the regularity of the forward solution of hyDOT
and the optical parameters in the spectral domain and show how this can be exploited
to apply model reduction to the forward and inverse problems. We show that the
solution at only a few wavelengths is sufficient to interpolate the solution at any
other wavelength. We combine this with the inherent sparsity of DOT in the spatial
domain, applying a sparsity term in the inversion algorithm that incorporates the
wavelength dependence of the parameters.

This dissertation is set up as follows. In Chapter 2 we establish the existence
and uniqueness of a solution for the DOT and hyDOT forward problems, and demon-
strate the well-posedness of each. We also discuss the regularity necessary for each
parameter and variable. In Chapter 3 we provide the analytical formulation for the
DOT and hyDOT inverse problems. Further, we suggest several cost functionals for
the minimization problem and describe the inversion algorithm. In Chapter 4 we
introduce the Reduced Basis Method and show how it may be applied to the hyDOT
forward and inverse problems. Finally, in Chapter 5 we give the simulated results of
applying the Reduced Basis Method to the hyDOT forward problem and applying the
reconstruction algorithm to the inverse problem for two relatively simple geometries.
Chapter 2

Analytical Formulation of the Forward Problem

In this chapter we will provide the analytical rigor for the hyDOT forward problem that provides the foundation for the simulation and experimental verification presented in Chapter 5. We will begin by proving the existence and uniqueness of a solution to the DOT forward problem and then prove the same for the hyDOT forward problem. This will help us to show that the forward problem of hyDOT is well-posed according to the definition of Hadamard [44]:

Definition 2.1. (Well-Posedness) A problem is said to be well-posed if

(i) a solution exists,

(ii) the solution is unique, and

(iii) the solution depends continuously on the data.

The third condition is also known as the sensitivity condition. The inverse problem for both DOT and hyDOT are ill-posed because they fail the third condition.
The solution to the inverse problem is very sensitive to small variations in the input, that is, the boundary measurements.

2.1 The DOT Forward Problem

The forward problem in DOT involves solving an elliptic partial differential equation with Robin boundary conditions where $\mu_a$ and $D$ are known. The solution, $u$, describes the photon density of the scattered light arriving at the detectors. The complete DOT experiment is given in the frequency domain as

\[-\text{div}(D \nabla u) + (\mu_a + ik)u = 0 \quad \text{in } \Omega, \quad (2.1)\]
\[u + 2D \frac{\partial u}{\partial n} = f \quad \text{on } \partial \Omega \quad (2.2)\]
\[-D \frac{\partial u}{\partial n} = g \quad \text{on } \partial \Omega, \quad (2.3)\]

where $D$ is the diffusion coefficient, $\mu_a$ the absorption coefficient, $k$ is the wave number of the modulation frequency of the laser, $f$ the source, $g$ the measurements of the scattered photons on the boundary, and $\Omega \subset \mathbb{R}^n$, $n = 2, 3$ a bounded, connected, Lipschitz domain.

More specifically, as discussed in the introduction, the interaction of the light photons being absorbed and scattered by the tissue is primarily modeled through the radiative transport equation (RTE), given in (1.1), which describes the transport of the photons through the tissue. The parameters of interest in the RTE are the diffusion and absorption parameters which are \textit{a priori} unknown. The difficulties of working with the RTE has prompted the use of the first order diffusion approximation to the RTE. This approximation is found using a $P_N$ approximation (specifically, $P_0$), which involves expanding the photon density $u$ and the source $g$ in spherical harmonics.
and retaining the first order terms. The time domain diffusion approximation is given by

\[
\frac{1}{c} \frac{\partial u}{\partial t}(x, t) - \nabla \cdot D(x) \nabla u(x, t) + \mu_a(x) u(x, t) = h(x, t) \tag{2.4}
\]

\[
u(x, 0) = 0 \quad \text{in } \Omega \tag{2.5}
\]

\[
u(x, t) + 2D(x) \frac{\partial u}{\partial \nu}(x, t) = 0, \quad x \in \partial \Omega \tag{2.6}
\]

where \(h\) is the interior forcing function, and the measurement is given by

\[
g(x, t) = -D(x) \nu(x) \cdot \nabla u(x, t) = -D(x) \frac{\partial u}{\partial \nu} \tag{2.7}
\]

In the time domain, this is a parabolic differential equation. In the frequency domain, (2.6) becomes

\[
-\nabla \cdot D(x) \nabla u(x, \omega) + \left( \mu_a(x) + \frac{i\omega}{c} \right) u(x, \omega) = h(x, \omega) \tag{2.8}
\]

through Fourier-transformation. Further, in the time-independent (or dc) case, the diffusion approximation is given by

\[
-\nabla \cdot D(x) \nabla u(x) + \mu_a(x) u(x) = h(x), \quad \text{in } \Omega \tag{2.9}
\]

\[
u(x) + 2D \frac{\partial u}{\partial \nu}(x) = f(x), \quad \text{on } \partial \Omega. \tag{2.10}
\]

For a complete derivation of the diffusion approximation from the radiative transport equation, see the Appendix. Note that \(D, \mu_a, u\) are all functions of the spatial variable \(x\). We also note that \(D, \mu_a\) are bounded. That is, there exist constants
$D_1, D_2$ and $\mu_1, \mu_2$ such that,

$$0 < D_1 \leq D \leq D_2 < \infty, \quad 0 < \mu_1 \leq \mu_a \leq \mu_2 < \infty.$$ (2.11)

Thus, $D, \mu_a \in L^\infty(\Omega)$. Finally, we define the parameter space to be

$$Q := \{(D, \mu) \in L^\infty(\Omega) \times L^\infty(\Omega) : 0 < D_0 < D < D_1, 0 < \mu_0 < \mu < \mu_1\}.$$ 

We define the Dirichlet trace,

$$\gamma_D : H^1(\Omega) \to H^{1/2}(\partial \Omega)$$

$$u \mapsto u|_{\partial \Omega}$$ (2.12)

the Robin trace,

$$\gamma_R : H^1(\Omega) \to H^{-1/2}(\partial \Omega)$$

$$u \mapsto (u + 2D \frac{\partial u}{\partial n})|_{\partial \Omega}$$ (2.13)

and the Neumann trace,

$$\gamma_N : H^1(\Omega) \to H^{-1/2}(\partial \Omega)$$

$$u \mapsto -D \frac{\partial u}{\partial n}|_{\partial \Omega}$$ (2.14)
where the spaces above are defined as

\[ H^1(\Omega) := \left\{ v \in L^2(\Omega) \mid \int_{\Omega} (|\nabla v|^2 + v^2) \, dx < \infty \right\} \]  
(2.15)

\[ H^1_0(\Omega) := \left\{ v \in H^1 \mid \int_{\partial\Omega} v \, ds = 0 \right\} \]  
(2.16)

\[ H^{1/2}(\partial\Omega) \cong \{ \gamma_D(v) \mid v \in H^1(\Omega)/H^1_0(\Omega) \} \]  
(2.17)

\[ H^{-1/2}(\partial\Omega) \cong \{ \gamma_N(v) \mid v \in H^1(\Omega)/H^1_0(\Omega) \}. \]  
(2.18)

We note that \( H^1_0(\Omega) \hookrightarrow H^1(\Omega) \hookrightarrow L^2(\Omega) \) and that \( H^{-1/2}(\partial\Omega) \) is the dual space of \( H^{1/2}(\partial\Omega) \). The inner product for the space \( H^1(\Omega) \) is

\[ \langle u, v \rangle_{H^1(\Omega)} = \int_{\Omega} (\nabla u \cdot \nabla \bar{v} + u \bar{v}) \, dx \]  
(2.19)

In general, these spaces are known as Sobolev spaces. The Sobolev space \( W^k_p(\Omega) \) is formally defined as

\[ W^m_p(\Omega) = \{ u \in L^p(\Omega) : D^\alpha u \in L^p(\Omega), \forall |\alpha| \leq m \}. \]

That is, \( W^k_p(\Omega) \) is the set of all functions in \( L^p(\Omega) \) whose \(|\alpha| \leq m \) weak partial derivatives are also in \( L^p(\Omega) \). It is convention to let \( W^m_2(\Omega) = H^m(\Omega) \), which we adopt here.

For DOT the measurement, \( g \), is typically considered to be in the Sobolev space \( H^{1/2}(\partial\Omega) \), the source in its dual space \( H^{-1/2}(\partial\Omega) \) and the photon density inside the medium in the Sobolev space \( H^1(\Omega) \), though in practice \( L^2(\partial\Omega) \) and \( L^2(\Omega) \), respectively, are used in their place [49, 22]. This replacement is partially due to the fact that the measurements, \( g \) are actually discrete and so we cannot truly say \( g \in H^{1/2}(\Omega) \) [49]. Though this replacement is done in practice, it has been shown
theoretically that for electrical impedance tomography (EIT) and DOT the choice of
inner product does make a difference in the reconstruction [49, 54]. Similarly, though
the coefficients $D(x), \mu_a(x)$ are generally assumed to be in $L^\infty(\Omega)$, in practice $D$ is
considered to be in $H^1(\Omega)$ and $\mu_a \in L^2(\Omega)$ for easier analysis for the uniqueness
arguments [22]. Thus, in this chapter we will assume $Q \in L^\infty(\Omega) \times L^\infty(\Omega)$ but
will need to consider the parameter space $\overline{Q} \in H^1(\Omega) \times L^2(\Omega)$ when proving results
regarding the inverse problem in Chapter 3. We also note that the results presented
here can be extended more generally for $D, \mu_a \in L^p(\Omega)$ and $u \in W^{1,q}$. While we do
not prove those results in this work, they are well-documented (see, e.g. [22]) and we
assume $L^p$ regularity to enforce the sparsity in Chapter 3.

To the show the first two conditions in Definition 2.1 hold, we will use the
Lax-Milgram Theorem for Sesquilinear Forms. A sesquilinear form is a generalization
of a bilinear form and is defined as follows.

**Definition 2.2.** (Sesquilinear form) A map $B : V \times V \to \mathbb{C}$ on a complex vector
space $V$ is called a sesquilinear form if

(i) $B(x + y, z + w) = B(x, z) + B(x, w) + B(y, z) + B(y, w)$, and

(ii) $B(ax, by) = \overline{a}bB(x, y)$

where $x, y, z, w \in V$, $a, b \in \mathbb{C}$ are constants and $\overline{b}$ is the complex conjugate of $b$.

**Theorem 2.3.** (Lax-Milgram Theorem) Let $B : H \times H \to \mathbb{C}$ be a sesquilinear form
on a Hilbert space, $H$, and $\langle \cdot, \cdot \rangle$ an inner product. If $B$ satisfies:

1. $|B(u, v)| \leq c_1 \|u\|_H \|v\|_H$ for all $u, v \in H$, and some constant, $c_1 > 0$ (bounded)

2. $B(u, u) \geq c_2 \|u\|_H^2$ for all $u \in H$, and some constant $c_2 > 0$ (coercive)
then there exists a unique bijective linear map $b : H \rightarrow H'$ that is continuous in both directions, uniquely determined by $B$, such that $B(u, v) = \langle Bu, v \rangle$ for all $u, v \in H$ and $B(b^{-1}w, v) = \langle w, v \rangle$ for all $v \in H$ and $w \in H'$, where $H'$ is the dual of $H$. In addition, $\|b\|_{\mathcal{L}(H, H')} \leq c_1$ and $\|b^{-1}\|_{\mathcal{L}(H', H)} \leq \frac{1}{c_2}$.

To obtain the sesquilinear form required in the Lax-Milgram Theorem, we find the weak formulation of equations (2.1) - (2.3). In fact, the weak formulation is necessary to ensure the existence of the required derivatives. That is, we cannot guarantee the appropriate smoothness of $u$ to guarantee the existence of $\nabla u$ and $\nabla \cdot (D\nabla u)$ in the strong sense [22, 34]. We require $u$ to be in the Sobolev space $H^1(\Omega)$ in order to guarantee the appropriate smoothness for this weak formulation, that is the existence of a derivative of $u$ in $L^2(\Omega)$ [22].

### 2.1.1 Well-Posedness of the Robin Problem

First we consider the Robin DOT problem which is to solve

$$\begin{align*}
-\text{div}(D\nabla u) + (\mu_a + ik)u &= 0 \quad \text{in } \Omega, \tag{2.20} \\
u + 2D\frac{\partial u}{\partial n} &= f \quad \text{on } \partial \Omega \tag{2.21}
\end{align*}$$

for $u \in H^1(\Omega)$. First, in order to use Theorem 2.3, we find the weak formulation of the Robin problem,

$$\begin{align*}
\int_{\Omega} (-\nabla \cdot (D\nabla u) + (\mu_a + ik)u)\bar{v}dx &= \int_{\Omega} 0 \cdot \bar{v}dx \\
\int_{\Omega} D\nabla u \nabla \bar{v}dx - \int_{\partial \Omega} D\gamma D\bar{v} \frac{\partial u}{\partial n}ds + \int_{\Omega} (\mu_a + ik)uv\bar{v}dx &= 0 \\
\int_{\Omega} D\nabla u \nabla \bar{v} + (\mu_a + ik)u\bar{v}dx + \int_{\partial \Omega} \frac{1}{2}D\gamma Duv = \int_{\partial \Omega} \frac{1}{2}f\gamma Dvds
\end{align*}$$

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through integration by parts and applying (2.21) and the Dirichlet trace, (2.12). From
the weak formulation we define

\[ B_R(u, v) = \int_\Omega D\nabla u \nabla \bar{v} + (\mu_a + ik)uv\bar{v}dx + \int_{\partial\Omega} \frac{1}{2} \gamma_D u \gamma_D \bar{v}ds \] (2.22)

\[ F_R(v) = \int_{\partial\Omega} \frac{1}{2} f \gamma_D \bar{v}ds. \] (2.23)

**Lemma 2.4.** \( B_R(u, v) \) is a sesquilinear form.

**Proof.**

\[ B_R(x + y, z + w) = \int_\Omega D\nabla (x + y) \nabla (z + w) + (\mu_a + ik)(x + y)(z + w)dx \]
\[ + \int_{\partial\Omega} \frac{1}{2} \gamma_D (x + y) \gamma_D (z + w)ds \]
\[ = \int_\Omega D(\nabla x + \nabla y)(\nabla z + \nabla w) + (\mu_a + ik)(x\bar{z} + x\bar{w} + y\bar{z} + y\bar{w})dx \]
\[ + \int_{\partial\Omega} \frac{1}{2}(\gamma_D x + \gamma_D y)(\gamma_D z + \gamma_D w)ds \]
\[ = \int_\Omega D(\nabla x \nabla z + \nabla x \nabla w + \nabla y \nabla z + \nabla y \nabla w)dx \]
\[ + \int_\Omega (\mu_a + ik)(x\bar{z} + x\bar{w} + y\bar{z} + y\bar{w})dx \]
\[ + \int_{\partial\Omega} \frac{1}{2}(\gamma_D x \gamma_D z + \gamma_D x \gamma_D w + \gamma_D y \gamma_D z + \gamma_D y \gamma_D w)ds \]
\[ = B_R(x, z) + B_R(x, w) + B_R(y, z) + B_R(y, w) \]

\[ B_R(c_1 u, c_2 v) = \int_\Omega \left( D\nabla (c_1 u) \nabla (c_2 \bar{v}) + (\mu_a + ik)(c_1 u)(c_2 \bar{v}) \right) dx + \int_{\partial\Omega} \frac{1}{2} \gamma_D (c_1 u) \gamma_d (c_2 \bar{v})ds \]
\[ = \int_\Omega (c_1 \bar{c}_2 D\nabla u \nabla \bar{v} + c_1 \bar{c}_2 (\mu_a + ik)u\bar{v}) dx + \int_{\partial\Omega} c_1 \bar{c}_2 \frac{1}{2} \gamma_D u \gamma_d \bar{v}ds \]
\[ = c_1 \bar{c}_2 B_R(u, v) \]
In order to use the Lax-Milgram Theorem, we need to show that $F_R(v)$ is a bounded linear functional. To do so, we will make use of a Riesz map, which is guaranteed by the Riesz Representation Theorem, given below as in [58].

**Theorem 2.5. (Riesz Representation)** Let $H_1, H_2$ be Hilbert spaces and $h : H_1 \times H_2 \to K$ a bounded sesquilinear form. Then, $h$ has a representation,

$$h(x, y) = \langle Sx, y \rangle$$

where $S : H_1 \to H_2$ is a bounded linear operator. Further, $S$ is uniquely determined by $h$ and has norm $||S|| = ||h||$.

**Lemma 2.6.** $F_R(v)$ is a bounded linear functional of $v$.

**Proof.** Note that $F_R(v)$ is the duality pairing

$$\frac{1}{2} \langle f, \gamma_D v \rangle_{H^{-1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)} = \langle f, v \rangle_{L^2(\partial\Omega)} = \int_{\partial\Omega} \frac{1}{2} f \gamma_D v ds$$

where $H^{-1/2}(\partial\Omega)$ is the dual space of $H^{1/2}(\partial\Omega)$. Now, making use Theorem 2.5, let $S : H^{-1/2}(\Omega) \to H^{1/2}(\Omega)$ be a Riesz map. Then,

$$\left| \frac{1}{2} \langle f, \gamma_D v \rangle_{H^{-1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)} \right| = \frac{1}{2} \left| \langle Sf, \gamma_D v \rangle_{H^{1/2}(\partial\Omega) \times H^{1/2}(\partial\Omega)} \right|$$

$$= |\langle F_D(0, Sf), v \rangle|_{H^1(\Omega)}$$

$$\leq ||F_D(0, Sf)||_{H^1(\Omega)} ||v||_{H^1(\Omega)} \leq c ||v||_{H^1(\Omega)}$$

where $F_D(\cdot, \cdot)$ is the forward Dirichlet operator. \qed
To show that the conditions of Theorem 2.3 are met, we now must show that \( B_R(u, v) \) is bounded and coercive. To make the proof easier, we define a norm that is more intuitive than the \( H^1 \) norm to use with our sesquilinear form. Let

\[
\|u\|_{H^1} = \left( \int_{\Omega} (D|\nabla u|^2 + \mu_a |u|^2) \, dx + \frac{1}{2} \int_{\partial \Omega} |\gamma D u|^2 \, ds \right)^{1/2}.
\] (2.24)

In order to prove the equivalence of this norm to the \( H^1 \) norm derived from (2.19), we need to make use of the Sobolev Trace Theorem.

**Theorem 2.7.** (Sobolev Trace Theorem) Given \( \Omega \), a bounded, simply connected Lipschitz domain, and \( \frac{1}{2} < s < \frac{3}{2} \), the trace operator \( \gamma|_{\partial \Omega} \) is a bounded linear operator from \( H^s(\Omega) \) to \( H^{s-\frac{1}{2}}(\partial \Omega) \).

Now we will prove the equivalence of the norms.

**Lemma 2.8.** The norms \( \|u\|_{H^1} = \left( \int_{\Omega} (|\nabla u|^2 + |u|^2) \, dx \right)^{1/2} \) and \( \|u\|_{H^1_*} \) (defined in (2.24)) are equivalent.

**Proof.** First, recall that \( D \) and \( \mu_a \) are bounded on \( \Omega \). That is, \( D_2 \geq D \) and \( \mu_2 \geq \mu_a \). Let \( C_1 = \max_{\Omega}\{D_2, \mu_2\} \). Then,

\[
\|u\|_{H^1_*}^2 = \int_{\Omega} (D|\nabla u|^2 + \mu_a |u|^2) \, dx + \frac{1}{2} \int_{\partial \Omega} |\gamma D u|^2 \, ds
\leq \int_{\Omega} (C_1|\nabla u|^2 + C_1 |u|^2) \, dx + \frac{1}{2} \int_{\partial \Omega} |\gamma D u|^2 \, ds
\leq C_1 \left( \int_{\Omega} |\nabla u|^2 + |u|^2 \, dx \right) + C \int_{\Omega} |\nabla u|^2 + |u|^2
= (C_1 + C)\|u\|_{H^1}.
\]

where \( C \) is the constant guaranteed by the Sobolev Trace Theorem (Theorem 2.7), that is, the constant that arises from \( \gamma_D \) being a bounded linear operator. Next, since
\( D_1 \leq D \) and \( \mu_1 \leq \mu \) in \( \Omega \),

\[
|u|_{H^1} = \int_{\Omega} (|\nabla u|^2 + |u|^2) dx
\]

\[
\leq \frac{1}{D_1} \int_{\Omega} D|\nabla u|^2 dx + \frac{1}{\mu_1} \int_{\Omega} \mu_a |u|^2 dx
\]

\[
\leq \max \left\{ \frac{1}{D_1}, \frac{1}{\mu_1} \right\} \left( \int_{\Omega} |\nabla u|^2 + |u|^2 dx \right) + \frac{1}{2} \int_{\partial \Omega} |\gamma_D u|^2 ds
\]

\[
\leq \max \left\{ \frac{1}{D_1}, \frac{1}{\mu_1} \right\} \left( \int_{\Omega} |\nabla u|^2 + |u|^2 dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D u|^2 ds \right)
\]

\[
= C_2 |u|_{H^1_*}
\]

That is,

\[
\frac{1}{C_1 + C} |u|_{H^1_*}^2 \leq |u|_{H^1} \leq C_2 |u|_{H^1_*}
\]

and so the two norms are equivalent. \( \square \)

Since we have defined \( H^1_*(\Omega) \), we will use its corresponding inner product to define an inner product on \( H^{1/2}(\partial \Omega) \). The spaces \( H^{1/2}(\partial \Omega) \) and \( H^{-1/2}(\partial \Omega) \) will then be connected by a Riesz map. In the following, we will denote the solution to the Dirichlet problem

\[
-\text{div}(D \nabla u) + \mu_a u = 0 \quad \text{in } \Omega
\]

\[
u = f \quad \text{on } \partial \Omega
\]

as \( F_D(0, f) \). Our inner product for \( H^{1/2}(\partial \Omega) \) is thus given by

\[
\langle f, g \rangle_{H^{1/2}(\partial \Omega)} = \langle F_D(0, f), F_D(0, g) \rangle_{H^1_*(\Omega)}
\]

\[
= \int_{\Omega} D\nabla F_D(0, f) \cdot \nabla \overline{F_D(0, g)} + \mu_a F_D(0, f)\overline{F_D(0, g)} dx
\]

\[
+ \frac{1}{2} \int_{\partial \Omega} \gamma_D F_D(0, f)\gamma_D \overline{F_D(0, g)} ds
\]

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\[
\begin{align*}
&= \int_\Omega (-\nabla \cdot (D\nabla F_D(0,f)) + \mu_a F_D(0,f))\overline{F_D(0,g)} \, dx \\
&\quad + \int_{\partial\Omega} \gamma_N(F_D(0,f))\gamma_D(\overline{F_D(0,g)}) \, ds + \frac{1}{2} \int_{\partial\Omega} \gamma_D F_D(0,f)\gamma_D(\overline{F_D(0,g)}) \, ds \\
&= \int_\Omega 0 \cdot \overline{F_D(0,g)} \, dx + \frac{1}{2} \int_{\partial\Omega} \gamma_R F_D(0,f)\gamma_D(\overline{F_D(0,g)}) \, ds \\
&= \frac{1}{2} \int_{\partial\Omega} \gamma_R F_D(0,f) \cdot \overline{g} \, ds.
\end{align*}
\]

It can be shown by a similar derivation (see, e.g., [22]) that

\[
\langle f, g \rangle_{H^{1/2}(\partial\Omega)} = \frac{1}{2} \int_{\partial\Omega} f\gamma_R F_D(0,g) \, ds.
\]

Thus, the \(H^{1/2}(\partial\Omega)\) inner product is given by the three equivalent definitions,

\[
\langle f, g \rangle_{H^{1/2}(\partial\Omega)} = \langle F_D(0,f), F_D(0,g) \rangle_{H^1_0(\Omega)} \\
= \frac{1}{2} \int_{\partial\Omega} \gamma_R F_D(0,f) \cdot \overline{g} \, ds \\
= \frac{1}{2} \int_{\partial\Omega} f\gamma_R F_D(0,g) \, ds.
\]  

(2.25)

We can verify quickly that this indeed is a valid inner product. First of all, the conjugate symmetry and linearity in the first term is guaranteed by the \(H^1_0(\Omega)\) inner product. Now consider \(f \in H^{1/2}(\partial\Omega)\) such that \(f = 0\). Then \(F_D(0,f) = 0\) and so

\[
\langle f, f \rangle_{H^{1/2}(\partial\Omega)} = \langle F_D(0,f), F_D(0,f) \rangle_{H^1_0(\Omega)} = 0.
\]

Since we are using the \(H^1_0(\Omega)\) inner product, \(\langle F_D(0,f), F_D(0,f) \rangle_{H^1_0(\Omega)}\) cannot be zero if \(F_D(0,f) \neq 0\) and thus if \(f \neq 0\), \(\langle F_D(0,f), F_D(0,f) \rangle_{H^1_0(\Omega)} \neq 0\). Therefore, (2.25) is a valid inner product.

Now we are prepared to prove that the hypotheses of the Lax-Milgram Theorem are met for the sesquilinear form \(B_R(u,v)\).
Theorem 2.9. $B_R(u, v)$ is bounded and coercive with respect to the $H^1$ norm.

Proof. We begin with the proof that $B_R(u, v)$ is bounded (that is, continuous) with respect to $H^1$.

$$|B_R(u, v)| = \left| \int_\Omega D\nabla u \nabla \bar{v} + (\mu_a + ik)u \bar{v}dx + \frac{1}{2}\int_{\partial \Omega} \gamma_D u \gamma_D vds \right|$$

$$\leq \int_\Omega D|\nabla u \nabla \bar{v}| + \mu_a |u \bar{v}| + |iku\bar{v}|dx + \frac{1}{2}\int_{\partial \Omega} |\gamma_D u \gamma_D v|ds$$

$$\leq D_2 \int_\Omega |\nabla u \nabla \bar{v}|dx + \mu_2 \int_\Omega |u \bar{v}|dx + |k| \int_\Omega |uv|dx + \frac{1}{2}\int_{\partial \Omega} |\gamma_D u \gamma_D v|ds$$

$$\leq D_2 \left( \int_\Omega (\nabla u)^2 dx \right)^{1/2} \left( \int_\Omega (\nabla v)^2 dx \right)^{1/2} + \mu_2 \left( \int_\Omega |u|^2 dx \right)^{1/2} \left( \int_\Omega |v|^2 dx \right)^{1/2}$$

$$+ |k| \left( \int_\Omega |u|^2 dx \right)^{1/2} \left( \int_\Omega |v|^2 dx \right)^{1/2} + \frac{1}{2} \left( \int_{\partial \Omega} |\gamma_D u|^2 \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 ds \right)^{1/2}$$

$$= (D_2 + \mu_2 + |k|) \left( \int_\Omega (\nabla u)^2 + |u|^2 dx \right)^{1/2} \left( \int_\Omega (\nabla v)^2 + |v|^2 dx \right)^{1/2}$$

$$+ \frac{1}{2} \left( \int_{\partial \Omega} |\gamma_D u|^2 \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 ds \right)^{1/2}$$

$$= (D_2 + \mu_2 + |k|) ||u||_{H^1(\Omega)} ||v||_{H^1(\Omega)} + \frac{1}{2} \left( \int_{\partial \Omega} |\gamma_D u|^2 ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 ds \right)^{1/2}$$

$$\leq (D_2 + \mu_2 + |k|) ||u||_{H^1(\Omega)} ||v||_{H^1(\Omega)}$$

$$+ \frac{1}{2} C \left( \int_\Omega |\nabla u|^2 + |u|^2 \right)^{1/2} \left( \int_\Omega |\nabla v|^2 + |v|^2 \right)^{1/2}$$

$$= (D_2 + \mu_2 + |k| + \frac{1}{2} C) ||u||_{H^1(\Omega)} ||v||_{H^1(\Omega)}$$
using Hölder’s Inequality and the Sobolev Trace Theorem. Now we will show that $B_R(u, v)$ is coercive with respect to $H^1$.

$$|B_R(u, u)| \geq |Re(B_R(u, u))|$$

$$= \left| \int_{\Omega} D^2|\nabla u|^2 + (\mu + ik)|u|^2 dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D u|^2 ds \right| = ||u||^2_{H^1(\Omega)} \geq \frac{1}{C_2} ||u||_{H^1}$$

where $C_2$ is defined as in the proof of Lemma 2.8.

Now that we have proven that all the conditions are met, we can conclude from Theorem 2.3 that (2.22) has a unique solution. More specifically, we can say $B_R(u, v) = \langle Au, v \rangle_{H^1(\Omega)}$ for $u, v \in H^1_*$(Ω) and a unique bijective $A$. Thus, since we have that $B_r(u, v) = F_R(v)$, a bounded linear functional, for all $v \in H^1_*$(Ω), then we also have

$$B_R(u, v) = \langle Au, v \rangle_{H^1(\Omega)} = F_R(v), \quad \forall v \in H^1_*$(Ω)$$

by the Lax-Milgram Theorem. Further, the Riesz Representation Theorem allows us to describe any element of $(H^1_*(\Omega))^*$ as an inner product and thus,

$$F_R(v) = \langle z, v \rangle_{H^1(\Omega)}, \quad \forall v \in H^1_*(\Omega).$$

Combining the above we thus have

$$B_R(u, v) = \langle Au, v \rangle_{H^1(\Omega)} = \langle z, v \rangle_{H^1(\Omega)} = F_R(v), \quad \forall v \in H^1_*$(\Omega).$$

Since this equality holds for all $v \in H^1_*(\Omega)$, we can conclude that $Au = z$ and thus $u = A^{-1}z$ since $A$ is bijective and thus, invertible. Since $A$ is also unique, this $u$ is the only solution to $B_R(u, v) = F_R(v)$ on $H^1(\Omega)$. Recall that the Lax-Milgram Theorem
also gives bounds on $A$ (see Theorem 2.3), given by
\[
\|A\|_{H^1_0(\Omega)} \leq c_1, \quad \|A^{-1}\|_{H^1_0(\Omega)} \leq \frac{1}{c_2}.
\]

In the proofs of Lemma 2.8 and Theorem 2.9, we found that
\[
c_1 = D_2 + \mu_2 + |k| + \frac{1}{2} C, \quad \frac{1}{c_2} = \max \{D_1, \mu_1\}
\]
and so
\[
\|A\|_{H^1_0(\Omega)} \leq D_2 + \mu_2 + |k| + \frac{1}{2} C, \quad \|A^{-1}\|_{H^1_0(\Omega)} \leq \max \{D_1, \mu_1\}.
\]

Then, for $u = A^{-1}z$ where $z$ is the representation of $F_R$ given by the Riesz Representation Theorem (and thus $\|z\| = \|f\|$), the solution $u$ has bound
\[
\|u\|_{H^1_0(\Omega)} = \|A^{-1}z\|_{H^1_0(\Omega)} \leq \|A^{-1}\||z||_{H^1_0(\Omega)} \leq \max \{D_1, \mu_1\} \|f\|_{H^1_0(\Omega)}.
\]

Since we have shown the existence and uniqueness of the Robin forward problem, all that remains to prove that is well-posed is to show that the solution depends continuously on the data. Note that if $f$ is the source and $g$ is the measurement for a DOT experiment, the whole experiment can be described by the system
\[
-\nabla \cdot (D \nabla u) + (\mu + ik)u = 0 \quad \text{in } \Omega \quad (2.26)
\]
\[
u + 2D \frac{\partial u}{\partial n} = f \quad \text{on } \partial \Omega \quad (2.27)
\]
\[
-D \frac{\partial u}{\partial n} = g \quad \text{on } \partial \Omega \quad (2.28)
\]
which represents a Robin-to-Neumann map given by $F_{RN}(D, \mu)f = g$, for any source.
Thus, the forward problem that we need to analyze is

\[ -\nabla \cdot (D \nabla u) + (\mu + ik)u = 0 \quad \text{in } \Omega \quad (2.29) \]

\[ u + 2D \frac{\partial u}{\partial n} = g \quad \text{on } \partial \Omega. \quad (2.30) \]

We are now prepared to prove that the last condition of Hadamard (Definition 2.1) for well-posedness is met.

