SOME APPLICATIONS OF MINIMIZING VARIATIONAL PRINCIPLES FOR THE COMPLEX HELMHOLTZ EQUATION

by

Russell Bingham Richins

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STATEMENT OF DISSERTATION APPROVAL

The dissertation of **Russell Bingham Richins**

has been approved by the following supervisory committee members:

David Dobson	, Chair	**5/4/2010**
Graeme Milton	, Member	**5/4/2010**
Andrej Cherkaev	, Member	**5/4/2010**
Ken Golden	, Member	**5/17/2010**
Marian Bocea	, Member	**4/23/2010**

and by [redacted], Chair of the Department of **Mathematics**

and by Charles A. Wight, Dean of The Graduate School.

ABSTRACT

This work is based on the work of Milton, Seppecher, and Bouchitté on variational principles for lossy media. I will describe several applications of the variational principle for the complex Helmholtz equation.

First, I will describe a finite element method for solving the Helmholtz equation based on the minimization variational principle. The matrix in the linear system that results from the finite element method is symmetric positive definite, due to the minimization variational principle upon which it is based. I also present an error bound for the finite element method and an effective preconditioning strategy that can be used when the linear system is solved with the preconditioned conjugate gradient method.

Another application is the extension of the variational principles to handle more general boundary conditions, such as Robin boundary conditions. We base the Robin formulation on the natural boundary conditions. The importance of the Robin condition is that it can be thought of as a first order approximation to a transmission boundary condition, which is useful for scattering problems.

Next, I use the minimization variational principle to formulate a method for the tomography problem for Helmholtz equation. The tomography problem is to determine the coefficients of the Helmholtz equation from knowledge of the essential to natural map. The basic idea behind this method is to minimize the L^2 distance between the solutions to the essential and natural problems for a given set of essential and natural data. However, instead of solving the natural and essential problems, we add the functionals for which the solutions are minimizers as constraints in the minimization problem outlined above. Then all the parameters in the minimization (solutions and material coefficients) are considered as independent. Then the minimization is performed with respect to all the parameters. A regularization term on the material

coefficients is added to stabilize the solution.

The final application will be to provide some elementary bounds on the essential to natural map by applying the variational principles with simple test functions. These bounds can be especially useful in determining volume fraction information from the measurements of current and potential on the boundary.

To my wife Nicole, for all your hard work and patience.

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CHAPTER 1

INTRODUCTION AND OVERVIEW

In this chapter we present some motivation for the problems to be studied and an overview of the chapters, including which chapters may be skipped by those already familiar with the material.

1.1 Motivation for the Method

There are many dissipative wave propagation problems that can be modeled via the complex Helmholtz equation

$$-\nabla \cdot \rho^{-1} \nabla P - \frac{\omega^2}{\kappa} P = 0,$$

and so there is much interest in its solution. Traditionally, the solution P of this problem has been thought of as a stationary point of the functional

$$\int_\Gamma \left[\rho^{-1} \nabla P \cdot \nabla \bar{P} - \frac{\omega^2}{\kappa} |P|^2 \right] dx$$

(assuming Dirichlet boundary conditions to fix ideas). The obvious lack of coercivity that this functional suffers from in general prevents one from taking advantage of the many benefits that come from having a minimization variational principle rather than simply a stationary principle. For example, when one attempts to find a numerical solution to this problem using a finite element discretization, the resulting system of equations has a coefficient matrix A with entries

$$(A)_{ij} = \int_\Gamma \left[\rho^{-1} \nabla \psi_i \cdot \nabla \psi_j + \frac{\omega^2}{\kappa} \psi_i \psi_j \right] dx,$$

where $\{\psi_1, \psi_2, \ldots, \psi_M\}$ is the finite element basis. For a vector $x \in \mathbb{C}^M$, we have

$$x^* A x = \int_\Gamma \left[\rho^{-1} \left(\sum_{j=1}^M x_j \nabla \psi_j \right) \cdot \left(\sum_{j=1}^M \bar{x}_j \nabla \psi_j \right) - \frac{\omega^2}{\kappa} \left(\sum_{j=1}^M x_j \psi_j \right) \left(\sum_{j=1}^M \bar{x}_j \psi_j \right) \right] dx.$$

In general, this last expression will be complex, and even when it is real it may be positive or negative. Therefore, the coefficient matrix is indefinite, and this makes the corresponding system of equations much more difficult to solve. Much effort has been put into finding effective preconditioning schemes ([23], [29], [32]) so that Krylov subspace methods that apply to indefinite systems (such as GMRES) can be used, since simpler methods, such as conjugate gradient, do not apply.

On the other hand, when solving the Dirichlet boundary value problem for the real conductivity equation $-\nabla \cdot \sigma \nabla u = 0$, where $\sigma \geq \alpha I$ for some $\alpha > 0$, one seeks to minimize the functional

$$\int_\Gamma \sigma \nabla u \cdot \nabla u \, dx,$$

which is convex as a function of u because of the assumption on σ. For $x \in \mathbb{R}^M$, the matrix that results from finite element discretization satisfies

$$x^T A x = \int_\Gamma \sigma \left(\sum_{j=1}^M \nabla \psi_j \right) \cdot \left(\sum_{j=1}^M x_j \nabla \psi_j \right) \, dx \geq C \| \sum_{j=1}^M x_j \psi_j \|^2_{H_0^1(\Gamma)} \geq 0,$$

where we have used the Poincaré inequality. Therefore, the matrix is symmetric positive definite, and conjugate gradient can be applied.

The next logical question is whether or not we can modify the problem formulation of the complex Helmholtz equation so that the solution can be seen as the minimizer of a minimization variational principle, and thereby retain all the advantages that come from minimization. This is the work that is found in [37].

In this thesis, we apply the minimization variational principles for the Helmholtz equation to several problems. As in the discussion above, we use them to formulate a finite element method that results in a symmetric positive definite system of equations, which allows for the use of simple iterative methods. Also, we use the minimization principles as constraints in an optimization problem. This simplifies matters considerably and saves work, since it negates the need to solve large adjoint problems in order to implement a gradient descent algorithm to solve the optimization problem.

We now present an overview of the chapters contained in the thesis.

1.2 Background

Chapter 2 gives some background on the Calculus of Variations, which is the study of minimization problems and their solution. It contains several examples and some basic theorems on minimizing real-valued functionals over Banach spaces, as well as information specific to quadratic integral functionals, which will be the focus throughout this thesis. Much of the information in this chapter follows the presentation of [17]. This chapter can be skipped by those already familiar with the methods of the Calculus of Variations.

In Chapter 3, we outline the original work done on minimization variational principles for complex equations, that of Cherkaev and Gibiansky for the conductivity equation. The importance of this chapter is that it demonstrates the methods employed in deriving a minimization principle on an equation that is simpler than the full Helmholtz equation, and motivates the approach in the following chapter. This chapter should also be skipped by those already acquainted with the material.

Chapter 4 presents the generalization of the concepts in Chapter 3 to the complex Helmholtz equation, which is the work of G.W. Milton, P. Seppecher, and G. Bouchitté. Also, some of the results from Chapter 2 are applied to these variational principles to derive the Euler-Lagrange equation. This is the most important of the background chapters as these variational principles will be used throughout the rest of the thesis, but can of course be skipped by those already familiar with this work. Chapter 5 illustrates the different boundary conditions that can be enforced by slight modification of the minimization functional, work appearing originally in [38].

1.3 The Numerical Method

Beginning with Chapter 6, we present the new work contained in this thesis. Chapter 6 describes a bound on the error that is incurred when the variational principles of Chapter 4 are solved over a finite dimensional subspace of the infinite dimensional Sobolev spaces where the true solution lies. The error bound depends only on the grid spacing used and how well the finite dimensional subspaces are able to approximate the solutions, which is measured by the highest degree of polynomials

contained in them.

Chapter 7 outlines the implementation of the finite element method, specifically detailing the finite element spaces over which the functionals are minimized in the numerical method. The block structure of the resulting system of equations is described, and an effective method for preconditioning is introduced, which exploits this block structure. Some numerical examples and numerical evidence of the error bound are also presented.

Chapter 8 shows how a Robin boundary condition can be enforced by suitably manipulating the functional for the natural boundary condition presented in Chapter 5. The importance of this particular boundary condition is that it serves as a first-order approximation to the transmission boundary conditions described in [40].

1.4 Inverse Problem

Section 9.1 of contains a condensed version of the opening sections of [7], which gives a background on the problem of electrical impedance tomography, as well as an accounting of many results and methods developed for the problem. The purpose of this chapter is to familiarize the reader with the properties of the Dirichlet to Neumann map for the conductivity problem, and like the other background chapters, may be skipped by those familiar with the subject. Section 9.2 generalizes the idea of the Dirichlet to Neumann map for the conductivity equation to define a "essential to natural" map for the complex Helmholtz equation. Most of the important properties possessed by the Dirichlet to Neumann map also hold for the essential to natural map.

In Section 9.3 an algorithm for determining the coefficients in the complex Helmholtz equation from measurements of the fields on the boundary of the domain is presented. The main idea of the algorithm is to minimize the L^2 distance between the solutions of the complex Helmholtz equation with two different types of boundary conditions (essential and natural). Then, the minimization functionals associated with these boundary conditions are added as constraints, thus allowing us to consider all the variables in the minimization as independent and negating the necessity of solving

adjoint problems in order to calculate gradients. Section 9.4 explains some of the details involved in implementing the gradient descent method described in the previous chapter.

1.5 Bounds

Chapter 10 gives some very elementary upper bounds on the quadratic form generated by the essential to natural map. These bounds come from inequalities found in [38], which are derived by comparing the value of the minimization functional for the natural boundary value problem evaluated at the solution with the value when evaluated at test fields. The value is that there are no assumptions on the boundary conditions satisfied by the test fields.

CHAPTER 2

INTRODUCTION TO THE CALCULUS OF VARIATIONS

The purpose of this chapter is to give some simple examples of problems that can be set in a variational framework and present some of the basic results from the Calculus of Variations as they pertain to the functionals that will be used later on.

2.1 Motivation, and Examples

2.1.1 Why Minimization?

Minimization problems arise naturally in many applications, and can even be seen in one's own life. We are constantly faced with optimization problems, such as how to minimize the amount of time spent on a commute, for example. In nature there are many examples of physical and biological processes that can be thought of as minimizing some quantity, such as the structure of the circulatory system being designed to minimize the amount of blood vessel necessary to transport blood throughout the body. It can be observed that in nature there is a tendency to minimize, and for this reason the mathematics of minimization have been studied for centuries.

Euler gave the methods developed to study certain minimization problems the name of Calculus of Variations, but the study of these methods and problems goes back centuries before Euler. The study of the Calculus of Variations has aided in and benefitted from the development of many mathematical theories, such as the theories of functional analysis, partial differential equations, optimization, and control. The value of the Calculus of Variations is shown in that it is still an area of active research and development after centuries of work and contributions by some of the most notable mathematicians of history (Euler, Lagrange, Bernoulli, Newton, Hilbert,

Lebesgue, to name a few). In this thesis, I will apply the Calculus of Variations to minimization problems in order to develop numerical methods for the complex Helmholtz equation and to formulate optimization methods for solving an inverse problem, among other applications.

2.1.2 Classical Examples

In this section, we present two examples of physical problems that can be formulated in terms of minimizing an integral functional. The first of these is one that easy to visualize and experiment with. Here is the setup: take a length of wire and bend it into a loop with any desired shape. Then take the wire loop and dip it into a solution of dish soap and water. When the loop is removed from the soap solution, there should be a soap film that occupies the interior of the loop. If the configuration of the loop is changed and it is dipped in the soap again, the soap film that forms will also change. The natural question to ask is, given the configuration of the wire loop, what is the shape of the soap film that will form when it is dipped? In order to find the answer to this question, we must first decide what is being minimized here. It should be reasonable that the soap molecules that form the film do not want to stretch any farther than is absolutely necessary, and we can turn this idea into a minimization.

Let Γ be the domain in $\mathbb{R}^2$ whose boundary is formed by projecting the wire loop onto the plane. We can then think of a given configuration of the wire as a real-valued function u_0 defined on the boundary $\partial\Gamma$ of Γ. Then all possible shapes of the soap film that might be created when the loop is dipped can be thought of as a functions $v : \Gamma \to \mathbb{R}$. We can interpret the idea that the soap molecules do not want to stretch any more than is necessary mathematically by saying that the surface area of the actual configuration function u over Γ should be as small as possible. Recall from calculus that the surface area of a function v is

$$\int_\Gamma \sqrt{1 + |\nabla v|^2}\, dx.$$

Then the problem of finding the actual configuration of the soap film that forms is that of finding u such that

$$\int_\Gamma \sqrt{1+|\nabla u|^2}\,dx = \min_{v\in\mathcal{A}} \int_\Gamma \sqrt{1+|\nabla v|^2}\,dx,$$

where $\mathcal{A}$ is the set of all admissible functions. In this case for a function v to be admissible, it must have the right boundary values, i.e., it must touch the wire on the boundary. Also, it must be smooth enough to have a gradient that is square integrable. Therefore, for this problem, the admissible set is

$$\mathcal{A} = \left\{ v : \int_\Gamma |\nabla v|^2\,dx < \infty \text{ and } v|_{\partial\Gamma} = u_0 \right\}.$$

The shape of the soap film that will form in practice is therefore the surface of the function that has the smallest surface area and also has the right values on the boundary of the domain Γ. This example is a good illustration of how a physical situation can be seen as a minimization problem once the correct quantity to minimize is found.