**Theorem 2.10.** The solution, \( u \), to (2.20)-(2.21) depends continuously on the data \( g \).

**Proof.** By our previous calculation of the weak formulation of the forward problem given by (2.22), (2.23), we have that the weak formulation of (2.29), (2.30) is

\[
\int_{\Omega} D \nabla u \nabla \bar{v} + (\mu_a + ik)u \bar{v} dx + \int_{\partial \Omega} \frac{1}{2} \gamma_D u \gamma_D v = \frac{1}{2} \int_{\partial \Omega} g \gamma_D \bar{v} ds
\]

for all \( v \in H^1(\Omega) \). This can also be represented by

\[
a[u, v] = \frac{1}{2} \langle g, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)}, \quad \forall v \in H^1(\Omega). \]

Thus, as we have described above, if we can show that \( \frac{1}{2} \langle g, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} \) can be considered as a bounded linear functional on \( H^1_s(\Omega) \) (or, equivalently, \( H^1(\Omega) \)), then we can show the existence of a unique solution. As this is currently a duality pairing and not an element of the dual space of \( H^1_s(\Omega) \), we will have to do some work to connect it to an inner product in \( H^1_s(\Omega) \). By the Riesz map \( S : H^{-1/2}(\partial \Omega) \rightarrow H^{1/2}(\partial \Omega) \) defined in the proof of Lemma 2.6, we have that

\[
\langle g, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} = \langle Sg, \gamma_D v \rangle_{H^{1/2}(\partial \Omega)}. \]
Additionally, by the inner product for $H^{1/2}(\partial \Omega)$ defined in (2.25), we have

$$\langle g, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} = \langle F_D(0, g), F_D(0, \gamma_D v) \rangle_{H^1(\Omega)}$$

$$= \langle F_D(0, \gamma_D F_R(0, g)), F_D(0, \gamma_D v) \rangle_{H^1(\Omega)}$$

$$= \langle F_D(0, \gamma_D F_R(0, g)), v \rangle_{H^1(\Omega)}$$

where $F_R(0, g)$ is the forward Robin map and $F_D(0, g)$ the forward Dirichlet map. We now consider the extension operator $\pi : H^{1/2}(\partial \Omega) \to H^1_*(\Omega)$, where $\pi f = F_d(0, f)$. Thus, by the Riesz map $S$ we have,

$$\langle g, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} = \langle \pi S g, v \rangle_{H^1_*(\Omega)}.$$  

This is a quantity that we can consider as a linear functional in $(H^1_*(\Omega))^*$. We only need to show that it is bounded to be able to use the argument above. But by the Cauchy Schwarz Inequality we have

$$\frac{1}{2} \langle \pi S g, v \rangle_{H^1_*(\Omega)} \leq \|\pi S g\|_{H^1_*(\Omega)} \|v\|_{H^1_*(\Omega)} < \infty$$

since $\pi S g, v \in H^1_*(\Omega)$. Now since

$$B_R(u, v) = \langle Au, v \rangle_{H^1_*(\Omega)} = \frac{1}{2} \langle \pi S g, v \rangle_{H^1_*(\Omega)}$$

where $\pi S g, v \in H^1_*(\Omega)$. Now since

by the above argument, the Lax Milgram Theorem gives us that $Au = \frac{1}{2} \pi S g$ gives
\[ u = A^{-\frac{1}{2}} \pi Sg, \] a unique solution. Thus we have that
\[
\| u \|_{H^1_*(\Omega)} = \| A^{-\frac{1}{2}} \pi Sg \|_{H^1_*(\Omega)} \\
\leq \frac{1}{2} \| A^{-1} \| \| \pi Sg \|_{H^1_*(\Omega)} \\
= \frac{1}{2} \| \pi Sg \|_{H^1_*(\Omega)} < \infty
\]

because \( \pi Sg \in H^1_*(\Omega) \) by construction. So, finally,
\[
\| u \|_{H^1_*(\Omega)} \leq \frac{1}{2} \| \pi Sg \|_{H^1_*(\Omega)} \\
\leq \| \pi \| \| S \| \| g \|_{H^{-1/2}(\partial\Omega)} \\
= C \| g \|_{H^{-1/2}(\partial\Omega)}
\]

for some constant \( C \), and so \( u \) depends continuously on the data, \( g \).

Thus, having already shown the existence and unique of \( u \), we conclude that the DOT forward problem is well-posed.

### 2.2 The hyDOT Forward Problem

The forward problem for hyDOT has the same form as that for DOT, but the optical coefficients \( D \) and \( \mu_a \) are now dependent on a continuous parameter, \( \lambda \).

\[
- \text{div}(D(x, \lambda) \nabla u) + (\mu_a(x, \lambda) + ik)u = 0 \quad \text{in } \Omega, \quad (2.31)
\]
\[
u + 2D(x, \lambda) \frac{\partial u}{\partial n} = f \quad \text{on } \partial \Omega \quad (2.32)
\]

The optical wavelength, \( \lambda \), is in \( \Lambda = [\lambda_{\text{min}}, \lambda_{\text{max}}] \), a closed, bounded subset of \( \mathbb{R} \).
2.2.1 Spectral Dependence

In discovering how the spectral dependence of the optical parameters affects the hyDOT inverse problem, we wish to examine the behavior of the governing PDE with respect to its spectral dependence. To do this, we first consider (2.1) - (2.2) evaluated at a fixed \( q_0 \) where

\[
q_0 = \begin{pmatrix}
D_0(x_0, \lambda) \\
\mu_{a,0}(x_0, \lambda)
\end{pmatrix}.
\]

This PDE is given by,

\[
\begin{align*}
-\text{div}(D_0 \nabla u_0) + (\mu_{a,0} + ik)u_0 &= 0 \quad \text{in } \Omega, \\
u_0 + 2D_0 \frac{\partial u_0}{\partial n} &= f \quad \text{on } \partial \Omega. 
\end{align*}
\] (2.33)

Next, we take the derivative with respect to \( \lambda \). We obtain,

\[
\begin{align*}
-\text{div} \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) + (\mu_{a,0} + ik)\frac{\partial u_0}{\partial \lambda} &= \text{div} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \quad \text{in } \Omega, \\
\frac{\partial u_0}{\partial \lambda} + 2D_0 \frac{\partial}{\partial n} \left( \frac{\partial u_0}{\partial \lambda} \right) &= \frac{\partial f}{\partial \lambda} - 2\frac{\partial D_0}{\partial \lambda} \frac{\partial u_0}{\partial n} \quad \text{on } \partial \Omega. 
\end{align*}
\] (2.34)

We see that this new equation has the same form as (2.33). Hoping to see a pattern, we take the derivative with respect to \( \lambda \) again to obtain,

\[
\begin{align*}
-\text{div} \left( D_0 \nabla \frac{\partial^2 u_0}{\partial \lambda^2} \right) + (\mu_{a,0} + ik)\frac{\partial^2 u_0}{\partial \lambda^2} &= \text{div} \left( \frac{\partial^2 D_0}{\partial \lambda^2} \nabla u_0 \right) - \frac{\partial^2 \mu_{a,0}}{\partial \lambda^2} u_0 \\
&\quad + 2\text{div} \left( \frac{\partial D_0}{\partial \lambda} \nabla \frac{\partial u_0}{\partial \lambda} \right) - 2\frac{\partial \mu_{a,0}}{\partial \lambda} \frac{\partial u_0}{\partial n} \quad \text{in } \Omega, \\
\frac{\partial^2 u_0}{\partial \lambda^2} + 2D_0 \frac{\partial}{\partial n} \left( \frac{\partial^2 u_0}{\partial \lambda^2} \right) &= \frac{\partial^2 f}{\partial \lambda^2} - 2\frac{\partial^2 D_0}{\partial \lambda^2} \frac{\partial u_0}{\partial n} - 4\frac{\partial D_0}{\partial \lambda} \frac{\partial}{\partial n} \left( \frac{\partial u_0}{\partial \lambda} \right) \quad \text{on } \partial \Omega.
\end{align*}
\] (2.35)
Upon taking the derivative with respect to $\lambda$ the third time, a pattern emerges. Mainly, the $n^{th}$ derivative with respect to $\lambda$ of (2.33) is,

$$-	ext{div} \left( D_0 \nabla \frac{\partial^n u_0}{\partial \lambda^n} \right) + (\mu_{a,0} + i k) \frac{\partial^n u_0}{\partial \lambda^n} = \text{div} \left( \frac{\partial^n D_0}{\partial \lambda^n} \nabla u_0 \right) - \frac{\partial^n \mu_{a,0}}{\partial \lambda^n} u_0$$

$$+ n \sum_{k=1}^{n-1} \left[ \text{div} \left( \frac{\partial^{n-k} D_0}{\partial \lambda^{n-k}} \nabla \frac{\partial^k u_0}{\partial \lambda^k} \right) - \frac{\partial^{n-k} \mu_{a,0}}{\partial \lambda^{n-k}} \frac{\partial^k u_0}{\partial \lambda^k} \right] \text{ in } \Omega \quad (2.36)$$

The formula for the $n$th derivative of the boundary condition is harder to write compactly, but there is a pattern there as well. While we will not use the $n$th derivative of the PDE with respect to $\lambda$ in this dissertation, this helps us to see the regularity of the solution $u$ with respect to $\lambda$.

Since the governing equations of hyDOT must take into account the spectral dependence of the solution as well as its spatial dependence, the forward problem of hyDOT can be given by the coupled system of equations,

$$-\text{div} (D_0 \nabla u_0) + (\mu_{a,0} + i k) u_0 = 0 \quad \text{in } \Omega \quad (2.37)$$

$$-\text{div} \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) + (\mu_{a,0} + i k) \frac{\partial u_0}{\partial \lambda} = \text{div} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \quad \text{in } \Omega \quad (2.38)$$

$$u_0 + 2D_0 \frac{\partial u_0}{\partial \mathbf{n}} = f \quad \text{on } \partial \Omega \quad (2.39)$$

$$\frac{\partial u_0}{\partial \lambda} + 2D_0 \frac{\partial}{\partial \mathbf{n}} \left( \frac{\partial u_0}{\partial \lambda} \right) = \frac{\partial f}{\partial \lambda} - 2 \frac{\partial D_0}{\partial \lambda} \frac{\partial u_0}{\partial \mathbf{n}} \quad \text{on } \partial \Omega. \quad (2.40)$$

We seek to examine the regularity of the solutions to this system. We have already proven the existence and uniqueness of the solution to (2.37), (2.39) in Chapter 2. Thus, we must only examine the regularity of $\frac{\partial u_0}{\partial \lambda}$ in (2.38), (2.40). We proceed as we did in Section 2.1. As before, we seek to use the Lax-Milgram Theorem (Theorem 2.3) and so must find the weak formulation of (2.38).

First, we note that (2.38) depends on, $u_0$, the solution to (2.37), (2.39). Thus,
we must solve this coupled system sequentially. First, we must find a solution, $u_0$ to (2.37) using the boundary condition (2.39). Then, we plug $u_0$ into the righthand side of (2.38) and solve it using boundary condition (2.40). So, we find the the weak formulation of (2.38) by multiplying by a test function, $v \in H^1(\Omega)$ and applying integration by parts and the Dirichlet trace, (2.12) to obtain,

\[
\int_{\Omega} \left( -\nabla \cdot \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) + (\mu_{a,0} + ik) \frac{\partial u_0}{\partial \lambda} \right) \bar{v} dx = \int_{\Omega} \left( \nabla \cdot \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \right) \bar{v} dx
\]

\[
\int_{\Omega} \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) \nabla \bar{v} + (\mu_{a,0} + ik) \frac{\partial u_0}{\partial \lambda} \bar{v} dx - \int_{\partial \Omega} D_0 \gamma_D \bar{v} \frac{\partial}{\partial n} \left( \frac{\partial u_0}{\partial \lambda} \right) ds = \int_{\Omega} \left( \nabla \cdot \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \right) \bar{v} dx
\]

\[
\int_{\Omega} \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) \nabla \bar{v} dx + \int_{\Omega} (\mu_{a,0} + ik) \frac{\partial u_0}{\partial \lambda} \bar{v} dx + \int_{\partial \Omega} \frac{1}{2} \gamma_D \frac{\partial u_0}{\partial \lambda} \gamma_D \bar{v} ds
\]

\[
+ \int_{\partial \Omega} \left( \nabla \cdot \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \right) \bar{v} dx = 1/2 \int_{\partial \Omega} \bar{v} ds
\]

Thus, our bilinear form for (2.38),(2.40) is,

\[
B_{\lambda} \left( \frac{\partial u_0}{\partial \lambda}, v \right) = \int_{\Omega} \left( D_0 \nabla \frac{\partial u_0}{\partial \lambda} \right) \nabla \bar{v} dx + \int_{\Omega} (\mu_{a,0} + ik) \frac{\partial u_0}{\partial \lambda} \bar{v} dx + \int_{\partial \Omega} \frac{1}{2} \gamma_D \frac{\partial u_0}{\partial \lambda} \gamma_D \bar{v} ds
\]

where $B_{\lambda}(u,v) : H^1(\Omega) \times H^1(\Omega) \rightarrow \mathbb{C}$. We also define the operator for the righthand
side of the weak formulation, (2.41),

\[ F_\lambda(v) = \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds - \int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \nabla \bar{v} + \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \bar{v} \right) dx. \]  

(2.43)

In other words,

\[ B_\lambda(u, v) = \frac{1}{2} \langle \frac{\partial f}{\partial \lambda}, \gamma_D v \rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} - \int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \nabla \bar{v} + \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \bar{v} \right) dx, \forall v \in V \]  

(2.44)

In order to prove the existence and uniqueness of a solution, we will use the Lax-Milgram Theorem (Theorem 2.3). Thus, we must show that the conditions of this theorem are satisfied. First we show that \( F_\lambda(v) \) is a bounded linear functional of \( v \).

\textbf{Lemma 2.11.} \( F_\lambda(v) \) is a bounded linear functional.

\textit{Proof.} To begin with, we examine the first term of \( F_\lambda(v) \), \( \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds \). We note that this term is given by the duality pairing,

\[ \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds = \frac{1}{2} \left\langle \frac{\partial f}{\partial \lambda}, v \right\rangle_{L^2(\partial \Omega)} = \frac{1}{2} \left\langle \frac{\partial f}{\partial \lambda}, \gamma_D v \right\rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} \]

noting that \( H^{-1/2}(\partial \Omega) \) is the dual space of \( H^{1/2}(\Omega) \). Now, making use Theorem 2.5, let \( S : H^{-1/2} \to H^{1/2} \) be a Riesz map. Then,

\[ \left| \frac{1}{2} \left\langle f, \gamma_D v \right\rangle_{H^{-1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} \right| = \frac{1}{2} \left| \langle Sf, \gamma_D v \rangle_{H^{1/2}(\partial \Omega) \times H^{1/2}(\partial \Omega)} \right| = \left| \langle F_D(Sf), v \rangle_{H^1(\Omega)} \right| \leq \| F_D(Sf) \|_{H^1(\Omega)} \| v \|_{H^1(\Omega)} \leq c \| v \|_{H^1(\Omega)}. \]

Next, we examine the second term of \( F_\lambda(v) \). We know that \( \frac{\partial D_0}{\partial \lambda}, \frac{\partial \mu_{a,0}}{\partial \lambda} \in L^\infty(\Omega) \).
and that $u \in H^1(\Omega)$ thus we have that
\[
\left| \int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \nabla \bar{v} + \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \bar{v} \right) \, dx \right| \leq C_1 ||u_0||_{H^1(\Omega)} ||v||_{H^1(\Omega)}
\leq C_1 C_2 ||v||_{H^1(\Omega)}
\]

by Hölder’s Inequality, where
\[
C_1 = \max \left\{ \left| \frac{\partial D_0}{\partial \lambda} \right|_{L^\infty(\Omega)}, \left| \frac{\partial \mu_{a,0}}{\partial \lambda} \right|_{L^\infty(\Omega)} \right\}.
\]

So, $\int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \nabla \bar{v} + \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \bar{v} \right) \, dx$ is a bounded functional of $v$. \qed

Next, we must first show that $B_\lambda \left( \frac{\partial u}{\partial \lambda}, v \right)$ is a sesquilinear form.

**Lemma 2.12.** $B_\lambda(u,v)$ is a sesquilinear form.

**Proof.**

\[
B_\lambda(x+y, z+w) = \int_{\Omega} D_0 \nabla \frac{\partial (x+y)}{\partial \lambda} \nabla (z+w) + (\mu_{a,0} + ik) \frac{\partial (x+y)}{\lambda} (z+w) \, dx
\]
\[
+ \int_{\partial \Omega} \frac{1}{2} \gamma_D \frac{\partial (x+y)}{\partial \lambda} \gamma_D (z+w) \, ds
\]
\[
= \int_{\Omega} D \left( \nabla \frac{\partial x}{\partial \lambda} + \nabla \frac{\partial y}{\partial \lambda} \right) (\nabla z + \nabla \bar{w})
\]
\[
+ (\mu_a + ik) \left( \frac{\partial x}{\partial \lambda} \frac{\partial x}{\partial \lambda} + \frac{\partial x}{\partial \lambda} \frac{\partial y}{\partial \lambda} z + \frac{\partial y}{\partial \lambda} \bar{w} \right) dx
\]
\[
+ \int_{\partial \Omega} \frac{1}{2} \left( \gamma_D \frac{\partial x}{\partial \lambda} + \gamma_D \frac{\partial y}{\partial \lambda} \right) \left( \gamma_D z + \gamma_D \bar{w} \right) ds
\]
\[
= \int_{\Omega} D \left( \nabla \frac{\partial x}{\partial \lambda} \nabla z + \nabla \frac{\partial x}{\partial \lambda} \nabla \bar{w} + \nabla \frac{\partial y}{\partial \lambda} \nabla z + \nabla \frac{\partial y}{\partial \lambda} \nabla \bar{w} \right)
\]
\[
+ (\mu_a + ik) \left( \frac{\partial x}{\partial \lambda} \frac{\partial x}{\partial \lambda} \frac{\partial x}{\partial \lambda} + \frac{\partial x}{\partial \lambda} \frac{\partial y}{\partial \lambda} z + \frac{\partial y}{\partial \lambda} \bar{w} \right) dx
\]
\[
+ \int_{\partial \Omega} \frac{1}{2} \left( \gamma_D \frac{\partial x}{\partial \lambda} \gamma_D z + \gamma_D \frac{\partial x}{\partial \lambda} \gamma_D \bar{w} + \gamma_D \frac{\partial y}{\partial \lambda} \gamma_D z + \gamma_D \frac{\partial y}{\partial \lambda} \gamma_D \bar{w} \right) ds
\]

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\[ B_\lambda(x, z) + B_\lambda(x, w) + B_\lambda(y, z) + B_\lambda(y, w) \]

\[ B_\lambda(c_1 u, c_2 v) = \int_\Omega \left( D_0 \nabla \left( c_1 \frac{\partial u}{\partial \lambda} \nabla (c_2 v) + (\mu_a + ik) \left( c_1 \frac{\partial u}{\partial \lambda} (c_2 v) \right) \right) dx \right. \]
\[ + \int_{\partial \Omega} \frac{1}{2} \gamma_D \left( c_1 \frac{\partial u}{\partial \lambda} \gamma_d (c_2 v) \right) ds \]
\[ = \int_\Omega \left( c_1 c_2 D \nabla \frac{\partial u}{\partial \lambda} \nabla v + c_1 c_2 (\mu_a + ik) \frac{\partial u}{\partial \lambda} v \right) dx + \int_{\partial \Omega} c_1 c_2 \frac{1}{2} \gamma_D u \gamma_d v ds \]
\[ = c_1 c_2 B_\lambda(u, v) \]

Next, we must show that \( B_\lambda(u, v) \) is bounded and coercive in order to be sure the conditions of Theorem 2.3 are satisfied. We must first assume that \( \frac{\partial u}{\partial \lambda} \in H^1(\Omega) \), which is reasonable as long as \( u_0 \) is sufficiently smooth in \( \lambda \) since \( u_0 \in H^1(\Omega) \). As before, we will use the modified \( H^1 \) norm, \( || \cdot ||_{H^1} \) given in (2.24), (which is shown to be equivalent to the \( H^1 \) norm in Lemma 2.8) for our proof.

**Theorem 2.13.** \( B_\lambda(u, v) \) is bounded and coercive with respect to the \( H^1 \) norm.

**Proof.** First, we will show that \( B_\lambda(u, v) \) is bounded with respect to \( H^1 \). Recall that \( D, \mu_a \) are bounded, and thus \( 0 < D_1 \leq D_0 \leq D_2 < \infty \) and \( 0 < \mu_1 \leq \mu_{a,0} \leq \mu_2 < \infty \).

\[ |B_\lambda(u, v)| = \left| \int_\Omega D_0 \nabla \left( \frac{\partial u}{\partial \lambda} \nabla \bar{v} + (\mu_{a,0} + ik) \frac{\partial u}{\partial \lambda} \bar{v} \right) dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u}{\partial \lambda} \gamma_D v ds \right| \]
\[ \leq \int_\Omega D_0 \left| \nabla \frac{\partial u}{\partial \lambda} \nabla \bar{v} \right| + \mu_{a,0} \left| \frac{\partial u}{\partial \lambda} \bar{v} \right| + \left| ik \frac{\partial u}{\partial \lambda} \bar{v} \right| dx + \frac{1}{2} \int_{\partial \Omega} \left| \frac{\partial u}{\partial \lambda} \gamma_D v \right| ds \]
\[ \leq D_2 \int_\Omega \left| \nabla \frac{\partial u}{\partial \lambda} \nabla \bar{v} \right| dx + \mu_2 \int_\Omega \left| \frac{\partial u}{\partial \lambda} \bar{v} \right| dx \]
\[ + |k| \int_\Omega \left| \frac{\partial u}{\partial \lambda} \bar{v} \right| dx + \frac{1}{2} \int_{\partial \Omega} \left| \frac{\partial u}{\partial \lambda} \gamma_D v \right| ds \]
\[ \leq D_2 \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 \, dx \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 \, dx \right)^{1/2} + \mu_2 \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 \, dx \right)^{1/2} \left( \int_{\Omega} |v|^2 \, dx \right)^{1/2} + \frac{1}{2} \left( \int_{\partial \Omega} \left| \gamma_D \frac{\partial u}{\partial \lambda} \right|^2 \, ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 \, ds \right)^{1/2} \]

\[ \leq D_2 \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 \, dx + \left| \frac{\partial u}{\partial \lambda} \right|^2 \, dx \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 + |v|^2 \, dx \right)^{1/2} + \mu_2 \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 \, dx + \left| \frac{\partial u}{\partial \lambda} \right|^2 \, dx \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 + |v|^2 \, dx \right)^{1/2} + |k| \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 \, dx + \left| \frac{\partial u}{\partial \lambda} \right|^2 \, dx \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 + |v|^2 \, dx \right)^{1/2} + \frac{1}{2} \left( \int_{\partial \Omega} \left| \gamma_D \frac{\partial u}{\partial \lambda} \right|^2 \, ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 \, ds \right)^{1/2} \]

\[ = (D_2 + \mu_2 + |k|) \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 + \left| \frac{\partial u}{\partial \lambda} \right|^2 \, dx \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 + |v|^2 \, dx \right)^{1/2} + \frac{1}{2} \left( \int_{\partial \Omega} \left| \gamma_D \frac{\partial u}{\partial \lambda} \right|^2 \, ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 \, ds \right)^{1/2} \]

\[ = (D_2 + \mu_2 + |k|) \left\| \frac{\partial u}{\partial \lambda} \right\|_{H^1(\Omega)} \left\| v \right\|_{H^1(\Omega)} + \frac{1}{2} \left( \int_{\partial \Omega} \left| \gamma_D \frac{\partial u}{\partial \lambda} \right|^2 \, ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D v|^2 \, ds \right)^{1/2} \]

\[ \leq (D_2 + \mu_2 + |k|) \left\| \frac{\partial u}{\partial \lambda} \right\|_{H^1(\Omega)} \left\| v \right\|_{H^1(\Omega)} + \frac{1}{2} C \left( \int_{\Omega} \left( \nabla \frac{\partial u}{\partial \lambda} \right)^2 + \left| \frac{\partial u}{\partial \lambda} \right|^2 \right)^{1/2} \left( \int_{\Omega} (\nabla v)^2 + |v|^2 \right)^{1/2} \]

\[ = (D_2 + \mu_2 + |k| + \frac{1}{2} C) \left\| \frac{\partial u}{\partial \lambda} \right\|_{H^1(\Omega)} \left\| v \right\|_{H^1(\Omega)} \]

using Hölder’s Inequality and the Sobolev Trace Theorem. Now we will show that
$B_\lambda(u,v)$ is coercive with respect to $H^1$.

\[ |B_\lambda(u,u)| \geq |\text{Re}(B_\lambda(u,u))| \]
\[ = \left| \int_\Omega D_0 \left| \frac{\partial u}{\partial \lambda} \right|^2 + \mu_a \left| \frac{\partial u}{\partial \lambda} \right|^2 \, dx + \frac{1}{2} \int_{\partial \Omega} \left| \gamma_p \frac{\partial u}{\partial \lambda} \right|^2 \, ds \right| \]
\[ = \left| \left| \frac{\partial u}{\partial \lambda} \right|_{H^1(\Omega)}^2 \right| \geq \frac{1}{C_2} \| u \|_{H^1} \]

where $C_2$ is defined as in the proof of Lemma 2.8. \hfill \Box

Now, as in Section 2.1.1 we can apply the Lax-Milgram Theorem and conclude that (2.38), (2.40) has a unique solution. Further, following an argument very similar to that in Theorem 2.10, we can show that $\frac{\partial u}{\partial \lambda}$ depends continuously on the data, and thus that the forward problem for hyDOT is well-posed.

### 2.2.2 Regularity

The weak formulation given in (2.41) also gives us insight into the appropriate function spaces for the solutions and parameters in which we are interested. We have already stated that the solution to (2.20), (2.21), $u$, is considered to be in $H^1(\Omega)$ in order to guarantee the existence of a derivative in $L^2(\Omega)$ and apply Green’s Identity (integration by parts) in deriving the weak formulation. By the same logic, $\frac{\partial u}{\partial \lambda}$ must also be in $H^1(\Omega)$. Since we require $\frac{\partial u}{\partial \lambda}$ to exist, $u_0 \in C^1(\Lambda)$ where $\Lambda = [\lambda_{\text{min}}, \lambda_{\text{max}}] \subset \mathbb{R}$. Thus, we have $u \in C^1(H^1(\Omega); \Lambda)$.

Now that we have defined the space in which $u$ lives, we must define the norm that we will use on that space. Ultimately, we would like to show that $u$ is continuous with respect to $\lambda$. Since $u \in H^1(\Omega)$ our norm will incorporate the $H^1$ norm. Since we wish to include the spectral regularity of $u$ in our norm, we will include a term
involving $\frac{\partial u}{\partial \lambda}$. In order to get a clear idea of how the norm should be constructed, we will first give some continuity proofs.

The parameters of interest in the reconstruction problem are given as

$$q = \begin{pmatrix} D \\ \mu_a \end{pmatrix}$$

Later, when considering the spectral dependence, it will also be useful to examine the extended parameter space, which is given by

$$\hat{q} = \begin{pmatrix} D \\ \mu_a \\ \frac{\partial D}{\partial \lambda} \\ \frac{\partial \mu_a}{\partial \lambda} \end{pmatrix}$$

We have previously asserted that $D, \mu_a \in L^\infty(\Omega)$, which was integral to the proof of Theorem 2.9. We must now determine the appropriate function spaces in the spectral domain, $\Lambda$. As stated in the introduction, experimental results (see, e.g., [89, 101]) seem to indicate that the optical parameters $D, \mu_a$ are quite smooth respect to $\lambda$ (see Figures 1.3, 1.4). In order for the solution to (2.37)- (2.40) to exist, $\frac{\partial D}{\partial \lambda}, \frac{\partial \mu_a}{\partial \lambda}$ must exist. That is, $D, \mu_a$ must at least be in $C^1(\Lambda)$. So, $D, \mu_a \in C^1(L^\infty(\Omega); \Lambda)$. Thus, we have by definition that $q$ is continuous with respect to $\lambda$. We further assume that $\frac{\partial D}{\partial \lambda}, \frac{\partial \mu_a}{\partial \lambda} \in L^\infty(\Omega)$.

Now we prepared to prove the continuity of $u, \frac{\partial u}{\partial \lambda}$ with respect to the parameters $q$ and, ultimately, with respect to the implicit parameter, $\lambda$. First, in the proof that follows we will need to make use of the Poincaré Inequality, which is stated below as given by [69].

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Lemma 2.14. (Poincaré Inequality) Let $\Omega$ be a connected, bounded domain in $\mathbb{R}^n$ with $C^1$-boundary and $1 \leq p < \infty$. Then,

$$
||u - u\Omega||_p \leq C(n, p, \Omega)||\nabla u||_p
$$

for all $u \in H^{1,p}(\Omega)$, where

$$
u\Omega = \frac{1}{|\Omega|} \int_{\Omega} u(x)dx
$$

is the average value of $u$ over $\Omega$.

Theorem 2.15. The solution to (3.9) is continuous with respect to $q$ (as given in (2.45)).

Proof. We will prove that $u$ is continuous with respect to $q$ by showing that there exists a constant $c > 0$ such that $||u(q_1) - u(q_1 + \delta q)||_{H^1(\Omega)} \leq c||\delta q||_{L^\infty(\Omega)}$ where $||\delta q||_{L^\infty(\Omega)} = \max(||\delta D||_{L^\infty(\Omega)}, ||\delta \mu||_{L^\infty(\Omega)})$.

We will denote $u(q_1)$ as $u_1$ and $u(q_1 + \delta q) = u(q_2) = u_2$ in what follows. Also $q_1 = (D_1, \mu_{a,1})'$ and $q_2 = (D_2, \mu_{a,2})'$. First, note that the weak solutions of $u_1$ and $u_2$ satisfy

$$
\int_{\Omega} D_1 \nabla u_1 \nabla \bar{v} + (\mu_{a,1} + ik)u_1 \bar{v}dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_1 \gamma_D \bar{v}ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \bar{v}ds
$$

$$
\int_{\Omega} D_2 \nabla u_2 \nabla \bar{v} + (\mu_{a,2} + ik)u_2 \bar{v}dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_2 \gamma_D \bar{v}ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \bar{v}ds
$$

Expanding $q_2 = q_1 + \delta q$ and subtracting the second equation from the first we are left with

$$
\int_{\Omega} D_1 \nabla (u_2 - u_1) \nabla \bar{v} + (\mu_{a,1} + ik)(u_2 - u_1) \bar{v}dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D (u_2 - u_1) \gamma_D \bar{v}ds
$$

$$
= -\int_{\Omega} \delta D \nabla u_2 \nabla \bar{v} + \delta \mu_{a} u_2 \bar{v}dx.
$$

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Since this equality must hold for any \( v \in H^1(\Omega) \), let \( v = u_2 - u_1 \). Then we have

\[
\int_{\Omega} D_1 \nabla |u_2 - u_1|^2 dx + (\mu_{a,1} + ik)|u_2 - u_1|^2 + \frac{1}{2} \int_{\partial \Omega} |\gamma_D(u_2 - u_1)|^2 ds
= -\int_{\Omega} \delta D \nabla u_2 \nabla (u_2 - u_1) + \delta \mu_a u_2 (u_2 - u_1) dx.
\]

Now, using this information, the equality of the norms \( ||\cdot||_{H^1} \) and \( ||\cdot||_{H^1}^* \), Hölder’s Inequality, and the Poincaré Inequality we have,

\[
c_1 ||u_2 - u_1||^2_{H^1(\Omega)} \leq ||u_2 - u_1||^2_{H^1}
= \int_{\Omega} (D_1 \nabla |u_2 - u_1|^2 + \mu_{a,1}|u_2 - u_1|^2) dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D(u_2 - u_1)|^2 ds
\leq \int_{\Omega} (D_1 \nabla |u_2 - u_1|^2 + (\mu_{a,1} + ik)|u_2 - u_1|^2) dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D(u_2 - u_1)|^2 ds
= -\int_{\Omega} \delta D \nabla u_2 \nabla (u_2 - u_1) + \delta \mu_a u_2 (u_2 - u_1) dx
\leq ||\delta D||_{L^\infty(\Omega)} ||\nabla u_2||_{L^2(\Omega)} ||\nabla (u_2 - u_1)||_{L^2(\Omega)}
+ ||\delta \mu_a||_{L^\infty(\Omega)} ||u_2||^2_{L^2(\Omega)} ||u_2 - u_1||_{L^2(\Omega)}
\leq ||\delta D||_{L^\infty(\Omega)} ||\nabla u_2||_{L^2(\Omega)} ||\nabla (u_2 - u_1)||_{L^2(\Omega)}
+ C(\Omega) ||\delta \mu_a||_{L^\infty(\Omega)} ||\nabla u_2||_{L^2(\Omega)} ||\nabla (u_2 - u_1)||_{L^2(\Omega)}
\leq \max\{1, C(\Omega)\} ||\delta q||_{L^\infty(\Omega)} ||u_2||_{H^1(\Omega)} ||\nabla (u_2 - u_1)||_{L^2(\Omega)}
\leq c_2 \max\{1, C(\Omega)\} ||\delta q||_{L^\infty(\Omega)} ||u_2 - u_1||_{H^1(\Omega)}
\]

where \( c_1, c_2 > 0 \) are constants and \( C(\Omega) \) is the constant given by the Poincaré Inequality. Thus, we have

\[
||u_2 - u_1||_{H^1(\Omega)} \leq C_1 ||\delta q||_{L^\infty(\Omega)}
\]

where \( C_1 = \frac{c_2 \max\{1, C(\Omega)\}}{c_1} \).

\( \square \)
Since we want to include information about the solution’s dependence on \( \lambda \) in our norm, we will also prove the continuity of \( \frac{\partial u}{\partial \lambda} \) with respect to \( q \).

**Theorem 2.16.** The solution to (2.38), (2.40), \( \frac{\partial u}{\partial \lambda} \), is continuous with respect to \( \hat{q} \).

**Proof.** This proof will follow that of Theorem 2.15. We will denote \( \frac{\partial u}{\partial \lambda}(\hat{q}_1) \) as \( \frac{\partial u_1}{\partial \lambda} \) and \( \frac{\partial u}{\partial \lambda}(\hat{q}_1 + \delta \hat{q}) = \frac{\partial u(\hat{q}_2)}{\partial \lambda} = \frac{\partial u_2}{\partial \lambda} \) in what follows. Here we must consider the extended set of parameters, \( \hat{q} \), given in (2.46), where \( \hat{q}_1, \hat{q}_2, \delta \hat{q} \) are given analogously to \( q_1, q_2, \delta q \) in the proof of Theorem 2.15. Here, we will specifically denote

\[
\hat{q}' = \begin{pmatrix}
\frac{\partial D}{\partial \lambda} \\
\frac{\partial u}{\partial \lambda}
\end{pmatrix}
\]

and \( \hat{q}'_1, \hat{q}'_2, \delta \hat{q}' \) analogously to the corresponding values of \( q \) and \( \hat{q} \). Recall that the weak solutions of \( \frac{\partial u_1}{\partial \lambda} \) and \( \frac{\partial u_2}{\partial \lambda} \) satisfy

\[
\int_{\Omega} \left( D_1 \nabla \frac{\partial u_1}{\partial \lambda} \right) \nabla \tilde{v} + (\mu_{a,1} + ik) \frac{\partial u_1}{\partial \lambda} \tilde{v} \, dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_1}{\partial \lambda} \gamma_D \tilde{v} \, ds
\]

\[
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \tilde{v} \, ds - \int_{\Omega} \left( \frac{\partial D_1}{\partial \lambda} \nabla u_1 \nabla \tilde{v} + \frac{\partial \mu_{a,1}}{\partial \lambda} u_1 \tilde{v} \right) \, dx
\]

\[
\int_{\Omega} \left( D_2 \nabla \frac{\partial u_2}{\partial \lambda} \right) \nabla \tilde{v} + (\mu_{a,2} + ik) \frac{\partial u_2}{\partial \lambda} \tilde{v} \, dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_2}{\partial \lambda} \gamma_D \tilde{v} \, ds
\]

\[
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \tilde{v} \, ds - \int_{\Omega} \left( \frac{\partial D_2}{\partial \lambda} \nabla u_2 \nabla \tilde{v} + \frac{\partial \mu_{a,2}}{\partial \lambda} u_2 \tilde{v} \right) \, dx
\]

Expanding \( \hat{q}_2 = \hat{q}_1 + \delta \hat{q} \) and subtracting the second equation from the first we are...
left with

\[ \int_{\Omega} D_1 \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \nabla \tilde{v} + (\mu_{a,1} + ik) \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \tilde{v} \, dx \]

\[ + \frac{1}{2} \int_{\partial \Omega} \gamma_D \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \gamma_D \tilde{v} \, ds \]

\[ = \int_{\Omega} \left( \frac{\partial D_1}{\partial \lambda} \nabla (u_1 - u_2) \nabla \tilde{v} + \frac{\partial \mu_{a,1}}{\partial \lambda} (u_1 - u_2) \tilde{v} \right) \, dx \]

\[ - \int_{\Omega} \left( \delta \left( \frac{D}{\partial \lambda} \right) \nabla u_2 \nabla \tilde{v} + \delta \left( \frac{\partial \mu}{\partial \lambda} \right) u_2 \tilde{v} \right) \, dx \]

\[ - \int_{\Omega} \delta D \nabla \frac{\partial u_2}{\partial \lambda} \nabla \tilde{v} + \delta \mu_a \frac{\partial u_2}{\partial \lambda} \tilde{v} \, dx \]

Since this equality must hold for any \( v \in H^1(\Omega) \), let \( v = \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \). Then we have

\[ \int_{\Omega} D_1 \nabla \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2 \, dx + (\mu_{a,1} + ik) \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right)^2 \, dx \]

\[ + \frac{1}{2} \int_{\partial \Omega} \gamma_D \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \gamma_D \tilde{v} \, ds \]

\[ = \int_{\Omega} \frac{\partial D_1}{\partial \lambda} \nabla (u_1 - u_2) \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \, dx \]

\[ + \int_{\Omega} \frac{\partial \mu_{a,1}}{\partial \lambda} (u_1 - u_2) \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \, dx \]

\[ - \int_{\Omega} \delta \left( \frac{D}{\partial \lambda} \right) \nabla u_2 \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \, dx \]

\[ - \int_{\Omega} \delta \left( \frac{\partial \mu}{\partial \lambda} \right) u_2 \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \, dx \]

\[ - \int_{\Omega} \delta D \nabla \frac{\partial u_2}{\partial \lambda} \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) + \delta \mu_a \frac{\partial u_2}{\partial \lambda} \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \, dx \]

Now, using this information, the equality of the norms \( \| \cdot \|_{H^1} \) and \( \| \cdot \|_{H^1} \), Hölder’s
Inequality, the Poincaré Inequality, and the continuity of \( u \) with respect to \( q \) we have,

\[
c_1 \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2_{H^1(\Omega)} \leq \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2_{H^1(\Omega)}
\]

\[
= \int_\Omega \left( D_1 \nabla \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2 + \mu a_1 \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2 \right) dx
\]

\[
+ \frac{1}{2} \int_{\partial \Omega} \gamma_D \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right)^2 ds
\]

\[
\leq \int_\Omega \left( D_1 \nabla \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2 + (\mu a_1 + i \kappa) \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|^2 \right) dx
\]

\[
+ \frac{1}{2} \int_{\partial \Omega} \gamma_D \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right)^2 ds
\]

\[
= \int_\Omega \frac{\partial D_1}{\partial \lambda} \nabla (u_1 - u_2) \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) dx
\]

\[
+ \int_\Omega \frac{\partial \mu a_1}{\partial \lambda} (u_1 - u_2) \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) dx
\]

\[
- \int_\Omega \delta \left( \frac{\partial D}{\partial \lambda} \right) u_2 \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) dx
\]

\[
- \int_\Omega \delta \left( \frac{\partial \mu}{\partial \lambda} \right) u_2 \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) dx
\]

\[
\leq \left| \frac{\partial D_1}{\partial \lambda} \right|_{L^\infty(\Omega)} \left| \nabla (u_1 - u_2) \right|_{L^2(\Omega)} \left| \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \right|_{L^2(\Omega)}
\]

\[
+ \left| \frac{\partial \mu a_1}{\partial \lambda} \right|_{L^\infty(\Omega)} \left| u_1 - u_2 \right|_{L^2(\Omega)} \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|_{L^2(\Omega)}
\]

\[
- \left| \delta \left( \frac{\partial D}{\partial \lambda} \right) \right|_{L^\infty(\Omega)} \left| \nabla u_2 \right|_{L^2(\Omega)} \left| \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \right|_{L^2(\Omega)}
\]

\[
- \left| \delta \left( \frac{\partial \mu}{\partial \lambda} \right) \right|_{L^\infty(\Omega)} \left| u_2 \right|_{L^2(\Omega)} \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|_{L^2(\Omega)}
\]

\[
- \left| \delta D \right|_{L^\infty(\Omega)} \left| \nabla \frac{\partial u_2}{\partial \lambda} \right|_{L^2(\Omega)} \left| \nabla \left( \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right) \right|_{L^2(\Omega)}
\]

\[
- \left| \delta \mu \right|_{L^\infty(\Omega)} \left| \frac{\partial u_2}{\partial \lambda} \right|_{L^2(\Omega)} \left| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right|_{L^2(\Omega)}
\]
where \( c_i > 0, i = 1, \ldots, 5 \) are constants, \( C_1(\Omega), C_2(\Omega), C_3(\Omega) \) are the constants given by the Poincaré Inequality, and

\[
C_6 = \max\{c_2c_3 \max\{1, C_1(\Omega)\}, c_4 \max\{1, C_2(\Omega)\}, c_5 \max\{1, C_3(\Omega)\}\}. 
\]
Thus, we have
\[ \left\| \frac{\partial u_2}{\partial \lambda} - \frac{\partial u_1}{\partial \lambda} \right\|_{H^1(\Omega)} \leq C\left( \| \delta \hat{q}' \|_{L^\infty(\Omega)} + 2\| \delta q \|_{L^\infty(\Omega)} \right) \]
where \( C = \frac{C_6}{c_1} \) plus the constant that comes from the bound on \( \| \hat{q}' \|_{L^\infty(\Omega)} \).

Noticing the results of the theorems above, we are now ready to define our norm. Let the norm on \( C^1(H^1(\Omega); \Lambda) \) be given by
\[ \| u \|_{C^1_\lambda} = \left( \| u \|_{H^1(\Omega)}^2 + \left\| \frac{\partial u}{\partial \lambda} \right\|^2_{H^1(\Omega)} \right)^{1/2} \]

(2.47)

**Lemma 2.17.** \( \| \cdot \|_{C^1_\lambda} : H^1(\Omega) \to [0, \infty) \) is a norm.

**Proof.** Let \( u, v \in H^1(\Omega) \) and \( \alpha \in \mathbb{R} \). Since \( \| \cdot \|_{H^1(\Omega)} \) is a norm, it follows that

(i)
\[ \| u + v \|_{C^1_\lambda} = \left( \| u + v \|_{H^1(\Omega)}^2 + \left\| \frac{\partial u}{\partial \lambda} + \frac{\partial v}{\partial \lambda} \right\|_{H^1(\Omega)}^2 \right)^{1/2} \]
\[ \leq \left( \| u \|_{H^1(\Omega)}^2 + \| v \|_{H^1(\Omega)}^2 + \left\| \frac{\partial u}{\partial \lambda} \right\|^2_{H^1(\Omega)} + \left\| \frac{\partial v}{\partial \lambda} \right\|^2_{H^1(\Omega)} \right)^{1/2} \]
\[ \leq \left( \| u \|_{H^1(\Omega)}^2 + \left\| \frac{\partial u}{\partial \lambda} \right\|^2_{H^1(\Omega)} \right)^{1/2} + \left( \| v \|_{H^1(\Omega)}^2 + \left\| \frac{\partial v}{\partial \lambda} \right\|^2_{H^1(\Omega)} \right)^{1/2} \]
\[ = \| u \|_{C^1_\lambda} + \| v \|_{C^1_\lambda} \]
(ii) \[ \|\alpha u\|_{C^1_\lambda} = \left(\|\alpha u\|_{H^1(\Omega)}^2 + \left|\alpha\right| \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2\right)^{1/2} = \left(\alpha^2\|u\|_{H^1(\Omega)}^2 + \alpha^2 \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2\right)^{1/2} = |\alpha| \left(\|u\|_{H^1(\Omega)}^2 + \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2\right)^{1/2} = |\alpha|\|u\|_{C^1_\lambda} \]

(iii) Assume \(\|u\|_{C^1_\lambda} = 0\). Then,
\[
\left(\|u\|_{H^1(\Omega)}^2 + \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2\right)^{1/2} = 0
\implies \|u\|_{H^1(\Omega)}^2 + \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2 = 0
\]

Thus since \(\|u\|_{H^1(\Omega)}^2 \geq 0\) and \(\|\frac{\partial u}{\partial \lambda}\|_{H^1(\Omega)}^2 \geq 0\), it must be that \(\|u\|_{H^1} = 0\) and \(\|\frac{\partial u}{\partial \lambda}\|_{H^1(\Omega)} = 0\) and so, since \(\|\cdot\|_{H^1(\Omega)}\) is a norm, \(u = 0\) for all \(\lambda \in \Lambda\).

Now assume that \(u = 0\) for all \(\lambda \in \Lambda\). Then \(\frac{\partial u}{\partial \lambda} = 0\) for all \(\lambda \in \Lambda\). Thus, since \(\|\cdot\|_{H^1(\Omega)}\) is a norm, \(\|u\|_{C^1_\lambda} = \left(\|u\|_{H^1(\Omega)}^2 + \left\|\frac{\partial u}{\partial \lambda}\right\|_{H^1(\Omega)}^2\right)^{1/2} = 0\).

So \(\|\cdot\|_{C^1_\lambda}\) is a norm.

Now we are ready to prove that \(u\) is continuous with respect to \(q\), with respect to its dependence on \(\lambda\) using this new norm.

**Theorem 2.18.** There exists constants, \(c_1, c_2 > 0\) such that
\[
\|u(q_{\lambda,2}) - u(q_{\lambda,1})\|_{C^1_\lambda} \leq c_1\|\delta \lambda q\|_{L^\infty(\Omega)} + c_2\|\delta \lambda \hat{q}'\|_{L^\infty(\Omega)}
\]
where \( \|\delta_{\lambda}q\|_{L^\infty(\Omega)} = \max\{\|\delta_{\lambda}D\|_{L^\infty(\Omega)}, \|\delta_{\lambda}\mu_a\|_{L^\infty(\Omega)}\} \) and \( D(\lambda_2) = D(\lambda_1) + \delta_{\lambda}D, \mu_a(\lambda_2) = \mu_a(\lambda_1) + \delta_{\lambda}\mu_a. \)

**Proof.** To simplify notation, in what follows let \( u(\lambda_1) = u_{\lambda,1} \) and \( u(\lambda_2) = u_{\lambda,2}. \) Additionally, 

\[
q_{\lambda,1} = \begin{pmatrix} D(\lambda_1) \\ \mu_a(\lambda_1) \end{pmatrix} = \begin{pmatrix} D_{\lambda,1} \\ \mu_{\lambda,1} \end{pmatrix}
\]

and similarly for \( q_{\lambda,2}. \) We will follow this same notation to define \( \frac{u_{\lambda,1}}{\partial_{\lambda}}, \frac{u_{\lambda,2}}{\partial_{\lambda}}, \) and \( \hat{q}'_{\lambda,1}, \hat{q}'_{\lambda,2}, \delta_{\lambda}q'. \)

First, note that the weak solutions of \( u_{\lambda,1} \) and \( u_{\lambda,2} \) satisfy

\[
\int_{\Omega} D_{\lambda,1} \nabla u_{\lambda,1} \nabla \tilde{v} + (\mu_{\lambda,1} + ik)u_{\lambda,1} \tilde{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_{\lambda,1} \gamma_D \tilde{v} ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \tilde{v} ds
\]

\[
\int_{\Omega} D_{\lambda,2} \nabla u_{\lambda,2} \nabla \tilde{v} + (\mu_{\lambda,2} + ik)u_{\lambda,2} \tilde{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_{\lambda,2} \gamma_D \tilde{v} ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \tilde{v} ds
\]

Expanding \( q_{\lambda,2} = q_{\lambda,1} + \delta_{\lambda}q \) and subtracting the second equation from the first we are left with

\[
\int_{\Omega} D_{\lambda,1} \nabla (u_{\lambda,2} - u_{\lambda,1}) \nabla \tilde{v} + (\mu_{\lambda,1} + ik)(u_{\lambda,2} - u_{\lambda,1}) \tilde{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D (u_{\lambda,2} - u_{\lambda,1}) \gamma_D \tilde{v} ds
\]

\[
= -\int_{\Omega} \delta_{\lambda}D \nabla u_{\lambda,2} \nabla \tilde{v} + \delta_{\lambda}\mu_a u_{\lambda,2} \tilde{v} dx
\]

Since this equality must hold for any \( v \in H^1(\Omega), \) let \( v = u_2 - u_1. \) Then we have

\[
\int_{\Omega} D_{\lambda,1} \nabla |u_{\lambda,2} - u_{\lambda,1}|^2 dx + (\mu_{\lambda,1} + ik)|u_{\lambda,2} - u_{\lambda,1}|^2 dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D (u_{\lambda,2} - u_{\lambda,1})|^2 ds
\]

\[
= -\int_{\Omega} \delta_{\lambda}D \nabla u_{\lambda,2} \nabla (u_{\lambda,2} - u_{\lambda,1}) + \delta_{\lambda}\mu_a u_{\lambda,2} (u_{\lambda,2} - u_{\lambda,1}) dx
\]
Similarly, the weak solutions of $\frac{\partial u_\lambda,1}{\partial \lambda}$ and $\frac{\partial u_\lambda,2}{\partial \lambda}$ satisfy

\[
\int_\Omega \left( D_{\lambda,1} \nabla \frac{\partial u_\lambda,1}{\partial \lambda} \right) \nabla \bar{v} + (\mu_{\lambda,1} + ik) \frac{\partial u_\lambda,1}{\partial \lambda} \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_\lambda,1}{\partial \lambda} \gamma_D \bar{v} ds
\]

\[
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds - \int_{\Omega} \left( \frac{\partial D_{\lambda,1}}{\partial \lambda} \nabla u_\lambda,1 \nabla \bar{v} + \frac{\partial \mu_{\lambda,1}}{\partial \lambda} u_\lambda,1 \bar{v} \right) ds
\]

\[
\int_\Omega \left( D_{\lambda,2} \nabla \frac{\partial u_\lambda,2}{\partial \lambda} \right) \nabla \bar{v} + (\mu_{\lambda,2} + ik) \frac{\partial u_\lambda,2}{\partial \lambda} \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_\lambda,2}{\partial \lambda} \gamma_D \bar{v} ds
\]

\[
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds - \int_{\Omega} \left( \frac{\partial D_{\lambda,2}}{\partial \lambda} \nabla u_\lambda,2 \nabla \bar{v} + \frac{\partial \mu_{\lambda,2}}{\partial \lambda} u_\lambda,2 \bar{v} \right) dx
\]

Expanding $\hat{q}_{\lambda,2} = \hat{q}_{\lambda,1} + \delta_{\lambda} \hat{q}$ and subtracting the second equation from the first we are left with

\[
\int_\Omega D_{\lambda,1} \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \nabla \bar{v} + (\mu_{\lambda,1} + ik) \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \bar{v} dx
\]

\[
+ \frac{1}{2} \int_{\partial \Omega} \gamma_D \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \gamma_D \bar{v} ds
\]

\[
= \int_{\Omega} \frac{\partial D_{\lambda,1}}{\partial \lambda} \nabla (u_{\lambda,1} - u_{\lambda,2}) \nabla \bar{v} dx
\]

\[
+ \int_{\Omega} \frac{\partial \mu_{\lambda,1}}{\partial \lambda} (u_{\lambda,1} - u_{\lambda,2}) \bar{v} dx
\]

\[
- \int_{\Omega} \delta_{\lambda} \left( \frac{\partial D}{\partial \lambda} \nabla u_{\lambda,2} \nabla \bar{v} + \delta_{\lambda} \left( \frac{\partial \mu_a}{\partial \lambda} \right) u_{\lambda,2} \bar{v} \right) dx
\]

\[
- \int_{\Omega} \delta_{\lambda} D \nabla \frac{\partial u_{\lambda,2}}{\partial \lambda} \nabla \bar{v} + \delta_{\lambda} \mu_a \frac{\partial u_{\lambda,2}}{\partial \lambda} \bar{v} dx
\]

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Since this equality must hold for any \( v \in H^1(\Omega) \), let \( v = \frac{\partial u}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \). Then we have

\[
\int_{\Omega} D_{\lambda,1} \nabla \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|^2 + (\mu_{\lambda,1} + ik) \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|^2 \, dx \\
+ \frac{1}{2} \int_{\partial \Omega} \left| \gamma_D \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right|^2 \, ds \\
= \int_{\Omega} \frac{\partial D_{\lambda,1}}{\partial \lambda} \nabla (u_{\lambda,1} - u_{\lambda,2}) \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
+ \int_{\Omega} \frac{\partial \mu_{\lambda,1}}{\partial \lambda} (u_{\lambda,1} - u_{\lambda,2}) \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
- \int_{\Omega} \delta \left( \frac{\partial D}{\partial \lambda} \right) \nabla u_{\lambda,2} \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \\
+ \delta \left( \frac{\partial \mu}{\partial \lambda} \right) u_{\lambda,2} \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
- \int_{\Omega} \delta_D \nabla \frac{\partial u_{\lambda,2}}{\partial \lambda} \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \\
+ \delta \mu \frac{\partial u_{\lambda,2}}{\partial \lambda} \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx
\]

Now, using this information, the equality of the \( H^1 \) and \( H^1_* \) norms, Hölder’s Inequality, and the Poincaré Inequality we have

\[
c_1 \| u_{\lambda,2} - u_{\lambda,1} \|_C^2 = c_1 \| u_{\lambda,2} - u_{\lambda,1} \|^2_{H^1(\Omega)} + c_1 \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|^2_{H^1(\Omega)} \\
\leq \| u_{\lambda,2} - u_{\lambda,1} \|^2_{H^1(\Omega)} + \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|^2_{H^1(\Omega)} \\
= \int_{\Omega} D_{\lambda,1} \nabla |u_{\lambda,2} - u_{\lambda,1}|^2 \, dx + \mu_{\lambda,1} |u_{\lambda,2} - u_{\lambda,1}|^2 \\
+ \frac{1}{2} \int_{\partial \Omega} |\gamma_D (u_{\lambda,2} - u_{\lambda,1})|^2 \, ds \\
+ \int_{\Omega} D_{\lambda,1} \nabla \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|^2 + \mu_{\lambda,1} \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|^2 \, dx \\
+ \frac{1}{2} \int_{\partial \Omega} \left| \gamma_D \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right|^2 \, ds
\]

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\[ \begin{align*}
&= - \int_{\Omega} \delta_{\lambda} D \nabla u_{\lambda,2} \nabla (u_{\lambda,2} - u_{\lambda,1}) + \delta_{\lambda} \mu_{a} u_{\lambda,2} (u_{\lambda,2} - u_{\lambda,1}) \, dx \\
&+ \int_{\Omega} \frac{\partial D_{\lambda,1}}{\partial \lambda} \nabla (u_{\lambda,1} - u_{\lambda,2}) \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
&+ \int_{\Omega} \frac{\partial \mu_{\lambda,1}}{\partial \lambda} (u_{\lambda,1} - u_{\lambda,2}) \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
&- \int_{\Omega} \delta_{\lambda} \left( \frac{\partial D}{\partial \lambda} \right) \nabla u_{\lambda,2} \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \\
&+ \delta_{\lambda} \left( \frac{\partial \mu_{\lambda}}{\partial \lambda} \right) u_{\lambda,2} \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx \\
&- \int_{\Omega} \delta_{\lambda} D \nabla \frac{\partial u_{\lambda,2}}{\partial \lambda} \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \\
&+ \delta_{\lambda} \mu_{a} \frac{\partial u_{\lambda,2}}{\partial \lambda} \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \, dx
\end{align*} \]

\[ \leq \left\| \delta_{\lambda} D \right\|_{L^{\infty}(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \nabla (u_{\lambda,2} - u_{\lambda,1}) \right\|_{L^{2}(\Omega)} \\
+ \left\| \delta_{\lambda} \mu_{a} \right\|_{L^{\infty}(\Omega)} \left\| u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| u_{\lambda,2} - u_{\lambda,1} \right\|_{L^{2}(\Omega)} \\
+ \left\| \frac{\partial D_{\lambda,1}}{\partial \lambda} \right\|_{L^{\infty}(\Omega)} \left\| \nabla (u_{\lambda,1} - u_{\lambda,2}) \right\|_{L^{2}(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^{2}(\Omega)} \\
+ \left\| \frac{\partial \mu_{\lambda,1}}{\partial \lambda} \right\|_{L^{\infty}(\Omega)} \left\| u_{\lambda,1} - u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{L^{2}(\Omega)} \\
+ \left\| \delta_{\lambda} \left( \frac{\partial D}{\partial \lambda} \right) \right\|_{L^{\infty}(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^{2}(\Omega)} \\
+ \left\| \delta_{\lambda} \left( \frac{\partial \mu_{\lambda}}{\partial \lambda} \right) \right\|_{L^{\infty}(\Omega)} \left\| u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{L^{2}(\Omega)} \\
\leq \left\| \delta_{\lambda} D \right\|_{L^{\infty}(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \nabla (u_{\lambda,2} - u_{\lambda,1}) \right\|_{L^{2}(\Omega)} \\
+ C_{1}(\Omega) \left\| \delta_{\lambda} \mu_{a} \right\|_{L^{\infty}(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^{2}(\Omega)} \left\| \nabla (u_{\lambda,2} - u_{\lambda,1}) \right\|_{L^{2}(\Omega)} \\
+ \left\| \frac{\partial D_{\lambda,1}}{\partial \lambda} \right\|_{L^{\infty}(\Omega)} \left\| \nabla (u_{\lambda,1} - u_{\lambda,2}) \right\|_{L^{2}(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^{2}(\Omega)} \\
+ C_{2}(\Omega) \left\| \frac{\partial \mu_{\lambda,1}}{\partial \lambda} \right\|_{L^{\infty}(\Omega)} \left\| \nabla (u_{\lambda,1} - u_{\lambda,2}) \right\|_{L^{2}(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^{2}(\Omega)}
\]
+ \left\| \delta_\lambda \left( \frac{\partial D}{\partial \lambda} \right) \right\|_{L^\infty(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^2(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
+ C_3(\Omega) \left\| \delta_\lambda \left( \frac{\partial u_a}{\partial \lambda} \right) \right\|_{L^\infty(\Omega)} \left\| \nabla u_{\lambda,2} \right\|_{L^2(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
+ ||\delta_\lambda D||_{L^\infty(\Omega)} \left\| \nabla \frac{\partial u_{\lambda,2}}{\partial \lambda} \right\|_{L^2(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
+ C_4(\Omega) \left\| \delta_\lambda \mu_a \right\|_{L^\infty(\Omega)} \left\| \nabla \frac{\partial u_{\lambda,2}}{\partial \lambda} \right\|_{L^2(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
\leq \max\{1, C_1(\Omega)\} \left\| \delta_\lambda q \right\|_{L^\infty(\Omega)} \left\| u_{\lambda,2} \right\|_{H^1(\Omega)} \left\| \nabla \left( u_{\lambda,2} - u_{\lambda,1} \right) \right\|_{L^2(\Omega)}
+ \max\{1, C_2(\Omega)\} \left\| \dot{q}_1 \right\|_{L^\infty(\Omega)} \left\| u_{\lambda,1} - u_{\lambda,2} \right\|_{H^1(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
+ \max\{1, C_3(\Omega)\} \left\| \delta_\lambda \dot{q} \right\|_{L^\infty(\Omega)} \left\| u_{\lambda,2} \right\|_{H^1(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}
+ \max\{1, C_4(\Omega)\} \left\| \delta_\lambda q \right\|_{L^\infty(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} \right\|_{H^1(\Omega)} \left\| \nabla \left( \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right) \right\|_{L^2(\Omega)}

Note that if we follow the same argument as the proof of Theorem 2.16 but replace the spatial perturbations of \( \frac{\partial u}{\partial \lambda}, \dot{q} \) with the spectral perturbations described at the beginning of this proof, then we can show that

\[ \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{H^1(\Omega)} \leq C \left( \left\| \delta_\lambda \dot{q} \right\|_{L^\infty(\Omega)} + 2 \left\| \delta_\lambda q \right\|_{L^\infty(\Omega)} \right). \]

Using this fact, we continue the reasoning above to obtain,

\[ c_1 \left\| u_{\lambda,2} - u_{\lambda,1} \right\|_{C^2} \leq c_2 \max\{1, C_1(\Omega)\} \left\| \delta_\lambda q \right\|_{L^\infty(\Omega)} \left\| u_{\lambda,2} - u_{\lambda,1} \right\|_{H^1(\Omega)}
+ \max\{1, C_2(\Omega)\} \left\| \dot{q}_1 \right\|_{L^\infty(\Omega)} \left\| u_{\lambda,1} - u_{\lambda,2} \right\|_{H^1(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{H^1(\Omega)}
+ c_3 \max\{1, C_3(\Omega)\} \left\| \delta_\lambda \dot{q} \right\|_{L^\infty(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{H^1(\Omega)}
+ c_4 \max\{1, C_4(\Omega)\} \left\| \delta_\lambda q \right\|_{L^\infty(\Omega)} \left\| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right\|_{H^1(\Omega)} \]
\[
\leq c_2 \max \{1, C_1(\Omega)\} \|\delta_\lambda \mathbf{q}\|_{L^\infty(\Omega)} \|u_{\lambda,2} - u_{\lambda,1}\|_{H^1(\Omega)} + c_5 \max \{1, C_2(\Omega)\} \|\tilde{\mathbf{q}}_1\|_{L^\infty(\Omega)} (\|\delta_\lambda \tilde{\mathbf{q}}_1\|_{L^\infty(\Omega)} \|u_{\lambda,1} - u_{\lambda,2}\|_{H^1(\Omega)}
\]
\[
+ c_5 \max \{1, C_2(\Omega)\} \|\tilde{\mathbf{q}}_1\|_{L^\infty(\Omega)} (2\|\delta_\lambda \mathbf{q}\|_{L^\infty(\Omega)} \|u_{\lambda,1} - u_{\lambda,2}\|_{H^1(\Omega)}
\]
\[
+ c_3 \max \{1, C_3(\Omega)\} \|\delta_\lambda \tilde{\mathbf{q}}'_1\|_{L^\infty(\Omega)} \left( \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|_{H^1(\Omega)}^2 \right)^{1/2}
\]
\[
+ c_4 \max \{1, C_4(\Omega)\} \|\delta_\lambda \mathbf{q}\|_{L^\infty(\Omega)} \left( \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|_{H^1(\Omega)}^2 \right)^{1/2}
\]
\[
+ C_9 \|\delta_\lambda \tilde{\mathbf{q}}'_2\|_{L^\infty(\Omega)} \left( \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|_{H^1(\Omega)}^2 \right)^{1/2}
\]
\[
+ C_9 \|\delta_\lambda \mathbf{q}\|_{L^\infty(\Omega)} \left( \left| \frac{\partial u_{\lambda,2}}{\partial \lambda} - \frac{\partial u_{\lambda,1}}{\partial \lambda} \right|_{H^1(\Omega)}^2 \right)^{1/2}
\]
\[
\leq (\max \{C_6, C_9\} \|\delta_\lambda \mathbf{q}\|_{L^\infty} + \max \{C_7, C_8\} \|\delta_\lambda \tilde{\mathbf{q}}'_1\|_{L^\infty}) \|u_{\lambda,2} - u_{\lambda,1}\|_{C^1_\lambda}
\]

Thus, we are left with

\[
\|u_{\lambda,2} - u_{\lambda,1}\|_{C^1_\lambda} \leq C_{10} \|\delta_\lambda \mathbf{q}\|_{L^\infty} + C_{11} \|\delta_\lambda \tilde{\mathbf{q}}'_1\|_{L^\infty}
\]

where \(C_{10} = \frac{\max \{C_6, C_9\}}{c_1}\) and \(C_{11} = \frac{\max \{C_7, C_8\}}{c_1}\). □

Finally, we consider the spaces that govern the boundary, \(\partial \Omega\) of the spatial domain of the medium, \(\Omega\). Since we have Robin boundary conditions, we cannot say
that \( u \) or \( \frac{\partial u}{\partial \lambda} \) are 0 on \( \partial \Omega \) and thus in \( H^1_0(\Omega) \). Instead, we note that the Sobolev Trace Theorem (Theorem 2.7) guarantees the existence of a bounded linear trace operator, denoted here as \( \gamma_D \), that takes \( u \) and \( \frac{\partial u}{\partial \lambda} \) to from \( \Omega \) to \( \partial \Omega \) using the Dirichlet trace (see (2.12)). According to Theorem 2.7, this operator takes \( u, \frac{\partial u}{\partial \lambda} \) from \( H^1(\Omega) \) to \( H^{1/2}(\partial \Omega) \). Further, we have asserted that \( f \in H^{-1/2}(\partial \Omega) \). We claim that \( \frac{\partial f}{\partial \lambda} \in H^{-1/2}(\partial \Omega) \) as well.