Another problem that can be very naturally formulated as a minimization is that of finding the electric field in a material. Recall that the electric field $E(x)$ is a vector function whose values are the force per unit charge acting at a given point. In symbols, this says that $F(x) = qE(x)$, where F is the force acting on a particle of charge q at location x. Coulomb's law states that

$$F = kq_1q_2\frac{x_1 - x_2}{|x_1 - x_2|^3}$$

is the force between two charged particles of charges q_1 and q_2 located at positions x_1 and x_2, where k is a constant. Therefore, the electric field at a point x due to a point charge q_1 located at x_1 is

$$E(x) = kq_1\frac{x - x_1}{|x - x_1|^3}.$$

By adding forces, we see that the electric field at x due to a system of point charges q_i located at points x_i, $i = 1, \ldots, n$ is

$$E(x) = k\sum_{i=1}^{n} q_i\frac{x - x_i}{|x - x_i|^3}.$$

In the limit where the charge distribution becomes a continuous function $\rho(x)$, the expression for the electric field becomes

$$E(x) = k \int \rho(y) \frac{x-y}{|x-y|^3} \, dy.$$

Since

$$\frac{x-y}{|x-y|^3} = -\nabla_x \left(\frac{1}{|x-y|} \right),$$

we can write

$$E(x) = -k \nabla_x \int \frac{\rho(y)}{|x-y|} \, dy.$$

We can now define a potential u such that $E = -\nabla u$ by

$$u(x) = k \int \frac{\rho(y)}{|x-y|} \, dy. \tag{2.1}$$

Stepping back for a moment to our discrete distribution of charges, we see that the work done on one of the charges by moving it along a path C from a point A to another point B is given by

$$W = -\int_C F \cdot dl = -q \int_C E \cdot dl = q \int_C \nabla u \cdot dl = q(u(B) - u(A)).$$

Therefore, assuming that the potential u vanishes at infinity, the work that must be done to bring a charge q_i from infinity to the point x_i (and therefore its potential energy) is $W_i = q_i u(x_i)$. In the discrete case, the potential satisfies

$$u(x_i) = k \sum_{j=1}^{n-1} \frac{q_j}{|x - x_j|^2},$$

where there are $n-1$ charges q_j located at points x_j already in the charge distribution. The potential of the charge q_i is then

$$W_i = k q_i \sum_{j=1}^{n-1} \frac{q_j}{|x_i - x_j|},$$

and the total potential energy is

$$W = \frac{k}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{n} \frac{q_i q_j}{|x_i - x_j|}.$$

In the case of a continuous distribution of charge $\rho(x)$, using (2.1) we have

$$W = \frac{k}{2}\int\int \frac{\rho(x)\rho(y)}{|x-y|}\,dy\,dx = \frac{1}{2}\int \rho(x)u(x)\,dx. \tag{2.2}$$

Recall that the equations governing the electromagnetic response of a body are Maxwell's equations

$$\begin{aligned} \nabla \cdot D &= \rho \\ \nabla \times H - \frac{\partial D}{\partial t} &= J \\ \nabla \times E + \frac{\partial B}{\partial t} &= 0 \\ \nabla \cdot B &= 0, \end{aligned}$$

where D is the electrical displacement, B is the magnetic field, H is the induction field, and J is the current density. Also recall that we have the constitutive relations $D = \varepsilon E$ and $B = \mu H$, where ε is the permittivity and μ is the permeability of the material. If we assume that the fields do not depend on time, then the equations involving E are

$$\nabla \cdot D = \rho,\ \nabla \times E = 0,\ \text{and}\ D = \varepsilon E.$$

As we have already seen, E can be written as the gradient of a potential, and this fact also asserted by the equation $\nabla \times E = 0$. We can combine the three equations above into one equation concerning the potential by writing

$$-\nabla \cdot \varepsilon \nabla u = \rho.$$

Using this result we see that (2.2) becomes

$$W = \frac{1}{2}\int \nabla \cdot D(x)u(x)\,dx = -\frac{1}{2}\int (\nabla \cdot \varepsilon \nabla u)u\,dx$$

Integrating by parts, this becomes

$$W = \frac{1}{2}\int \varepsilon \nabla u \cdot \nabla u\,dx.$$

Experience and experiment tell us that nature will seek to minimize this potential energy. This means that the electrical potential u satisfies

$$\frac{1}{2}\int \varepsilon \nabla u \cdot \nabla u\,dx = \min_{v} \frac{1}{2}\int \varepsilon \nabla v \cdot \nabla v\,dx,$$

where the functions v must vanish at infinity.

These examples illustrate two of the many situations which call for the minimization of an integral functional. However, even once a problem has been formulated as a minimization, it still often an open question as to whether or not there is a minimizer, and if there is whether or not it is unique. Under some basic assumptions, which are satisfied by a large class of integral functionals, we can prove the existence of a minimizer.

2.2 Minimizing Integral Functionals

2.2.1 Direct Methods

The ideas used to find a minimizer to a variational problem involving an integral functional are familiar ones, much the same as those learned in any first semester calculus class. In such a class you learn how to solve the problem of finding the minimum of a differentiable function $f(x)$ defined on a closed interval $[a, b]$. In the setting of a variational problem, these ideas translate into solving the Euler-Lagrange equation, which will be treated in the next section. As far as determining the existence of a minimizer for f on $[a, b]$, a little knowledge about topology tells us that the hypothesis of differentiability of f is stronger than absolutely necessary, and that continuity is enough to guarantee that a function has a minimizer on a compact set. We will use these ideas of continuity and compactness to provide hypotheses under which an integral functional has a minimizer.

Since both continuity and compactness are ideas that are highly dependent on the topology that we use, we need first to fix ideas about the kind of topological space over which we intend to minimize.

Definition 1 *Let X be a vector space. A function $\|\cdot\|_X : X \to \mathbb{R}$ is a norm on X if*

- $\|f\|_X > 0$ *for all* $x \neq 0$ *and* $\|0\|_X = 0$,
- $\|cx\|_X = |c|\|x\|_X$ *for all* $x \in X$ *and all scalars* c,
- $\|x + y\|_X \leq \|x\|_X + \|y\|_X$ *for all* $x, y \in X$.

Definition 2 *A sequence $\{x_n\}$ in a normed vector space X is called a Cauchy sequence if for every $\varepsilon > 0$ there exists N such that $i, j \geq N$ implies*

$$\|x_i - x_j\|_X < \varepsilon.$$

Definition 3 *A normed vector space $(X, \|\cdot\|_X)$ is called a Banach space if every Cauchy sequence in X converges in X. In other words, if $\{x_n\} \subset X$ is a Cauchy sequence, then there exists $x \in X$ such that for every $\varepsilon > 0$ there is an N so that $n \geq N$ implies*

$$\|x_n - x\|_X < \varepsilon.$$

With these ideas in place, we can formulate our abstract minimization problem. Let X be a Banach space and let $I : X \to \mathbb{R}$. We seek to find $x_0 \in X$ such that

$$I(x_0) = \min_{x \in X} I(x). \tag{2.3}$$

As was mentioned, the key to being able to guarantee a solution to this problem was compactness. Unfortunately, if X is infinite dimensional, as it is in most meaningful applications, a closed and bounded set need not be compact in the topology that X inherits from its norm $\|\cdot\|_X$. In order to remedy this problem, we introduce a topology that has fewer open sets, and therefore more compact sets (because there are fewer possible open covers). This topology is called the weak topology on X, and the topology of the metric is referred to as the strong toplolgy. Although we could build this topology from the ground up, for our purposes all that is needed is the definition of convergence in the weak topology. For a full account of the details involved in the definition of the weak topology, see [11].

Definition 4 *Let X be a Banach space. If $f : X \to \mathbb{R}$ is linear and*

$$\sup_{\|x\|_X \leq 1} |f(x)| < \infty,$$

then f is called a bounded linear functional on X. The set of all such f is called the dual space of X and is denoted by X'.

It should be clear that X' is a vector space. In fact, if we define

$$\|f\|_{X'} = \sup_{\|x\|_X \leq 1} |f(x)|,$$

then X' is a Banach space with respect to this norm (see [11]). We are now ready to define convergence in the weak topology.

Definition 5 *A sequence $\{x_n\} \subset X$ converges weakly to $x \in X$ (denoted by $x_n \rightharpoonup x$) if*

$$\lim_{n\to\infty} f(x_n) = f(x)$$

for all $f \in X'$.

There is no reason to stop with defining just one dual space. Since X' is a Banach space, it also has a dual, which we will denote by X''. In fact, some of the simplest elements of X'' are the most useful. Define $g_x : X' \to \mathbb{R}$ by $g_x(f) = f(x)$. Then for scalars α and β and $f, h \in X'$, we have

$$g_x(\alpha f + \beta h) = \alpha f(x) + \beta h(x) = \alpha g_x(f) + \beta g_x(h)$$

and

$$|g_x(f)| = |f(x)| \leq \|f\|_{X'}\|x\|_X \;\Rightarrow\; \|g_x\|_{X''} \leq \|x\|_X,$$

which implies that $g_x \in X''$. If we denote by J the mapping $x \mapsto g_x$, we see that $J(X) \subset X''$.

Definition 6 *If $J(X) = X''$, then X is called a reflexive space.*

A reflexive space is exactly the type of space that we want to work in, since we have the following theorem.

Theorem 1 (Kakutani) *A normed vector space X is reflexive if and only if the closure in the strong topology of the unit ball is weakly compact.*

In particular, this theorem tells us that bounded sequences in a reflexive Banach space have convergent subsequences.

Now that we have the compactness properties that we want, the next problem to tackle is that of continuity.

Definition 7 *A function $I : X \to \mathbb{R}$ is said to be sequentially weakly lower semicontinuous if*

$$\liminf_{n\to\infty} I(x_n) \geq I(x)$$

whenever $x_n \rightharpoonup x$ in X.

We are now in a position to prove

Theorem 2 *Let X be a reflexive Banach space, and let $I : X \to \mathbb{R}$ be weakly lower semicontinuous and coercive over X, i.e., there exist constants $\alpha > 0$ and $\beta \in \mathbb{R}$ such that*

$$I(x) \geq \alpha \|x\|_X + \beta$$

for every $x \in X$. Then there exists $x_0 \in X$ such that

$$I(x_0) = \inf\{I(x) : x \in X\}.$$

Proof : Let $\{x_n\}$ be a minimizing sequence for the problem, i.e., a sequence such that

$$I(x_n) \to \inf\{I(x) : x \in X\}.$$

The coercivity of I implies that $\beta \leq \inf\{I(x) : x \in X\} < \infty$, and the coercivity also implies that the minimizing sequence $\{x_n\}$ must be bounded, since otherwise $\lim_{n\to\infty} I(x_n) = \infty$. Since X is reflexive, we can extract a subsequence $\{x_{n_k}\}$ and a limit x_0 such that $x_{n_k} \rightharpoonup x_0$ in X. The weak lower semicontinuity of I implies that

$$\inf\{I(x) : x \in X\} = \liminf_{k\to\infty} I(x_{n_k}) \geq I(x_0),$$

which gives the result.

Under the assumptions that our function I is weakly lower semicontinuous and coercive, and that the underlying Banach space X is reflexive, we have the existence of a solution to our minimization problem. However, we do not have as yet a method for finding the minimizer. The purpose of the next section will be to derive an equation which the minimizer must satisfy.

2.2.2 The Euler-Lagrange Equation

We continue in our general framework of trying to find a solution to the problem (2.3). As was pointed out at the beginning, the methods for finding this solution x_0 are generalizations of the methods learned in a beginning calculus class for the case when $X = \mathbb{R}$. It follows then that we will need a suitable definition of a derivative.

Definition 8 *Let X be a Banach space and $I : X \to \mathbb{R}$. We define the directional or Gâteau derivative of I at a point u in the direction v as the limit*

$$I'_v(u) = \lim_{\lambda \to 0} \frac{I(u + \lambda v) - I(u)}{\lambda}$$

if this limit exists. If the limit exists for every $v \in X$, then I is said to be differentiable at u.

When the term differentiable is used below, it is to be in this sense. Again relying on our Calculus intuition, it should not be surprising that we have the following result.

Theorem 3 *Let X be a Banach space and let $I : X \to \mathbb{R}$ be differentiable at $\hat{u}$, where*

$$I(\hat{u}) = \inf\{I(u) : u \in X\}.$$

Then

$$I'_v(\hat{u}) = 0 \text{ for all } v \in X.$$

Proof : Fix $v \in X$ and define a function $\varphi : \mathbb{R} \to \mathbb{R}$ by $\varphi(t) = I(\hat{u} + tv)$. Then φ is differentiable, and since it has a minimum at $t = 0$, we must have

$$0 = \varphi'(0) = \frac{d}{dt} I(\hat{u} + tv)|_{t=0} = I'_v(\hat{u}).$$

The converse of this theorem is true also under the additional assumption that I is convex. The convexity of I allows us to use the following lemma.

Lemma 1 (Supporting Hyperplanes) *Let $I : X \to \mathbb{R}$ be differentiable and convex. Then for every $u, v \in X$,*

$$I(v) \geq I(u) + I'_{v-u}(u).$$

Proof : Let $\lambda \in [0,1]$. From the definition of convexity, it follows that

$$\frac{1}{\lambda}\left[I(u+\lambda(v-u)) - I(u)\right] \leq I(v) - I(u).$$

Now simply let $\lambda \to 0$.

Theorem 4 *Let $I : X \to \mathbb{R}$ be differentiable and convex, and assume that $\hat{u} \in X$ is such that*

$$I'_v(\hat{u}) = 0 \text{ for all } v \in X.$$

Then

$$I(\hat{u}) = \inf\{I(u) : u \in X\}.$$

Proof : The previous lemma implies that for any $v \in X$

$$I(v) \geq I(\hat{u}) + I'_{v-\hat{u}}(\hat{u}) = I(\hat{u}),$$

which gives the result.

The equation $I'_v(\hat{u}) = 0$ for all $v \in X$ is known as the Euler-Lagrange equation for the minimization problem (2.3). In effect, it gives us a way to find the minimizer by solving an equation. In the next section, we will focus on the special case when $I(u)$ is an integral functional.

2.2.3 Integral Functionals

As we now move from the general to the specific, it is necessary to recount some of the results that justify the choices of Banach spaces and functionals that we are going to use in what follows. The ultimate goal of this section is to apply the results of the previous two sections to functionals of the form

$$I(u) = \int_\Gamma A(x)\nabla u \cdot \nabla u \, dx, \tag{2.4}$$

where $A(x)$ is a symmetric positive definite matrix-valued function on a smooth domain Γ in $\mathbb{R}^d$. We also assume that $(A(x))_{ij} \in L^\infty(\Gamma)$. The results that apply to functionals of this form can be generalized in a very straightforward way to the functionals that apply to the complex Helmholtz equation.

In order to treat the minimization of integral functionals such as the one above, it is necessary to minimize over spaces of functions such that $I(u)$ makes sense. In other words, we need a Banach space containing functions that have a gradient, and whose gradients are integrable, but we do not want to impose any more restrictions on the space than are absolutely necessary.

Definition 9 *Let $f \in L^p(\Gamma)$, where $\Gamma \subset \mathbb{R}^d$ is open. If there exist functions $f_1, f_2, \ldots, f_d$ in $L^p(\Gamma)$ such that*

$$\int_\Gamma f_i \varphi \, dx = -\int_\Gamma f \frac{\partial \varphi}{\partial x_i} \, dx, \;\; i = 1, 2, \ldots, d \tag{2.5}$$

for all $\varphi \in C_0^\infty(\Gamma)$, then we say $f \in W^{1,p}(\Gamma)$.

Equation (2.5) says that the functions in $W^{1,p}(\Gamma)$ have derivatives in the sense of distributions that are in $L^p(\Gamma)$. Even though the functions in $W^{1,p}(\Gamma)$ may not be differentiable in the classical sense, the integration by parts formula holds for a dense subset of $L^p(\Gamma)$. In this weak sense we can define the gradient of a function $f \in W^{1,p}(\Gamma)$ by $\nabla f = (f_1, \ldots, f_n)^T$. The space $W^{1,p}(\Gamma)$ is a Banach space with norm

$$\|f\|_{W^{1,p}(\Gamma)} = \left(\int_\Gamma |f|^p \, dx + \int_\Gamma |\nabla f|^p \, dx \right)^{\frac{1}{p}}$$

for $1 \leq p < \infty$ and

$$\|f\|_{W^{1,\infty}(\Gamma)} = \text{ess sup}_{x \in \Gamma} |f(x)| + |\nabla f(x)|.$$

for details, see [11].

When $p = 2$, we write $W^{1,2}(\Gamma) = H^1(\Gamma)$. This is a special case because $H^1(\Gamma)$ is a Hilbert space, which is a Banach space whose norm is generated by an inner product. The inner product in $H^1(\Gamma)$ is given by

$$\langle f, g \rangle_{H^1(\Gamma)} = \int_\Gamma fg \, dx + \int_\Gamma \nabla f \cdot \nabla g \, dx.$$

The fact that $H^1(\Gamma)$ is a reflexive space is a simple corollary to the following theorem.