### 2.2.3 Linearization

The application of the Reduced Basis Method to the hyDOT forward problem (see Chapter 4) reveals the regularity of hyDOT with respect to the wavelength, \( \lambda \). We seek to exploit this regularity in \( \lambda \) in the inverse problem as we already have in the forward problem. In order to exploit this regularity in the inverse problem as well, we wish to incorporate the sensitivity of the solution \( u \) with respect to \( \lambda \) into the minimization problem. Solving this minimization problem will require use of a gradient method, so in order to find this gradient we must first find the linearization of the problem. Linearization is often used as a regularization technique to solve the DOT inverse problem because the discretized form of the governing PDE (given by (2.1)-(2.2)) is severely ill-posed (due to the highly scattering nature of the medium) and ill-conditioned. We now apply it to the system (2.37) - (2.40). We will do this sequentially, as we did when deriving the weak formulation, first linearizing (2.37), (2.39) and then applying this to the linearization of (2.38), (2.40).

Give a fixed \( \lambda \), we consider a perturbation \( \delta \hat{q} \) of \( \hat{q}_0 \) such that \( \hat{q} = \hat{q}_0 + \delta \hat{q} \) where \( \hat{q}_0 \) is the value of the unknown optical parameters for a homogeneous background. Note that \( \delta \hat{q} \) is an arbitrary direction for the variation of \( \hat{q} \) that vanishes on \( \delta \Omega \). That
is,
\[ \hat{q} = \begin{bmatrix} D \\ \mu_a \\ \frac{\partial D}{\partial \lambda} \\ \frac{\partial \mu_a}{\partial \lambda} \end{bmatrix} = \begin{bmatrix} D_0 + \delta D \\ \mu_{a,0} + \delta \mu_a \\ \frac{\partial D_0}{\partial \lambda} + \frac{\partial}{\partial \lambda}(\delta D_0) \\ \frac{\partial \mu_{a,0}}{\partial \lambda} + \frac{\partial}{\partial \lambda}(\delta \mu_{a,0}) \end{bmatrix}. \] (2.48)

Since the solution, \( \hat{u} \), to the coupled system (2.37)- (2.40) is dependent on \( \hat{q} \), we can rewrite \( \hat{u} \) as
\[ \hat{u} = \begin{pmatrix} u_1 \\ \frac{\partial u_1}{\partial \lambda} \end{pmatrix} = \begin{pmatrix} u_0 \\ \frac{\partial u_0}{\partial \lambda} \end{pmatrix} + \begin{pmatrix} \delta u(q_0)[\delta q] \\ \frac{\partial}{\partial q} \frac{\partial u(q_0)}{\partial \lambda} \left[ \delta \left( \frac{\partial q}{\partial \lambda} \right) \right] \end{pmatrix}. \] (2.49)

From now on we will refer to \( \delta u(q_0)[\delta q] \) as \( \delta u \) and \( \frac{\partial}{\partial q} \frac{\partial u(q_0)}{\partial \lambda} \left[ \delta \left( \frac{\partial q}{\partial \lambda} \right) \right] \) as \( \frac{\partial (\delta u)}{\partial \lambda} \) for simplicity. We seek to find the partial differential equations of which \( \delta u \) and \( \frac{\partial (\delta u)}{\partial \lambda} \) are solutions, given a fixed value \( q_0 \) of \( \hat{q} \).

First, we will find the linearization of (2.37), (2.39). To do this, we examine the Robin forward problem at a fixed \( \lambda \) given by (2.1) - (2.2). Note that (2.48) substituted into (2.1) - (2.2) is given by
\[ \begin{align*}
\text{in } \Omega, \\
u + 2[D_0 + \delta D] \frac{\partial u}{\partial n} = f \text{ on } \partial \Omega
\end{align*} \] (2.50)

Additionally, (2.1) - (2.2) evaluated at \( q_0 \) is
\[ \begin{align*}
\text{in } \Omega, \\
u_0 + 2D_0 \frac{\partial u_0}{\partial n} = f \text{ on } \partial \Omega
\end{align*} \] (2.51)

Note that since \( u = u_0 + \delta u \), then \( \delta u = u - u_0 \). Thus, if we subtract (2.51) from
(2.50), we obtain,

\[-\text{div}(D_0 \nabla (u - u_0)) - \text{div}(\delta D \nabla u) + [\mu_{a,0} + ik](u - u_0) + \delta \mu_a u = 0 \quad \text{in } \Omega\]

\[(u - u_0) + 2 \left[ D_0 \left( \frac{\partial u}{\partial n} - \frac{\partial u_0}{\partial n} \right) + \delta D \frac{\partial u}{\partial n} \right] = 0 \quad \text{on } \partial \Omega \quad (2.52)\]

Now, substituting \( u = u_0 + \delta u \), ignoring the resulting quadratic terms, moving terms that do not include \( \delta u \) to the righthand side, and noting that \( \delta D \) and \( \delta \mu_a \) are 0 on the boundary, we are left with,

\[-\text{div}(D_0 \nabla \delta u) + (\mu_{a,0} + ik)\delta u = \text{div}(\delta D \nabla u_0) - \delta \mu_a u_0 \quad \text{in } \Omega \quad (2.53)\]

\[\delta u + 2D_0 \frac{\partial (\delta u)}{\partial n} = 0 \quad \text{on } \partial \Omega \quad (2.54)\]

We have found a PDE for which \( \delta u \) is a solution. We note that the mapping from \( \delta q \) to \( u \) defines a linear operator and is the linearization of \( F(q) \) about \( q \). We denote this linearization \( F'(q) \). Note that (2.53)-(2.54) is also known as the sensitivity equation.

We now find the weak form of (2.53) in order to investigate its properties analytically and numerically. We find the weak formulation as in Section 2.1.1 by multiplying both sides of (2.53) by a test function \( v \in H^1(\Omega) \), integrating, applying integration by parts, and the Dirichlet trace given in (2.12), and (2.54). We are left with

\[
\int_{\Omega} (D_0 \nabla \delta u) \nabla \bar{v} dx + \int_{\Omega} (\mu_{a,0} + ik)(\delta u)\bar{v} dx + \int_{\partial \Omega} \frac{1}{2} \gamma_D \delta u \gamma_D \bar{v} ds
\]

\[= - \int_{\Omega} (\delta D \nabla u_0) \nabla \bar{v} dx - \int_{\partial \Omega} \delta \mu_a u_0 \bar{v} ds. \quad (2.55)\]

Now we wish to show that \( \delta u \) is acting as the derivative of the forward solution \( u \).

That is, we will show that the derivative of \( u \) with respect to the parameter set \( q \) is \( \delta u(q_0)[\delta q] \).
Theorem 2.19. The solution, \( u \), to (2.37), (2.39) is differentiable. That is, for \( \{q_0, q_0 + \delta q\} \in Q \) (where \( Q \) is the parameter space) we have

\[
\frac{\| u(q_0 + \delta q) - u(q_0) - \delta u(q_0)[\delta q] \|_{H^1(\Omega)}}{\| \delta q \|_{L^\infty(\Omega)}} \to 0 \quad \text{as} \quad \| \delta q \|_{L^\infty(\Omega)} \to 0.
\]

Proof. As before, we will simplify notation by letting \( \delta u = \delta u(q_0)[\delta q] \), \( u_0 = u(q_0) \), and \( u_1 = u_0 + \delta q \). Additionally, we define

\[
w = u(q_0 + \delta q) - u(q_0) - \delta u(q_0)[\delta q] = u_1 - u_0 - \delta u.
\]

We seek to find a weak formulation for \( w \). First, we derive a weak formulation for (2.51). Multiplying by a test function \( v \in H^1(\Omega) \) and then applying integration by parts and the boundary condition we are left with,

\[
\int_{\Omega} D_0 \nabla u_0 \nabla \bar{v} dx + \int_{\Omega} (\mu a, 0 + ik) u_0 \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_0 \gamma_D \bar{v} ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \bar{v} ds. \tag{2.56}
\]

Next, we derive a weak formulation for (2.50). We obtain,

\[
\int_{\Omega} (D_0 + \delta D) \nabla u_1 \nabla \bar{v} dx + \int_{\Omega} (\mu a, 0 + \delta \mu a + ik) u_1 \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D u_1 \gamma_D \bar{v} ds = \frac{1}{2} \int_{\partial \Omega} f \gamma_D \bar{v} ds. \tag{2.57}
\]

Now, to find the weak formulation for \( w \), we subtract the weak formulation (2.56) from (2.57) and then subtract (2.55) from the result to obtain,

\[
\int_{\Omega} D_0 \nabla w \nabla \bar{v} dx + \int_{\Omega} (\mu a, 0 + ik) w \bar{v} dx = - \int_{\Omega} \delta D \nabla (\delta u) \nabla \bar{v} dx - \int_{\Omega} \delta \mu (\delta u) \bar{v} dx - \frac{1}{2} \int_{\partial \Omega} \gamma_D (\delta u) \gamma_D \bar{v} ds. \tag{2.58}
\]
Now, applying Hölder’s Inequality, the Sobolev Trace Theorem (Theorem 2.7), Theorem 2.15, and Poincaré’s Inequality we have,

\[ \min \left\{ D_0, \mu_0 \right\} ||w||^2_{H^1(\Omega)} \leq \frac{\int_\Omega D_0 |\nabla w|^2 + \mu_{a,0} |w|^2 \, dx}{||\delta q||_{L^\infty(\Omega)}} \]

\[ \leq -\int_\Omega \delta D \nabla (\delta u) \nabla \delta \bar{w} + \delta \mu (\delta u) \delta \bar{w} \, dx \]

\[ \leq -\int_\Omega \delta D \nabla (\delta u) \nabla \delta \bar{w} + \delta \mu (\delta u) \delta \bar{w} \, dx \]

\[ + \frac{1}{2} \left( \int_\Omega |\gamma_D (\delta u)|^2 ds \right)^{1/2} \left( \int_{\partial \Omega} |\gamma_D \delta \bar{w}|^2 ds \right)^{1/2} \]

\[ \leq -\int_\Omega \delta D \nabla (\delta u) \nabla \delta \bar{w} + \delta \mu (\delta u) \delta \bar{w} \, dx \]

\[ + \frac{1}{2} \int_\Omega |\nabla (\delta u)|^2 + |\delta u|^2 \, dx \]

\[ \leq \frac{||\delta q||_{L^\infty(\Omega)} \left( ||\nabla u||_{L^2(\Omega)} ||\nabla w||_{L^2(\Omega)} + ||u||_{H^1(\Omega)} ||w||_{H^1(\Omega)} \right)}{||\delta q||_{L^\infty(\Omega)}} \]

\[ + \frac{1}{2} ||\delta q||_{L^\infty(\Omega)} ||\delta u||_{H^1(\Omega)} ||w||_{H^1(\Omega)} \]

\[ \leq ||\delta u||_{H^1(\Omega)} ||\nabla w||_{L^2(\Omega)} + ||\delta u||_{H^1(\Omega)} ||w||_{L^2(\Omega)} \]

\[ + ||\delta u||_{H^1(\Omega)} ||w||_{H^1(\Omega)} \]

\[ \leq 3C_1(\Omega) ||\nabla w||_{L^2(\Omega)} ||\delta u||_{H^1(\Omega)} \]

\[ \leq C_2 ||\nabla w||_{L^2(\Omega)} ||\delta q||_{L^\infty(\Omega)} \]

where \( C_2 > 0 \) is a constant and \( C_1(\Omega) \) is the constant arising from use of the Poincaré Inequality. Thus, \( ||w||_{H^2(\Omega)} \to 0 \) as \( ||\delta q||_{L^\infty(\Omega)} \to 0 \).

Now we will find the linearized version of (2.38), (2.40). As before, we substitute the expansions of the parameters given by (2.48) into (2.38), (2.40) to obtain
Now, subtracting (2.38), (2.40) from (2.59) we are left with

\[
-\text{div} \left( [D_0 + \delta D] \nabla \frac{\partial {u_1}}{\partial \lambda} \right) + ([\mu_{a,0} + \delta \mu_a] + i k) \frac{\partial {u_1}}{\partial \lambda} = \text{div} \left( \left[ \frac{\partial D_0}{\partial \lambda} + \delta \left( \frac{\partial D}{\partial \lambda} \right) \right] \nabla {u_1} \right) - \left[ \frac{\partial {\mu_{a,0}}}{\partial \lambda} + \delta \left( \frac{\partial {\mu_a}}{\partial \lambda} \right) \right] {u_1} \quad \text{in } \Omega
\]

\[
\frac{\partial u_1}{\partial \lambda} + 2(D_0 + \delta D) \frac{\partial}{\partial n} \left( \frac{\partial {u_1}}{\partial \lambda} \right) = \frac{\partial f}{\partial \lambda} - 2 \left( \frac{\partial D_0}{\partial \lambda} + \delta \frac{\partial D}{\partial \lambda} \right) \frac{\partial {u_1}}{\partial n} \quad \text{on } \partial \Omega.
\]

Expanding \( u_1 = u_0 + \delta u \), ignoring quadratic terms, and using the fact that \( \delta D = 0 \)
on the boundary, \( \partial \Omega \), we have

\[
- \text{div} \left( D_0 \nabla \frac{\partial (\delta u)}{\partial \lambda} \right) + (\mu_{a,0} + ik) \frac{\partial (\delta u)}{\partial \lambda} = \text{div} \left( \delta D \nabla \frac{\partial u_0}{\partial \lambda} \right) - \delta \mu_a \frac{\partial u_0}{\partial \lambda} \\
+ \text{div} \left( \delta \left( \frac{\partial D}{\partial \lambda} \right) \nabla u_0 \right) - \delta \left( \frac{\partial \mu_a}{\partial \lambda} \right) u_0 \\
+ \text{div} \left( \frac{\partial D_0}{\partial \lambda} \nabla (\delta u) \right) - \frac{\partial \mu_{a,0}}{\partial \lambda} \delta u \quad \text{in } \Omega
\]

\[
\frac{\partial (\delta u)}{\partial \lambda} + 2 D_0 \frac{\partial}{\partial \mathbf{n}} \left( \frac{\partial (\delta u)}{\partial \lambda} \right) + 2 \frac{\partial D_0}{\partial \lambda} \frac{\partial}{\partial \mathbf{n}} u_0 = 0 \quad \text{on } \partial \Omega.
\]

(2.60)

We seek to prove a theorem similar to Theorem 2.20 for the solution \( \frac{\partial u}{\partial \lambda} \) to (2.38), (2.40). We define

\[
w_{\lambda} = \frac{\partial u(q_0 + \delta q)}{\partial \lambda} - \frac{\partial u_0}{\partial \lambda} - \frac{\partial (\delta u)}{\partial \lambda} = \frac{\partial u_1}{\partial \lambda} - \frac{\partial u_0}{\partial \lambda} - \frac{\partial (\delta u)}{\partial \lambda}.
\]

(2.61)

In order to proceed as before, we first must find the weak form of (2.38), (2.40). As before, we multiply both sides of (2.38) by a test function \( v \in H^1(\Omega) \) and apply integration by parts and the boundary condition (2.40) to obtain,

\[
\int_{\Omega} D_0 \nabla \frac{\partial u_0}{\partial \lambda} \nabla \bar{v} dx + \int_{\Omega} (\mu_{a,0} + ik) \frac{\partial u_0}{\partial \lambda} \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_0}{\partial \lambda} \gamma_D \bar{v} ds \\
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds - \int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} \nabla u_0 \nabla \bar{v} + \frac{\partial \mu_{a,0}}{\partial \lambda} u_0 \bar{v} \right) dx
\]

(2.62)

Next, we must find the weak form of (2.59). Proceeding as before we find,

\[
\int_{\Omega} [D_0 + \delta D] \nabla \frac{\partial u_1}{\partial \lambda} \nabla \bar{v} dx + \int_{\Omega} (\mu_{a,0} + \delta \mu_a + ik) \frac{\partial u_1}{\partial \lambda} \bar{v} dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \frac{\partial u_1}{\partial \lambda} \gamma_D \bar{v} ds \\
= \frac{1}{2} \int_{\partial \Omega} \frac{\partial f}{\partial \lambda} \gamma_D \bar{v} ds - \int_{\Omega} \left( \frac{\partial D_0}{\partial \lambda} + \delta \frac{\partial D}{\partial \lambda} \right) \nabla u_1 \nabla \bar{v} dx \\
- \int_{\Omega} \left( \frac{\partial \mu_{a,0}}{\partial \lambda} + \delta \left( \frac{\partial \mu_a}{\partial \lambda} \right) \right) u_1 \bar{v} dx
\]

(2.63)
Finally, we find the weak formulation of (2.60) to be

$$
\int_{\Omega} D_0 \nabla \frac{\partial (\delta u)}{\partial \lambda} \nabla \bar{v} \, dx + \int_{\Omega} (\mu_{a,0} + ik) \frac{\partial (\delta u)}{\partial \lambda} \bar{v} \, dx + \int_{\partial \Omega} \frac{1}{2} \mu \frac{\partial (\delta u)}{\partial \lambda} \gamma_D \bar{v} \, ds
$$

$$
= - \int_{\Omega} \delta D \nabla \frac{\partial u_0}{\partial \lambda} \nabla \bar{v} \, dx - \int_{\Omega} \mu \frac{\partial u_0}{\partial \lambda} \bar{v} \, dx
$$

$$
- \int_{\Omega} \frac{\partial (\delta D)}{\partial \lambda} \nabla u_0 \nabla \bar{v} \, dx - \int_{\Omega} \frac{\partial (\delta u_0)}{\partial \lambda} u_0 \bar{v} \, dx
$$

$$
- \int_{\Omega} \frac{\partial D_0}{\partial \lambda} \nabla (\delta u) \nabla \bar{v} \, dx - \int_{\Omega} \frac{\partial \mu_{a,0}}{\partial \lambda} \partial u \bar{v} \, dx
$$

$$
(2.64)
$$

We are now ready to derive the weak formulation of \( w_\lambda \). We define the weak formulation of \( w_\lambda \) by subtracting (2.62) from (2.63) and then subtracting (2.64) from the result. We thus obtain,

$$
\int_{\Omega} D_0 \nabla w_\lambda \nabla \bar{v} \, dx + \int_{\Omega} (\mu_{a,0} + ik) w_\lambda \bar{v} \, dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \partial w_\lambda \gamma_D \bar{v} \, ds
$$

$$
= - \int_{\Omega} \frac{\partial D_0}{\partial \lambda} \nabla w \nabla \bar{v} \, dx - \int_{\Omega} \frac{\partial \mu_{a,0}}{\partial \lambda} w \bar{v} \, dx
$$

$$
- \int_{\Omega} \frac{\partial (\delta D)}{\partial \lambda} \nabla \delta u \nabla \bar{v} \, dx - \int_{\Omega} \frac{\partial (\delta u_0)}{\partial \lambda} \delta u \bar{v} \, dx
$$

$$
+ \int_{\Omega} \frac{\partial D_0}{\partial \lambda} \nabla (\delta u) \nabla \bar{v} \, dx + \int_{\Omega} \frac{\partial \mu_{a,0}}{\partial \lambda} \partial \delta u \bar{v} \, dx
$$

$$
(2.65)
$$

where \( w \) and \( \delta u \) are defined as in the proof of Theorem 2.20. We are now prepared to solve an analogous theorem to Theorem 2.20 for \( \frac{\partial u}{\partial \lambda} \).

**Theorem 2.20.** The solution, \( \frac{\partial u}{\partial \lambda} \), to (2.38), (2.40) is differentiable. That is, for \( \mathbf{q}_0, \mathbf{q}_0 + \delta \mathbf{q}, \mathbf{q}_0' \), \( \mathbf{q}_0' + \delta \mathbf{q}' \) we have

$$
\left\| \frac{\partial u(\mathbf{q}_0 + \delta \mathbf{q})}{\partial \lambda} - \frac{\partial u(\mathbf{q}_0)}{\partial \lambda} - \frac{\partial u(\mathbf{q}_0)}{\partial \lambda} \delta \mathbf{q} \right\|_{H^1(\Omega)} \to 0 \quad \text{as} \quad \|\delta \mathbf{q}\|_{L^\infty(\Omega)} + \|\delta \mathbf{q}'\|_{L^\infty(\Omega)} \to 0.
$$

**Proof.** To simplify notation, let \( \frac{\partial (\delta u(\mathbf{q}_0))}{\partial \lambda} \delta \mathbf{q} = \frac{\partial (\delta u)}{\partial \lambda} \). Also, let \( w_\lambda \) be defined as in

64
equality we have,

$$c_1 \min \{D_0, \mu_0\} \|w_\lambda\|_{H^1(\Omega)}^2 + \|\hat{q}\|_{L^\infty(\Omega)} + \|\hat{q}'\|_{L^\infty(\Omega)} \leq \frac{\int_\Omega D_0 |\nabla w_\lambda|^2 + \mu_{a,0} |w_\lambda|^2 dx + \frac{1}{2} \int_{\partial \Omega} |\gamma_D w_\lambda|^2 ds}{\|\delta q\|_{L^\infty(\Omega)} + \|\hat{q}'\|_{L^\infty(\Omega)}}$$

$$= - \int_\Omega \frac{\partial D_0}{\partial x} \nabla w \nabla w_\lambda dx - \int_\Omega \frac{\partial \mu_{a,0}}{\partial x} w w_\lambda dx - \int_\Omega \frac{\partial (\delta D_0)}{\partial x} \nabla \delta u \nabla w_\lambda dx$$

$$+ \int_\Omega \delta D \nabla \frac{\partial (\delta u)}{\partial x} \nabla w_\lambda dx + \int_\Omega \delta \mu \frac{\partial (\delta u)}{\partial x} w w_\lambda dx$$

$$\leq \|\hat{q}\|_{L^\infty(\Omega)} (||\nabla w||_{L^2(\Omega)} ||\nabla w_\lambda||_{L^2(\Omega)} + ||w||_{L^2(\Omega)} ||w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \left| \nabla \frac{\partial (\delta u)}{\partial x} \right|_{L^2(\Omega)} ||\nabla w_\lambda||_{L^2(\Omega)}$$

$$\leq \|\hat{q}\|_{L^\infty(\Omega)} (||w||_{H^1(\Omega)} ||\nabla w_\lambda||_{L^2(\Omega)} + C_2(\Omega) ||w||_{H^1(\Omega)} ||w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \left| \nabla \frac{\partial (\delta u)}{\partial x} \right|_{L^2(\Omega)} ||\nabla w_\lambda||_{L^2(\Omega)}$$

$$\leq c_3 \max \{1, C_2(\Gamma)\} \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)} (||\nabla w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)}$$

$$\leq c_3 \max \{1, C_2(\Omega)\} \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)} (||w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)}$$

$$\leq c_3 \max \{1, C_2(\Omega)\} \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)} (||w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)}$$

$$\leq c_3 \max \{1, C_2(\Omega)\} \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)} (||w_\lambda||_{L^2(\Omega)})$$

$$+ \|\delta q\|_{L^\infty(\Omega)} \|\hat{q}'\|_{L^\infty(\Omega)}$$
\[ + \frac{(|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)})}{|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)}} \left( |\nabla \delta u|_{L^2(\Omega)} |\nabla w_\lambda|_{L^2(\Omega)} \right) \]

\[ + \frac{(|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)})}{|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)}} \left( \left| \frac{\nabla (\delta u)}{\partial \lambda} \right|_{L^2(\Omega)} |\nabla w_\lambda|_{L^2(\Omega)} \right) \]

\[ \leq c_3 \max\{1, C_2(\Omega)\} |\delta q|_{L^\infty(\Omega)} |\delta q'|_{L^\infty(\Omega)} (|\nabla w_\lambda|_{L^2(\Omega)}) \]

\[ + c_3 \max\{1, C_2(\Omega)\} |\delta q|_{L^\infty(\Omega)} |\delta q'|_{L^\infty(\Omega)} (|w_\lambda|_{L^2(\Omega)}) \]

\[ + |\nabla \delta u|_{L^2(\Omega)} |\nabla w_\lambda|_{L^2(\Omega)} + |\delta u|_{L^2(\Omega)} |w_\lambda|_{L^2(\Omega)} \]

\[ + \left( \left| \frac{\nabla (\delta u)}{\partial \lambda} \right|_{L^2(\Omega)} |\nabla w_\lambda|_{L^2(\Omega)} + \left| \frac{\partial (\delta u)}{\partial \lambda} \right|_{L^2(\Omega)} |w_\lambda|_{L^2(\Omega)} \right) \]

\[ \leq c_3 \max\{1, C_2(\Omega)\} C_4(\Omega) |\delta q|_{L^\infty(\Omega)} |\delta q'|_{L^\infty(\Omega)} |w_\lambda|_{H^1(\Omega)} \]

\[ + c_5 C_6(\Omega) C_7(\Omega) |\delta q|_{L^\infty(\Omega)} |w_\lambda|_{H^1(\Omega)} \]

\[ + c_8 |\delta q'|_{L^\infty(\Omega)} |w_\lambda|_{H^1(\Omega)} + c_9 C_{10}(\Omega) |\delta q'|_{L^\infty(\Omega)} |w_\lambda|_{H^1(\Omega)} \]

\[ \leq (|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)}) |w_\lambda|_{H^1(\Omega)} \]

\[ \cdot \left[ (c_3 \max\{1, C_2(\Omega)\} C_4(\Omega) |\delta q'|_{L^\infty(\Omega)}) \right. \]

\[ + c_5 C_6(\Omega) C_7(\Omega) + c_8 + c_9 C_{10}(\Omega) \]

where \(c_1, c_3, c_5, c_8, c_9 > 0\) are constants and \(C_2(\Omega), C_4(\Omega), C_6(\Omega), C_7(\Omega), C_{10}(\Omega)\) are the constants arising from use of the Poincaré Inequality. Thus, \(\|w_\lambda\|_{H^1(\Omega)} \rightarrow 0\) as \(|\delta q|_{L^\infty(\Omega)} + |\delta q'|_{L^\infty(\Omega)}| \rightarrow 0\). \(\square\)

Now that we have linearized the governing equations for the forward problem of hyDOT given by (2.37)-(2.40), and proven that the linearized solutions are in fact derivative operators, we have the necessary tools to solve the image reconstruction.
problem. In the next chapter, we will use these operators and their adjoints to implement a gradient algorithm to recover the spatial maps of the optical parameters with respect to each of the wavelengths. The small number of basis elements needed for an accurate estimation of the forward solution at any given wavelength using the Reduced Basis Method also suggests that regularity in the spectral domain can be effectively used in the inverse problem.
Chapter 3

Analytical Formulation of the Inverse Problem

Inverse problems are important because of their abundance in application. Many of the problems we encounter in daily life are inverse problems: given an observed or desired effect, what was the original cause [16]? Mathematically, we represent a general inverse problem with the equation $F(x) = y$, where the output $y$ is known, as well as the transformation function $F$, but the input data $x$ are unknown. Such problems are relatively straightforward mathematically if $F$ has an inverse. However, as mathematicians know, inverses often do not exist or can only be approximated numerically. In addition, such inverses are very unstable in the sense that a small change to the input data can lead to a large change in the output. Another way to say this is that inverse problems are often sensitive, they do not depend continuously on the data, violating the third condition of Hadamard (see Definition 2.1) and thus, are ill-posed.

Inverse problems arise naturally in medical imaging as the unknowns are the geometry and physiological properties of the tissue being imaged. In the case of optical
imaging like DOT, the “output data” \( y \) is the data about the scattered photons read by the detectors at the boundary of the tissue. Due to the sensitivity of the unknown parameter values to small perturbations in the data measurements at the boundary, this problem is ill-posed and can only be solved through numerical optimization. Further, due to the sensitivity of the solution, regularization is needed.

In this chapter we will discuss, analyze, and present some techniques for solving the inverse (or image reconstruction) problem for hyDOT. We will start by analyzing and solving the inverse problem for DOT and then will investigate how the parameterization with respect to wavelength changes the problem.

### 3.1 The DOT Inverse Problem

In diffuse optical tomography (DOT), light in the visible to near-infrared range from a laser source enters the tissue to be imaged and interacts with it primarily through the scattering and absorption of the photons. As stated in the previous chapter, this interaction is modeled in the time-independent (or dc) case, by the diffusion approximation

\[
-\nabla \cdot D(x) \nabla u(x) + \mu_a(x) u(x) = h(x), \quad \text{in } \Omega \tag{3.1}
\]

\[
u(x) + 2D \frac{\partial u}{\partial \nu}(x) = f(x), \quad \text{on } \partial \Omega. \tag{3.2}
\]

Note that in this case, it has been shown that the unique recovery diffusion and absorption coefficients cannot occur simultaneously [6].

In the inverse, or image reconstruction, problem we seek to estimate the unknown optical parameters, \( D \) and \( \mu_a \), and reconstruct a spatial map of them given the data of the scattered photons collected by the detectors at the boundary of the
medium. Put simply, the inverse problem can be stated as: given data \( g \) on \( \partial \Omega \) find \( \{D, \mu_a\} \). In other words, if \( F(q) \) is the forward operator and \( g \) are measurements then we wish to find \( q = (D, \mu_a) \in Q \) such that \( F(q) = g^\delta \), and \( ||F - F^\delta|| \leq \delta \) where \( g^\delta \) is the perturbed measurement from the data given by

\[
g^\delta = \gamma_N F(q^*) + \xi
\]

where \( \gamma_N \) is the Neumann trace, \( q^* \) are the true optical parameters, \( \xi \) is the data noise, and \( \delta \) is an upper bound on the noise. For a finite data set, as is the case experimentally, this problem is ill-posed (see Definition 2.1) since it is an underdetermined system.

We will denote \( q = (D, \mu_a) \) to represent the values of the optical parameters, and \( q_0 = (D_0, \mu_0) \) to represent their values on a homogeneous background that may represent, for example, healthy tissue. Thus, in the image reconstruction problem, we would like to determine \( q \) knowing the complete Robin-to-Neumann map given by

\[
\begin{align*}
-\text{div}(D \nabla u) + (\mu_a + ik)u &= 0 & \text{in } \Omega, \\
u + 2D \frac{\partial u}{\partial n} &= f & \text{on } \partial \Omega \\
-D \frac{\partial u}{\partial n} &= g & \text{on } \partial \Omega,
\end{align*}
\]

where for the purposes of this dissertation we are considering \( h(x) = 0 \).

Reconstructing this map involves minimizing the cost functional

\[
\min_{q \in Q} J_\alpha(q) = \frac{1}{2} \|\gamma_N F_R(0, f) - g\|^2_{H^{-1/2}(\partial \Omega)} + \alpha_1 \|q - q_0\|^2 + \alpha_2 \sum_{i=1}^{\infty} |c_i - \hat{c}_i|
\]  

(3.6)
where $F_R(0, f)$ is the forward Robin operator. The second term in the sum is the smoothing term, which helps smooth the final image, with regularization parameter given by $\alpha_1$. The third term in the sum is a sparsity term, with sparsity parameter $\alpha_2$. If $q, \hat{q}$ are rewritten as

$$
q = \sum_{j=1}^{\infty} c_i \phi_i, \quad q_0 = \sum_{j=1}^{\infty} \hat{c}_i \phi_i,
$$

(3.7)

respectively, where $\{\phi_i\}_{i=1}^{\infty}$ is a basis for $Q$, then the sparsity term enforces the homogeneity of the optical parameters at all but a small number of locations. This sparsity is natural in the physical domain since we can expect that cancerous cells, for example, will only be present at a small number of locations in the tissue being imaged. Enforcing sparsity in the inverse problem is further discussed in Section 3.3.

A good overview of numerical reconstruction schemes for DOT is given by [32, 33].

### 3.1.1 Existence and Uniqueness

The inverse problem for DOT is ill-posed because it does not depend continuously on the data. For finitely many data, as is the case experimentally, this is due to the fact that the problem is underdetermined. For the infinite data theoretical case, the problem is still unstable because of the noise in the data [33]. Since the forward problem of DOT is well-posed, it was sufficient to consider $q \in \{L^\infty(\Omega) \times L^\infty(\Omega), 0 < D_0 \leq D \leq D_1 < \infty, 0 < \mu_0^a \leq \mu_a \leq \mu_1^a < \infty\}$. However, we will need to assume more smoothness in the parameter space to prove the uniqueness of the solution to the inverse problem. Thus, we will consider $q \in \{H^2(\Omega) \times L^2(\Omega), 0 < D_0 \leq D \leq D_1 < \infty, 0 < \mu_0^a \leq \mu_a \leq \mu_1^a < \infty\}$. Given this higher regularity, it can be shown that Hadamard’s first two conditions for well-posedness are met.
Theorem 3.1. A solution $q$ to the DOT inverse problem exists and is unique. That is, given measurements on the boundary, we can reconstruct a unique spatial map for the parameters $q = (D, \mu_a)$.

The proof of this theorem is well established in the literature (see, e.g. the classical work [96] and the proof for the two-dimensional case given by [40]), so we will only outline it here. The proof uses a Liouville transformation to convert the PDE to a Schrödinger type equation and the Robin-to-Neumann map to a Dirichlet-to-Neumann map. It then concludes that if we have knowledge of $D$ on the boundary, $\partial \Omega$, full knowledge of the Robin-to-Neumann map implies full knowledge of the Dirichlet-to-Neumann map. From this point, the proof invokes the classical theory on uniqueness for inverse scattering problems.

3.2 The hyDOT Inverse Problem

The hyDOT inverse problem has the same goal as the DOT inverse problem, namely estimating the parameters $D$ and $\mu_a$. However, in hyDOT, these parameters have both spatial and spectral dependence. Thus, we seek not only a spatial map of the unknown parameters, but a spatial map for each wavelength. In hyDOT the first-order diffusion approximation to the radiative transport equation that describes the transport of the photons through the tissue is given in the frequency domain as:

$$-\nabla \cdot D(x, \lambda) \nabla u(x) + (\mu_a(x, \lambda) + ik)u(x) = h(x, \lambda), \quad \text{in } \Omega$$

$$u(x) + 2D \frac{\partial u}{\partial \nu}(x) = f(x, \lambda), \quad \text{on } \partial \Omega. \quad (3.8)$$

Note that the source function, $h$, also has spectral dependence. This function, which describes the optical energy of the laser source per unit time, is usually described
using a delta function (to indicate a pulsed laser source) and is given by $h(x, \lambda) = h_0(\lambda)\delta(x - x_s)$ where $h_0(\lambda)$ is the power of the source at wavelength $\lambda$ [61, 89]. Here, we will consider the simplified case,

$$-
abla \cdot D(x, \lambda) \nabla u(x) + (\mu_a(x, \lambda) + ik)u(x) = 0, \quad \text{in } \Omega$$

$$u(x) + 2D \frac{\partial u}{\partial \nu}(x) = f(x, \lambda), \quad \text{on } \partial \Omega. \quad (3.9)$$

As in DOT, a reconstruction of a spatial map of the optical parameters will require minimization of a cost functional, similar to (3.6). In hyDOT, however, the spectral dependence of the optical parameters must also be taken into account. Thus, the minimization functional is now dependent on $\lambda$ as well. Note that, in this case, the regularization and sparsity parameters are wavelength dependent and so they may be different for each value of $\lambda$. A couple different cost functionals for hyDOT will be proposed in Section 3.4.

Now that we have the linearized forms of the coupled PDE governing the forward problem, (2.37)-(2.40), we would like to use them to solve the inverse problem. There are several methods to do this and an overview of several discretization techniques and reconstruction algorithms is given in [4]. These techniques include linear back projection methods [10] and Newton-type iterative methods [86, 90]. We present here a sparsity-promoting Tikhonov based regularization method, similar to the one presented in [53] for electrical impedance tomography. Most of these methods use the gradient in the iterative scheme. The sparsity term in (3.6) is not differentiable, but the least squares term is. So it is from this term that we will calculate the gradient to use in the algorithm to minimize the cost functionals by stepping in the negative gradient direction.

Specifically, consider the generalized forward operator $F : X \rightarrow Y$. In hyDOT,
$X$ is the parameter space $Q_\lambda = L^\infty(\Omega) \times L^\infty(\Omega)$. To introduce more regularity to the problem in order for the inner products below to be well-defined, we will consider $\overline{Q}_\lambda = H^1(\Omega) \times L^2(\Omega)$, where $H^1(\Omega) \subseteq L^2(\Omega) \subseteq L^\infty(\Omega)$, and $\Omega \subseteq \mathbb{R}^n$, $n = 2, 3$ is open and bounded. The space $Y$ is the measurement space $H^{-1/2}(\partial\Omega)$. Note that the operator $F$ is equivalent to $\gamma_N u$ in the DOT and hyDOT forward problems, where $\gamma_N$ is the Neumann trace given in (2.14). In practice, since finding the Neumann trace of the solution numerically requires taking a derivative a large amount of error may be introduced. Thus, since $u$ satisfies the Robin boundary condition (2.39), we have

$$-2D \frac{\partial u}{\partial n} = u - f \quad \text{on } \partial\Omega$$

which is a Neumann condition describing the measurement of the scattered photons leaving the tissue. So, instead of calculating $\gamma_N$, in practice we can use $\gamma_D u - f$ to find the measurements $g$ where $\gamma_D$ is the Dirichlet trace given by (2.12). That is

$$(\gamma_N F_R)[\delta q] = \gamma_D \delta u,$$

where $F_R$ is the forward Robin operator and $\delta u$ is the solution of the sensitivity equation (2.55). We proved in Theorem 2.20 that this is the derivative in the $\delta q$ direction. With this definition of $F$, we need to find

$$\nabla J(q) = \nabla \|Fq - g\|^2_Y.$$

Note that here we have not considered the sparsity-promoting term, but we will include it later and discuss how to address it when using the gradient to find the step size and direction.

The directional derivative of $J$ in the direction $\delta q$ is thus given by

$$J'(q)[\delta q] = \langle F'(q)[\delta q], Fq - g \rangle_Y.$$
Finally, since the gradient can be defined by a Riesz map to obtain,

$$\langle \delta \mathbf{q}, \nabla J(q) \rangle_Y = J'(f)[\delta \mathbf{q}]$$

we have,

$$\langle \delta \mathbf{q}, \nabla J(f) \rangle_Y = \langle F'(\mathbf{q})[\delta \mathbf{q}], F\mathbf{q} - g \rangle_Y$$

$$= \langle \delta \mathbf{q}, (F'(\mathbf{q})[\delta \mathbf{q}])^*(F\mathbf{q} - g) \rangle_X.$$ 

Thus, in order to find the gradient, $\nabla J(q) = (F'(\mathbf{q})[\delta \mathbf{q}])^*(F\mathbf{q} - g)$, we must first calculate the adjoint of the linearized derivative operators $\delta u(q_0)[\delta \mathbf{q}]$, which is the solutions to (2.53)-(2.54).

Although the theorem below can be proved in a discretized setting (see e.g. the corresponding DOT proof in [33]), we will assume the continuous case here. Additionally, as previously mentioned, in solving the inverse problem we are interested in $F(q) = \gamma_N u$ but we will show the results using just $u$ below. The proof for $\gamma_N u$ follows easily.

**Theorem 3.2. (Adjoint of the hyDOT derivative operator)** Let $u$ be the solution to the system (2.37) - (2.39) and let $\delta \mathbf{q} := (\delta D, \delta \mu_a)$. Let $w_1$ be the solution of the adjoint problem

$$-\text{div}(D_0 \nabla w_1) + (\mu_{a,0} - ik)w_1 = 0 \quad \text{in } \Omega \quad (3.10)$$

$$w_1 + 2D_0 \frac{\partial w_1}{\partial n} = g \quad \text{on } \partial \Omega \quad (3.11)$$
Further, define $\delta u(q_0)^* g : L^2(\partial \Omega) \to H^1(\Omega) \times L^2(\Omega)$ such that

$$g \rightarrow \begin{bmatrix} R(-\nabla u \cdot \nabla w_1) \\ -u \cdot w_1 \end{bmatrix}$$

(3.12)

where

$$R(h) = \tilde{h}, \quad h \in L^2(\Omega), \quad \tilde{h} \in H^1(\Omega)$$

(3.13)

and $\tilde{h}$ solves the partial differential equation,

$$-\Delta \tilde{h} + \tilde{h} = h \quad \text{in } \Omega$$

$$\gamma_D \tilde{h} = 0 \quad \text{on } \partial \Omega.$$  

(3.14)

Then $\delta u(q_0)^*$ is the adjoint operators of $\delta u(q_0)$. That is,

$$\langle \delta u(q_0)[\delta q], g \rangle_{\mathbb{R}^d} = \langle \delta q, \delta u(q_0)^* g \rangle_{H^1(\Omega; \mathbb{R}) \times L^2(\Omega; \mathbb{R})}$$

(3.15)

holds for all $D \in H^1(\Omega; \mathbb{R})$ and $\mu_a \in L^2(\Omega; \mathbb{R})$.

**Proof.** The weak formulation of (3.10), (3.11), using $\delta u$ as the test function, is given by

$$\int_\Omega D_0 \nabla w_1 \nabla \delta u + (\mu_{a,0} - ik) w_1 \delta u dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D w_1 \gamma_D \overline{\delta u} ds = \frac{1}{2} \int_{\partial \Omega} g \gamma_D \overline{\delta u} ds.$$  

(3.16)

Note that the conjugate of (3.16) is given by,

$$\int_\Omega D_0 \nabla \delta u \nabla \bar{w}_1 + (\mu_{a,0} + ik) \delta u \bar{w}_1 dx + \frac{1}{2} \int_{\partial \Omega} \gamma_D \delta u \gamma_D \bar{w}_1 ds = \frac{1}{2} \int_{\partial \Omega} \bar{g} \gamma_D \delta u ds.$$  

(3.17)

If we use $w_1$ as the test function for the weak form of the linearized PDE, (2.55), we
\[
\int_{\Omega} D_0 \nabla \delta u \nabla \bar{w}_1 \, dx + \int_{\Omega} (\mu_{\alpha,0} + i k)(\delta u)\bar{w}_1 \, dx + \int_{\partial \Omega} \frac{1}{2} \gamma_D \delta u \gamma_D \bar{w}_1 \, ds \\
= - \int_{\Omega} (\delta D \nabla u_0) \nabla \bar{w}_1 \, dx - \int_{\Omega} \delta \mu_0 \bar{w}_1 \, dx.
\]

Thus by (2.55) and (3.16) we have,

\[
\frac{1}{2} \int_{\partial \Omega} \bar{g} \gamma_D \delta u \, ds = - \int_{\Omega} (\delta D \nabla u_0) \nabla \bar{w}_1 \, dx - \int_{\Omega} \delta \mu_0 \bar{w}_1 \, dx
\]

which is equivalent to

\[
\langle \gamma_N \delta u, g \rangle_{L^2(\partial \Omega)} = \langle \delta D, -\nabla u_0 \cdot \nabla w_1 \rangle_{L^2(\Omega)} + \langle \delta \mu, -u_0 \cdot w_1 \rangle_{L^2(\Omega)}
\]  

(3.19)

Now, to get the required smoothness on \( \delta D \) we apply (3.13), (3.14) to the first term on the righthand side of (3.19), giving

\[
\langle \delta D, -\nabla u_0 \cdot \nabla w_1 \rangle_{L^2(\Omega)} = \int_{\Omega} \delta D (\nabla u_0 \nabla w_1) \, dx
\]

\[
= \int_{\Omega} (\delta D) \cdot (-\Delta R (-\nabla u_0 \nabla w_1)) \, dx + \int_{\Omega} \delta D R (-\nabla u_0 \nabla w_1) \, dx
\]

\[
= \int_{\Omega} \nabla (\delta D) \nabla R (-\nabla u_0 \nabla w_1) \, dx + \int_{\Omega} (\delta D) R (-\nabla u_0 \nabla w_1) \, dx
\]

\[
= \langle \delta D, R (-\nabla u_0 \nabla w_1) \rangle_{H^1(\Omega)}
\]

Thus, plugging this back into (3.19) we have

\[
\langle \gamma_N \delta u, g \rangle_{L^2(\partial \Omega)} = \langle \delta D, R (-\nabla u_0 \nabla w_1) \rangle_{H^1(\Omega)} + \langle \delta \mu, -u_0 \cdot w_1 \rangle_{L^2(\Omega)}
\]

\[
= \langle \delta q, (\gamma_N \delta u)^* g \rangle_{H^1(\Omega) \times L^2(\Omega)}
\]
for all $\delta q \in Q$. Therefore, $(\gamma_N \delta u) * g$ as given by (3.12) holds true and $\delta u(q_0)^*$ is the adjoint operator of $\delta u$.

In sum, to find the gradient needed in the algorithm described in Section 3.5, we must first solve the sensitivity problems (2.53)- (2.54) and/or (2.64) (depending on our $J$). Then we will take the Neumann trace to get $F'(q)$. Finally we will calculate the adjoint to get from the measurement space $L^2(\partial \Omega)$ back to the parameter space $H^1(\Omega) \times L^2(\Omega)$.

3.3 Sparsity

Sparsity is a term used to describe the situation when only a few solutions to a problem are significantly different from the others. The significance level of this difference is predetermined and sparsity is exploited in the minimization problems given above by setting all solution values below that level to zero, creating a homogeneous “background” value and leaving a small number of nonzero solutions. To explain sparsity a bit more precisely, but still generally, we will follow the explanation given in [14]. We can consider our inverse problem as finding $x$ in the equation $b = Ax$ where $A \in \mathbb{R}^{n \times m}$ is an underdetermined system, that is, $n < m$. When seeking a sparse solution we look specifically for the solution $x$ that has small values. That is, we seek to solve

$$\min_x J(x) \quad \text{s.t.} \quad b = Ax.$$ \hspace{1cm} (3.20)

The standard least squares solution of this problem is given by

$$\|x\|_2^2 = A^T(AA^T)^{-1}b.$$
But the $\ell_2$ norm is a measure of energy instead of sparsity. Based on our previous explanation, a natural measure of sparsity would be the $\ell_0$ norm, which counts the number of nonzero entries in $x$. If $||x||_0 \ll m$ we say that $x$ is sparse.

However, the problem

$$\min_x ||x||_0 \quad \text{s.t.} \quad b = Ax$$

(3.21)

has been shown to be NP-Hard in general [71]. So an alternative way of promoting sparsity must be sought. Typically, the $\ell_1$ norm is considered where

$$||x||_1 = \sum_i |x_i|$$

and thus we have

$$\min_x ||x||_1 \quad \text{s.t.} \quad b = Ax$$

(3.22)

This is a convex optimization problem that is close to (3.21) and that can be solved using standard optimization tools, such as linear programming. In fact, if the matrix $A$ has incoherent columns and (3.21) has a sufficiently sparse solution, the solution is unique and is equal to (3.22) [14, 28, 29, 48].

Another way of saying this is that we seek to add a sparsity-promoting regularization term to our minimization functional when solving the inverse problem. As described in [13], if $Ku = f$ is our inverse problem we wish to find $u$ by solving a minimization problem of the form

$$J(u) = \min_{u \in H} ||Ku - f||^2 + \sum_n w_n |\langle u, \phi_n \rangle|^p$$

(3.23)

where $H$ is a Hilbert space, $\{w_n\}$ are a sequence of nonnegative weights, and $\{\phi_n\}$ is
an orthonormal basis for $H$. Changing the value of $p$ changes the penalty we place on the coefficients. As demonstrated in Figure 3.1, decreasing $p$ from 2 to 1, for example, increases the penalty on small coefficients ($\langle u, \phi_n \rangle < 1$) and decreases the penalty on large coefficients ($\langle u, \phi_n \rangle > 1$). In general, the penalty promotes sparse solutions and maintains the convexity of the functional (3.23) for $1 \leq p < 2$. Since small coefficients have a high penalty, while large coefficients have a small penalty, the solution to (3.23) favors those with only a few large coefficients, which is a sparse solution.

Figure 3.1: Demonstrating the effect of different values of $p$ for the sparsity-promoting regularization term in (3.23)

In this dissertation we will focus only on the case where $p = 1$. In that case the functional is convex, but a minimizer is not immediately clear. In [26], however, an iterative approach using a surrogate functional has been shown to find a minimizer for (3.23) in the linear case. Assuming, as in [26], that $\|K\| < 1$, the surrogate functional
is defined by

\[ J_{SUR}(u; a) = ||Ku - f||^2 + \alpha \sum_n w_n |\langle u, \phi_n \rangle|^p - ||K(u - a)||^2 + ||u - a||^2 \quad (3.24) \]

where if \( a = u \) the surrogate functional reduces to the original. \( J_{SUR} \) has minimizer

\[ u = S(\alpha(a + K^* (f - Ka))). \quad (3.25) \]

where \( S(\alpha) = \sum_n S(\alpha) \phi_i \) and \( S(\alpha) \) is the soft shrinkage functional

\[ S(\alpha)(x) = \begin{cases} 
  x - \alpha, & x \geq \alpha \\
  0, & |x| < \alpha \\
  x + \alpha, & x \leq \alpha 
\end{cases} \quad (3.26) \]

or in other words,

\[ S(\alpha)(x) = \text{sign}(x) \max\{|x| - \alpha, 0\}. \]

That is, if the coefficients are small, \( S(\alpha)(x) \) takes them to 0, and otherwise \( S(\alpha)(x) \) shrinks them. So, starting with a guess \( u_0 \), the iterative scheme

\[ u^n = S(\alpha)(u^{n-1} + K^* (g - Ku^{n-1})) \]

will converge to the minimizer of (3.23).

It is well-known that the DOT inverse problem is very sparse in the spatial domain [22, 53] (note that [53] discusses EIT, but this is a very similar problem mathematically to DOT and the methods used there can be applied to DOT as well). This is due to the high optical contrast between tumors and healthy tissues since the
chromophores scatter and absorb light very differently at these wavelengths for these types of tissue.

In the following chapters, we will see several pieces of evidence that suggest that the solution to the hyDOT inverse problem will not only be sparse spatially, but we can also exploit that sparsity with respect to wavelength. That is, the sparsity promoting penalty term will be different for each wavelength. Further, the successful implementation of the Reduced Basis Method in Chapter 5 to a simple application of the hyDOT forward problem suggests that the solution at only a small number of wavelengths is needed to approximate the solution to the forward problem at any wavelength. Additionally, experimental results such as those given by Jacques [50] in Figure 5.3 and Cerussi et al. [18] in Figure 5.2 show that the absorption coefficient \( \mu_a \) follows roughly the same profile with respect to wavelength for both healthy and cancerous tissue, the profiles differing in shape only at a small number of wavelengths. Thus, since the optical parameters are very smooth in the spectral domain, we can exploit this smoothness by only finding the reconstruction at a few wavelengths instead of the for the whole spectrum.

### 3.4 Proposed Functionals

In this section we will propose functionals \( J \) to be minimized to get the best possible image for the image reconstruction problem in hyDOT. While we do not outline the theoretical rigor and verify the effectiveness of each of these functionals in this dissertation, we will pursue this in our future work. For the simulations presented in Chapter 5 we will focus on the most basic of these functionals, that introduces the dependence of the optical parameters on \( \lambda \), but does not incorporate \( \frac{\partial u}{\partial \lambda} \). This chapter included the results for finding the gradient and adjoint with respect to \( \frac{\partial u}{\partial \lambda} \), however,
to demonstrate that solving the inverse problem with functionals that do include this
term will be possible. The functional that we will be focusing on in this section and
in Chapter 5 is given by

\[
J_\alpha(q(\lambda)) = \int_{\lambda_{\min}}^{\lambda_{\max}} \omega(\lambda) \| \gamma Nu - g \|_2^2 d\lambda + \int_{\lambda_0}^{\lambda_f} \sum_{k=1}^{\infty} \alpha_k(\lambda) |c_{k,\lambda} - \hat{c}_{k,\lambda}| d\lambda \quad (3.27)
\]

where the \( c_k \) are the coefficients of the basis functions used to represent \( q \), as in (3.7).
We note that this functional contains a sparsity term, but no smoothing term. If we
wished to add more smoothing, we could easily add a smoothing term. This may in
fact be the wiser choice, but as the focus of this dissertation is on sparsity, we will
examine the effect of a sparsity term alone on the image reconstruction. We also note
that the sparsity parameter \( \alpha_k \) is wavelength dependent, recognizing that the spatial
differences in the values of the optical parameters are more pronounced for certain
wavelengths over others. For wavelengths where the differences are more pronounced,
\( \alpha_k \) will be a larger value, promoting sparsity. For wavelengths where the difference
between the optical parameters in the healthy and cancerous tissue is less obvious,
\( \alpha_k \) will be smaller, making the solution less sparse, to distinguish those parameters
more clearly.

The discretization of (3.27) is given by

\[
J_\alpha(q(\lambda)) = \sum_{j=1}^{N_\lambda} \omega_j(\lambda_j) \| (\gamma Nu - g)(\lambda_j) \|_2^2 \Delta \lambda + \sum_{j=1}^{N_\lambda} \sum_{k=1}^{\infty} \alpha_k(\lambda_j) |c_{k,j} - \hat{c}_{k,j}| \Delta \lambda \quad (3.28)
\]

We wish to show that our functional indeed has a minimizer. To do this, we
need to strengthen the regularity of the parameter space so that it is a subspace of a
Hilbert space. We will consider $q \in \overline{Q}$ where

$$
\overline{Q} = \{ H^1(\Omega) \times L^2(\Omega), 0 < D_0 \leq D \leq D_1, 0 < \mu_{a,0} \leq \mu_a \leq \mu_{a,1} \} \quad (3.29)
$$

We have already proven that the forward Robin operator is (weakly) continuous with respect to the parameter $q$ in Theorem 2.15 with respect to the parameter space $Q$. We can also show continuity (and compactness) of the forward operator with respect to this Hilbert space formulation (see e.g. [32]). We cannot guarantee that $\overline{Q}$ is compact, but we can show that it is weakly closed, that is, closed and convex.

**Lemma 3.3.** $\overline{Q}$ is weakly closed. That is, it is closed and convex.

**Proof.** First, we show that $\overline{Q}$ is closed. Consider a sequence $\{q_n\} \in \overline{Q}$ that converges to $q = (D, \mu_a)$. Assume, for proof by contradiction, that $q \notin \overline{Q}$. So $q = (D, \mu_a)$ is such that $D > D_1$, $D < D_0$, $\mu_a > \mu_{a,1}$, or $\mu_a < \mu_{a,0}$. But then $||q_n - q||_{H^1(\Omega) \times L^2(\Omega)} > \epsilon$ for all $n$ and some $\epsilon$ where $\epsilon$ is determined by the distance between $D$ and $D_0$ or $D_1$ or between $\mu_a$ and $\mu_{a,1}$ or $\mu_{a,0}$. Thus, $q \in \overline{Q}$ and so $\overline{Q}$ is closed.

Now we show that $\overline{Q}$ is convex. Let $t \in [0, 1]$ and $q_n = (D_n, \mu_n)$, $q_m = (D_m, \mu_m) \in \overline{Q}$. Then,

$$
(1 - t)D_m + tD_n \leq (1 - t)D_1 + tD_1 = D_1
$$

$$
(1 - t)D_m + tD_n \geq (1 - t)D_0 + tD_0 = D_0
$$

$$
(1 - t)\mu_m + t\mu_n \leq (1 - t)\mu_{a,1} + t\mu_{a,1} = \mu_{a,1}
$$

$$
(1 - t)\mu_m + t\mu_n \geq (1 - t)\mu_{a,0} + t\mu_{a,0} = \mu_{a,0}
$$

and thus $(1 - t)q_m + tq_n \in \overline{Q}$ for all $t \in [0, 1]$. Therefore, $\overline{Q}$ is convex, and so, weakly closed. \qed
We need to verify one more property to prove that our cost functional has a minimizer. Let $F_R(0, f)$ represent the forward Robin operator for the hyDOT problem.

**Lemma 3.4.** The operator $\gamma_N F_R(0, f)$ is weakly sequentially closed. That is, if $q_n \rightharpoonup q$ then $q \in \overline{Q}$ and $\gamma_N F_R(0, f) \rightharpoonup \gamma_N F_R(0, f)$.

**Proof.** We will not give a full proof here but refer the reader to [32]. We have already proved enough to show that since $\overline{Q}$ is weakly closed, $\gamma_N F_R(0, f)$ is weakly closed and continuous. \hfill \Box

In this Hilbert space setting, we can consider our (discretized) optimization problem for one wavelength as

$$\min_{q \in \overline{Q}} J_H^\alpha(q) = \min_{q \in \overline{Q}} \frac{1}{2} \sum_{i=1}^M \| \gamma_N F_R(0, f_i)[\lambda] - g_i(\lambda) \|_{H^{-1/2}(\partial\Omega)}^2. \quad (3.30)$$

**Theorem 3.5.** There exists a minimizer to (3.30).

**Proof.** Since $J_H^\alpha(q)$ is bounded below by 0, there exists a minimizing sequence that converges monotonically to $\inf_{q \in \overline{Q}} J_H^\alpha(q)$. Since the sequence is in a separable Hilbert space and is uniformly bounded due to the conditions in (2.11), the minimizing sequence has a weakly convergent subsequence $q_n \rightharpoonup q \in \overline{Q}$ since $\overline{Q}$ is weakly closed. Similarly, $\gamma_N F_R(0, f)[q_n] \rightharpoonup y$ and since $\gamma_N F_R(0, f)$ is weakly sequentially closed, $y = \gamma_N F_R(0, f)[q]$. Thus, $J_H^\alpha(q)$ is weakly lower semicontinuous. That is, $\lim_{n \to \infty} \inf J_H^\alpha(\tilde{q}_n) \geq J_H^\alpha(\tilde{q})$ for any $\tilde{q}_n \rightharpoonup \tilde{q}$. Therefore,

$$J_H^\alpha(q) \leq \lim_{n \to \infty} \inf J_H^\alpha(\tilde{q}_n) = \inf \{ J_H^\alpha(q) : q \in \overline{Q} \}. $$

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By definition of the infimum, we also have $J^H_\alpha(q) \geq \inf \{ J^H_\alpha(q) : q \in \overline{Q} \}$. Thus,

$$J^H_\alpha(q) = \inf \{ J^H_\lambda(q) : q \in \overline{Q} \}$$

and so $q$ is the minimizer of $J^H_\alpha(q)$ over $\overline{Q}$ and further $q$ exists in $\overline{Q}$. $\square$

So we have shown that the minimization problem given by (3.27) does indeed have a solution when it is reduced to the minimization problem involving only one wavelength. Since we can show the existence of a minimum solution to the functional at each wavelength, when using (3.27) in practice we would like to optimize over each $\lambda$ and then sum up the solution. We conjecture that if $\{q\}_i=1,\ldots,\infty$ are minimizers for (3.30) evaluated at wavelengths $\lambda_i, i = 1, \ldots, \infty$ then $\{q\}$ is a minimizer for (3.27).

We will not rigorously prove this here, but the proof should follow from the regularity of $\alpha$ with respect to $\lambda$, and thus the uniform convergence of sequences in the spectral parameter space.

In order to include more of the wavelength dependence of $q$ in the functional $J$, an alternative to (3.27) would be

$$J_1(q(\lambda)) = \int_{\lambda_0}^{\lambda_f} \omega(\lambda)\|\gamma_0 u - g\|^2 d\lambda + \int_{\lambda_0}^{\lambda_f} \sum_{k=1}^{\infty} \alpha_k(\lambda) \left( \|q\|^2_{L^\infty(\Omega)} + \left\| \frac{\partial q}{\partial \lambda} \right\|^2_{L^\infty(\Omega)} \right) d\lambda$$

where $\|q\|_{L^\infty(\Omega)} = \max \{ \|D\|_{L^\infty(\Omega)}, \|\mu_a\|_{L^\infty(\Omega)} \}$ and $\left\| \frac{\partial q}{\partial \lambda} \right\|_{L^\infty(\Omega)} = \max \left\{ \left\| \frac{\partial D}{\partial \lambda} \right\|_{L^\infty(\Omega)}, \left\| \frac{\partial \mu}{\partial \lambda} \right\|_{L^\infty(\Omega)} \right\}$, as before.

### 3.5 Our Algorithm

We wish to use a gradient descent algorithm but, as previously stated, the sparsity term in (3.27) is not differentiable, though it is convex. For this reason, the
descent will only be used on the least-squares data-fitting term, while a shrinkage operator (given by [26]) will be applied to the sparsity term as in [13, 22]. As in our solution to the forward problem, we will assume that the values for the reduced scattering coefficient $\mu'_s$ are known and constant, as this makes the problem a little easier. An overview of the suggested algorithm, based on the DOT reconstruction algorithm given in [22], is given in Algorithm 1. Note that since $D, \mu_a, u$ are all functions of $\lambda$, each of the steps will be preformed for each value of $\lambda$. Recall that it was noted in Section 3.2 that calculating $\gamma_N u$ introduces a lot of error, so in practice the equivalent calculation $\gamma_D u - f$ is used instead.

As described in Section 3.2, computing the gradient $\nabla J_\alpha(q_j)$ involves calculating the residual

$$r(\lambda) = (\gamma_N u(q_j) - g)(\lambda) \quad (3.32)$$

for each source-detector pair $(f_i, g^\delta_i)$, and for each $\lambda$. Then, the adjoint problem for each must be solved (as given in (3.10)-(3.11)) so that the gradient is given by the

---

**Algorithm 1 Reconstruction Algorithm**

Give $\alpha_k, q_0$, and let $\delta q = 0$;

for $i = 1 : N_S$
  
  Simulate data $q^i$ for each $\lambda \in [\lambda_s, \lambda_f]$ using source $i$

for $j = 1 : n$
  Compute $q_{j+1} = q_j + \delta q_j$
  
  for $i = 1 : N_S$
    Compute the gradient $\nabla J^{(i)}_\alpha(q_j)$;
    Let $\nabla J_\alpha(q_j) = \sum_i \nabla J^{(i)}_\alpha(q_j)$;
    Compute the smoothed gradient $\nabla J_s(q_j)$
    Determine the step size $s^j = [s^j_D, s^j]\$
    Update $\delta q_{j+1} = \delta q_j - s^j \nabla J_s(q_j)$
    Apply the shrinkage operator, $S_{s^j/\alpha_k}(\delta q_{j+1})$

Check Stopping Criterion.
sum over all \((f_i, g_i^\delta)\) of

\[
\begin{bmatrix}
    R(-\nabla u \cdot \nabla w_1) \\
    -u \cdot w_1
\end{bmatrix}
\]

where \(R\) is defined as in (3.13) in Theorem 3.2.