Theorem 5 (Riesz Representation Theorem) *Let H be a Hilbert space with inner product $\langle \cdot, \cdot \rangle_H$. For any bounded linear functional $f : H \to \mathbb{R}$, there exists a unique $y \in H$ so that $\langle f, x \rangle_{H',H} = \langle x, y \rangle_H$.*

Here $\langle \cdot, \cdot \rangle_{H',H}$ denotes the action of an element of H' on an element of H.

Proof : Let N be the null space of f. If $N = H$, take $y = 0$. Otherwise, $N \neq \{0\}$ is a closed subspace of H. Take $y_0 \in N^{\perp}$ such that $\|y_0\|_H = 1$ and let $y = y_0 \langle f, y_0 \rangle_{H',H}$. Fix $x \in H$ and define $z = y_0 \langle f, x \rangle_{H',H} - x \langle f, y_0 \rangle_{H',H}$. Notice that $z \in N$, so $\langle z, y_0 \rangle_H = 0$. Therefore,

$$\begin{aligned} \langle f, x \rangle_{H',H} &= \langle f, x \rangle_{H',H} \langle y_0, y_0 \rangle_H = \langle \langle f, x \rangle_{H',H} y_0, y_0 \rangle_H \\ &= \langle z + x \langle f, y_0 \rangle_{H',H}, y_0 \rangle_H = \langle x, y \rangle_H. \end{aligned}$$

If there exist $y, \tilde{y} \in H$ such that $\langle f, x \rangle_{H',H} = \langle x, y \rangle_H = \langle x, \tilde{y} \rangle_H$ for all $x \in H$, then $\langle x, y - \tilde{y} \rangle_H = 0$ for all $x \in H$, and in particular for $x = y - \tilde{y}$. Therefore $y = \tilde{y}$.

It is convenient to define another function space at this point which shall be used extensively later on. We define

$$H(\mathrm{div}, \Gamma) = \{v \in L^2(\Gamma, \mathbb{R}^d) : \nabla \cdot v \in L^2(\Gamma)\}.$$

Here the derivatives are again taken in the sense of distribution. The space $H(\mathrm{div}, \Gamma)$ is a Hilbert space with inner product

$$\langle p, v \rangle_{H(\mathrm{div},\Gamma)} = \int_\Gamma p \cdot v \; dx + \int_\Gamma \nabla \cdot p \nabla \cdot v \; dx.$$

Recall from the previous section that if u minimizes I, then u must satisfy the Euler-Lagrange equation $I'_v(u) = 0$ for all $v \in X$. The converse is also true since the functional (2.4) is convex. To see this, note that since A is symmetric positive definite, we have that $0 \leq A(\nabla u - \nabla v) \cdot (\nabla u - \nabla v)$, which, when expanded and rearranged, becomes $A\nabla u \cdot \nabla v \leq (1/2) A\nabla u \cdot \nabla u + (1/2) A\nabla v \cdot \nabla v$. This in turn implies that

$$\begin{aligned} I(tu + (1-t)v) &= \int_\Gamma A(t\nabla u + (1-t)\nabla v) \cdot (t\nabla u + (1-t)\nabla v) \; dx \\ &= \int_\Gamma \left[t^2 A\nabla u \cdot \nabla u + 2t(1-t) A\nabla u \cdot \nabla v + (1-t)^2 A\nabla v \cdot \nabla v \right] \; dx \\ \leq \int_\Gamma \left[t^2 A\nabla u \cdot \nabla u + t(1-t) A\nabla u \cdot \nabla u + t(1-t)\nabla v \cdot \nabla v + (1-t)^2 A\nabla v \cdot \nabla v \right] \; dx \\ &= tI(u) + (1-t)I(v). \end{aligned}$$

Therefore, if we can find u that satisfies the Euler-Lagrange equation, we will have found the minimizer of (2.4).

For a fixed $v \in H^1(\Gamma)$, we have that

$$I'_v(u) = \lim_{t\to 0} \frac{1}{t}\left\{\int_\Gamma A(\nabla u + t\nabla v)\cdot(\nabla u + t\nabla v)\ dx - \int_\Gamma A\nabla u\cdot\nabla u\ dx\right\}$$

$$= \lim_{t\to 0} \frac{1}{t}\left\{\int_\Gamma \left[A\nabla u\cdot\nabla u - 2tA\nabla u\cdot\nabla v + t^2 A\nabla v\cdot\nabla v - A\nabla u\cdot\nabla u\right]\ dx\right\}$$

$$= 2\int_\Gamma A\nabla u\cdot\nabla v\ dx.$$

Therefore, the Euler-Lagrange equation that the minimizer u must satisfy is

$$\int_\Gamma A\nabla u\cdot\nabla v\ dx = 0\ \forall\ v \in \mathcal{A}, \tag{2.6}$$

where $\mathcal{A}$ is the set of admissible functions for the problem. Now that we know the equation that our minimizer u must satisfy, the next question to answer is whether or not the equation has a unique solution. If we define

$$a(u,v) = \int_\Gamma A\nabla u\cdot\nabla v\ dx,$$

then for fixed v, $a(u,v)$ is a linear function of u and vise-versa, so it is called a bilinear form. The equation (2.6) can then be written

$$a(u,v) = \langle f, v\rangle_{H^{-1}(\Gamma),H^1(\Gamma)},$$

where $H^{-1}(\Gamma) = (H^1(\Gamma))'$ is the dual space of $H^1(\Gamma)$ and $\langle\cdot,\cdot\rangle_{H^{-1}(\Gamma),H^1(\Gamma)}$ denotes the action of an element of $H^{-1}(\Gamma)$ on an element of $H^1(\Gamma)$. In (2.6) we have $f = 0$. The following theorem gives the needed result.

Theorem 6 (Lax-Milgram) *Let H be a Hilbert space and $a : H\times H \to \mathbb{R}$ a bilinear form for which there exist constants $\alpha, \beta > 0$ such that*

$$|a(u,v)| \le \alpha\|u\|_H\|v\|_H\ \forall\ u,v \in H\ (a\ \textit{is bounded})$$

and

$$a(u,u) \ge \beta\|u\|_H^2\ \forall u \in H\ (a\ \textit{is coercive}).$$

Finally, let $f \in H'$. Then there exists an element $u \in H$ such that

$$a(u,v) = \langle f, v\rangle_{H',H}$$

for all $v \in H$.

This theorem is powerful in that all it requires is boundedness and coercivity of the bilinear form a. However, if a is also symmetric, i.e., if $a(u, v) = a(v, u)$ for all $u, v \in H$, then the proof of the Lax-Milgram theorem can be simplified significantly. Since all the functionals that we will work with in the sequel are symmetric, we will prove the theorem under that additional assumption.

Proof : Since the bilinear form a is symmetric, bounded and coercive, it is easy to check that $a(\cdot, \cdot)$ defines an inner product on H. Then the Riesz Representation Theorem implies that for each $f \in H'$ there exists an element $u \in H$ such that

$$a(u, v) = \langle f, v \rangle_{H',H}$$

for all $v \in H$.

Now we know conditions under which we can solve the Euler-Lagrange equation, and since the functional is convex, this is equivalent to finding a minimizer to the problem (2.3).

These techniques and results will form the basis for our analysis of the minimization variational principles for the solution of the Helmholtz equation.

CHAPTER 3

VARIATIONAL PRINCIPLES FOR CONDUCTIVITY

We now present the variational principles introduced by Cherkaev and Gibiansky in [16] (see also [15]). The derivation of these principles demonstrates the idea of rearranging the constitutive relation in order to obtain a minimization problem, and the derivation of the minimization principles for the complex Helmholtz equation will follow many of the same basic steps. As will be seen, these principles are quadratic, and therefore the methods described in the previous chapter apply with very little modification.

3.1 The Conductivity Problem

Consider a conducting body occupying a region $\Gamma \in \mathbb{R}^d$ whose conductivity at a point $x \in \Gamma$ is given by the complex matrix-valued function $\sigma : \Gamma \to \mathbb{C}^{d\times d}$. Then the current density $J : \Gamma \to \mathbb{C}^d$ and the electrical field $E : \Gamma \to \mathbb{C}^d$ are related by the constitutive relation

$$J = \sigma E.$$

The fields also satisfy the differential constraints

$$\nabla \cdot J = 0 \text{ and } \nabla \times E = 0.$$

The differential constraint on E implies the existence of a complex-valued potential $u : \Gamma \to \mathbb{C}$ such that $E = -\nabla u$. The differential constraints along with the constitutive relation imply that the potential u satisfies the equation

$$-\nabla \cdot \sigma \nabla u = 0.$$

We would like to think of this equation as the Euler-Lagrange equation for a minimization variational principle. Unfortunately, when we multiply through the equation

by the conjugate of a test function $v \in H_0^1(\Gamma)$ and integrate by parts, the functional that results is

$$\int_\Gamma \sigma \nabla u \cdot \nabla \bar{v} \, dx,$$

which is complex valued. In order to circumvent this difficulty, we will derive a new constitutive relation which relates the real and imaginary parts of the fields. Then the quadratic functional corresponding to this constitutive relation will be real valued and it will again at least make sense to talk about minimization.

3.2 The Real Constitutive Relation

Throughout what follows, let $'$ denote the real part of a complex quantity, and let $''$ denote the imaginary part. Starting from the constitutive relation $J = \sigma E$ and equating the real and imaginary parts of both sides of the equation, we find that

$$J' = \sigma' E' - \sigma'' E'' \text{ and } J'' = \sigma' E'' + \sigma'' E', \tag{3.1}$$

or in matrix form

$$\begin{pmatrix} -J' \\ J'' \end{pmatrix} = \begin{pmatrix} -\sigma' & \sigma'' \\ \sigma'' & \sigma' \end{pmatrix} \begin{pmatrix} E' \\ E'' \end{pmatrix}.$$

As was demonstrated in section 2.2.3, the fact that the matrix in the constitutive relation is positive definite is necessary for minimization, since this makes the integral functional convex. It is clear that the matrix above cannot be positive definite, since

$$\begin{pmatrix} E' \\ E'' \end{pmatrix} \cdot \begin{pmatrix} -\sigma' & \sigma'' \\ \sigma'' & \sigma' \end{pmatrix} \begin{pmatrix} E' \\ E'' \end{pmatrix} = -\sigma' E' \cdot E' + 2\sigma'' E' \cdot E'' + \sigma' E'' \cdot E'',$$

and the right-hand side cannot be guaranteed to be positive for all choices of E' and E'' (for example, take E' to be a eigenvector corresponding to a positive eigenvalue of σ' and $E'' = 0$, or if all the eigenvalues of σ' are negative, reverse the roles of E' and E'').

Even though the matrix in the constitutive relation as it stands is not positive definite, we can rearrange the constitutive relation so that this will be the case. Solving for E'' in the first equation in (3.1), we find that

$$E'' = (\sigma'')^{-1} \sigma' E' - (\sigma'')^{-1} J'.$$

Substituting this into the second equation from (3.1), we find that

$$J'' = \sigma' \left[(\sigma'')^{-1}\sigma' E' - (\sigma'')^{-1} J'\right] + \sigma'' E = (\sigma'' + \sigma'(\sigma'')^{-1}\sigma')E' - \sigma'(\sigma'')^{-1} J'.$$

In matrix form, this reads

$$\begin{pmatrix} J'' \\ E'' \end{pmatrix} = \mathcal{L} \begin{pmatrix} E' \\ -J' \end{pmatrix}, \tag{3.2}$$

where

$$\mathcal{L} = \begin{pmatrix} \sigma'' + \sigma'(\sigma'')^{-1}\sigma' & \sigma'(\sigma'')^{-1} \\ (\sigma'')^{-1}\sigma' & \sigma'' \end{pmatrix}.$$

3.2.1 Positivity of the Tensor

The matrix in (3.2) is positive definite as long as σ'' is, since if we take any field $(E', -J')^T$ and define $(J'', E'')^T$ by (3.2), then we have

$$\begin{pmatrix} E' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} E' \\ -J' \end{pmatrix} = \begin{pmatrix} E' \\ -J' \end{pmatrix} \cdot \begin{pmatrix} J'' \\ E'' \end{pmatrix} = E' \cdot J'' - J' \cdot E''.$$

Referring back to (3.1), this becomes

$$\begin{aligned} \begin{pmatrix} E' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} E' \\ -J' \end{pmatrix} &= \sigma' E'' \cdot E' + \sigma'' E' \cdot E' - \sigma' E' \cdot E'' + \sigma'' E'' \cdot E'' \\ &= \sigma'' E' \cdot E' + \sigma'' E'' \cdot E'' \geq 0, \end{aligned}$$

as long as σ'' is positive definite.

3.2.2 Dissipation

In the case of the steady state oscillations of the dissipative medium caused by a monochromatic excitation, the electric field $e(x,t)$ and the current $j(x,t)$ satisfy

$$j(x,t) = (J(x)e^{i\omega t})' \text{ and } e(x,t) = (E(x)e^{i\omega t})'.$$

The energy dissipation in the material averaged over a period of oscillation and integrated over the body Γ is equal to

$$\begin{aligned} \frac{\omega}{2\pi} \int_\Gamma \int_0^{\frac{2\pi}{\omega}} j(x,t) \cdot e(x,t)\, dt\, dx &= \int_\Gamma \frac{1}{2} \left[J' \cdot E' + J'' \cdot E''\right] dx \\ &= \frac{1}{2} \int_\Gamma \left[\sigma' E' \cdot E' + \sigma' E'' \cdot E''\right] dx. \end{aligned}$$

Therefore, for the heat dissipated into energy to be positive, we must have $\sigma' > 0$.

3.3 Minimization Functional

The differential constraints for the conductivity problem are

$$\nabla \cdot J = 0 \text{ and } \nabla \times E = 0,$$

so we may assume that $E = \nabla u$ for some scalar potential u, which will automatically enforce the differential constraint on E. If we desire, we can also enforce the constraint on J by writing it as $J = \nabla \times A$ for some vector potential A, but we will not do so in order to make the notation used here match more closely with that of later sections.

Assuming that $\sigma'' > 0$, the matrix $\mathcal{L}$ in (3.2) is positive definite, and therefore the functional

$$Y(u', J') = \int_\Gamma \begin{pmatrix} \nabla u' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \nabla u' \\ -J' \end{pmatrix} \, dx$$

is convex. Also, we see that if u and J are solutions to

$$\begin{cases} -\nabla \cdot \sigma \nabla u = 0 & \text{in } \Gamma \\ u' = u'_0 & \text{on } \partial\Gamma \\ J' \cdot n = J'_0 \cdot n & \text{on } \partial\Gamma \end{cases}, \tag{3.3}$$

where n denotes the outward unit normal to Γ, and if s is a scalar function such that $s = 0$ on $\partial\Gamma$ and T is a vector function such that $T \cdot n = 0$ on $\partial\Gamma$ and $\nabla \cdot T = 0$ in Γ, we have

$$Y(u' + s, J' + T) = Y(u', J') + 2 \int_\Gamma \begin{pmatrix} \nabla u' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \nabla s \\ -T \end{pmatrix} \, dx + Y(s, T).$$

Because of the homogeneous boundary conditions satisfied by s and T and the fact that $\nabla \cdot T = 0$, we have that

$$2 \int_\Gamma \begin{pmatrix} \nabla u' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \nabla s \\ -T \end{pmatrix} \, dx = 2 \int_\Gamma \begin{pmatrix} J'' \\ \nabla u'' \end{pmatrix} \cdot \begin{pmatrix} \nabla s \\ -T \end{pmatrix} \, dx$$

$$= 2 \int_\Gamma \left[J'' \cdot \nabla s - \nabla u'' \cdot T \right] dx = 2 \int_\Gamma \left[-\nabla \cdot J'' s + \nabla \cdot T u'' \right] dx = 0.$$

Since $Y(s, T) \geq 0$ and $Y(s, T) = 0$ if and only if $s = 0$ and $T = 0$, we have that (u', J') minimizes Y over all functions satisfying the same boundary conditions and the differential constraint $\nabla \cdot J' = 0$.

On the other hand, if (u', J') is the minimizer of Y, then let $t \in \mathbb{R}$. The function $\varphi(t) = Y(u' + ts, J' + tT)$, where s and T are any fields satisfying the homogeneous boundary conditions and $\nabla \cdot T = 0$, has a minimum at $t = 0$, so

$$0 = \varphi'(0) = 2\int_\Gamma \begin{pmatrix} \nabla u' \\ -J' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \nabla s \\ -T \end{pmatrix} dx = 2\int_\Gamma \begin{pmatrix} J'' \\ \nabla u'' \end{pmatrix} \cdot \begin{pmatrix} \nabla s \\ -T \end{pmatrix} dx$$

$$= 2\int_\Gamma [J'' \cdot \nabla s - \nabla u'' \cdot T]\, dx$$

Integrating by parts, we have that

$$0 = \int_\Gamma -\nabla \cdot J'' s \; dx$$

for all s satisfying the homogeneous boundary conditions, since $\nabla \cdot T = 0$. Therefore,

$$\nabla \cdot J'' = 0 \;\Leftrightarrow\; (\nabla \cdot \sigma \nabla u)'' = 0,$$

which is just the imaginary part of equation (3.3).

3.3.1 Dual Variational Principle for the Imaginary Parts

We can rewrite the the constitutive relation (3.2) as

$$\begin{pmatrix} E' \\ -J' \end{pmatrix} = \mathcal{L}^{-1} \begin{pmatrix} J'' \\ E'' \end{pmatrix}.$$

Because of the form of the matrix $\mathcal{L}$, we have that

$$\mathcal{L}^{-1} = \begin{pmatrix} \sigma'' & -\sigma'(\sigma'')^{-1} \\ -(\sigma'')^{-1}\sigma' & \sigma'' + \sigma'(\sigma'')^{-1}\sigma' \end{pmatrix}.$$

Following the same arguments as in the section above, we arrive at the functional

$$\int_\Gamma \begin{pmatrix} J'' \\ E'' \end{pmatrix} \cdot \begin{pmatrix} \sigma'' & -\sigma'(\sigma'')^{-1} \\ -(\sigma'')^{-1}\sigma' & \sigma'' + \sigma'(\sigma'')^{-1}\sigma' \end{pmatrix} \begin{pmatrix} J'' \\ E'' \end{pmatrix} dx,$$

which we can rearrange to read

$$\int_\Gamma \begin{pmatrix} E'' \\ -J'' \end{pmatrix} \cdot \begin{pmatrix} \sigma'' + \sigma'(\sigma'')^{-1}\sigma' & \sigma'(\sigma'')^{-1} \\ (\sigma'')^{-1}\sigma' & \sigma'' \end{pmatrix} \begin{pmatrix} E'' \\ -J'' \end{pmatrix} dx,$$

which implies that this variational principle is self-dual, making it very convenient to solve for both the real and imaginary parts of the solution via minimization variational principles.

CHAPTER 4

VARIATIONAL PRINCIPLES FOR THE HELMHOLTZ EQUATION

Before presenting the variational principles of Milton, Seppecher, and Bouchitté for the complex Helmholtz equation, we will study some examples of situations in which the Helmholtz equation arises.

4.1 Helmholtz Equation

Many systems that result in steady state oscillations can be modeled with the Helmholtz equation

$$-\nabla \cdot A(x)\nabla u - k(x)u = 0,$$

where $A(x)$ is a matrix-valued function and $k(x)$ is scalar valued, but of particular interest are acoustic waves and transverse electric or transverse magnetic electromagnetic waves. We will give a brief review of how the Helmholtz equation results from each of these situations

4.1.1 Transverse Electric Mode in Electromagnetism

The time harmonic version of Maxwell's equations (2.3) are

$$\nabla \times E = -i\omega\mu H,\ \nabla \times H + i\omega\varepsilon E = 0.$$

Let us assume that μ and ε are scalar functions that are independent of x_1. We will look for a solution with $E_2 = E_3 = 0$ and E_1 that does not depend on x_1. Then we have

$$\nabla \times E = \begin{pmatrix} 0 \\ \dfrac{\partial E_1}{\partial x_3} \\ -\dfrac{\partial E_1}{\partial x_2} \end{pmatrix},$$

so it must be that $H_1 = 0$, and the only nonzero components of H are

$$H_2 = \frac{1}{i\omega\mu}\frac{\partial E_1}{\partial x_3} \text{ and } H_3 = -\frac{1}{i\omega\mu}\frac{\partial E_1}{\partial x_2},$$

neither of which depend on x_1. The curl of H is therefore

$$\nabla \times H = \begin{pmatrix} \frac{\partial H_3}{\partial x_2} - \frac{\partial H_2}{\partial x_3} \\ \frac{\partial H_1}{\partial x_3} - \frac{\partial H_3}{\partial x_1} \\ \frac{\partial H_2}{\partial x_1} - \frac{\partial H_1}{\partial x_2} \end{pmatrix} = \begin{pmatrix} \frac{i}{\omega}\left(\frac{\partial}{\partial x_2}\frac{1}{\mu}\frac{\partial E_1}{\partial x_2} + \frac{\partial}{\partial x_3}\frac{1}{\mu}\frac{\partial E_1}{\partial x_3}\right) \\ 0 \\ 0 \end{pmatrix}.$$

Let $\bar{\nabla} = \left(\frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}\right)^T$. Then we can write the line above as

$$\nabla \times H = \begin{pmatrix} \frac{i}{\omega}\bar{\nabla} \cdot \frac{1}{\mu}\bar{\nabla}E_1 \\ 0 \\ 0 \end{pmatrix},$$

which implies that

$$\bar{\nabla} \cdot \frac{1}{\mu(x_2, x_3)}\bar{\nabla}E_1 + \omega^2\varepsilon(x_2, x_3)E_1 = 0.$$

4.1.2 The Acoustic Equation

In elastodynamics, we have the relation

$$C\nabla u = G(\nabla u + (\nabla u)^T) + \lambda(\nabla \cdot u)I,$$

where C is the elasticity tensor, u is the displacement, λ is the Lamé modulus, and G is the shear modulus. In a fluid we have

$$G = 0 \text{ and } \lambda = \kappa - \frac{2}{3}G = \kappa,$$

where κ is the bulk modulus. Therefore, the stress field σ satisfies

$$\sigma = C\nabla u = \kappa I(\nabla \cdot u) = -PI,$$

where $P = -\kappa\nabla \cdot u$ is the pressure. We can write the equation of elastodynamics

$$\nabla \cdot \sigma + \omega^2\rho u = 0$$

as

$$\nabla P = \omega^2 \rho u,$$

where ρ is the density and ω is the frequency, and we also have

$$\nabla \cdot u = \nabla \cdot \frac{1}{\omega^2 \rho} \nabla P = -\frac{1}{\kappa} P,$$

which implies the acoustic wave equation

$$-\nabla \cdot \rho^{-1} \nabla P - \frac{\omega^2}{\kappa} P = 0.$$

Of course, we are interested in the case where both ρ and κ are complex-valued. For a discussion of the meaning of complex mass-density and some examples of materials with such characteristics, see [39].

4.2 Minimization Variational Principle

Throughout the rest of this thesis, we will express the Helmholtz equation in the form of the acoustic equation

$$-\nabla \cdot \rho^{-1} \nabla P - \frac{\omega^2}{\kappa} P = 0.$$

We are interested in the case where ρ, κ, and P are complex. By the usual methods (multiplying by a test function an integrating by parts), we can derive a weak form for this equation (assuming Dirichlet boundary conditions in order to fix ideas),

$$\int_\Gamma \left[\rho^{-1} \nabla P \cdot \nabla \bar{v} - \frac{\omega^2}{\kappa} P \bar{v} \right] dx \ \forall \ v \in H_0^1(\Gamma).$$

However, this Euler-Lagrange equation corresponds to a stationary principle and not a minimization principle, since the bilinear form is not coercive even when the variables are real. Our goal is to follow the process in Chapter 3 to derive a minimization variational principle for the Helmholtz equation. This process can be done in much more generality than will be done here, and can be applied to any complex equation of the form

$$\nabla \cdot (L \nabla u + K u) = h + K^T \nabla u + M u,$$

where L is a fourth-order tensor and K and M are matrices, with L and M symmetric. For details see [37].

First we define a dual variable v, called the complex velocity, by

$$i\omega v = \rho^{-1}\nabla P,$$

and then we define two complex-valued fields and a matrix by

$$\mathcal{F} = \begin{pmatrix} \nabla P \\ P \end{pmatrix},\ \mathcal{G} = \begin{pmatrix} -i\omega v \\ -i\omega \nabla \cdot v \end{pmatrix} \text{ and } Z = \begin{pmatrix} -\rho^{-1} & 0 \\ 0 & \frac{\omega^2}{\kappa} \end{pmatrix}.$$

Then we have

$$\begin{pmatrix} -\rho^{-1} & 0 \\ 0 & \frac{\omega^2}{\kappa} \end{pmatrix} \begin{pmatrix} \nabla P \\ P \end{pmatrix} = \begin{pmatrix} -\rho^{-1}\nabla P \\ \frac{\omega^2}{\kappa} P \end{pmatrix} = \begin{pmatrix} -i\omega v \\ -i\omega \nabla \cdot v \end{pmatrix},$$

which is equivalent to the constitutive relation

$$\mathcal{G} = Z\mathcal{F}.$$

We are still working with complex-valued quantities, and we need to move to real-valued quantities in order to talk about minimization. For this reason, we take the real and imaginary parts of the equation above to find (recall that $'$ denotes a real part and $''$ denotes an imaginary part)

$$\mathcal{G}' = Z'\mathcal{F}' - Z''\mathcal{F}'' \text{ and } \mathcal{G}'' = Z'\mathcal{F}'' + Z''\mathcal{F}',$$

which in matrix form reads

$$\begin{pmatrix} \mathcal{G}'' \\ \mathcal{G}' \end{pmatrix} = \begin{pmatrix} Z'' & Z' \\ Z' & -Z'' \end{pmatrix} \begin{pmatrix} \mathcal{F}' \\ \mathcal{F}'' \end{pmatrix}.$$

The matrix in this constitutive relation is obviously not positive definite, but if $Z'' > \alpha I$, then we may use this relation to build saddle point variational principles, as detailed in [37].

In order to get a matrix that is positive definite, and therefore a minimization variational principle, we rearrange this equation, solving for the imaginary parts of $\mathcal{G}$ and $\mathcal{F}$. We find that

$$\mathcal{F}'' = (Z'')^{-1}Z'\mathcal{F}' - (Z'')^{-1}\mathcal{G}'$$

and

$$\mathcal{G}'' = Z'((Z'')^{-1}Z'\mathcal{F}' - (Z'')^{-1}G') + Z''\mathcal{F}' = (Z'' + Z'(Z'')^{-1}Z')\mathcal{F}' - Z'(Z'')^{-1}\mathcal{G}'$$

In matrix form, the new constitutive relation is

$$\begin{pmatrix} \mathcal{G}'' \\ \mathcal{F}'' \end{pmatrix} = \mathcal{L} \begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix}, \tag{4.1}$$

where

$$\mathcal{L} = \begin{pmatrix} Z'' + Z'(Z'')^{-1}Z' & Z'(Z'')^{-1} \\ (Z'')^{-1}Z' & (Z'')^{-1} \end{pmatrix}.$$

The matrix $\mathcal{L}$ is positive definite as long as Z'' is . Indeed, given a vector $(\mathcal{F}', -\mathcal{G}')^T$, define $(\mathcal{G}'', \mathcal{F}'')^T$ by (4.1). Then

$$\begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix} = \begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix} \cdot \begin{pmatrix} \mathcal{G}'' \\ \mathcal{F}'' \end{pmatrix} = \mathcal{F}' \cdot \mathcal{G}'' - \mathcal{G}' \cdot \mathcal{F}''$$

$$= \mathcal{F}' \cdot (Z'\mathcal{F}'' + Z''\mathcal{F}') - (Z'\mathcal{F}' - Z''\mathcal{F}'') \cdot \mathcal{F}'' = \mathcal{F}' \cdot Z''\mathcal{F}' + \mathcal{F}'' \cdot Z''\mathcal{F}''.$$

In the constitutive relation (4.1), it is convenient to separate the scalar variables from the vector variables. Let $r = -\rho^{-1}$ and $k = \kappa^{-1}$. Then

$$Z = \begin{pmatrix} r & 0 \\ 0 & \omega^2 k \end{pmatrix},$$

so

$$Z' = \begin{pmatrix} r' & 0 \\ 0 & \omega^2 k' \end{pmatrix}, \; Z'' = \begin{pmatrix} r'' & 0 \\ 0 & \omega^2 k'' \end{pmatrix} \text{ and } (Z'')^{-1} = \begin{pmatrix} (r'')^{-1} & 0 \\ 0 & \frac{1}{\omega^2}(k'')^{-1} \end{pmatrix}.$$

Therefore,

$$\mathcal{L} = \begin{pmatrix} r'' + r'(r'')^{-1}r' & 0 & r'(r'')^{-1} & 0 \\ 0 & \omega^2(k'' + k'(k'')^{-1}k') & 0 & k'(k'')^{-1} \\ (r'')^{-1}r' & 0 & (r'')^{-1} & 0 \\ 0 & (k'')^{-1}k' & 0 & \frac{1}{\omega^2}(k'')^{-1} \end{pmatrix},$$

and we can rearrange the rows and columns in $\mathcal{L}$ so that (4.1) reads

$$\begin{pmatrix} -\omega v' \\ \nabla P'' \\ -\omega \nabla \cdot v' \\ P'' \end{pmatrix}$$

$$= \begin{pmatrix} r'' + r'(r'')^{-1}r' & r'(r'')^{-1} & 0 & 0 \\ (r'')^{-1}r' & (r'')^{-1} & 0 & 0 \\ 0 & 0 & \omega^2(k'' + k'(k'')^{-1}k') & k'(k'')^{-1} \\ 0 & 0 & (k'')^{-1}k' & \frac{1}{\omega^2}(k'')^{-1} \end{pmatrix} \begin{pmatrix} \nabla P' \\ -\omega v'' \\ P' \\ -\omega \nabla \cdot v'' \end{pmatrix}. \tag{4.2}$$