The operator \(R\) is actually a Riesz map that performs what is known as Sobolev smoothing. Given a measurement pair \((f, g)\), taking a gradient step in the direction

\[
\begin{bmatrix}
    -\nabla u \cdot \nabla w_1 \\
    -u \cdot w_1
\end{bmatrix}
\]

is only valid if \(q \in L^2(\Omega) \times L^2(\Omega)\). However, in order to ensure that \(D\) does not have an unbounded gradient so that the iterations will not converge, we require that \(D \in H^1(\Omega)\). In fact, we will consider that the parameter space \(Q = H_0^1(\Omega) \times L^2(\Omega)\) since we assume that \(\delta D = 0\) on the boundary, that is that \(D\) is equal to the homogeneous background there. In this case we define the Sobolev gradient [73]

\[
\nabla J_s(q) = (\nabla J_{sD}(q), \nabla J_{s\mu}(q))
\]

by [22]

\[
\nabla J(q)[\delta q] = \begin{bmatrix}
    \langle \delta D, \nabla J_{sD}(q) \rangle_{H_0^1(\Omega)} \\
    \langle \delta u, \nabla J_{s\mu}(q) \rangle_{L^2(\Omega)}
\end{bmatrix}. \tag{3.33}
\]

If we integrate by parts in the first entry we are left with

\[-\Delta(\nabla J_{sD}(q)) + \nabla J_{sD}(q) = \nabla J_D(q) \quad \text{in } \Omega.\]

This corresponds to the definition we gave for the adjoint using \(R\) that we gave in
Theorem 3.2, and thus the gradient step with the necessary smoothness is given by
\[ \nabla J_s(q) = \begin{bmatrix} R(-\nabla u \cdot \nabla w_1) \\ -u \cdot w_1 \end{bmatrix}. \]

As previously stated, we minimize the sparsity term not through the gradient step, but by applying the shrinkage operator introduced in [26] and given by (3.26) in Section 3.3. For this algorithm, two shrinkage steps will be made in each iteration, one for \( D \) and one for \( \mu_a \), both as a function of \( \lambda \). These steps are given by

\[ S_{s_D^{j\alpha_D,\lambda}}(\delta D) = \text{sign}(\delta D) \max\{|\delta D| - s_D^{j\alpha_D,\lambda}, 0\} \]

and

\[ S_{s_{\mu}^{j\alpha_\mu,\lambda}}(\delta \mu) = \text{sign}(\delta D) \max\{|\delta \mu| - s_{\mu}^{j\alpha_\mu,\lambda}, 0\} \]

where \( \alpha_\lambda \) is the wavelength dependent regularization parameter and \( s^j \) is the step size, both given for \( D \) and \( \mu_a \).

We note that the original values of the regularization parameter \( \alpha_k(\lambda) \) and the step size were the same for all wavelengths, but were updated differently for each wavelength in the algorithm. The step size could have been kept constant, but since gradient algorithms often have slow convergence, we followed the example of [22, 53] and used a Barzilai-Borwein (BB) [12] guess for the step size given by

\[ s_D^{j} = \frac{\langle \delta D^j - \delta D^{j-1}, \nabla J_s(q^j) - \nabla J_s(q^{j-1}) \rangle_{H^1(\Omega)}}{\langle \delta D^j - \delta D^{j-1}, \delta D^j - \delta D^{j-1} \rangle_{H^1(\Omega)}} \tag{3.34} \]

\[ s_{\mu}^{j} = \frac{\langle \delta \mu_a^j - \delta \mu_a^{j-1}, \nabla J_s(q^j) - \nabla J_s(q^{j-1}) \rangle_{L^2(\Omega)}}{\langle \delta \mu_a^j - \delta \mu_a^{j-1}, \delta \mu_a^j - \delta \mu_a^{j-1} \rangle_{H^1(\Omega)}} \tag{3.35} \]

\[ \text{(3.36)} \]
Using this step size ensures a weak monotonicity rather than simple monotone convergence of the functional so that the speed of the convergence due to the step is maintained.

The stopping criterion is given by two elements. The first is the number of iterations. The second is given by bounds put on the step size guess. That is, given $s_{\text{min}}, s_{\text{max}}$, if the step size does not fall within $[s_{\text{min}}, s_{\text{max}}]$, then the algorithm is assumed to have stagnated and the iterations end. Algorithm 1 was applied to a couple basic profiles and these initial results are given in Chapter 5.
Chapter 4

Reduced Basis Method

The main problem with the additional consideration of the dependence of the parameters on the variable $\lambda$ in hyDOT is the addition of another dimension to the problem. In short, we now have a discretization of size $N_s \times N_x \times N_\lambda$ where $N_s$ is the number of chromophore species, $N_x$ is the number of pixels, and $N_\lambda$ is the number of wavelengths. Clearly this problem is computationally expensive, if not intractable, so model reduction methods must be used. Specifically, any algorithm used to solve the inverse problem in hyDOT requires the forward problem to be solved hundreds, if not thousands, of times in the iterative procedure. Thus, any reduction of the computational effort required to solve the forward problem of hyDOT will greatly reduce the computational burden of the inverse problem. In this section we focus on a specific model reduction technique applied to the forward problem.

There are several viable and well-researched model reduction techniques that could be applied to the hyDOT forward problem. These techniques include Proper Orthogonal Decomposition [30, 93] and the Empirical Interpolation Method [11, 64]. The Empirical Interpolation Method is often used in conjunction with the RBM, especially to serve as an approximate replacement to the affine decomposition assumption.
(discussed below) when it cannot be met [17]. The effectiveness of these methods is well-established, but we the ill-posed nature of the hyDOT problem, specifically with respect to the parameter $\lambda$, suggest that a different model reduction technique will be more effective.

One model reduction technique that applies specifically to partial differential equations with parameter dependence is the reduced basis method (RBM). A parameter (variable or constant for which there is not a derivative given) can appear in a differential equation as a coefficient to a variable (often in application characterizing a physical property, such as frequency), as a coefficient in the parameterization of the domain of the problem (describing the geometry), or in the definition of the right-hand side, as part of a forcing or boundary condition [63, 85]. The reduced basis method was first developed in the late 1970s and was initially applied to the nonlinear structural analysis of beams and arches [2, 70, 75] but was later applied to differential algebraic equation systems [83] and finally to a variety of parametric PDEs, including the linear Helmholtz-elasticity equation [25, 87] and the nonlinear Navier-Stokes equations [42, 78, 79, 82].

Reduced basis methods are used in conjunction with finite element models to give a discretization of a problem of very large dimension [87]. The idea is that the state variable in a PDE is not actually a member of the infinite-dimensional space in which the partial differential equation resides, but rather exists on a finite-dimensional manifold induced by its parametric dependence [38, 68]. Thus, the RBM seeks to consider the problem only on this manifold, and find an approximate solution to the PDE using a linear combination of basis functions for this manifold (see Figure 4.1). This reduced basis, $\{u(\mu_i)\}_{i=1}^N$, consists of finite element solutions, $u$, to the PDE evaluated a finite number of parameter values, with $N$ hopefully much smaller than the number of basis functions needed for a finite element approximation [43].
The PDE is discretized on the approximation space (the manifold) spanned by these vectors and the reduced basis approximation is to find solutions to the PDE from the approximation space [68].

\[
\mathcal{M} \quad X(\Omega) \quad u(\mu_1) \quad u(\mu) \quad u(\mu_2) \quad u(\mu_3) \quad u(\mu_4) \quad u(\mu_5) \quad X(\Omega) \quad M
\]

Figure 4.1: The graph on the left represents the 3-D finite element space, \( X(\Omega) \) of a PDE with solution \( u \) and domain \( \Omega \), and a 2-D manifold, \( \mathcal{M} \) in red, on which the reduced basis approximation is calculated. On the right, the solution \( u \) at unknown parameter \( \mu \) is approximated by the RBM using a linear combination of basis functions for \( \mathcal{M} \), \( \{u(\mu_i)\}_{i=1}^{N} \) for \( N \ll \dim(X) \).

### 4.1 Theory

The RBM applies only to parameterized PDEs, that is, the input vector is discretized to lie in \( \mathbb{R}^d \) for some \( d \in \mathbb{N} \) [38]. In its strong formulation, the PDE is defined on an infinite dimensional space, \( \Omega \) and, in general, a solution, \( u \) can not be calculated exactly. Therefore, before a reduced basis approximation can be calculated, the problem must be discretized. Most often the finite element method is used to give what is known as a “truth approximation” of the solution

\[
w^{fe}(\mu) = \sum_{i=1}^{N} c_i(\mu) \phi_i \tag{4.1}
\]

where the \( \phi_i \) form a basis for the finite element approximation space, \( X \), of dimension \( \mathcal{N} \), where \( \mathcal{N} \) is large [68]. Note that \( X \) is a Hilbert space over the bounded spatial
domain $\Omega \subseteq \mathbb{R}^d$. From its weak formulation, the PDE is defined as an input-output operator given as a bilinear form. In general, for input parameter $\mu$ (where $\mu$ may be a vector if there is more than one parameter), this is given as

$$a(u(\mu), v; \mu) = f(v), \quad \forall v \in X.$$  

(4.2)

The bilinear (or sesquilinear in the complex case) form is continuous with respect to $X$, as well as coercive. That is, there exists a coercivity constant, $\alpha(\mu)$ and continuity constant $\gamma(\mu)$ defined by,

$$0 < \alpha_0 \leq \alpha(\mu) \equiv \inf_{v \in X} \frac{a(v, v; \mu)}{||v||^2_X}, \quad \forall \mu \in \Lambda$$  

(4.3)

$$\sup_{v \in X} \frac{a(v, v; \mu)}{||v||^2_X} \equiv \gamma(\mu) < \infty, \quad \forall \mu \in \Lambda$$  

(4.4)

respectively [24]. Often, $a(u, v; \mu)$ is also assumed to be symmetric in the real case to prove convergence of the reduced basis approximate solution to the finite element solution [24]. The existence and uniqueness of a solution to (4.2) are proved using the Lax-Milgram Theorem. We prove these for the hyDOT problem in Chapter 2.

The output is a functional of the field variable $u(\mu)$ and is given by $s(\mu) = \ell(u(\mu))$. Problems where $\ell = f$ are commonly called “compliant”; otherwise, the problem is known as “noncompliant”. The theory addressed here assumes a compliant case, though some results have been shown for noncompliant cases. The set of all possible solutions to the parameterized PDE is a manifold of dimension $N$ given by

$$\mathcal{M} = \{u(\mu)| \mu \in \Lambda \subset \mathbb{R}\}$$

where $\Lambda$ is the parameter space. The idea is to find an approximation to the solution,
$u$, on an approximation to $\mathcal{M}$ instead of on the whole space $X$ [38]. Thus, the reduced basis approximation is not an approximation to the infinite dimensional problem, but rather an approximation to its finite element discretization, which is still of large and unmanageable dimension [87].

To construct a basis for $\mathcal{M}$, first a sample set of parameters $S_N = \{\mu_i|i = 1, \ldots, N\}$ is chosen, usually using a greedy algorithm, choosing the parameters that give the most significant information about the structure of the manifold. Note that $N \ll N$. There have been several methods suggested to find these $\mu_i$, trying to balance finding the most relevant samples and computational efficiency. We discuss some of these methods further in the next section. From this sample parameter space, we define a basis space for the manifold,

$$W_{N}^{L} = \text{span}\{u(\mu_i)|\mu_i \in S_N\}$$

where the $u(\mu_i)$ are found using the finite element approximation given in (4.1). This type of approximation space is known as a Lagrange subspace [79, 82] and was used, for example, by Almroth et al. in their development of numerical solutions in nonlinear structural analysis [2]. An alternative approximation subspace, known as the Taylor subspace or moving frame, is defined as

$$W_{N}^{T} = \text{span}\left\{u^j : u^j = \left. \frac{\partial^j u}{\partial \mu^j}\right|_{\mu=0}, j = 1, \ldots, N \right\}.$$

That is, $\mathcal{M}$ is a subspace of dimension $N \ll N$ spanned by the first $N$ partial derivatives of $u$ evaluated at $\mu = 0$ or any value of $\mu$ for which the solution $u$ is known [79, 82]. The Taylor space has been used to solve finite element discretizations by Noor et al. to solve nonlinear structural shell problems [74, 76] and Peterson to
find a numeric solution to the stationary Navier-Stokes equations [78]. An obvious
downside of this method is having to evaluate several derivatives of the solution with
respect to the parameter. Once an appropriate method is chosen and the approxima-
tion space is constructed, the reduced basis approximation of the solution for a new
\( \mu \) is given by

\[
u_N(\mu) = \sum_{j=1}^{N} \hat{c}_j(\mu) u(\mu_j) \in W_N.
\]

(4.5)

The coefficients \( \hat{c}_j \) are found by solving the state equations in \( W_N \) [43].

The state equations are solved using some type of projection, usually a Galerkin
or Petrov-Galerkin projection [15]. A Galerkin projection (or approximation) con-
structs a weak solution for a PDE by finding approximate solutions that satisfy
projections of the PDE onto a finite-dimensional subspace spanned by smooth or-
thonormal basis functions [34]. In the RBM, the Galerkin projection with respect to
\( W_N \) is to find a solution to

\[
a \left( \sum_{j=1}^{N} \hat{c}_j(\mu) u(\mu_j), v; \mu \right) = f(v), \quad \forall v \in W_N
\]

\[
\Rightarrow \sum_{j=1}^{N} \hat{c}_j(\mu) a(u(\mu_j), v; \mu) = f(v)
\]

with respect to \( \hat{c}_j(\mu) \). Since \( W_N = \text{span}\{u(\mu_i) | \mu_i \in S_N\} \), \( a(\cdot, \cdot) \) is bilinear and \( f(\cdot) \)
is linear, it is sufficient to solve

\[
\sum_{i=1}^{N} \hat{c}_j(\mu) a(u(\mu_i), u(\mu_j); \mu) = f(u(\mu_j)), \quad \forall j \in \{1, 2, \ldots, N\}.
\]

(4.6)

This problem is ill-conditioned because the basis vectors \( u(\mu_i) \) are usually pointing in
similar directions due to the smoothness of the low-dimensional \( \mathcal{M} \) and thus are not
sufficient to solve for the unknown \( \hat{c}_i \). Thus, the Gram-Schmidt procedure is often
applied to make the \( u(\mu_i) \) orthogonal [38].

The RBM has both an offline stage and an online stage when it is implemented computationally. In order for the RBM to have the full benefit of computational efficiency, as much as possible should be precomputed and stored in the offline stage. In this stage, the sample set \( S_N \) is constructed, and the basis functions \( u(\mu_i) \) of the space \( W_N \) are precomputed using the FEM approximation [17].

A significant source of computational effort for the RBM is the dependence of the bilinear form \( a(u(\mu_i), u(\mu_j); \mu) \) on the parameter \( \mu \), which results in it having to be calculated for each pair \( (u(\mu_i), u(\mu_j)) \) in the Galerkin projection (4.6) during the online stage [38]. If that parameter dependence can be removed, then the bilinear form can be precomputed and stored in the offline stage. For some PDEs, the bilinear form can be decomposed as

\[
a(u, v; \mu) = \sum_{q=1}^{Q} \Theta^q(\mu)a^q(u, v)
\]

where the \( \Theta^q : \Lambda \rightarrow \mathbb{R} \) are differentiable and, in general, very smooth functions depending on \( \mu \), and the \( a^q : X \times X \rightarrow \mathbb{R} \) are parameter-independent, continuous (with respect to \( X \)) bilinear forms [24, 87]. Given this decomposition, the reduced basis approximation involves solving (plugging (4.7) into (4.6)),

\[
\sum_{i=1}^{N} \sum_{q=1}^{Q} \hat{c}_i(\mu)\Theta^q(\mu)a^q(u(\mu_i), u(\mu_j)) = f(u(\mu_j)) \quad \forall j = 1, 2, \ldots, N
\]

for the coefficients \( \hat{c}_i(\mu) \) for each new value of the parameter \( \mu \). Since they no longer depend on the parameter, the \( a^q(u(\mu_i), u(\mu_j)) \) can be precomputed in the offline stage, reducing the computational burden significantly. Note that \( f \) may also be affinely parameter dependent, and so there may also exist a similar decomposition for \( f \) [87].
In this case, \( f(v; \mu) \) is expressed as the sum of \( Q_f \) elements and the approximation (4.8) can be written in matrix form as

\[
\sum_{q=1}^{Q_a} \Theta^a_q(\mu)A_q \hat{C} = \sum_{\hat{q}=1}^{Q_f} \Theta^f_{\hat{q}}(\mu)F_{\hat{q}} \tag{4.9}
\]

where \( A_q \) is an \( N \times n \) matrix with entries \((A_q)_{i,j} = a^q(u(\mu_j), u(\mu_i))\), \( \hat{C} \) is of dimension \( N \times 1 \) and is the vector of unknown coefficients (the reduced solution), and \( F_{\hat{q}} \) is an \( N \times 1 \) vector of entries \((F_{\hat{q}})_i = f_q(u(\mu_i))\) [63]. If the bilinear form cannot be affinely decomposed, the empirical interpolation method (EIM) has been proposed to approximate them in the form (4.7) so that the computational efficiency can be (relatively) maintained [11, 35, 39, 46].

Examining the operation counts of the offline and online stages helps to reveal the computation complexity of this method. In the offline stage, we form and store the matrices \( A_q \) (where \((A_q)_{i,j} = a^q(\phi_j, \phi_i)\)) and \( F_{\hat{q}} \) (where \((F_{\hat{q}})_i = f_q(u(\mu_i))\)). Note that this is only performed once since none of the quantities computed are dependent on the parameter \( \mu \). This computation requires \( N \) finite-element solutions and \( O(QN^2) \) finite-element vector inner products where \( Q = Q_a + Q_f \) if both \( a(u, v; \mu) \) and \( f(v; \mu) \) can be affinely decomposed [24]. In the online stage, the matrix \( \sum_{q=1}^{Q_a} \Theta^a_q A_q \), known as the stiffness matrix, must be assembled and inverted for each new value of \( \mu \). Since the \( A_q \) are precomputed and stored, the assembly requires only evaluation of the \( \Theta^a_q \), and then matrix multiplication and addition. The stiffness matrix is a full \( N \times N \) matrix so this requires \( O(N^3) \) operations. Since the \( F_{\hat{q}} \) are precomputed, evaluating the output inner product requires \( O(N) \) operations [24].

The great benefit of the RBM is that all operation counts in the online stage are independent of \( \mathcal{N} \gg N \) and so the computational burden is greatly reduced from a procedure that would require finding the finite element solution for each new
value of \( \mu \). Note that significant computational reduction is only possible if the affine decomposition of the bilinear form given in (4.7) is possible. In summary, Algorithm 2 describes how to solve a partial differential equation using the reduced basis method.

**Algorithm 2 Reduced Basis Method**

1: procedure **Offline Stage**
2: Choose parameter samples: \( \mu_1, \ldots, \mu_N, N \ll N \)
3: Define \( W_N = \text{span}\{u(\mu_k), k = 1, \ldots, N\} \), where \( u(\mu_k) = \sum_{i=1}^{N} c_i(\mu_k)\phi_i \)
4: Compute and store \( \sum_{i=1}^{N} a^q(u(\mu_i), u(\mu_j)) \), for \( q = 1, \ldots, Q^a \) (and \( \sum_{i=1}^{N} f^\hat{q}(u(\mu_j)) \) for \( \hat{q} = 1, \ldots, Q_f \), where applicable) for \( j = 1, 2, \ldots, N \)
5: procedure **Online Stage**
6: Find a solution with respect to \( \hat{c}_i \) for \( \sum_{i=1}^{N} \sum_{q=1}^{Q} \hat{c}_i(\mu)\Theta^q(\mu)a^q(u(\mu_i), u(\mu_j)) = f(u(\mu_j)) \quad \forall j = 1, 2, \ldots, N \)
7: Reduced Basis approximation: \( u_N(\mu) = \sum_{i=1}^{N} \hat{c}_i u(\mu_i) \)

Finally, we will show the convergence of the RBM approximation in the norm governing the approximation space \( X \). First, it is known that the finite element approximation converges to the exact solution in this norm (see, e.g., [55]). We have by the triangle inequality,

\[
||u^e - u_N||_X \leq ||u^e - u||_X ||u - u_N||_X \tag{4.10}
\]

where \( u^e \) is the exact solution, so we only need to show the convergence of the reduced basis solution to the finite element solution in order to prove the convergence of the reduced basis solution to the exact solution. The smoothness of the manifold \( M \) suggests that \( u_N(\mu) \) converges rapidly to \( u^f(\mu) \), and we used this assumption to construct \( S_N \) such that \( N \ll N \). In fact, this assumption has been demonstrated numerically [66], and the convergence has been shown to be exponential when the parameter values in \( S_N \) are chosen to be logarithmically (quasi-) uniformly distributed [67, 84]. The following proposition and its proof is standard in the a priori
convergence theory of the RBM (see, e.g., [24, 84]).

**Proposition 4.1.** The reduced basis approximation $u_N(\mu)$ is optimal in the $X$-norm in the sense

$$||u(\mu) - u_N(\mu)||_X \leq \sqrt{\frac{\gamma(\mu)}{\alpha(\mu)}} \inf_{w_N \in W_N} ||u(\mu) - w_N||_X.$$ 

*Proof.* For this proof, we assume that the bilinear form $a(\cdot, \cdot; \mu)$ is symmetric. Since we have that $a(u(\mu), v; \mu) = f(v)$ and $a(u_N(\mu), v; \mu) = f(v)$ for all $v \in W_N$, it follows that

$$a(u(\mu) - u_N(\mu), v; \mu) = 0, \quad \forall v \in W_N.$$ 

Consider $w_N = u_N + v_N \in W_N$ for some $v_N \neq 0$. Then,

$$a(u - w_N, u - w_N; \mu) = a(u - u_N - v_N, u - u_N - v_N; \mu)$$

$$= a(u - u_N, u - u_N - v_N; \mu) - a(v_N, u - u_N - v_N; \mu)$$

$$= a(u - u_N, u - u_N; \mu) - a(u - u_N, v_N; \mu) - a(v_N, u - u_N - v_N; \mu)$$

$$= a(u - u_N, u - u_N; \mu) - 2a(u - u_N, v_N; \mu) + a(v_N, v_N; \mu)$$

$$> a(u - u_N, u - u_N; \mu).$$

Using (4.3) and (4.4), we have

$$\alpha(\mu)||u - u_N||^2_X \leq a(u - u_N, u - u_N; \mu)$$

$$< a(u - w_N, u - w_N; \mu)$$

$$\leq \gamma(\mu) \inf_{w_N \in W_N} ||u - w_N||^2_X.$$ 

Thus, $||u(\mu) - u_N(\mu)||_X \leq \sqrt{\frac{\gamma(\mu)}{\alpha(\mu)}} \inf_{w_N \in W_N} ||u(\mu) - w_N||_X$. \qed
A similar argument can be used to show the convergence of the output operator.

### 4.2 Choice of Sample Set

A key element in the RBM, specifically when using a Lagrange space, is choosing an appropriate sample set $S_N$ of parameters from which to form a basis for the approximation space $W_N$. The goal is to choose the parameters that yield the most sensitive solutions, that is, solutions that illustrate the most significant features of the solution space. Enough parameter samples must be chosen to yield reduced basis approximations that converge to the truth solution (which in turn converges to the exact solution), but the number of samples must be far fewer than the dimension of the finite element approximation space and small enough to preserve computational efficiency.

For problems in which the bilinear form $a(u, v; \mu)$ has an affine decomposition of the form,

$$ a(u, v; \mu) = a_0(u, v) + \mu a_1(u, v) $$

where $a_0(u, v)$ is symmetric, coercive and continuous, and the parameter space is given by $D = [0, \mu_{\text{max}}] \subset \mathbb{R}$, it has been shown that if the sample points are chosen according to a logarithmic point distribution, then the reduced basis approximation will converge exponentially to the truth solution for all $N$ greater than some value $N_{\text{crit}}$ [68]. Further, it has been numerically demonstrated that using a logarithmic versus a uniform or Chebyshev distribution in the choosing of points results in a much smaller maximum relative error [98]. These considerations suggest that $N$ can be chosen to be very small.
4.2.1 Greedy Algorithms

The most common sampling procedure for generating a Lagrange reduced basis space is a greedy algorithm based on \textit{a posteriori} error bounds that allows for an efficient sampling of $\mathcal{M}$ that is independent of $\mathcal{N}$ [24, 25, 87, 91]. First, the smallest anticipated error tolerance, $\epsilon_{\text{tol, min}}$ is calculated \textit{a priori} offline where

$$\epsilon_{\text{tol, min}} = \min \epsilon_{\text{tol}}$$

Next, $\epsilon_{\text{tol}}$ is calculated as

$$||u^f(\mu) - u_N(\mu)||_X \leq \epsilon_{\text{tol}}$$

Next, a very fine mesh $\Xi$ of the parameter space $\Lambda$ is created, containing the surrogate values of $\Lambda$ from which the greedy algorithm will draw to generate a set of “training” samples, $S_N$. This mesh is usually generated using a Monte Carlo method with respect to a uniform or log-uniform density and must be sufficiently fine to ensure that further refinement does not significantly improve the results [87].

Next, $N_{\text{max}}$, the maximum allowable dimension of the reduced basis space, is defined, such that the desired accuracy of the reduced basis approximation is attained [87, 91]. $N_{\text{max}}$ can also be adaptively determined during the greedy algorithm [25]. A sample $\mu_1$ is chosen at random to be the first sample added to $S_1$ such that $S_1 = \{\mu_1\}$, and then $W_1 = \{u(\mu_1)\}$ is calculated. The next sample, $\mu_2$ is calculated as

$$\mu_2 = \arg \max_{\mu \in \Xi} \epsilon^*_1(\mu)$$

where

$$\epsilon^*_k = \Delta^*_k(\mu)/s_k(\mu) \quad (4.11)$$

is the relative error bound [24, 91]. That is, a bound on the error in approximating $u(\mu)$ by a linear combination of elements in the set $\{u(\mu_1), \ldots, u(\mu_k)\}$. Note that $s_k(\mu)$ is the reduced basis approximation with $k$ basis functions of the desired output.
at $\mu$.

The estimate $\Delta^s_k(\mu)$ is an online error bound and must be calculated for each new value of $\mu$. To calculate $\Delta^s_k(\mu)$, first a positive lower bound, $\hat{\alpha}(\mu)$ for the stability constant, $\alpha(\mu)$, of the bilinear form $a(u, v; \mu)$ must be determined. Note that if the bilinear form is symmetric and coercive, that $\alpha(\mu)$ is simply the coercivity constant,

$$\alpha(\mu) := \inf_{w \in X} \frac{a(w, w; \mu)}{||w||^2_X}$$

Otherwise, $\alpha(\mu)$ is the inf-sup stability constant given by

$$\alpha(\mu) = \inf_{w \in X} \sup_{v \in X} \frac{a(w, v; \mu)}{||w||_X||v||_X}$$

a generalized minimum singular value. For theory on how to calculate this bound in general see [24]. Then, the residual associated with $u_N(\mu)$,

$$r(v; \mu) := f(v) - a(u_N(\mu), v; \mu) \quad v \in X$$

is calculated to define the dual norm of the residual

$$\varepsilon_N(\mu) = ||r(\cdot; \mu)||_{X'} = \sup_{v \in X} \frac{r(v; \mu)}{||v||_X}$$

Thus, for the compliant problem, we define

$$|s(\mu) - s_N(\mu)| \leq \Delta^s_n(\mu) := \frac{\varepsilon^2_N(\mu)}{\hat{\alpha}}$$

A sharper bound with more rapid convergence of the reduced basis output approximation can be obtained using the dual problem for noncompliant ($\ell \neq f$) problems [91].
Thus, in calculating each new $\mu_i$, we are looking for the parameter value in $\Xi$ that will give us the largest scaled residual, that is, the parameter that affects the most significant change in the solution. It is important to note that $\Delta_n^*\Delta^*$ is reliable (an upper bound of the true error), and as a surrogate, truly represents the true error, $||u(\mu) - u_N(\mu)||_X$ (and thus is sharp) [91]. Further, since it is computed online, it must be computed inexpensively, that is, independently of $N$. Clearly, this step will be the most expensive step in the sampling procedure, so it is essential that the computational effort is as low as possible. Further, this sampling procedure is very similar to the proper orthogonal decomposition (POD) economization procedure, it is more efficient because the unused or “rejected” snapshots are never constructed [24].

Note that other types of error estimators can be used in the definition of $\mu_i$, see, e.g. [46, 87]. Then it must be verified that $\varepsilon^*_2 = \epsilon_1(\mu_2)$ is greater than $\epsilon_{tol,\ min}$. If it is not, then the current set $S_1$ is the final sample set and the process is terminated. Otherwise, $S_2 = S_1 \cup \mu_2$ and $W_2 = W_1 + \{u(\mu_2)\}$. The process then continues until we reach $N_{max}$ or an error estimate goes below $\epsilon_{tol,\ min}$. Hesthaven, et al. have adapted this algorithm to cases where the parameter space is of high dimension [46]. The greedy algorithm described here is summarized in Algorithm 3.

Algorithm 3 Greedy Sampling Algorithm

for $k = 2 : n_{max}$ do
2: $\mu_k = \arg \max_{\mu \in \Xi} \epsilon^*_{k-1}(\mu)$
3: $\varepsilon_k^* = \epsilon_k^* (\mu_k)$
4: if $\varepsilon_k^* \leq \epsilon_{tol,\ min}$ then
5: $n_{max} = k - 1$
6: exit
7: $S_k = S_k \cup \mu_k$
8: $W_k = W_k + \{u(\mu_k)\}$

Recall that the set of basis functions $\{u(\mu_1), u(\mu_2), \ldots, u(\mu_N)\}$ are usually pointing in similar directions, so in order to make (4.6) well-conditioned, the basis
functions need to be orthogonalized. This process can be incorporated into Algorithm 3 for efficiency.

Algorithm 3 is generally sufficient for finding an appropriate sample space for parameters of low-dimension, but since the algorithm requires calculating $\epsilon_k^*(\mu)$ for all $\mu \in \Xi$, it can be very expensive. Thus, Hesthaven et al. [46] have developed alternative sampling algorithms, modifications of the greedy algorithms above, that decrease computational complexity and increase the likelihood that the set of basis functions accurately represents the manifold. The first modification relies on what Hesthaven calls a *saturation assumption*. The saturation assumption is said to be satisfied if

$$
\epsilon^*(\mu, W_m) \leq C \epsilon^*(\mu; W_k)
$$

for some $C > 0$ for all $m > k > 0$

where $\epsilon^*(\mu; W_m)$ is an $\mu$-dependent error estimator, used in the determination of the next parameter in the standard greedy algorithm. The choice of the constant $C$ does not need to be theoretically rigorous in order for the modified greedy algorithm to work [46]. A simple consideration of the error estimator is sufficient to determine an appropriate $C$. The standard greedy algorithm previously described assumes that the error estimator will converge to zero as $k$ approaches infinity and thus we can assume that $\epsilon^*(\mu, W_k)$ will overall be decreasing as $k$ increases. If we set $C < 1$, then we assume that $\epsilon^*(\mu, W_k)$ is strictly decreasing. A choice of $C = 1$ implies only that $\epsilon^*(\mu, W_k)$ is not increasing for a fixed $\mu$ as $k$ increases. The most relaxed assumption is that $C > 1$, in which case we allow for $\epsilon^*(\mu, W_k)$ to oscillate periodically, though decrease in the long run. Hesthaven et al. state that $C = 1$ is usually a good choice for projection based methods (as in the RBM), whereas $C > 1$ is better for interpolation based methods such as the EIM [46].
We can use the saturation assumption to prevent $\epsilon^*(\mu, W_k)$ from having to be calculated for each $\mu \in \Xi$ and for each value of $k$. Instead, we store an error profile $\epsilon_\ast^s(\mu) = \epsilon^*(\mu, W_\ell)$ for each $\mu$ such that $\ell < k$. Each time we loop through each value of $\mu$ in $\Xi$, we use the stored error profiles to set a temporary maximum error. The saturation assumption states $\epsilon^*(\mu, w_k) \leq C\epsilon_\ast^s(\mu, W_\ell)$ for $\ell < k$ and thus, $\epsilon^*(\mu, W_k)$ cannot be greater than the temporary maximum as long as $C\epsilon_\ast^s(\mu, W_\ell)$ is less than the temporary max. If $C\epsilon_\ast^s(\mu, W_\ell)$ is greater than the temporary maximum, then it is a candidate for the new temporary maximum error. To verify if we should update the temporary maximum, we must calculate $\epsilon^*(\mu, W_k)$, update $\epsilon_\ast^s(\mu)$ and then compare it to the current temporary maximum. Note that $\epsilon_\ast^s(\mu, W_\ell)$ for some $\ell < k$ is maintained for each $\mu$ if we continue in this manner.