We can then rewrite the quadratic form generated by $\mathcal{L}$ as

$$\begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix} = \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix},$$

where

$$\mathcal{R} = \begin{pmatrix} r'' + r'(r'')^{-1}r' & r'(r'')^{-1} \\ (r'')^{-1}r' & (r'')^{-1} \end{pmatrix} \text{ and } \mathcal{K} = \begin{pmatrix} k'' + k'(k'')^{-1}k' & k'(k'')^{-1} \\ (k'')^{-1}k' & (k'')^{-1} \end{pmatrix}.$$

A calculation similar to the one done above shows that the matrices $\mathcal{R}$ and $\mathcal{K}$ are positive definite as long as there exist constants $\alpha > 0$ and $\beta < 0$ such that

$$\rho''(x) \geq \alpha I \text{ and } \kappa''(x) < \beta \ \forall \ x \in \Gamma. \tag{4.3}$$

Assuming that this condition holds, we define the functional

$$Y(P', v'') = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \right] dx.$$

Then if $P' \in H^1(\Gamma)$ and $v'' \in H(\text{div}, \Gamma)$ are solutions to the Helmholtz equation satisfying the constitutive relation (4.2), let $s \in H_0^1(\Gamma)$ and $T \in H_0(\text{div}, \Gamma)$ (the subscript 0 connotes the idea of zero boundary conditions $s = 0$ and $T \cdot n = 0$ on $\partial\Gamma$, but the exact definitions of these spaces are more complicated). We have

$$Y(P' + s, v'' + T) = Y(P', v'')$$
$$+2 \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx + Y(s, T).$$

Since

$$\int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx$$
$$= \int_\Gamma \left[\begin{pmatrix} \omega v' \\ \nabla P'' \end{pmatrix} \cdot \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \nabla \cdot v' \\ \omega P'' \end{pmatrix} \cdot \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx$$
$$= \int_\Gamma \left[\omega v' \cdot \nabla s - \omega \nabla P'' \cdot T + \omega \nabla \cdot v' s - \omega P'' \nabla \cdot T \right] dx$$
$$= \int_\Gamma \left[\omega \nabla \cdot (s v') - \omega \nabla \cdot (P'' T) \right] dx = \int_{\partial\Gamma} \left[\omega s v' \cdot n - \omega P'' T \cdot n \right] dS = 0$$

because of the homogeneous boundary conditions satisfied by s and T, we have that

$$Y(P' + s, v'' + T) = Y(P', v'') + Y(s, T) \geq Y(P', v''),$$

so (P', v'') minimizes Y over all functions satisfying the same boundary conditions.

Conversely, if (P', v'') minimizes Y over all functions satisfying the same boundary conditions, then define a function $\varphi : \mathbb{R} \to \mathbb{R}$ by

$$\varphi(t) = Y(P' + ts, v'' + tT),$$

where s and T are as before, and let

$$\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} = \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \text{ and } \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} = \mathcal{K} \begin{pmatrix} \omega P' \\ -\omega \nabla \cdot v'' \end{pmatrix}.$$

Since φ has a minimum at $t = 0$, it must be true that

$$\begin{aligned} 0 = \varphi'(0) &= 2 \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx. \\ &= \int_\Gamma \left[\begin{pmatrix} A_1 \\ A_2 \end{pmatrix} \cdot \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} B_1 \\ B_2 \end{pmatrix} \cdot \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx \\ &= \int_\Gamma \left[A_1 \cdot \nabla s - \omega A_2 \cdot T + \omega B_1 s - B_2 \nabla \cdot T \right] dx. \end{aligned}$$

Integrating by parts and using the homogeneous boundary conditions satisfied by s and T, we have

$$0 = \int_\Gamma \left[(-\nabla \cdot A_1 + \omega B_1) s + (-\omega A_2 + \nabla B_2) \cdot T \right] dx,$$

so it must be that the vector

$$\begin{pmatrix} A_1 \\ \omega B_1 \\ \omega A_2 \\ B_2 \end{pmatrix}$$

satisfies the same differential constraint as the vector on the right-hand side of the constitutive relation (4.1), namely, that the second component is the divergence of the first and the third component is the gradient of the fourth. In particular, we have found that by applying the constitutive relation to the vector $(\nabla P', -\omega v'', P', -\omega \nabla \cdot v'')^T$, we get a vector that satisfies the correct differential constraint, so the pair (P', v'') that minimizes Y over all such pairs satisfying the same boundary conditions must be a solution to the Helmholtz equation.

4.3 Rotation

It is important to note that the requirements (4.3) on ρ and κ must be satisfied in order for the minimization variational principles to remain valid. Unfortunately, one consequence of this requirement is that the variational principles do not apply to the Helmholtz equation with real coefficients. However, the observation is made in [37] that such a problem can be rotated to that the coercivity bounds hold. To accomplish this, we fix an angle θ, and multiply the Helmholtz equation through by $e^{-i\theta}$ to obtain

$$-\nabla \cdot (e^{i\theta}\rho)^{-1}\nabla P + \frac{\omega^2}{e^{i\theta}\kappa}P = 0.$$

In effect, we are replacing the old coefficients ρ and κ with new coefficients $e^{i\theta}\rho$ and $e^{i\theta}\kappa$, without changing the solution of the equation. Care should be taken that the boundary condition satisfied by v should also be rotated accordingly.

For example, in solving the Helmholtz equation with coefficients $\rho = 1$ and $\kappa = -1$, one might apply the rotation $\theta = \pi/2$ so that $e^{i\theta}\rho = i$ and $e^{i\theta}\kappa = -i$. Unfortunately, this process is not always effective, such as in a problem where $\rho = \kappa = 1$.

CHAPTER 5

BOUNDARY CONDITIONS

Before outlining the numerical method, it is important to note that the variational principles of the last chapter can be used to solve the Helmholtz equation with several sets of boundary conditions, as was noticed by Milton and Willis in [38]. In the next sections we will see that each of these different sets of boundary conditions can be realized by properly modifying the functional Y from the last chapter.

5.1 Essential Boundary Conditions

As we saw in the last chapter, in order to find (P', v'') of the solution to the boundary value problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P' = P_0' & \text{on } \partial\Gamma \\ v'' \cdot n = v_0'' \cdot n & \text{on } \partial\Gamma, \end{cases}$$

we minimize the functional

$$Y(P', v'') = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \right] dx$$

over all functions in the admissible class

$$\mathcal{A} = \left\{ (P', v'') \in H^1(\Gamma) \times H(\mathrm{div}, \Gamma) : P' = P_0' \text{ and } v'' \cdot n = v_0'' \cdot n \text{ on } \partial\Gamma \right\}.$$

One way to accomplish this is to minimize $Y(\psi_R + P', \varphi_I + v'')$ over $(P', v'') \in H_0^1(\Gamma) \times H_0(\mathrm{div}, \Gamma)$, where ψ_R and φ_I satisfy $\psi_R = P_0'$ and $\varphi_I \cdot n = v_0'' \cdot n$ on $\partial\Gamma$. Unfortunately, these boundary conditions are not usually encountered in practice, so it is important to be able to modify the functional Y to handle more usual boundary conditions, such as Dirichlet or Neumann conditions. The first step is to define a minimization functional to solve for the natural boundary conditions.

5.2 Natural Boundary Conditions

Instead of specifying boundary conditions on P' and v'', we can specify boundary conditions on their dual variables P'' and v' and solve the boundary value problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P'' = P_0'' & \text{on } \partial\Gamma \\ v' \cdot n = v_0' \cdot n & \text{on } \partial\Gamma \end{cases}$$

If (P'', v') are parts of a solution to the problem above, then for any choice of functions $s \in H^1(\Gamma)$ and $T \in H(\text{div}, \Gamma)$, we have

$$0 = \int_\Gamma \left[-\omega(-\nabla \cdot v' + \nabla \cdot v')s - \omega(\nabla P'' - \nabla P'') \cdot T \right] dx$$

$$= \int_\Gamma \left[-\omega v' \cdot \nabla s - \omega \nabla \cdot v' s - \omega \nabla P'' \cdot T - \omega P'' \nabla \cdot T \right] dx + \int_{\partial\Gamma} \left[\omega s v' \cdot n + \omega T \cdot n P'' \right] dS$$

$$= \int_\Gamma \left[\begin{pmatrix} -\omega v' \\ \nabla P'' \end{pmatrix} \cdot \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} -\nabla \cdot v' \\ \omega P'' \end{pmatrix} \cdot \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx + \int_{\partial\Gamma} \left[\omega s v' \cdot n + \omega T \cdot n P'' \right] dS$$

$$= \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega P \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx + \omega \int_{\partial\Gamma} \left[s v' \cdot n + T \cdot n P'' \right] dS. \tag{5.1}$$

This is just the weak form of the Euler-Lagrange equation for the variational problem

$$\inf_{(P', v'') \in H^1(\Gamma) \times H(\text{div}, \Gamma)} \tilde{Y}(P', v''),$$

where

$$\tilde{Y}(P', v'') = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \right] dx + 2\omega \int_{\partial\Gamma} \left[P' v_0' \cdot n + v'' \cdot n P_0'' \right] dS. \tag{5.2}$$

We will refer to these boundary conditions as the natural boundary conditions for the complex Helmholtz equation. These still are not boundary conditions that are often encountered, but we can combine the problem formulations for the essential and natural boundary conditions to derive minimization functionals for the Dirichlet and Neumann boundary value problems.

5.3 Dirichlet and Neumann Conditions

5.3.1 Dirichlet Conditions

In order to solve the Dirichlet boundary value problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P = P_0 & \text{on } \partial\Gamma, \end{cases}$$

we solve the variational problem

$$\inf_{(P',v'') \in H_0^1(\Gamma) \times H(\mathrm{div},\Gamma)} \tilde{Y}(P' + P_0', v'').$$

Since we are enforcing zero boundary values on the P', variable, we have that

$$\tilde{Y}(P' + P_0', v'') = \int_\Gamma \left[\begin{pmatrix} \nabla P_0' + \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P_0' + \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega(P_0' + P) \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega(P_0' + P') \\ -\nabla \cdot v'' \end{pmatrix} \right] dx + 2\omega \int_{\partial\Gamma} v'' \cdot n P_0'' \, dS.$$

5.3.2 Neumann Conditions

The minimization functional for the Neumann problem is derived in an analogous manner. To solve the problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ v \cdot n = v_0 \cdot n & \text{on } \partial\Gamma, \end{cases}$$

we solve the variational problem

$$\inf_{(P',v'') \in H^1(\Gamma) \times H_0(\mathrm{div},\Gamma)} \tilde{Y}(P', v'' + v_0'').$$

In this case, since we are enforcing zero normal component on v'', we have that

$$\tilde{Y}(P', v'' + v_0'') = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega(v'' + v_0'') \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega(v'' + v_0'') \end{pmatrix} + \begin{pmatrix} \omega P \\ -\nabla \cdot v'' - \nabla \cdot v_0'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' - \nabla \cdot v_0'' \end{pmatrix} \right] dx + 2\omega \int_{\partial\Gamma} P' v_0' \cdot n \, dS.$$

CHAPTER 6

THE ERROR BOUND

In this chapter we give a bound on the error incurred by solving any of the minimization problems above over a finite dimensional subspace of the specified Sobolev spaces. We will give a more detailed account of exactly what the finite dimensional space looks like later on; in this chapter all that will matter is the highest degree of polynomials that the finite dimensional space (referred to as the finite element space) contains. We will use the Bramble-Hilbert lemma to give a bound on the error.

In this chapter we will return to the notation of $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{L}$ and drop the primes used to denote real and imaginary parts. Note that what follows applies to any of the boundary value problems discussed previously, since the bounds depend only on the corresponding bilinear form. Throughout this chapter, C is a constant independent of the solution (P, v) and the grid spacing h.

6.1 Bilinear Form

Define the bilinear form B by

$$B(P, v; s, T) = \int_\Gamma \begin{pmatrix} \mathcal{F} \\ -\mathcal{G} \end{pmatrix} \cdot \mathcal{L} \begin{pmatrix} \mathcal{S} \\ -\mathcal{T} \end{pmatrix} \, dx, \tag{6.1}$$

where as before, $\mathcal{F} = (\nabla P, P)^T$, $\mathcal{G} = (-i\omega v, -i\omega \nabla \cdot v)^T$, and $\mathcal{S}$ and $\mathcal{T}$ are generated from test function $s \in H^1(\Gamma)$ and $T \in H(\mathrm{div}, \Gamma)$ in the same fashion. Assume that there exist constants $\gamma_1, \gamma_2 > 0$ such that $\mathcal{L} > \gamma_2 I$ and that $[\mathcal{L}(x)]_{ij} \leq \gamma_1$ for a.e. $x \in \Gamma$. Let $V = H_0^1(\Gamma) \times H(\mathrm{div}, \Gamma)$, endowed with the norm

$$\|(u, G)\|_V = (\|u\|^2_{H^1(\Gamma)} + \|G\|^2_{H(\mathrm{div},\Gamma)})^{\frac{1}{2}}.$$

Then it follows immediately from (6.1) that

$$B(P, v; s, T) \leq C\gamma_1 \|(P, v)\|_V \|(s, T)\|_V \tag{6.2}$$

and

$$B(P,v;P,v) \geq \gamma_2 \|(P,v)\|_V^2. \tag{6.3}$$

6.2 Minimization Inequality

Define the energy by

$$f(s,T) = \frac{1}{2}B(s,T;s,T) - F(s,T),$$

where $F : H^1(\Gamma) \times H(\mathrm{div},\Gamma) \to \mathbb{R}$ (in practice, F is usually composed of terms resulting from an inhomogeneous term and enforcement of the desired boundary conditions). If (u,G) is the minimizer of the energy, then this pair must satisfy the Euler-Lagrange equation

$$B(P,v;s,T) = F(s,T) \quad \forall s \in H_0^1(\Gamma),\ \forall\ T \in H(\mathrm{div},\Gamma),$$

so that

$$f(s,T) = f(P,v) + \frac{1}{2}B(P-s,v-T;P-s,v-T) \quad \forall\ s \in H_0^1(\Gamma)\ \forall\ T \in H(\mathrm{div},\Gamma).$$

Consider a finite dimensional subspace $V_N = V_{N1} \times V_{N2}$ of V, where V_{N1} is a finite dimensional subspace of $H^1(\Gamma)$ and V_{N2} is a finite dimensional subspace of $H(\mathrm{div},\Gamma)$. If (P_N, v_N) is such that

$$f(P_N,v_N) = \min_{(s,T)\in V_N} f(s,T),$$

then

$$[B(P-P_N,v-v_N;P-P_N,v-v_N)]^{\frac{1}{2}} = \min_{(s,T)\in V_N} [B(P-s,v-T;P-s,v-T)]^{\frac{1}{2}}.$$

Inequalities (6.2) and (6.3) imply that

$$\sqrt{\gamma_2}\|(s,T)\|_V \leq \sqrt{B(s,T;s,T)} \leq C\sqrt{\gamma_1}\|(s,T)\|_V \quad \forall\ (s,T) \in V,$$

so we have

$$\sqrt{\gamma_2}\|(P,v)-(P_N,v_N)\|_V \leq \min_{(s,T)\in V_N} C\sqrt{\gamma_1}\|(P,v)-(s,T)\|_V. \tag{6.4}$$

Let F_1 be the orthogonal projection from $H^1(\Gamma)$ onto V_{N1}. Since F_1 is an orthogonal projection, it has $\|F_1\|_{B(H^1(\Gamma),H^1(\Gamma))} = 1$, where $B(H^1(\Gamma),H^1(\Gamma))$ is the set of bounded

linear functions from $H^1(\Gamma)$ to $H^1(\Gamma)$. Also, define an operator $F_2 : H(\mathrm{div}, \Gamma) \to V_{N2}$ by the solution of the variational inequality

$$\langle F_2 G, Q - F_2 G \rangle_{L^2(\Gamma, \mathbb{R}^d)} \geq \langle G, Q - F_2 G \rangle_{L^2(\Gamma, \mathbb{R}^d)} \ \forall\ Q \in E_G,$$

over the set $E_G = \{v \in V_{N2} : \|\nabla \cdot v\|_{L^2(\Gamma)} \leq \|\nabla \cdot G\|_{L^2(\Gamma)}\}$, which is a closed, convex subset of $L^2(\Gamma, \mathbb{R}^d)$. We then have

$$\|F_2 G\|^2_{L^2(\Gamma, \mathbb{R}^d)} = \langle F_2 G, F_2 G \rangle_{L^2(\Gamma, \mathbb{R}^d)} \leq \langle G, F_2 G \rangle_{L^2(\Gamma, \mathbb{R}^d)} \leq \|G\|_{L^2(\Gamma, \mathbb{R}^d)} \|F_2 G\|_{L^2(\Gamma, \mathbb{R}^d)}.$$

If we take $s = F_1 P$ and $T = F_2 v$ in (6.4), then we have

$$\|(P, v) - (P_N, v_N)\|_V \leq C \|(P - F_1 P, v - F_2 v)\|_V. \tag{6.5}$$

6.2.1 Seminorm bounds

We will discretize the domain Γ by by subdividing it into smaller regions, each of which can be seen as a suitable shifting and scaling of a "reference element". More precisely, if $\hat{e}$ is our reference element, there exist affine changes of variables $F_l(x) = Bx + x_l$ such that $F_l(\hat{e}) = e_l$, where e_l is the lth element (subdivision) in the finite element decomposition of Γ. In the case of rectangular elements in $\mathbb{R}^d$, for example, we can take $\hat{e} = (0, 1)^d$, and then we have $B = hI_d$. In this section a hat will denote the corresponding function defined over the reference element.

Let

$$[u, w]_s = \sum_{|\alpha| = s} \int_{\hat{e}} D^\alpha u \cdot D^\alpha w \ dx \quad \text{and} \quad |w|_s^2 = [w, w]_s, \tag{6.6}$$

where for vector functions we define

$$D^\alpha w = \begin{pmatrix} D^\alpha w_1 \\ D^\alpha w_2 \\ \vdots \\ D^\alpha w_d \end{pmatrix}.$$

From [12] we get the inequalities

$$\begin{aligned} &c^{-1} h^{s - \frac{d}{2}} |w|_{s, e_l} \leq |\hat{w}|_s \leq c h^{s - \frac{d}{2}} |w|_{s, e_l} \\ &h^{s + \frac{d}{2} - 1} |q|_{s, e_l} \leq |\hat{q}|_s \leq h^{s + \frac{d}{2} - 1} |q|_{s, e_l} \\ &h^{s + \frac{d}{2}} |\nabla \cdot q|_{s, e_l} \leq |\nabla \cdot \hat{q}|_s \leq h^{s + \frac{d}{2}} |\nabla \cdot q|_{s, e_l} \end{aligned} \tag{6.7}$$

for scalar functions w and vector functions q, where $w = \hat{w} \circ F^{-1}$ and $q = \hat{q} \circ F^{-1}$ and $|\cdot|_{s, e_l}$ denotes (6.6) with e_l in place of $\hat{e}$.

We now recall the following lemma from [3], which will be used in what follows.

Lemma 2 (Bramble-Hilbert Lemma) *For some region $\Omega \subset \mathbb{R}^2$ and some integer $k \geq -1$, let there be given a bounded linear functional*

$$f : H^{k+1}(\Omega) \to \mathbb{R},$$

satisfying $|f(u)| \leq \delta \|u\|_{H^{k+1}(\Omega)}$ for all $u \in H^{k+1}(\Omega)$ for some δ independent of u. Suppose that $f(u) = 0$ for all $u \in P_k(\bar{\Omega})$. Then there exists a constant C, dependent only on Ω such that

$$|f(u)| \leq C\delta |u|_{k+1}, \quad u \in H^{k+1}(\Omega).$$

Let us suppose that $\hat{P} \in H^{k+1}(\hat{e})$ and $\hat{v} \in H^j(\mathrm{div}, \hat{e}) = \{q \in H^j(\hat{e}, \mathbb{R}^d) : \nabla \cdot q \in H^j(\hat{e})\}$. For fixed elements $w \in H^s(\hat{e})$ and $Q \in H^s(\mathrm{div}, \hat{e})$ define the functionals

$$f_1(u) = [u - F_1 u, w]_s, \ f_2(G) = [G - F_2 G, Q]_0, \ f_3(\nabla \cdot G) = [\nabla \cdot G - \nabla \cdot F_2 G, \nabla \cdot Q]_0,$$

where $s = 0$ or $s = 1$. Then, since

$$|f_1(u)| \leq |u - F_1 u|_s |w|_s \leq (|u|_s + |F_1 u|_s)|w|_s \leq (\|u\|_{H^1(\Gamma)} + \|F_1 u\|_{H^1(\Gamma)})|w|_s$$

$$\leq 2\|u\|_{H^1(\Gamma)}|w|_s \leq 2\|u\|_{H^{k+1}(\Gamma)}|w|_s,$$

$$|f_2(G)| \leq |G - F_2 G|_0 |Q|_0 \leq (|G|_0 + |F_2 G|_0)|Q|_0 = (\|G\|_{L^2(\Gamma,\mathbb{R}^d)} + \|F_2 G\|_{L^2(\Gamma,\mathbb{R}^d)})|Q|_0$$

$$\leq 2\|G\|_{L^2(\Gamma),\mathbb{R}^d)}|Q|_0 \leq \|G\|_{H^j(\Gamma,\mathbb{R}^d)}|Q|_0,$$

$$|f_3(\nabla \cdot \ G)| \leq |\nabla \cdot G - \nabla \cdot F_2 G|_0 |\nabla \cdot Q|_0 \leq (|\nabla \cdot G|_0 + |\nabla \cdot F_2 G|_0)|\nabla \cdot Q|_0$$

$$= (\|\nabla \cdot G\|_{L^2(\Gamma)} + \|\nabla \cdot F_2 G\|_{L^2(\Gamma)})|\nabla \cdot Q|_0 \leq 2\|\nabla \cdot G\|_{L^2(\Gamma)}|\nabla \cdot Q|_0 \leq 2\|\nabla \cdot G\|_{H^j(\Gamma)}|\nabla \cdot Q|_0,$$

and $F_1 u = u$ for polynomials in V_{N1} and $F_2 G = G$ for vectors of polynomials from V_{N2}, we can apply the Bramble-Hilbert lemma to find that there exists a constant such that

$$|f_1(\hat{P})| \leq C|w|_s |\hat{P}|_{k+1}, \ |f_2(\hat{v})| \leq C|Q|_0 |\hat{v}|_j, \ |f_3(\nabla \cdot \hat{v})| \leq C|\nabla \cdot Q|_0 |\nabla \cdot \hat{v}|_j,$$

as long as k and j are small enough so that all polynomials of degree less than or equal to k are contained in the span of the basis functions representing $\hat{u}$ and all

polynomials of degree less than or equal to j are contained in the span of the basis functions representing $\hat{G}$. For the elements used in the implementation to follow, we will have $j = k = 1$. By choosing $w = \hat{P} - F_1\hat{P}$ and $Q = \hat{v} - F_2\hat{v}$, we find that

$$|\hat{P} - F_1\hat{P}|_s \leq C|\hat{P}|_{k+1},\ |\hat{v} - F_2\hat{v}|_0 \leq C|\hat{v}|_j,\ |\nabla\cdot\hat{v} - \nabla\cdot F_2\hat{v}| \leq C|\nabla\cdot\hat{v}|_j.$$

Employing (6.7), we find that for $h \leq 1$,

$$|P - F_1P|_{s,e_l} \leq Ch^{\frac{d}{2}-s}|\hat{P} - F_1\hat{P}|_s \leq Ch^{\frac{d}{2}-s}|\hat{P}|_{k+1} \leq Ch^{k-s+1}|P|_{k+1,e_l},$$

$$|v - F_2v|_{0,e_l} \leq h^{1-\frac{d}{2}}|\hat{v} - F_2\hat{v}|_0 \leq h^{1-\frac{d}{2}}C|\hat{v}|_j \leq Ch^j|v|_{j,e_l},$$

$$|\nabla\cdot v - \nabla\cdot F_2v|_{0,e_l} \leq h^{-\frac{d}{2}}|\nabla\cdot\hat{v} - \nabla\cdot F_2\hat{v}|_0 \leq h^{-\frac{d}{2}}C|\nabla\cdot\hat{v}|_j \leq Ch^j|\nabla\cdot v|_{j,e_l}.$$

Returning to inequality (6.5), we find that

$$\|(P,v) - (P_N,v_N)\|_V^2 \leq C\|(P,v) - (F_1P,F_2v)\|_V^2$$

$$= C\sum_{l=1}^{(N-1)^2}\left[|P - F_1P|_{0,e_l}^2 + |P - F_1P|_{1,e_l}^2 + |v - F_2v|_{0.e_l}^2 + |\nabla\cdot v - \nabla\cdot F_2v|_{0,e_l}^2\right]$$

$$\leq C\sum_{l=1}^{(N-2)^2}\left[h^{2k+2}|P|_{k+1,e_l}^2 + h^{2k}|P|_{k+1,e_l}^2 + h^{2j}|v|_{j,e_l}^2 + h^{2j}|\nabla\cdot v|_{j.e_l}^2\right]$$

$$\leq C(h^{2k}|P|_{k+1,\Gamma}^2 + h^{2j}(|v|_{j,\Gamma}^2 + |\nabla\cdot v|_{j,\Gamma}^2)).$$

Let $P_k(\bar{\Gamma})$ denote all polynomials of degree less than or equal to k on $\bar{\Gamma}$. We have now proved

Theorem 7 *If the solution $(P,v) \in H^{k+1}(\Gamma) \times H^{j+1}(div,\Gamma)$ and the finite element subspace used in the numerical method contains $P_k(\bar{\Gamma}) \times P_j(\bar{\Gamma})) \times P_j(\bar{\Gamma})$, then there is a constant C such that the error satisfies*

$$\|(P,v) - (P_N,v_N)\|_V^2 \leq C(h^{2k}|P|_{k+1,\Gamma}^2 + h^{2j}(|v|_{j,\Gamma}^2 + |\nabla\cdot v|_{j,\Gamma}^2)),$$

where $h \leq 1$ is the grid spacing.

CHAPTER 7

THE FINITE ELEMENT METHOD

For our model in the development of the numerical method, we will focus on the Dirichlet problem with functional

$$\hat{Y}(P', v'') = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \right] dx$$

$$+2 \int_{\partial\Gamma} \omega v'' \cdot n P'' \, dS,$$

where $\mathcal{R}$ and $\mathcal{K}$ are as previously defined. By taking the first variation of $\hat{Y}$, (see Section 4.2), we find that the Euler-Lagrange equation is

$$0 = \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx + \int_{\partial\Gamma} \omega T \cdot n P'' \, dS \tag{7.1}$$

for any $s \in H_0^1(\Gamma)$ and any $T \in H(\mathrm{div}, \Gamma)$.

7.1 Implementation of the Finite Element Method

Our goal is to test the efficacy of this new variational principle, so we will use a relatively simple implementation with a rectangular grid. Also, for simplicity, let us assume that $d = 2$ and $\Gamma = (0,1)^2$. In order to find a numerical solution for P', we introduce an $N \times N$ computational grid with equally spaced nodes (x_j, y_t) for $t, j = 1, 2, \ldots, N$ and grid spacing $h = 1/(N-1)$. We also introduce the finite element spaces

$$\begin{aligned}
\Psi &= \mathrm{span}\left\{ \left(1 - \tfrac{|x-x_j|}{h}\right)\left(1 - \tfrac{|y-y_t|}{h}\right) \chi_{tj} : 2 \le t, j \le N-1 \right\} \\
\Phi_1 &= \mathrm{span}\left\{ \begin{pmatrix} 1 - \frac{|x-x_j|}{h} \\ 0 \end{pmatrix} \zeta^{tj} : 1 \le j \le N,\ 1 \le t \le N-1 \right\}, \\
\Phi_2 &= \mathrm{span}\left\{ \begin{pmatrix} 0 \\ 1 - \frac{|y-y_t|}{h} \end{pmatrix} \zeta_{tj} : 1 \le t \le N,\ 1 \le j \le N-1 \right\}
\end{aligned}$$

where

$$\chi_{tj}(x,y) = \begin{cases} 1 & \text{if } |x-x_j|, |y-y_t| \le h \\ 0 & \text{otherwise} \end{cases}$$
$$\zeta^{tj}(x,y) = \begin{cases} 1 & \text{if} |x-x_j| \le h \text{ and } 0 \le y_t - y \le h \\ 0 & \text{otherwise} \end{cases} .$$
$$\zeta_{tj}(x) = \begin{cases} 1 & \text{if } |y-y_t| \le h \text{ and } 0 \le x - x_j \le h \\ 0 & \text{otherwise} \end{cases}$$

The basis functions in Ψ are simple piecewise bilinear elements. The basis functions in Φ_1 and Φ_2 are the so-called edge elements or Raviart-Thomas elements (see [12]).