The benefits of the saturation assumption can then be added to a procedure developed by Hesthaven et al. [46, 47] known as the adaptively enriching greedy algorithm (AEGA). This adaptation of the standard greedy algorithm adds in a “safety check” to ensure that the set $\Xi$ is rich enough and the errors are truly less than the desired tolerance, as well as adaptively changes and enriches the set $\Xi$ by removing useless points and adding new points. The set $\Xi$ is also initially chosen as a set of random points. The “safety check” involves testing the approximation from an initial set of basis functions on a larger, refined set of test parameters to see if the approximation errors are less than the prescribed tolerance on this refined set as well. If the basis set $W_k$ fails the test, the first failed parameter is added to the set $S_k$ and the check is performed again until it is passed. After a set, $W_k$, of basis functions is determined, the errors of some points in $\Xi$ will be below the prescribed tolerance and so, since the error is decreasing, these points will never be chosen. Thus, we can remove them from $\Xi$. New random points can then be added $\Xi$ so that it maintains the same cardinality. The general algorithm for the AEGA is given in Algorithm 4.
where $M$ is the number of parameter points in $\Xi$ and $N_{sc}$ is the number of sample points that must pass the safety check.

Algorithm 4 Adapively Enriching Greedy Algorithm (AEGA)

\begin{verbatim}
N_{safe} = \text{ceil}(N_{sc}/M)
Generate $\Xi$ with $M$ samples (randomly or otherwise)
3: Choose $\mu_1 \in \Xi$ and set $S_1 = \{\mu_1\}, k = 1$
    Set $\epsilon^*_s(\mu) = \infty$ for all $\mu \in \Xi$
    Set $W_1 = \{u(\mu_1)\}$, safe = 0, $err_{tmpmax} = 2 * tol$
6: while $err_{tmpmax} \geq tol$ or safe $\leq N_{safe}$ do
    $err_{tmpmax} = 0$
    for all $\mu \in \Xi$ do
9:      if $C\epsilon^*_s(\mu) > err_{tmpmax}$ then
        Compute $\epsilon^*(\mu; W_k)$, let $\epsilon^*_s(\mu) = \epsilon^*(\mu, W_k)$
        if $\epsilon^*_s(\mu) > err_{tmpmax}$ then
12:            $err_{tmpmax} = \epsilon^*_s(\mu)$, let $\mu_{max} = \mu$
        if $\epsilon^*_s(\mu) < tol$ then
15:            flag $\mu$ (to be removed later)
if $err_{tmpmax} > tol$ then
18:    Choose $\mu_{k+1} = \mu_{max}$, set $S_{k+1} = S_k \cup \{\mu_{k+1}\}$
    $W_{k+1} = W_k \cup \{u(\mu_{k+1})\}$
21:    Remove all flagged parameters from $\Xi$ and corresponding $\epsilon^*_s(\mu)$
    Generate $M - \text{size}(\Xi)$ new samples and add them to $\Xi$. Set $\epsilon^*_s(\mu^*) = \infty$
    for all new points $\mu^* \in \Xi$
    $k = k + 1$
else
24:    Discard $\Xi$ and generate $M$ new parameters to form a new $\Xi$, set $\epsilon^*_s(\mu) = \infty$
    for all $\mu \in \Xi$
\end{verbatim}

Hesthaven and Zhang [47] have also developed sample space generating algorithms which use ANOVA expansion to help identify the most important parameters through sensitivity analysis. These methods are especially useful in reducing the cost of problems with a high-dimensional parameter space.
4.2.2 Non-Greedy Alternatives

Recently, alternatives to the traditional greedy approach in finding $S_N$ have been suggested. In [41] both a Bayesian and a gradient approach are described and presented as effective alternatives to the basic greedy algorithm described in Algorithm 3. We will give an overview of both methods here and show the numerical results of [41] on a model problem in Chapter 5.

4.2.2.1 Gradient Algorithm

The gradient algorithm considered here (given in [41]) is an adaptation of the standard greedy algorithm. A gradient type algorithm can also be created as an adaptation to the Metropolis algorithm described below. Like the greedy algorithm, the gradient algorithm adds one new element to the basis each iteration, instead of updating the whole basis $S_N$ on every iteration as in Algorithm 6. The main idea is to solve the minimization problem,

$$\mu_k = \arg \min_{\mu \in \Lambda} \sum_{\tilde{\mu} \in \Upsilon} \frac{\|u^{fe}(\tilde{\mu}) - u_{N+1}(\tilde{\mu})\|_X}{\|u^{fe}(\tilde{\mu})\|_X}$$

in each iteration where $u_{N+1}(\tilde{\mu})$ is the reduced basis approximation of the solution evaluated at a new parameter $\tilde{\mu}$ in $S_{N+1} = S_N \cup \tilde{\mu}$, and $\Upsilon$ is a mesh over $\Lambda$. As in the greedy algorithm, the first sample is typically chosen randomly (as in [41]), but could also be chosen using a priori information. Since the gradient algorithm chooses the next element $\mu_k$ of the basis $S_N$ from the whole parameter space $\Lambda$, instead of from a fine mesh $\Xi$ of $\Lambda$ as in the greedy algorithm, it is able to improve $S_N$ more effectively at each iteration, reducing the dimension $N$. The size of $N$ is ultimately determined
by the \textit{a priori} error bound

\[ \|u_{fe}(\mu) - u_N(\mu)\|_X \leq \epsilon_{tol} \]

and the chosen maximum dimension, $N_{\text{max}}$, which are the same stopping criteria as the greedy algorithm.

The gradient algorithm is an iterative algorithm. To avoid clustering around local minima, the starting point for each iteration is generally varied. From a coarse mesh $\hat{\Xi}$ of $\Lambda$ the starting point of iteration $k$ is chosen as

\[ \mu_k^0 = \arg \min_{\mu \in \hat{\Xi}} \sum_{\tilde{\mu} \in \Upsilon} \frac{\|u_{fe}(\tilde{\mu}) - u_{N+1}(\tilde{\mu})\|_X}{\|u_{fe}(\tilde{\mu})\|_X}. \]

Choosing the starting point from a coarse mesh (an approach similar to the hill climbing algorithm [88]) reduces the likelihood of clustering and improves detection of a local minimum. As the name suggests, a gradient method is used to find this local minimum, although the Nealder-Mead (or simplex) algorithm can alternatively be used if all the requirements for the gradient method are not met [3]. The gradient algorithm requires $\Lambda$ to be closed and compact to ensure convergence using a penalty term, and the minimization function needs to be in $C^1(\Omega)$, to guarantee existence of a derivative, that is, a gradient.

The gradient algorithm used in [41] is given in Algorithm 5.

\subsection{Metropolis Algorithm}

While the greedy and gradient algorithms have the advantage of being able to create one new basis element at a time, [41] suggested the use of a Bayesian algorithm that depends on posterior distribution. Rather than finding one new element $\mu_{k+1}$ for
Algorithm 5 Gradient Sampling Algorithm

Initialize Setup
\( \mu_1 = \text{rand}(\Xi \subset \Lambda) \)

for \( k = 2 : N_{\text{max}} \) do
  Find starting point for minimization
  \( \mu_k^0 = \arg \min_{\mu \in \Lambda} \sum_{\tilde{\mu} \in \Upsilon} \frac{||u^{fe}(\tilde{\mu}) - u_{N+1}(\tilde{\mu})||_X}{||u^{fe}(\mu)||_X} \)
  Solve minimization problem
  \( \mu_k = \arg \min_{\mu \in \Lambda} \sum_{\tilde{\mu} \in \Upsilon} \frac{||u^{fe}(\tilde{\mu}) - u_{N+1}(\tilde{\mu})||_X}{||u^{fe}(\mu)||_X} \)
  \( \varepsilon_k = \max \)
  if \( \varepsilon_k \leq \epsilon_{\text{tol, min}} \) then
    \( N_{\text{max}} = k - 1 \)
    exit
  \( S_k = S_k \cup \mu_k \)
  \( W_k = \text{span}\{W_k, \{u(\mu_k)\}\} \)

the basis generating set \( S_N \) in each iteration, where \( N \) increases until the algorithm is terminated, the Metropolis algorithm can only be used for a fixed \( N \). Thus, we must know the desired size of the basis beforehand. In this case, the creation of \( S_N \) is set up as a minimization problem given as,

\[
\min_{S_N \in \Lambda^N} \sum_{\mu \in \Xi} \frac{||u^{fe}(\mu) - u_N(\mu; S_N)||_X}{||u^{fe}(\mu)||_X}. \tag{4.13}
\]

The Metropolis algorithm considers \( \tilde{\mu}_i \) as random variables of \( \mu_i \). It then finds the posterior probability density function of \( \{\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N\} \) using Bayes’ theorem, given the error or noise \( \delta = \{u^{fe}(\mu)\}_{\mu \in \Xi} \). If \( \tilde{\delta} \) is the random variable of \( \delta \), then posterior probability density function is given by,

\[
P_{\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N}(S_N|\delta) \propto P_{\tilde{\delta}|S_N}P_{\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N}(S_N), \tag{4.14}
\]
where $P_{\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N}(S_N)$ is the prior density and $P_\delta(\delta | S_N)$ is the density of the noise, in this case given by,

$$P_\delta(\delta | S_N) \propto \exp \left( -\sum_{\mu \in \Xi} \frac{||u^f_e(\mu) - u_N(\mu; S_N)||_X}{||u^f_e(\mu)||_X} \right).$$ (4.15)

The choice of the prior density could include prior knowledge of $\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N$ such as values found from $S_N$ from a previous algorithm.

The Metropolis algorithm seeks to find the Bayes’ estimate $E(\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N | \delta)$, approximating it using simulation as it is impossible to find directly. This approximation is found using a Monte Carlo method which generates a large random sample from the posterior density (4.14), of size $Y$. The approximation to the Bayes’ estimate is then given by the sample mean,

$$E(S_N | \delta) = \int_{\mathbb{R}^N} S_N P_{\tilde{\mu}_1, \tilde{\mu}_2, \ldots, \tilde{\mu}_N}(S_N | \delta) dS_N \approx \frac{1}{Y} \sum_{i=1}^{Y} S_{N_i}$$ (4.16)

where $S_{N_i}$ is the $i$th random sample (each sample is a basis generating set $S_N$). There are a few choices to generate these samples, but [41] uses an adaptive Metropolis Hastings algorithm (for explanation of the Metropolis Hastings algorithm see [20]).

In this algorithm (given in Algorithm 6), $\xi(S_{N_i}; A)$ is a transition kernel, a kernel that denotes the probability of moving from the current state $S_{N_i}$ to another state in $A$. We want to define the conditions of the transition kernel that allows convergence to an invariant distribution, $\pi$, where $\pi$ is the distribution of the posterior density $P(S_N | \delta)$. A transition kernel that converges to the distribution $\pi$ is given by

$$\xi_{MH}(S_{N_i}; A) := \int_A q(S_{N_i}, S_{N_{i+1}}) \alpha(S_{N_i}, S_{N_{i+1}}) dS_{N_{i+1}}$$

$$+ \left[ 1 - \int_{\mathbb{R}^N} q(S_{N_i}, S_{N_{i+1}}) \alpha(S_{N_i}, S_{N_{i+1}}) dS_{N_{i+1}} \right] \chi_A(S_{N_i}),$$ (4.17)
Algorithm 6 A Pilot Adaptive Metropolis Algorithm.

\[ j = 1; \]
\[ \text{for } i = 1 \text{ to } B+Y \text{ do} \]
\[ \quad \text{if } i \equiv 0 \mod m \text{ and } i \leq mM \text{ then} \]
\[ \quad \Sigma_j = \Lambda(\Sigma_{j-1}); \]
\[ \quad j++; \]
\[ \quad \text{Generate } S_{N_i} \text{ from } q_{C_j}(S_{N_{i-1}}, \cdot) \text{ and } u \text{ from } U(0, 1); \]
\[ \quad \text{if } u \leq \alpha(S_{N_i}, S_{N_e}) \text{ then} \]
\[ \quad S_{N_i} = S_{N_e}; \]
\[ \quad \text{else} \]
\[ \quad S_{N_i} = S_{N_{i-1}}; \]
\[ \text{Return } \{S_{N_1}, S_{N_2}, \ldots, S_{N_{B+Y}}\} \]

where \( \chi_A \) is an indicator function over \( A \), and \( q(S_{N_i}, S_{N_{i+1}}) \) is a density that generates a new candidate random sample \( S_{N_{i+1}} \) from the current sample \( S_{N_i} \). The probability of accepting this new random sample \( S_{N_{i+1}} \) is given by the acceptance ratio

\[
\alpha(\mu_i, \mu_{i+1}) = \begin{cases} 
\min \left[ \frac{P(\mu_{i+1}|\delta)q(\mu_{i+1}, \mu_i)}{P(\mu_i|\delta)q(\mu_i, \mu_{i+1})}, 1 \right], & \text{if } P(\mu_i|\delta)q(\mu_i, \mu_{i+1}) > 0 \\
1, & \text{otherwise}
\end{cases} \tag{4.18}
\]

In sum, the Metropolis Hastings algorithm generates new candidates for \( S_N \) using the proposed density \( q(\cdot, \cdot) \) and accept them as random samples of the posterior distribution with probability \( \alpha(S_{N_i}, S_{N_{i+1}}) \).

The choice of \( q(\cdot, \cdot) \) is essential to obtaining a reasonable result with an efficient running time of the algorithm. In general, a pilot adaptive Metropolis algorithm involves adapting the proposed distribution for a given amount of iterations and then starting the burn-in time after the last adaptation. Algorithm 6 trains the proposal distribution by changing the covariance matrix such that the acceptance ratio of the Markov chain after the last adaptation is close to the optimal acceptance ratio, \( a_0 \), of the chain. Once the algorithm comes to the end of the pilot time, during which
it modifies the covariance matrix until it approaches a covariance matrix with an optimal acceptance ratio, it starts the standard Metropolis Hastings algorithm with the latest state and proposal distribution given at the end of the pilot time. A more thorough explanation of this algorithm is given in [94], where the algorithm is first introduced.

4.3 Application to the hyDOT Inverse Problem

Application of the RBM to the inverse problem of hyDOT is not as straightforward as it is for the forward problem. Unfortunately, the geometry of the forward problem changes in each iteration of the inverse problem as the cost functional is minimized and the desired spatial map of the unknown optical coefficients is refined. As a result, the decomposition of the bilinear form necessary to reduce the computational complexity of the online stage of the RBM is not possible using the geometry as the means. We will demonstrate in Chapter 5, however, that the reduced basis for the DOT forward problem does not change very much as the geometry changes. Thus, we can run one of the basis generating algorithms in Section 4.2 only once before the inverse algorithm starts to iterate, and then use the same reduced basis every time the forward problem needs to be solved. Since new coefficients for the solution approximation given in (4.5) are found in the online stage, each iteration of the inverse problem will still yield a different approximate solution $u(\lambda)$.

Although we can use the same basis for all the iterations of the inverse problem, it is very difficult (and perhaps impossible) to apply the Reduced Basis Method to the inverse hyDOT problem. Each iteration of the inverse problem, in which the cost functional is minimized, requires the forward problem to be solved again. Unlike DOT, however, the forward problem at each iteration must be solved for each
wavelength in the spectrum that is being used since \( D(\lambda) \) and \( \mu_a(\lambda) \) can no longer be pulled out of the spatial integral in the weak formulation. It may be possible however, to use the Empirical Interpolation Method in conjunction with the RBM to get an approximation to this affine decomposition as suggested in [11, 35, 39, 46].

Further, in this work we have not investigated how using a reduced basis approximation for the solution at a given wavelength instead of the “exact” (or finite element) solution changes the final spatial resolution of the image. One of the main disadvantages of optical tomography is its low resolution (though it produces images with high contrast). If using the RBM in the inverse problem further degrades this resolution, it would not be advantageous to use it. Due to the regularity of the solution and optical parameters with respect to wavelength demonstrated in Chapter 2, however, we suspect that the resolution of an image using an approximate solution would not be much different than the exact solution. We hope to investigate this more thoroughly in future work.

We have shown in the previous sections, the RBM can be successfully applied to the forward problem so that the full problem need only be solved for a few wavelengths (those in the basis) and a reduced basis approximation of the solution be given for the other wavelengths. This greatly reduces the computational complexity of the forward problem for a given geometry. In our method, we cannot precompute the matrices that hold the finite element solutions of the elements of the reduced basis, however, we still reduce the computational complexity of the problem by only calculating the forward solution for the wavelengths in the reduced basis.
Chapter 5

Simulations

In this chapter we will present the results of the numerical simulations performed to confirm the theoretical results presented in the previous chapters. We begin by demonstrating an application of the reduced basis method to a simplified hyDOT forward model. We present the results using the three different basis selection methods described in Sections 4.2.1 and 4.2.2, to suggest alternatives to the traditional greedy method. Next we present numerical results of solving the hyDOT inverse problem for a simple two-dimensional simulation. The hyDOT simulations give initial confirmation to the ideas for solving the inverse problem discussed in Chapter 3 and demonstrate the robustness of the reconstruction algorithm presented there. All simulations were run on a MacBook Pro, OS X Version 10.9.5, with a 2.5 GHz Intel Core i5 processor, and 4 GB 1600 MHz memory.
5.1 Application of the RBM to the hyDOT Forward Problem

In general, the first-order diffusion approximation of the radiative transport equation that governs hyDOT is given in the frequency domain as

\[-\nabla \cdot (D \nabla u) + (\mu + ik)u = h \quad \text{in } \Omega \quad (5.1)\]

\[u + 2D \frac{\partial u}{\partial \nu} = f \quad \text{on } \partial \Omega \quad (5.2)\]

where \(h\) is the interior forcing function, and \(k\) is the wave number for the frequency modulation of the laser. To illustrate the application of this method, we consider a simplified version of the forward problem for hyDOT where \(k\) and \(h\) are considered to be zero and Neumann boundary conditions are used instead of Robin boundary conditions. The strong form of the governing PDE is thus given by

\[-\nabla \cdot (D(x, \lambda) \nabla u) + \mu_a(x, \lambda)u = 0 \quad \text{in } \Omega \quad (5.4)\]

\[D(x, \lambda) \frac{\partial u}{\partial n} = f \quad \text{on } \partial \Omega \quad (5.5)\]

The wavelength, \(\lambda\), is the parameter on which the PDE is dependent. We will consider the parameter space as \(\Lambda = [600, 1000] \subset \mathbb{R}\), with units nanometers. Note that \(\Lambda\) is a continuous subset theoretically, but discrete in practice.

We consider a simple geometry for \(\Omega\) in two dimensions given by a circle of radius 25 centimeters centered at the origin on a Cartesian grid, with a circular tumor of radius 5 centimeters located at the point \((-15, -10)\) (see Figure 5.1). The location of the tumor was chosen to be relatively close to the source to yield results that were
easier to visualize, since light does not penetrate very far into tissue. The domain \( \Omega \) was discretized using a finite element mesh of 2097 elements. We consider only Neumann boundary conditions with one Gaussian source given by

\[
f(x, y) = 15e^{-\frac{(x-x_1)^2+(y-y_1)^2}{10}}
\]

located at \((x_1, y_1) \approx (-24.5196, -4.8773)\), one of the finite element mesh points on the boundary. In the forward problem, the source \( f \) and the geometry and location of the area of interest, in our case a collection of cancerous cells, is known. Only the measurements of the scattered photons on the boundary are unknown and are derived from the solution, \( u \).

We will use the RBM to find an approximate solution \( u_N(x, \lambda) \) to (5.4) - (5.5). To apply the RBM, we must first consider the weak formulation of (5.4) - (5.5). To
find the weak form, we multiply both sides of (5.4) by a test function \( v \in V \) and integrate over the spatial domain, \( \Omega \) to obtain:

\[
\int_{\Omega} (-\nabla \cdot (D \nabla u) + \mu_a uv) \, dx = 0 \quad \forall v \in V
\]

Then, we integrate the lefthand side by parts and apply the boundary conditions to obtain the weak formulation:

\[
\int_{\Omega} (D \nabla u \cdot \nabla v + \mu_a uv) \, dx = \int_{\partial \Omega} f \gamma_D(v) \, ds \quad \forall v \in V \tag{5.6}
\]

with \( V \) the space of smooth test functions. From the weak formulation, we define the following bilinear and linear forms,

\[
a(u, v; \lambda) = \int_{\Omega} (D(\lambda) \nabla u \cdot \nabla v + \mu_a(\lambda) uv) \, dx \quad F(v) = \int_{\partial \Omega} f \gamma_D(v) \, ds \tag{5.7}
\]

where \( a(u, v) : H^1(\Omega) \times H^1(\Omega) \to \mathbb{R} \) and \( F(v) : H^1(\Omega) \to \mathbb{R} \), with the inner product induced by the bilinear form. Note that here we are in compliance (that is, the output functional \( \ell = f \)).

We created functions to represent \( \mu_a(\lambda) \) such that given \( \lambda \) the value of \( \mu_a \) would be one constant value anywhere in \( \Omega_0 \) and a different constant value anywhere in \( \Omega_1 \). Since

\[
D = \frac{1}{3(\mu_a + \mu'_a)}
\]

the value for the diffusion coefficient would follow a similar pattern as it is a function of \( \mu_a \). The function values were based on the graph showing the absorption coefficient as a function of wavelength given by Saibaba et al. in \cite{89} (Figure 1.4) and experimental values given by Yodh and Chance \cite{101} and Jiang \cite{52}. Cerussi et al. \cite{18} gave a similar
Figure 5.2: Graph of the absorption coefficient, $\mu_a$, (in mm$^{-1}$) as a function of wavelength, $\lambda$, (in nm), as found in [18].

The profile of the absorption coefficient with respect to wavelength, but with slightly lower values (see Figure 5.2). Given these experimental values, the function for $\mu_a$ in $\Omega_0$ was taken to be a quartic check function (found using interpolation through select data points) with Gaussian spikes at 725 and 950 nanometers. Since cancerous cells generally have higher absorption coefficients than healthy tissue, we followed the example of [18, 89] and made the profile of the absorption coefficient in $\Omega_1$ to be a positive perturbation of its profile in $\Omega_0$. This assumption is confirmed by [50, 51]. Jakubowski et al. [51] demonstrate that cancerous tissue has a higher water content and lower fat content than that of healthy tissue. Their results for breast tissue in particular, as reported in [50], are given in Table 5.1. Thus, in the graph given by [50] in Figure 5.3, we see that the profiles for the absorption coefficient for tissue with high water content and low fat content (cancerous cells) given in blue, and for tissue with low water content and high fat content (healthy tissue) in pink, follow roughly
Table 5.1: Results from [51] (summarized in [50]) describing the \textit{in vivo} tissue parameters of water and fat content that govern optical absorption.

The same shape and are only slight perturbations of one another. The functions used in this simulation for $\mu_a$ in $\Omega_0$ and $\Omega_1$ are given in Figure 5.4. The reduced scattering coefficient $\mu'_s$ was chosen to be 17 cm$^{-1}$ at all points in the spatial domain. This value was chosen because Yodh and Chance [101] reported that at 820 nm, they experimentally obtained $\mu'_s$ values of 16.5-18.5 cm$^{-1}$ in human brain tissue and values of 12.7-17.3 cm$^{-1}$ in human breast tissue. A review of the literature performed by Jacques [50], supports this by matching a fit line to the various experimental data that places the value of the reduced scattering coefficient in breast tissue and other soft tissues to be around 15-20 cm$^{-1}$ between wavelengths of about 750 and 1000 nm. Jacques reports the mean reduced scattering coefficient in breast tissue over eight published experiments to be 16.8 cm$^{-1}$ with a standard deviation of 8.1 cm$^{-1}$, while the mean value for $\mu'_s$ for other soft tissues, over eighteen published experimental values, was reported to be 18.9 cm$^{-1}$ with a standard deviation of 10.2 cm$^{-1}$ [50]. These values were recorded at a wavelength of 500 nm.

The first step of the offline stage of the RBM is to obtain a finite element solution to the problem

$$a(u, v; \lambda) = F(v)$$

at carefully chosen parameter values. We define the set of finite element basis func-
Figure 5.3: Graph of the absorption coefficient, $\mu_a$, (in cm$^{-1}$) as a function of wavelength, $\lambda$, (in nm), as found in [50] for tissues with a high water but low fat content (in blue) and those with low water but high fat content (in pink).
Figure 5.4: Graphs of the absorption coefficient, $\mu_a$, in (cm$^{-1}$) as a function of wavelength, $\lambda$, (in nm) in the healthy tissue, $\Omega_0$ (left) and in the cancerous tissue, $\Omega_1$ (right).

To choose the set of fixed, nested parameter samples, $S_N = \{\lambda_j\}_{j=1}^N$ where $N \ll N$, several techniques were tried including choosing the samples at linear intervals, on the logarithmic interval suggested by [98], by choosing only the samples at which there were significant changes in the graphs of the optical parameters $\mu_a$ and $D$, and by a simplified greedy algorithm. Compared to the linear and logarithmic interval techniques, the best results were found using the greedy algorithm given in Algorithm 3 where $\epsilon_k^*$ is the dual norm of the residual as given in (4.12), with the norm on $X$ the standard $H^1$ norm. Note that $\hat{\alpha}$ was assumed to be 1. The test space,
Ξ, was generated using a fine linear mesh of \( M = 400 \) equally spaced points between 600 and 1000 nanometers (in the visible to near infrared range).

Next, we compared Algorithms 6, 5 to the greedy algorithm given in Algorithm 3. The tolerance was set at 1e-5 for the greedy algorithm and 1e-7 for the gradient algorithm (to force the algorithm to choose a basis of a size \( N > 4 \)). The starting guess for the Metropolis algorithm was taken a vector of \( N \) linearly spaced values between 600 and 1000 nm. The number of samples was 1500 with a burn-in time of 3500 iterations, an alpha value of 1, a sigma value of 4e-7, and pilot time of 2500 iterations. We let \( N_{\text{max}} \) vary for bases of sizes in the set \( \{5, 6, 7, 8, 9, 10, 15, 20\} \).

We constructed and stored solutions for each value of the parameter in \( S_N \) using the finite element discretization,

\[
    u_j = u(\lambda_j) = \sum_{i=1}^{N} b_i(\lambda_j)\phi_i
\]

The finite element solution was found using the PDE Toolbox in Matlab over a mesh of 2097 elements [1]. Then we defined an approximation space \( W_N = \text{span}\{\hat{u}_j\}_{j=1}^N \). Note that \( W_N \) is constructed as a Lagrange approximation subspace since the derivatives of \( u \) with respect to \( \lambda \) are not known.

Since the efficiency of the RBM relies on the affine decomposition of the bilinear form, we must demonstrate that \( a(u, v; \lambda) \) given in (5.7) has affine parameter dependence. We first note that, although \( \lambda \) does not have spatial dependence, the diffusion coefficient \( D \) does. Thus, we must first decompose the bilinear form geometrically, considering the domain \( \Omega_0 = \{ (x_1, x_2) | x_1^2 + x_2^2 = 625 \} \setminus \Omega_1 \) of the healthy tissue, and the domain \( \Omega_1 = \{ (x_1, x_2) | (x_1 + 15)^2 + (x_2 + 10)^2 = 25 \} \) of the cancerous tissue. Since the diffusion and absorption are homogeneous within each of these domains by construction, we can consider the functions, \( D_0, \mu^0_a \) and \( D_1, \mu^1_a \) on \( \Omega_0 \) and
\( \Omega_1 \), respectively, that are functions of \( \lambda \) only (that is, they are spatially independent). Therefore, we can decompose the bilinear form as

\[
a(u, v; \lambda) = \sum_{q=1}^{Q} \Theta^q(\lambda) a^q(u, v) = D_0(\lambda) \int_{\Omega_0} \nabla u \cdot \nabla v dx + \mu_a^0(\lambda) \int_{\Omega_0} uv dx + D_1(\lambda) \int_{\Omega_1} \nabla u \cdot \nabla v dx + \mu_a^1(\lambda) \int_{\Omega_1} uv dx
\]

In this case, the linear form \( F \) has no explicit parameter dependence and so it does not need to be decomposed. The reduced basis approximation to the problem is then computed by solving the problem

\[
\hat{A}_{\lambda} \hat{C} = \hat{F}
\]

where \( \hat{C} \) is the vector of unknown coefficients, and \( \hat{A}_{\lambda} = C^T A_{\lambda} C \) where

\[
A_{\lambda} = D_0(\lambda) A_{00} + \mu_a^0(\lambda) A_{01} + D_1(\lambda) A_{10} + \mu_a^1(\lambda) A_{11} \quad (5.9)
\]

\[
(A_{00})_{i,j} = \int_{\Omega_0} \nabla u_i(x) \cdot \nabla u_j(x) dx \quad 1 \leq i, j \leq N \quad (5.10)
\]

\[
(A_{01})_{i,j} = \int_{\Omega_0} u_i(x) \cdot u_j(x) dx \quad 1 \leq i, j \leq N \quad (5.11)
\]

\[
(A_{10})_{i,j} = \int_{\Omega_1} \nabla u_i(x) \cdot \nabla u_j(x) dx \quad 1 \leq i, j \leq N \quad (5.12)
\]

\[
(A_{11})_{i,j} = \int_{\Omega_0} u_i(x) \cdot u_j(x) dx \quad 1 \leq i, j \leq N \quad (5.13)
\]

and \( C \) contains the coefficients for the finite element approximation, \( u_j \), for \( j = 1, \ldots, N \). Due to the decomposition of \( A \), the matrices \( A_{00}, A_{01}, A_{10}, A_{11} \) can be precomputed and stored in the offline stage. We note that orthogonalization of the basis functions using the Gram-Schmidt method with respect to the inner product
induced by the bilinear form was necessary for the conditioning of the matrix $A$. Without orthogonalization the condition number of the matrix was as high as order $10^{20}$ whereas with orthogonalization, mostly the condition number was around 1, and no higher than 10 at select wavelengths.

5.1.1 Results

To test the efficiency of the RBM on this simple example, given a basis generated by one of the three algorithms described above, the reduced basis approximation of the solution was computed for 100 linearly spaced values of $\lambda$ in $\mathcal{D}$. The finite element solution was computed for the same values and the total relative error, given by,

$$\text{total error} = \sum_{k=1}^{100} \frac{||u^{fe}(\lambda_k) - u_N(\lambda_k)||_{H^1(\Omega)}}{||u^{fe}(\lambda_k)||_{H^1(\Omega)}}$$

was used as a measure of the accuracy of the solution since we have shown in (4.10) that convergence to the finite element solution is sufficient to show convergence to the exact solution.

To give a general idea of the effectiveness of the RBM, the relative error at each of the 100 wavelengths for reduced basis approximations using 5, 10, 15, and 20 basis elements found using the standard greedy algorithm are given in Figure 5.5. The results presented as size of the reduced basis versus the average relative error over 100 wavelengths where the basis elements are found using the standard greedy algorithm are given in Figure 5.6.

As Figure 5.5 shows, only a small number of basis functions are needed to accurately approximate the solution at any value of $\lambda$. Figure 5.6 shows that $N = 10$ already gives a good estimate and after about $N = 20$, increasing the number of basis functions does little to nothing to improve the accuracy of the solution. This simple
Figure 5.5: Graphs depicting the relative error of the reduced basis approximation versus the finite element solution at each of 100 wavelengths for various reduced basis sizes, $N$. The greedy algorithm was used to choose $S_N$. The red X’s indicate where the basis elements are located.

example may demonstrate that only a relatively small number of wavelengths need to be used in the imaging process to get an accurate image with sufficient information, rather than the whole spectrum.