We can re-index these elements with a single index by setting

$$\psi_k = \left(1 - \tfrac{|x-x_j|}{h}\right)\left(1 - \tfrac{|y-y_t|}{h}\right)\chi_{tj}, \text{ where } k = (t-2)(N-2) + j + 1,\ k = 1, \ldots, (N-2)^2,$$
$$\phi_{1k} = \begin{pmatrix} 1 - \frac{|x-x_j|}{h} \\ 0 \end{pmatrix} \zeta^{tj} \text{ where } k = (t-1)N + j,\ k = 1, \ldots, N(N-1),$$
$$\phi_{2k} = \begin{pmatrix} 0 \\ 1 - \frac{|y-y_t|}{h} \end{pmatrix} \zeta_{tj} \text{ where } k = (t-1)(N-1) + j,\ k = 1, \ldots, N(N-1).$$

We assume that our finite element solution has the form

$$\begin{pmatrix} P' \\ v'' \end{pmatrix} = \begin{pmatrix} \psi_R + \sum_{k=1}^{(N-2)^2} \delta_k \psi_k \\ \sum_{k=1}^{N(N-1)} \beta_k \phi_{1k} + \sum_{k=1}^{N(N-1)} \gamma_k \phi_{2k} \end{pmatrix}.$$

Here ψ_R is any function that satisfies the desired Dirichlet boundary condition for P'. Making this substitution into (7.1), we get

$$\int_\Gamma \left[\begin{pmatrix} \sum \delta_k \nabla \psi_k \\ -\omega \sum \beta_k \phi_{1k} - \omega \sum \gamma_k \phi_{2k} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} \right.$$
$$\left. + \begin{pmatrix} \omega \sum \delta_k \psi_k \\ -\sum \beta_k \nabla \cdot \phi_{1k} - \sum \gamma_k \nabla \cdot \phi_{2k} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx$$

$$= -\int_\Gamma \left[\begin{pmatrix} \nabla \psi_0 \\ 0 \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ -\omega T \end{pmatrix} + \begin{pmatrix} \omega \psi_0 \\ 0 \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx$$
$$- \int_\Gamma \left[\omega \nabla \psi_I \cdot T + \omega \psi_I \nabla \cdot T \right] dx,$$

where we have used the divergence theorem on the boundary integral, ψ_I is any function on Γ satisfying the desired Dirichlet boundary condition for P'', and $s \in H_0^1(\Gamma),\ T \in H(\mathrm{div}, \Gamma)$ are arbitrary. In particular, this must hold when

$$s = \psi_k,\ T = 0 \text{ for } k = 1, \ldots, (N-2)^2$$

$$s = 0,\ T = \phi_{1k} \text{ for } k = 1, \ldots, N(N-1)$$

$$s = 0,\ T = \phi_{2k} \text{ for } k = 1, \ldots, N(N-1).$$

This gives rise to a system of equations of the form $A\alpha = b$, where A has the block form

$$A = \begin{pmatrix} A_1 & A_4 & A_6 \\ A_4 & A_2 & A_5 \\ A_6 & A_5 & A_3 \end{pmatrix} \tag{7.2}$$

and the blocks have entries

$$\begin{aligned}
(A_1)_{tj} &= \int_\Gamma \left[\begin{pmatrix} \nabla\psi_t \\ 0 \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla\psi_j \\ 0 \end{pmatrix} + \begin{pmatrix} \omega\psi_t \\ 0 \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega\psi_j \\ 0 \end{pmatrix} \right] dx \\
(A_2)_{tj} &= \int_\Gamma \left[\begin{pmatrix} 0 \\ -\omega\phi_{1t} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ -\omega\phi_{ij} \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{1t} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{1j} \end{pmatrix} \right] dx \\
(A_3)_{tj} &= \int_\Gamma \left[\begin{pmatrix} 0 \\ -\omega\phi_{2t} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ -\omega\phi_{2j} \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{2t} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{2j} \end{pmatrix} \right] dx \\
(A_4)_{tj} &= \int_\Gamma \left[\begin{pmatrix} 0 \\ -\omega\phi_{1t} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla\psi_j \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{1t} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega\psi_j \\ 0 \end{pmatrix} \right] dx \\
(A_5)_{tj} &= \int_\Gamma \left[\begin{pmatrix} 0 \\ -\omega\phi_{2t} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ -\omega\phi_{1j} \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{2t} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{1j} \end{pmatrix} \right] dx \\
(A_6)_{tj} &= \int_\Gamma \left[\begin{pmatrix} 0 \\ -\omega\phi_{2t} \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla\psi_j \\ 0 \end{pmatrix} + \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{2t} \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega\psi_j \\ 0 \end{pmatrix} \right] dx.
\end{aligned} \tag{7.3}$$

The right-hand side vector b is partitioned as

$$b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix},$$

where

$$\begin{aligned}
(b_1)_k = &- \int_\Gamma \left[\begin{pmatrix} \nabla\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla\psi_k \\ 0 \end{pmatrix} + \begin{pmatrix} \omega\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega\psi_k \\ 0 \end{pmatrix} \right] dx \\
(b_2)_k = &- \int_\Gamma \left[\begin{pmatrix} \nabla\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ -\omega\phi_{1k} \end{pmatrix} + \begin{pmatrix} \omega\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{1k} \end{pmatrix} \right] dx \\
&- \int_\Gamma \left[\omega\nabla\psi_I \cdot \phi_{1k} + \omega\psi_I \nabla\cdot\phi_{1k} \right] dx \\
(b_3)_k = &- \int_\Gamma \left[\begin{pmatrix} \nabla\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ -\omega\phi_{2k} \end{pmatrix} + \begin{pmatrix} \omega\psi_R \\ 0 \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ -\nabla\cdot\phi_{2k} \end{pmatrix} \right] dx \\
&- \int_\Gamma \left[\omega\nabla\psi_I \cdot \phi_{2k} + \omega\psi_I \nabla\cdot\phi_{2k} \right] dx.
\end{aligned} \tag{7.4}$$

The method for solving for P' and v'' can be easily modified to solve for P'' and v'. In this case the weak equation is

$$\int_\Gamma \left[\begin{pmatrix} \nabla P'' \\ \omega v' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla s \\ \omega T \end{pmatrix} + \begin{pmatrix} -\omega P'' \\ -\nabla \cdot v' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} -\omega s \\ -\nabla \cdot T \end{pmatrix} \right] dx + \int_{\partial\Gamma} \omega T \cdot n P' \, dS = 0,$$

and all the methods above still apply. In fact, to obtain the new matrix for this formulation, we simply change the signs of the blocks A_4 and A_6, and the changes in b are mostly reversing signs and the roles of the two auxiliary functions ψ_R and ψ_I.

7.2 Conditioning

Perhaps the greatest numerical advantage to having a minimization formulation for the Helmholtz equation is that the matrix produced by the finite element method is symmetric positive definite. This allows for the use of methods such as the conjugate gradient method to solve the system. Of course, the use of a preconditioning matrix in the conjugate gradient method can speed up the convergence considerably, which is especially important when solving the relatively large sparse systems generated by the finite element approach outlined above.

In our approach, there are three basic types of elements used: bilinear elements, first component edge elements, and second component edge elements. Each of these types of elements interacts with all of the other types, and these interactions are what give rise to the blocks in (7.2). Assuming that interactions among similar element types are most important, we choose the block Jacobi preconditioner

$$M = \begin{pmatrix} A_1 & 0 & 0 \\ 0 & A_2 & 0 \\ 0 & 0 & A_3 \end{pmatrix}.$$

Among all block diagonal preconditioners of this form, this choice of M minimizes the condition number of $M^{-\frac{1}{2}} A M^{-\frac{1}{2}}$ to within a factor of 3 of its minimum [18].

As one of the steps in the preconditioned conjugate gradient method (PCG) [19], a system of the form $Mr = y$ must be solved. In order to make solving this problem more efficient, we precondition the matrix M and use conjugate gradient to solve this system as well. The preconditioner used in this inner implementation of PCG was an incomplete Choleski factorization of M. Figure 7.2 shows the distribution of the

eigenvalues of the matrix A before and after preconditioning for $N = 30$. In Figure 7.1, we see the how the number of PCG iterations grows with N for several error tolerances.

A key component in ensuring that the system $A\alpha = b$ is well conditioned is for the matrix $\mathcal{L}$ (or equivalently $\mathcal{R}$ and $\mathcal{K}$) to have a coercivity constant that is as large as possible. For this reason, we expect better numerical results when the eigenvalues of $\mathcal{L}$ are bounded well away from zero. In the case of the Helmholtz equation, the matrix Z is diagonal, say $Z = \text{diag}(c_1, \ldots, c_{d+1})$, which makes it possible to calculate the eigenvalues of $\mathcal{L}$. If D is an invertible matrix, then we may factor a block diagonal matrix

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

as

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \begin{pmatrix} I & B \\ 0 & D \end{pmatrix} \begin{pmatrix} A - BD^{-1}C & 0 \\ D^{-1}C & I \end{pmatrix},$$

which implies that

$$\det \begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det(D)\det(A - BD^{-1}C).$$

Therefore,

$$\det(\mathcal{L} - \lambda I) = (-1)^{d+1}\det \begin{pmatrix} (Z'')^{-1}Z' & (Z'')^{-1} - \lambda I \\ Z'' + Z'(Z'')^{-1}Z' - \lambda I & Z'(Z'')^{-1} \end{pmatrix}$$

$$= (-1)^{d+1}\det(Z'(Z'')^{-1})\det((Z'')^{-1}Z' + [-(Z')^{-1} + \lambda Z''(Z')^{-1}][Z'' + Z'(Z'')^{-1}Z' - \lambda I])$$

$$= (-1)^{d+1}\det(Z'(Z'')^{-1})\det(\lambda^2[-Z''(Z')^{-1}] + \lambda[(Z')^{-1} + Z''(Z')^{-1}Z'' + Z'] - (Z')^{-1}Z'').$$

In the case of diagonal Z, this implies that

$$\lambda = \frac{-a_j \pm \sqrt{a_j^2 - b_j^2}}{-b_j} \quad j = 1, \ldots, d+1,$$

where

$$a_j = \frac{1}{c_j'} + \frac{(c_j'')^2}{c_j'} + c_j' \text{ and } b_j = 2\frac{c_j''}{c_j'}.$$

If $Z' = 0$, then $\mathcal{L}$ is diagonal, and its eigenvalues are those of Z'' and $(Z'')^{-1}$.

The above analysis tells us that the finite element problem will be better conditioned for those problems where the coefficients ρ and κ are such that Z is close to Ii, i.e., $\rho = iI$ and $\kappa = -Ii$ (this would correspond to the limiting case where $a_j = b_j$). In many cases when we are presented with a problem where the coercivity constant for $\mathcal{L}$ is small, we can apply an appropriate rotation and scaling to the problem in order to get a finite element matrix that is better conditioned. By multiplying the problem through by a complex constant $re^{i\theta}$, we effectively replace Z with $re^{i\theta}Z$, so we should choose r and θ so that $re^{i\theta}Z$ is as close as possible to iI. However, this may not always be possible, for example, when an isotropic $\rho(x)$ oscillates between values in the upper half of the complex plane that are close to 1 and -1.

As can be seen in Figure 7.2, there are many eigenvalues of the coefficient matrix A that are relatively small in magnitude. Even after preconditioning, the problem persists. The eigenfunctions that correspond to these eigenvalues are often nearly constant in the interior of Γ and highly oscillatory near the boundary. Some preliminary work has already been done towards eliminating this grouping of small eigenvalues. Indications are that using a higher order finite element space to approximate the v variable may improve this situation dramatically, perhaps reducing the condition number of the coefficient matrix by half or more.

7.3 Numerical Results

As an example, we demonstrate the error bound on the problem with parameters $\rho = (-5+5i)I$, $\kappa = 4-4i$ and $\omega = 2$. A solution is $P(x, y) = e^{2ix-3y}$. In this example we took

$$\psi_R = \mathrm{Re}(e^{2ix-3y}) + \sin(\pi x)\sin(\pi y),\ \ \psi_I = \mathrm{Im}(e^{2ix-3y}) + \sin(\pi x)\cdot 3\sin(\pi y)$$

and solved the problem on grids with $N = 3, \ldots, 100$. Table 7.1 shows the error in the finite element solution for various values of N. The errors were calculated using the trapezoidal rule with function evaluations on a grid with size $N = 1500$. Figure 7.3 demonstrates the method on a problem with non-constant coefficients, where the dissipation in the material is higher inside a disk centered in the unit square. The boundary conditions for the real part are oscillatory, while the boundary conditions

for the imaginary part are simply an affine function. Figure 7.4 demonstrates the solution of a problem with the same material coefficients, but with the two materials layered together.

Table 7.1. Error vs. Grid Size

N	h	$\|(P - P_N, v - v_N)\|_V$
30	0.0345	6.6204×10^{-4}
40	0.0256	3.6613×10^{-4}
50	0.0204	2.3197×10^{-4}
60	0.0169	1.5997×10^{-4}
70	0.0145	1.1701×10^{-4}
80	0.0127	8.9044×10^{-5}
90	0.0112	7.0308×10^{-5}
100	0.0101	5.6867×10^{-5}