To get a more accurate idea of the effectiveness of the reduced basis method, results were gathered by looking at three different basis generating parameter selection methods: the standard greedy algorithm, the gradient algorithm described in Algorithm 5 and the Metropolis algorithm described in Algorithm 6. In addition to the total relative error given by (5.14), the computational running time for all three parameter selection methods was also recorded for each value of $N$. The total relative
error and the timing for all the methods (averaged over 10 runs for the greedy and gradient algorithms due to the random selection of the first parameter) are given in Figures 5.7 and 5.8.

First we note that the gradient algorithm could only find a basis of size 9 at most. After this point it would get stuck at local minima and did not provide meaningful results. We see that for all basis sizes, the solutions generated using the Metropolis algorithm have a lower relative error than those generated by both the gradient and greedy algorithms, especially for small basis sizes. The error is almost a full order of magnitude lower than the greedy algorithm for small basis sizes, but was closer to that of the gradient algorithm. We also note that the accuracy of the reduced basis solution generated using both the gradient and greedy algorithms do not have a monotone decreasing error as the basis size increases. This sporadic result is due to the fact that the first wavelength chosen in both algorithms is chosen randomly. The rapid decline in the relative error for all three methods is expected,
as it has been shown numerically that the reduced basis approximation converges rapidly to the finite element solution [66]. This convergence has been proven to be exponential if the parameter values in $S_N$ are chosen to be logarithmically (quasi-) uniformly [67, 84]. The choice of basis generating values is fairly uniform for all three methods so the apparent exponential convergence of the relative error in our case is expected.

Finally, we see that the gradient algorithm has a significantly shorter running time than either of the other two algorithms. Comparatively, the MCMC algorithm has only a slightly shorter running time than the greedy algorithm for larger basis sizes since the greedy algorithm increases at a slightly faster rate. Although the running time for all three algorithms appears to increase linearly with $N$, the gradient algorithm increases the fastest. We note that this graph shows the running times for the algorithms given a fixed basis size. If we did not know the optimal or desired basis...
size up front, we note that the running time for the greedy and gradient algorithms to find a new basis element would be much faster since they store the previous elements and add one wavelength at a time. This is in contrast to the Metropolis algorithm which finds an optimal generating set from scratch for each new $N$.

We also changed the location of the tumor to see how that affected the choice of basis. Since light does not penetrate deeply into tissue, the solution should be less accurate for tumors that are located far from the source. In addition to the tumor located near the source, at (-15,-10), we found the reduced basis solution for tumors located at (0,0) and (15, 10) using bases generated from the greedy, Bayesian, and gradient algorithms. By examining the wavelengths chosen by all three algorithms to generate the basis, we observed that the algorithms chose very similar wavelengths for a given basis size for the location near the source, (-15,-10), in the center, (0,0), and far from the source (15,10). To measure just how close these bases were to each other, we note that the running time for the greedy and gradient algorithms to find a new basis element would be much faster since they store the previous elements and add one wavelength at a time. This is in contrast to the Metropolis algorithm which finds an optimal generating set from scratch for each new $N$.

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other, we computed the relative Euclidean distance between them using the formula

\[ \sqrt{\sum (\lambda_i^{(1)} - \lambda_j^{(1)})^2 + \ldots + (\lambda_i^{(N)} - \lambda_j^{(N)})^2} \]

\[ \frac{1}{\|\lambda_i\|_2} \]

(5.15)

where \( i, j \) represent the basis generating sets created by the same algorithm for two different tumor locations. Note that the sets were first sorted to be in ascending order. A summary of the results for each method for \( N = 9 \), is given in Table 5.2.

<table>
<thead>
<tr>
<th>Basis Location</th>
<th>Greedy</th>
<th>Metropolis</th>
<th>Gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>(-15,-10) to (15,10)</td>
<td>0.9461e-01</td>
<td>0.7100e-01</td>
<td>0.3217e-01</td>
</tr>
<tr>
<td>(-15,-10) to (0,0)</td>
<td>0.9364e-01</td>
<td>0.4820e-01</td>
<td>0.2715e-01</td>
</tr>
<tr>
<td>(15,10) to (0,0)</td>
<td>1.0935e-01</td>
<td>1.1217e-01</td>
<td>0.3238e-01</td>
</tr>
</tbody>
</table>

Table 5.2: Table describing the relative Euclidean distance between the basis generating sets found for each of the three algorithms for a tumor close to the source (centered at (-15,-10)), in the center of the healthy tissue (centered at (0,0)), and far from the source (centered at (15,10)).

We note the bases are very close to each other, no matter the location of the tumor, especially for the gradient algorithm. This demonstrates the lack of sensitivity of the hyDOT forward problem with respect to the parameter, \( \lambda \). This also indicates that the inverse problem of hyDOT is expected to be severely ill-posed in finding \( D \) and \( \mu_a \) in terms of the parameter \( \lambda \). We also compared the distances between the bases using a basis of size of \( N = 5 \), before the relative error converged (i.e. a non-optimal basis size) and obtained similar results which shows that the forward problem is not sensitive regardless of basis size. However, these results are promising for application of the RBM to the inverse problem. If the same reduced basis in terms of \( \lambda \) can be used for every iteration of the inverse problem, even when the geometry changes, then the computational burden of the inverse problem will be significantly reduced. In fact, our investigation indicates that hyperspectral imaging does not add
much additional meaningful information to DOT, where wavelength is held constant. Therefore, only a few strategic wavelengths should be chosen for the inversion to make hyDOT better posed and hopefully providing better resolution than single wavelength DOT. Only the solution a select number of wavelengths (possibly less than ten, as demonstrated by the apparent exponential decrease in the error for all three methods seen in Figure 5.7) gives significant information and the rest can be discarded.

We tested the hypothesis that the basis could remain the same, no matter the location of the tumor, by taking the basis generating set of size $N = 9$ found by all three algorithms for tumors located at $(15,10)$ and $(0,0)$, respectively, and using it to solve the problem with a tumor centered at $(-15,-10)$. The results are summarized in Table 5.3.

<table>
<thead>
<tr>
<th></th>
<th>Greedy</th>
<th>Metropolis</th>
<th>Gradient</th>
</tr>
</thead>
<tbody>
<tr>
<td>original error at $(-15,-10)$</td>
<td>$5.8268e-03$</td>
<td>$0.9474e-03$</td>
<td>$1.9719e-03$</td>
</tr>
<tr>
<td>error with basis from $(0,0)$</td>
<td>$0.9226e-03$</td>
<td>$1.7924e-03$</td>
<td>$1.7396e-03$</td>
</tr>
<tr>
<td>error with basis from $(15,10)$</td>
<td>$0.9172e-03$</td>
<td>$0.9464e-03$</td>
<td>$1.1413e-03$</td>
</tr>
<tr>
<td>difference $(-15,-10)$ to $(0,0)$</td>
<td>$4.9043e-03$</td>
<td>$0.8451e-03$</td>
<td>$0.2323e-03$</td>
</tr>
<tr>
<td>difference $(-15,-10)$ to $(15,10)$</td>
<td>$4.9096e-03$</td>
<td>$0.0010e-03$</td>
<td>$0.8306e-03$</td>
</tr>
</tbody>
</table>

Table 5.3: Table describing the relative error in approximating the solution at 100 different wavelengths using a reduced basis generated by each of the three algorithms for different tumor locations.

We can see that the relative error stays small no matter the basis for all three algorithms, and that the difference in error for using different wavelengths is very small, especially for the Metropolis and gradient algorithms. We note that the error actually appears to decrease as the bases for other tumor locations are used for both the greedy and gradient algorithms, while this does not occur for the Metropolis algorithm. This is to be expected since both the greedy and gradient algorithms can only guarantee semi-optimal solutions, whereas the Metropolis should find the global
minimum. The gradient is an improvement to the greedy algorithm, but both are set up such that they can get stuck in local minimums. We note that the a gradient version of the Metropolis algorithm could also be developed that would give better solutions. The data suggests that the choice of the wavelengths used to generate a reduced basis depends more on the behavior of $D, \mu_a$ then on the location of the tumor. Since $D, \mu_a$ do not change as the geometry changes, the basis should be able to be kept the same for several (if not all) iterations of the iterative algorithm used to solve the inverse problem.

5.1.2 Conclusions

The reduced basis method is an effective method for solving the forward problem in hyperspectral DOT, which is very insensitive to both the parameters $D$ and $\mu_a$ as a function of $\lambda$. HyDOT is also an example of a severely ill-posed inverse problem which utilizes wavelength information to better reconstruct $D$ and $\mu_a$. The relative error of the reduced basis approximate solution compared to the finite element solution is small for any wavelength in the range we tested. Further, for the hyDOT problem presented, the reduced basis did not appear to be dependent on the geometry of the problem, that is, the tumor location. This will have a significant impact on the application of the RBM to the inverse problem in hyDOT. Specifically, since each iteration of the inverse algorithm requires solving the forward problem for a different geometry, the reduced basis method may be used to significantly reduce computational time and effort as the same reduced basis may be used for several iterations.

The results presented here indicate that only a few wavelengths may be sufficient to improve the reconstruction of $D$ and $\mu_a$ in hyDOT since we have demonstrated
that hyDOT forward problem is very insensitive to the image parameters $D$ and $\mu_a$. Therefore, disregarding much of the ambiguity in $\lambda$ will help make the hyDOT inverse problem better posed and may help improve the image reconstruction in hyDOT. In fact, the RBM should be an excellent approach for identifying the critical wavelengths where the inverse problem should be solved and help introduce sparsity in the hyDOT image reconstruction process. Exploiting sparsity in the hyDOT inverse problem was discussed theoretically in Chapter 3 and we will investigate the use and effectiveness of sparsity in the spectral domain through simulation in Section 5.2.

In this section, we also proposed two alternatives to the greedy algorithm, mainly the Metropolis and gradient algorithms. We have demonstrated that both the Metropolis and gradient algorithms are viable alternatives to the traditional greedy approach when generating the set $S_N$ with which to construct a reduced basis. The relative error of the solution generated by the resulting reduced basis for the Metropolis algorithm can be as much as an order of magnitude more accurate than that generated by the greedy algorithm. Additionally, we have shown that the running time of the gradient algorithm is significantly smaller than the other two algorithms which makes a strong case for it being the preferred algorithm when the desired size of the basis is not known since the error of the basis it produces is only slightly larger of that generated by the Metropolis algorithm. We have also shown that once the dimension of the reduced basis method is somewhat determined, the Metropolis algorithm works really well and is very promising in finding a very good global minimum outperforming both greedy and gradient algorithms.
5.2 The hyDOT Image Reconstruction Problem

Before we begin applying Algorithm 1 to the inverse problem of hyDOT, we investigate the parameter dependence on wavelength for several different geometries. First, following the evidence from [18, 89] (see Figures 5.2, 1.4), we change the profile of $\mu_a$ in $\Omega_1$ to be slightly more different than an upward shift from the profile for $\Omega_0$. The differences in the two profiles are more biologically sound based on the experimental evidence, and have the added benefit of making the differences of the images in the spectral domain more obvious and easier to exploit. The updated profiles for $\mu_a$ are given in Figure 5.9. We also note that since $\mu'_s \gg \mu_a$ and $D = 1/(3*(\mu_a + \mu'_s))$, the values for $D$ do not change much with respect to wavelength and do not show much discernible difference between the tumor and healthy tissue. This is reflected in Figures 5.10, 5.11 which show the true $\mu_a$ and $D$ spatial maps for the simple geometric example explored in Section 5.1. In these figures we can see that the

Figure 5.9: The updated $\mu_a$ profile with respect to $\lambda$ for absorption in healthy (blue) and cancerous (red) tissue. This is the profile used in the image reconstruction problem.
cancerous tissue is clearly seen at some wavelengths, while it is barely distinguishable from the healthy tissue at other wavelengths. We also note, principally by observing the color scale that the difference are far less pronounced for the diffusion coefficient $D$ than they are for the absorption coefficient $\mu_a$. The small value of $D$ compared to $\mu_a$ makes the inversion even more ill-posed. Thus, even though the $\mu'_a$ value of 17 cm$^{-1}$ used in Section 5.1 is more biologically accurate, we used a value of $\mu'_a = 1$ cm$^{-1}$ to make $D$ and $\mu_a$ more comparable to each other and decrease the ill-posedness of the problem. That said, Figures 5.10, 5.11 were generated using $\mu_a = 17$ cm$^{-1}$.

We decided to test the image reconstruction algorithm on a slightly more complicated geometry than previously. Since tissue is a highly scattering medium almost none of the intensity of the light source is present on the other side of the medium, so only detectors that are close to the source can measure high enough intensity values. For this reason, we placed our tumors relatively close to the boundaries, knowing the light would not penetrate very deeply. The tumor from the previous example was still present, but another tumor of radius 7 was added 10 cm in the positive $x$-direction of the medium and 5 cm in the positive $y$-direction, as measured from the center of $\Omega$. There were 16 source-detector pairs around the boundary of the medium. The geometry and a diagram of the placement of the sources and detectors are given in Figure 5.12. The data was simulated using a fine mesh of 541 nodes with 1016 triangular elements, and the image was reconstructed on a coarse mesh of 2097 nodes with 4065 triangular elements. The two meshes are given in Figure 5.13.

Before incorporating the Reduced Basis Method into the inverse algorithm, we first tried solving the image reconstruction at ten different values for $\lambda$ to see the differences between them. The $\lambda$ values were chosen by applying the greedy algorithm using the solution to the forward problem as the solution with which to calculate the error estimate. The wavelengths at which the initial test was made were 695.2, 696.2,
Figure 5.10: The $\mu_a$ profile for the simple geometric example given in Section 5.1 at several wavelengths, $\lambda$. The tumor is more visibly seen at some wavelengths than at others.
Figure 5.11: The $D$ profile for the simple geometric example given in Section 5.1 at several wavelengths, $\lambda$. The tumor is more visibly seen at some wavelengths than at others, and overall the difference between the cancerous and healthy tissue is less pronounced than for $\mu_a$. 
Figure 5.12: A diagram of (a) the geometry of the domain for the image reconstruction problem, and (b) the placement of the 16 sources and 16 detectors placed around the boundary.

716.3, 717.3, 718.3, 719.3, 794.5, 798.5, 843.6, 961.9, all in nanometers. As noted in Section 3.5, a common initial regularization parameter and step size for both $D$ and $\mu_a$ were chosen for all wavelengths. The regularization parameter on the sparsity term was $1 \times 10^{-2}$ for both $D$ and $\mu_a$, while the initial step sizes were $s_\mu = 1.5 \times 10^{-5}$ and $s_D = 5 \times 10^{-5}$, and 400 iterations were used for each wavelength. The results for each of the ten wavelengths with no noise added in the simulation of the data measurements, is given in Figures 5.14-5.21.

We note that for each of the wavelengths chosen, the inversion algorithm correctly identified the two tumors present. As expected, the reconstruction for $\mu_a$ was a little bit better in the sense that the shape of the tumors was more clearly defined and matched the original better. In general, the reconstructed values for the tumor were too low and the background values to high for $D$, while for $\mu_a$ the tumor values were too low, especially near the boundary of the tumors, though the background
was fairly accurate. We suspect that with more iterations the reconstruction would have been more accurate.

We then tried adding noise to the simulation to see how robust the reconstruction algorithm was. First, we added 3% Gaussian white noise and noted that the reconstructions were still comparable to those without noise. The tumors are still clearly visible for both $D$ and $\mu_a$ and their boundaries are fairly well-defined. Some of the same issues of values of both the cancerous and healthy tissue for the reconstruction are present. We then added 10% noise and still got a good reconstruction that did not vary significantly from the reconstruction with 3% noise or no noise at all. The reconstruction results for 3% and 10% added noise, respectively, at a selected wavelength are given in Figures 5.22 - 5.23. Reconstructions this good for a comparable amount of added noise for other reconstruction algorithms that do not incorporate sparsity are rare. For example, we tried finding a reconstruction of the optical parameters using MATLAB’s lsnonlin.m, which uses a Levenberg-Marquardt algorithm. This algorithm ran very slowly and could not find even close to an accurate solution after the same number of iterations. Our algorithm is much more robust.
due to the added sparsity constraints.

Finally, we seek to implement the RBM in the inversion algorithm, by using the reduced basis approximation for solutions at any wavelength of the forward problem. We did not use the RBM for the adjoint and Sobolev smoothing steps, but we hope to do this in the future. As we noted in Chapter 4, applying the RBM to the inverse problem is not as straightforward as it was for the forward problem since the geometry changes on each iteration. However, even without the nice affine decomposition of the previous section, we can still exploit some of the advantages of the RBM in the inversion algorithm.

First of all, we confirm our suspicion in the previous chapter, further encouraged by the results in the previous section, that the parameter values to be included in the reduced basis need only be calculated once, before the iterations of the inversion algorithm begin. To demonstrate this experimentally, we ran the greedy algorithm on the forward problem at each of the 16 sources to find a separate basis generating set for each source. Though this took a long time (about 45 minutes) the basis generating sets that were created were all almost identical, except for the randomly chosen first element and a couple other elements. Now, since the reconstruction algorithm updates the solution vectors $u$ at each iteration as a new guess for the parameter values $q$ are made, the $u_j$ in the reduced basis must be updated at each iteration. Thus, the $A$ matrices outlined in (5.13) cannot be precomputed offline. Thus, before solving for the coefficients $\hat{c}_j$ in $u_N(\lambda) = \sum_{i=1}^{N} \hat{c}_j u_j$, at each iteration we need to recalculate $W_N$.
and the matrix $\hat{A}_\lambda = C^T A_\lambda C$ where

$$A_\lambda = A_0 + A_1 \quad (5.16)$$

$$(A_0)_{i,j} = \int_\Omega D(\lambda) \nabla u_i(x) \cdot \nabla u_j(x) dx \quad 1 \leq i, j, \leq N \quad (5.17)$$

$$(A_1)_{i,j} = \int_\Omega \mu(\lambda) u_i(x) \cdot u_j(x) dx \quad 1 \leq i, j, \leq N. \quad (5.18)$$

Using this implementation to solve the inverse problem for just one wavelength will thus be longer than just calculating the finite element solution to the forward problem, because it requires $N$ finite element solutions to be calculated each time the forward problem is solved, where $N$ is the size of the reduced basis. However, if the inverse problem is being solved for many wavelengths at once, as in for a number of wavelengths much greater than $N$, then the RBM reduces the computational burden by the forward problem having to be solved only $N$ times and then approximated for all other wavelengths.

### 5.2.1 Conclusions

The reconstruction algorithm given in Algorithm 1 was successful in exploiting the spatial sparsity at each wavelength. When run for 400 iterations, the reconstruction at each wavelength took an average of 93.58 seconds. Though the reconstruction values were too high for the background values for $D$ and too low for the tumor, and too low on the boundary of the tumor and healthy tissue for $\mu_a$, the reconstructions of both at all wavelengths still identified the correct shape and almost the correct size of the two tumors. We also note that when noise was added to the data, Algorithm 1 was still successful in producing a reconstruction of the image nearly identical to that.
without noise.

We were also able to demonstrate that application of the RBM to the inverse problem may be possible, despite not being able to geometrically decompose the bilinear form that describes the weak form of the hyDOT forward problem. We showed that the basis generating set need only be generated once to be used not only for all geometries (and hence, for all iterations) but also for all sources. We are hopeful that the RBM can be fully applied to the reconstruction algorithm in the future by making use of the reduced basis approximation in the adjoint and Sobolev smoothing steps as well.
Figure 5.14: The true values for $D$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.15: The true values for $D$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.16: The true values for $D$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.17: The true values for $D$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.18: The true values for $\mu_a$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
(a) True Value, \( \lambda = 717.3 \text{nm} \)
(b) Reconstruction, \( \lambda = 717.3 \text{nm} \)
(c) True Value, \( \lambda = 718.3 \text{nm} \)
(d) Reconstruction, \( \lambda = 718.3 \text{nm} \)
(e) True Value, \( \lambda = 719.3 \text{nm} \)
(f) Reconstruction, \( \lambda = 719.3 \text{nm} \)

Figure 5.19: The true values for \( \mu_a \) and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.20: The true values for $\mu_a$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.21: The true values for $\mu_a$ and the reconstruction, respectively, for each of the ten wavelengths found by the greedy algorithm with no noise added. We note the differences in the reconstruction between them.
Figure 5.22: The true values for $D$ and the reconstruction, respectively, at $\lambda = 716.3$ for 3% and 10% noise added, respectively. We note that added noise does not degrade the reconstruction significantly.
Figure 5.23: The true values for $\mu_a$ and the reconstruction, respectively, at $\lambda = 716.3$ for 3% and 10% noise added, respectively. We note that added noise does not degrade the reconstruction significantly.
Chapter 6

Conclusions and Future Work

This dissertation has formulated the hyDOT forward and inverse problems, previously unexplored in the literature, and has laid the mathematical framework from which future results in this area can be made. Most significantly, it has demonstrated the spectral regularity of the hyDOT solution, and how this regularity allows for application of model reduction techniques to reduce the computational burden of the inverse problem. Further, we have combined the spectral regularity with the sparsity in the spatial domain to propose a wavelength-dependent cost functional for the inverse problem that promotes sparsity. We have also shown that since the affine decomposition of the bilinear form found from the weak formulation of the forward solution is not possible in the inversion algorithm, at least not geometrically, there is not a clear way to effectively apply the RBM to the inverse problem.

Through simulation we have demonstrated that hyDOT is not any more effective or efficient in generating a good solution to the image reconstruction than multi-spectral DOT. That is, reconstructing the image at each of hundreds of wavelengths adds little to no information that is new and valuable compared to reconstructing the image at only a few wavelengths since the regularity in the spectral domain allows for
the solution at any intermediate wavelength to be interpolated from the few known solutions. That said, we have shown that application of the RBM to the reconstruction problem of hyDOT may be possible, making hyDOT more computationally feasible. By using the RBM, an approximation of the forward solution can be made at every wavelength that is much less expensive than finding an exact (finite element) solution. We have demonstrated in simulation that the variation in optical parameter values between wavelengths is subtle, a conclusion supported by the experimental evidence in the literature, adding to the ill-posedness of the problem in the spectral domain. The subtle difference between wavelengths, however, shows that the important optical features can be highlighted through use of a few select wavelengths, and thus the regularity in the spectral domain, as well as the sparsity in the spatial domain, can be exploited in the image reconstruction algorithm.

We have also presented a theoretical foundation for the forward and inverse problems in hyDOT. We have included results for the spectral regularity of the solution $u$ by taking the derivative of the governing PDE with respect to wavelength. We have proposed a cost functional that incorporates this regularity (by including the term $\frac{\partial u}{\partial \lambda}$) and hope to implement it in future work.

In the immediate future, we will continue to investigate ways to improve the image reconstruction in hyDOT, focusing specifically on exploiting the smoothness in the spectral domain and sparsity in the spatial domain. We seek to implement some of the functionals suggested in Section 3.4 computationally and to analyze them more thoroughly analytically. We will also continue to investigate the possible use of the RBM into the image reconstruction algorithm, using it to find approximations to the adjoint and Sobolev smoothing steps of the algorithm for every wavelength in addition to approximating the forward solution. We will examine how using an approximate solution for a given wavelength using the RBM at each step of the inversion algorithm,
though more expensive, compares to using the exact solution.

After extending the theory and application of sparsity regularization to hyperspectral OT, there are a few other areas we would like to explore. The first is to extend this theory to other imaging techniques, specifically hybrid techniques such as photoacoustic tomography (PAT) and ultrasound-modulated optical tomography (UMOT). Because these modalities have an acoustic, as well as an optical component, we suspect that the additional optical information would affect the image reconstruction differently than it does for DOT.
Appendices
Appendix A

Derivation of the First-Order Diffusion Approximation

As explained in the Introduction, the movement of light photons from the laser source through the tissue medium to the boundary is described by the Radiative Transport Equation (RTE), given in the Introduction by

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \hat{s} \cdot \nabla I + (\mu_a + \mu_s)I = \mu_s \int_{S^2} p(\hat{s}', \hat{s})I(x, \hat{s}')d\hat{s}'
\] (A.1)

where \( I(x, \hat{s}, t) \) is the specific intensity or spectral radiance at position \( x \), in the direction \( \hat{s} \) at time \( t \) and \( S^2 \) is the unit sphere in \( \mathbb{R}^2 \). We note that the scattering kernel \( p \) is normalized, giving

\[
\int_{S^2} p(\hat{s}', \hat{s})d\hat{s}' = 1.
\] (A.2)
This kernel describes the amount of Henyey-Greenstein scattering in the tissue and is given by

\[ p(\theta) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g\theta)^{3/2}} \]

where \( g \in (-1, 1) \) measures the anisotropy of the scattering, with \( g = 0 \) yielding isotropic scattering. The incoming flux is measured by the boundary condition

\[ I(\mathbf{x}, \hat{s}, t) = g^-(\mathbf{x}, \hat{s}, t), \quad \mathbf{x} \in \partial \Omega \quad (A.3) \]

and the DOT and hyDOT problems are to reconstruct the unknown optical parameters from the measurements of the outgoing flux given by

\[ g^+(\mathbf{x}, t) = \frac{1}{4\pi} \int_\mathcal{S} v(x) \cdot \hat{s} I(\mathbf{x}, \hat{s}, t) d\hat{s}, \quad \mathbf{x} \in \partial \Omega \quad (A.4) \]

where \( v \) is a vector that does not depend on \( \hat{s} \). This differential equation is too computationally expensive to use in practice, however. In fact, an analytical solution to the RTE is known only for simple cases [57]. The most common approximation to (A.1) is the diffusion approximation. There are several approaches to deriving the diffusion approximation from the RTE, such as using asymptotic methods [7, 57], but the most common approach is to use a \( P_N \) approximation, specifically the \( P_0 \) approximation. We will use this approach to derive it here, following the example of [22, 56, 72, 97].

The diffusion approximation holds if the scattering coefficient is large with respect to the absorption coefficient, as is the case in optical imaging since tissue is a highly scattering medium. We also assume that the point of observation is far from the boundary of the medium and that we have a sufficiently long time scale. Due to the highly scattering nature of the medium and the large distance from the source, we
can consider the radiance (or flux) to be isotropic, that is depending only linearly on \( \hat{s} \). Thus, the transport process can be adequately described by the first few moments of \( I \). That is,

\[
I(x, \hat{s}, t) = \alpha I_0(x, t) + \beta \hat{s} \cdot I_1(x, t) \tag{A.5}
\]

where

\[
I_0(x, t) = \frac{1}{4\pi} \int_{S^2} I(x, \hat{s}, t) d\hat{s} \tag{A.6}
\]
\[
I_1(x, t) = \frac{1}{4\pi} \int_{S^2} \hat{s} I(x, \hat{s}, t) d\hat{s}. \tag{A.7}
\]

If we plug these moments back into (A.5) and solve, we get \( \alpha = 1 \) and \( \beta = 3 \). That is,

\[
I(x, \hat{s}, t) = I_0(x, t) + 3\hat{s} \cdot I_1(x, t).
\]

We would like to obtain a closed system that relates \( I_0 \) and \( I_1 \). First, we integrate (A.1) over \( S^2 \) and apply (A.2) to obtain

\[
-\frac{1}{c} \frac{\partial I_0}{\partial t}(x, t) + \nabla \cdot I_1(x, t) + \mu_a(x) I_0(x, t) = 0. \tag{A.8}
\]

Then, we multiply (A.1) by \( \hat{s} \) and integrate over \( S^2 \) to obtain

\[
-\frac{1}{c} \frac{\partial I_1}{\partial t}(x, t) + \nabla \cdot I_2(x, t) + \mu(x) I_1(x, t) = \bar{\rho}_\beta \mu_s(x) u_1(x, t) \tag{A.9}
\]

where \( I_2(x, t) \) is the second moment, given by

\[
I_2(x, t) = \frac{1}{4\pi} \int_{S^2} \hat{s} \hat{s}^T I(x, \hat{s}, t) d\hat{s}
\]
and $\bar{p}$ is the mean scattering cosine given by

$$\bar{p} = \frac{1}{4\pi} \int_{S^2} \hat{s}' \cdot \hat{s} p(\hat{s} \cdot \hat{s}') d\hat{s}' .$$

Now we can simplify (A.8) and (A.9) by using the equation for the reduced scattering coefficient,

$$\mu'_s = (1 - \bar{p}) \mu_s$$

to obtain

$$\frac{1}{c} \frac{\partial I_0}{\partial t} (x, t) + \nabla \cdot I_1 (x, t) + \mu_a(x) I_0(x, t) = 0 \quad (A.10)$$

$$\frac{1}{c} \frac{\partial I_1}{\partial t} (x, t) + \nabla \cdot I_2 (x, t) + (\mu_a(x) + \mu'_s(x)) I_1(x, t) = 0 . \quad (A.11)$$

Finally, we can express $I_2$ in terms of $I_0, I_1$ using (A.5) to obtain

$$\nabla \cdot I_2 = \frac{1}{3} \nabla I_0$$

and thus we can simplify (A.11) even further to get,

$$\frac{1}{c} \frac{\partial I_0}{\partial t} (x, t) + \nabla \cdot I_1 (x, t) + \mu_a(x) I_0(x, t) = 0 \quad (A.12)$$

$$\frac{1}{c} \frac{\partial I_1}{\partial t} (x, t) + \frac{1}{3} \nabla I_0(x, t) + (\mu_a(x) + \mu'_s(x)) I_1(x, t) = 0 \quad (A.13)$$

which is called the $P_1$ approximation.

The $P_0$ approximation, also known as the diffusion approximation, further assumes that $\frac{\partial I_1}{\partial t}$ is negligible, which gives us

$$I_1 = -D \nabla I_0 \quad (A.14)$$
and Fick’s Law,
\[
D = \frac{1}{3(\mu_a + \mu_s)}.
\]  
(A.15)

Thus, substituting these quantities back into (A.13) and letting \( I = u \) (to better match notation in the rest of this work), we arrive at the diffusion approximation (in the time domain)
\[
\frac{1}{c} \frac{\partial u_0}{\partial t} - \nabla \cdot (D \nabla u_0) + \mu_a u_0 = 0.
\]  
(A.16)

We must also derive the boundary conditions. From (A.3) we have,
\[
\nu(x) \cdot \int_{\nu(x) \cdot \hat{s} \leq 0} \hat{s} u(x, \hat{s}, t) d\hat{s} = \nu(x) \cdot \int_{\nu(x) \cdot \hat{s} \leq 0} \hat{s} g^-(x, \hat{s}, t) d\hat{s}, \quad x \in \partial \Omega, \quad t \geq 0
\]
where \( \nu(x) \) is the outward unit normal. Then, (A.5), (A.14), and (A.15) yield
\[
u(x, \hat{s}, t) = \frac{1}{4\pi} u_0(x, t) - \frac{3}{4\pi} \hat{s} \cdot D \nu(x) \nabla u_0(x, t).
\]

We assume isotropic flux (so \( g^-(x, \hat{s}, t) = g^-(x, t) \)) and note that
\[
\nu \cdot \int_{\nu(x) \cdot \hat{s} \leq 0} \hat{s} d\hat{s} = -\pi, \quad \nu \cdot \int_{\nu(x) \cdot \hat{s} \leq 0} \hat{s}_i \hat{s}_j d\hat{s} = \begin{cases} 0, & i \neq j \\ \frac{2\pi}{3} \nu_i, & i = j \end{cases}
\]
to obtain
\[
-\pi u_0(x, t) - 3 \left( \frac{2\pi}{3} \right) D \nu(x) \cdot \nabla u_0(x, t) = -\pi g^-(x, t)
\]
which is equivalent to
\[
u_0 + 2D \frac{\partial u_0}{\partial \nu} = g^- \quad \text{on } \partial \Omega
\]  
(A.17)

which are Robin boundary conditions. We can also derive the equation for the mea-
surement from (A.4) by substituting in (A.14), (A.15) to obtain

\[ g^+(x, t) = \nu(x) \cdot u_1(x, t) = -D\nu(x) \cdot \nabla u_0(x, t) \]

or

\[ g^+ = -D \frac{\partial u_0}{\partial \nu} \ \text{on} \ \partial \Omega. \]
Bibliography