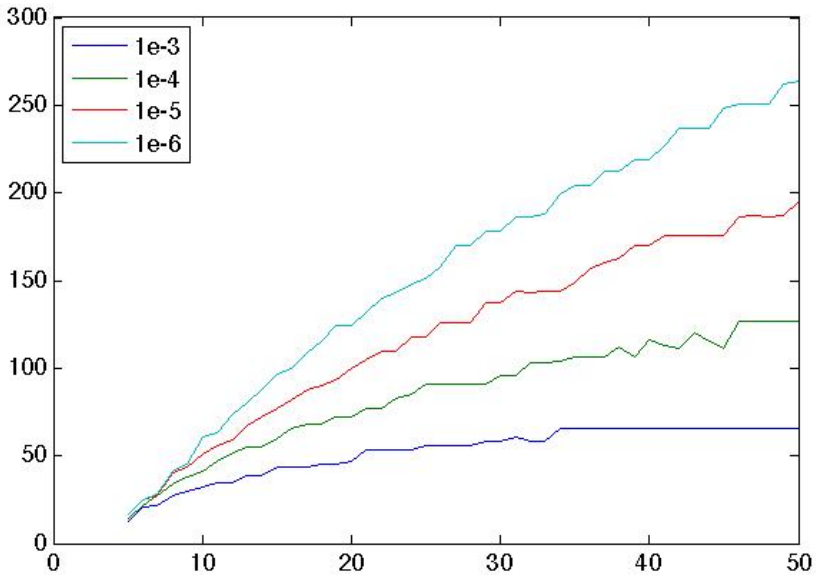

Figure 7.1. PCG Iterations

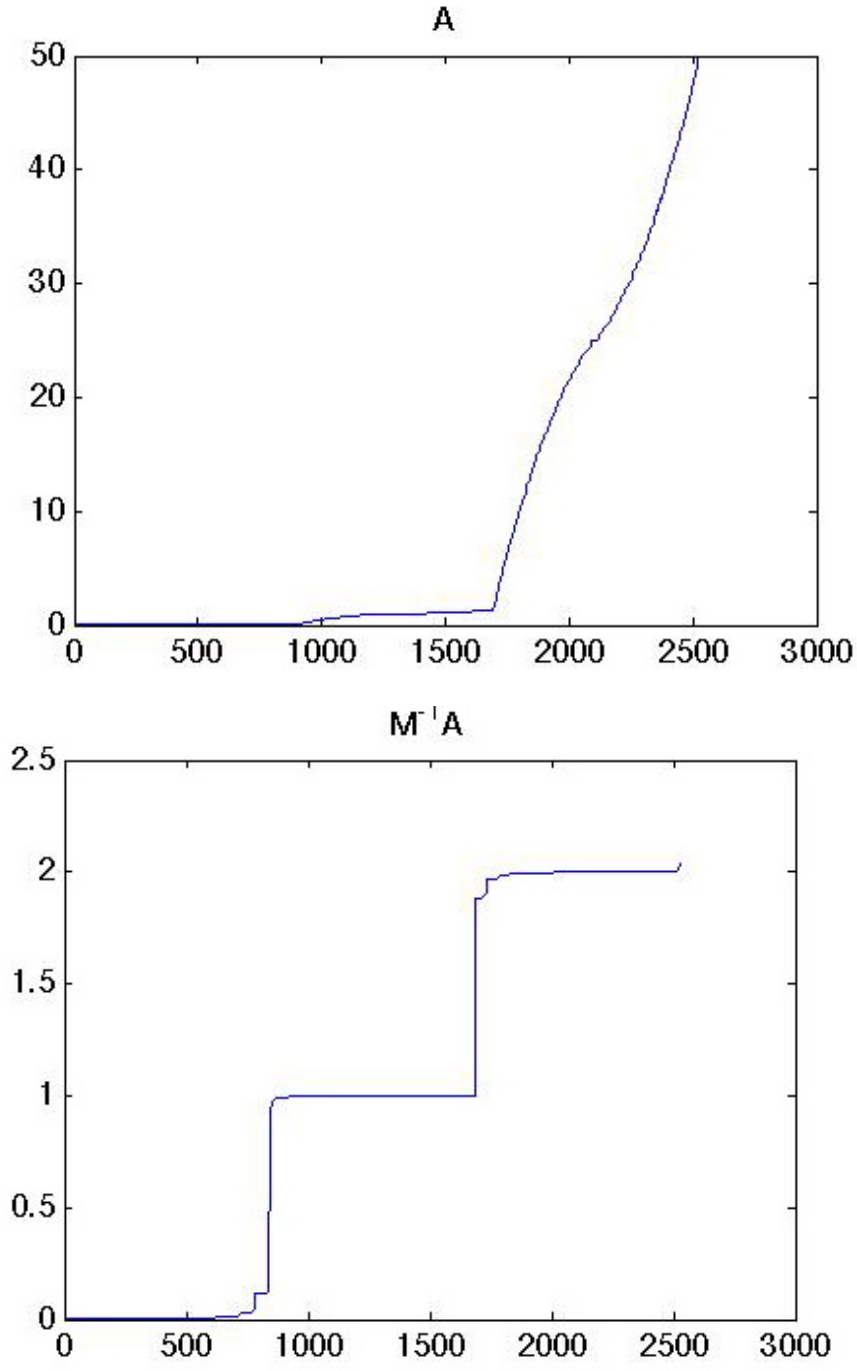

Figure 7.2. Eigenvalue Distribution

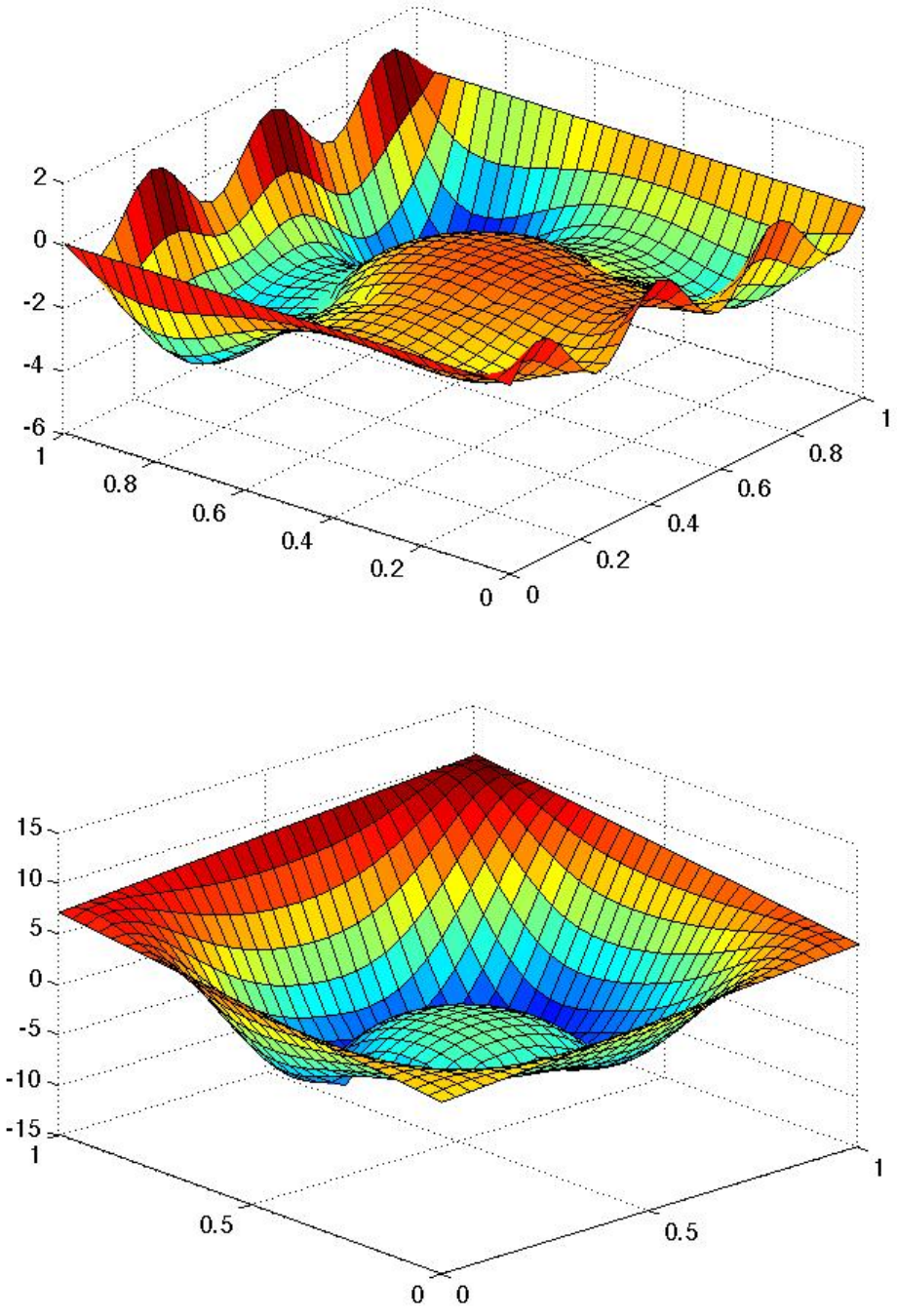

Figure 7.3. Circular Inclusion

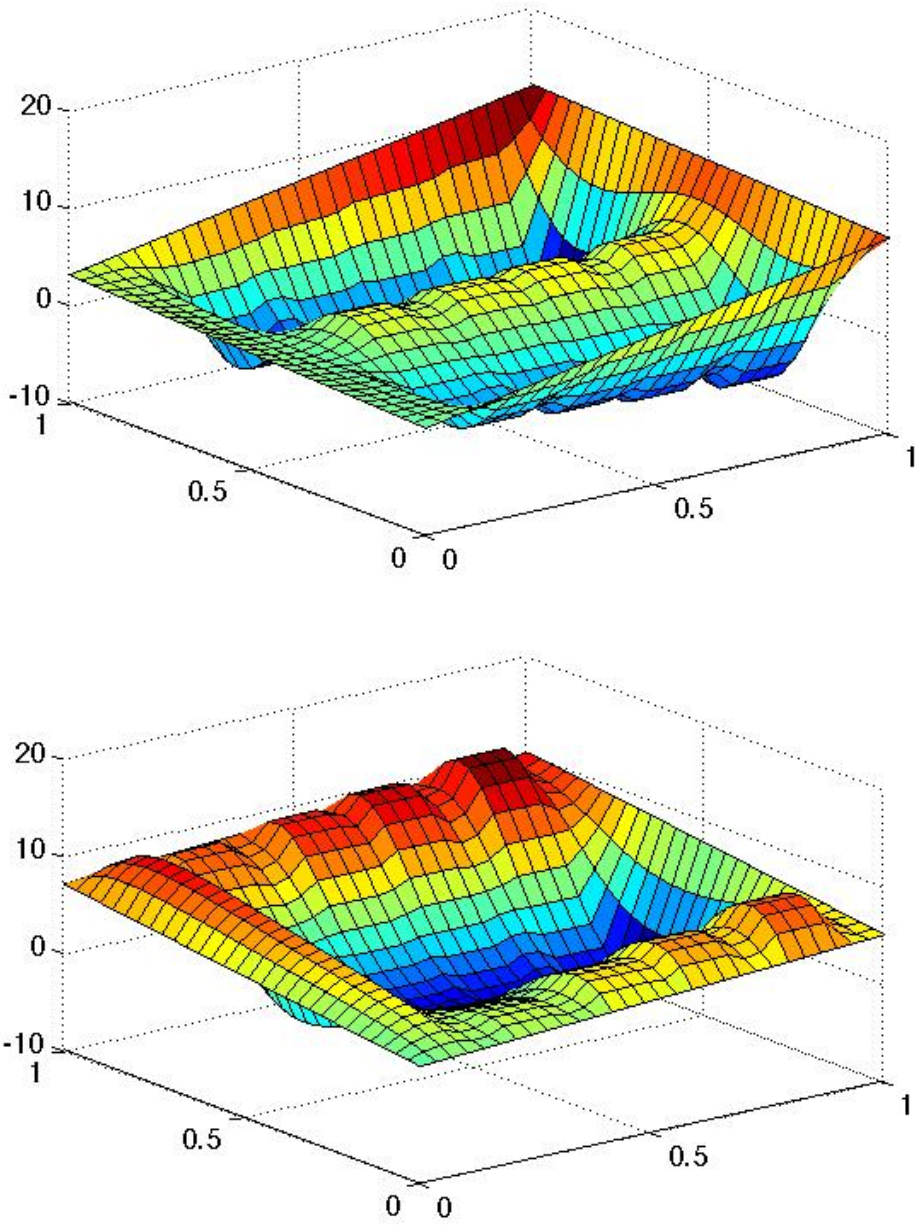

Figure 7.4. Layered Material

CHAPTER 8

ROBIN BOUNDARY CONDITIONS

In addition to the boundary conditions presented in Chapter 5, we present in this chapter a variational formulation for the Robin boundary condition along with the corresponding modifications to the numerical method.

8.1 Problem Formulation

Another boundary condition that often appears is the Robin problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P + av \cdot n = g & \text{on } \partial\Gamma \end{cases},$$

where $a \in \mathbb{C}$. In order to deal with this boundary condition which concerns both real and imaginary parts of the variables P and v simultaneously, we start with the minimization functional for the natural boundary conditions

$$Y(P', v'') + 2\omega \int_{\partial\Gamma} [P' v' \cdot n + P'' v'' \cdot n] \, dS.$$

The Euler-Lagrange Equation for the corresponding variational principle is

$$B(P', v'', s, T) = -\omega \int_{\partial\Gamma} [s v' \cdot n + P'' T \cdot n] \, dS.$$

where the bilinear form B is defined in (6.1). Notice that we can write the surface integral above as

$$-\omega \int_{\partial\Gamma} \begin{pmatrix} v' \cdot n \\ P'' \end{pmatrix} \cdot \begin{pmatrix} s \\ T \cdot n \end{pmatrix} \, dS.$$

The vector on the right contains the primary variables for which we would like to solve, and the vector on the left contains the dual variables which we would like to

eliminate using the Robin boundary condition. In terms of the vectors above, we can express the Robin condition as

$$M_1 \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} + M_2 \begin{pmatrix} v' \cdot n \\ P'' \end{pmatrix} = \begin{pmatrix} g' \\ g'' \end{pmatrix},$$

where

$$M_1 = \begin{pmatrix} 1 & -a'' \\ 0 & a' \end{pmatrix} \text{ and } M_2 = \begin{pmatrix} a' & 0 \\ a'' & 1 \end{pmatrix}.$$

Rearranging, we find that

$$\begin{pmatrix} v' \cdot n \\ P'' \end{pmatrix} = M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} - M_2^{-1} M_1 \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix},$$

so the surface integral term becomes

$$-\omega \int_{\partial\Gamma} \left[M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} - M_2^{-1} M_1 \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} \right] \cdot \begin{pmatrix} S \\ T \cdot n \end{pmatrix} \, dS$$

$$= -\omega \int_{\partial\Gamma} M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} \cdot \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} \, dS + \omega \int_{\partial\Gamma} M_2^{-1} M_1 \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} \cdot \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} \, dS.$$

The new Euler-Lagrange equation for the Robin boundary condition is therefore

$$B(P', v''; s, T) - \omega \int_{\partial\Gamma} M_2^{-1} M_1 \begin{pmatrix} P' \\ v'' \cdot n \end{pmatrix} \cdot \begin{pmatrix} s \\ T \cdot n \end{pmatrix} \, dS$$

$$= -\omega \int_{\partial\Gamma} M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} \cdot \begin{pmatrix} s \\ T \cdot n \end{pmatrix} \, dS.$$

Since

$$M_2^{-1} = \frac{1}{a'} \begin{pmatrix} 1 & 0 \\ -a'' & a' \end{pmatrix},$$

we have

$$M_2^{-1} M_1 = \frac{1}{a'} \begin{pmatrix} 1 & -a'' \\ -a'' & |a|^2 \end{pmatrix},$$

which is positive definite as long as $a' > 0$. The new bilinear form above is guaranteed to be coercive as long as ρ and κ satisfy (4.3) and $a' < 0$.

To find a numerical solution for the Robin boundary value problem, we discretize using the finite element scheme presented in the previous chapter. Unfortunately, the surface integrals can no longer be converted to volume integrals by integration by parts and must be computed as they stand. In this case, the finite element matrix is written as the sum of two matrices $A - \omega B$, where A is of the form (7.2), and the

blocks have entries (7.3), and another matrix B with the same block form and block entries

$$\begin{aligned}
(B_1)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} \psi_t \\ 0 \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} \psi_j \\ 0 \end{pmatrix} \, dS \\
(B_2)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{1t} \cdot n \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} 0 \\ \phi_{1j} \cdot n \end{pmatrix} \, dS \\
(B_3)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{2t} \cdot n \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} 0 \\ \phi_{2j} \cdot n \end{pmatrix} \, dS \\
(B_4)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{1t} \cdot n \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} \psi_j \\ 0 \end{pmatrix} \, dS \\
(B_5)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{2t} \cdot n \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} 0 \\ \phi_{1j} \cdot n \end{pmatrix} \, dS \\
(B_6)_{tj} &= \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{2t} \cdot n \end{pmatrix} \cdot M_2^{-1} M_1 \begin{pmatrix} \psi_j \\ 0 \end{pmatrix} \, dS.
\end{aligned}$$

The right-hand side vector b is also partitioned as $(b_1, b_2, b_3)^T$ with entries

$$\begin{aligned}
(b_1)_k &= -\omega \int_{\partial\Gamma} \begin{pmatrix} \psi_k \\ 0 \end{pmatrix} \cdot M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} \, dS \\
(b_2)_k &= -\omega \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{1k} \cdot n \end{pmatrix} \cdot M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} \, dS \\
(b_3)_k &= -\omega \int_{\partial\Gamma} \begin{pmatrix} 0 \\ \phi_{2k} \cdot n \end{pmatrix} \cdot M_2^{-1} \begin{pmatrix} g' \\ g'' \end{pmatrix} \, dS.
\end{aligned}$$

Assuming that the coercivity requirements mentioned above are satisfied, the system

$$(A - \omega B)\alpha = b$$

may be solved using the same preconditioned conjugate gradient approach as outlined in the previous chapter.

8.2 Numerical Examples

Here we present some numerical examples obtained by using the finite element method to solve problems with Robin boundary conditions. In these examples the Robin boundary conditions are imposed on $y = 0$ and $y = 1$, while on the other sides of the domain we have imposed periodic boundary conditions. Figure 8.1 shows the

solution with a circular scatterer with $\rho = 1+.011i$ outside the scatterer, $\rho = 2+.011i$ inside the scatterer, $\kappa = 1 + .011i$ everywhere, $a = -1 + .333i$ and $g = 3.33i$. In Figure 8.2, the circular scatterer is replaced by a bar angled across the domain, but the other parameters in the problem remain the same.

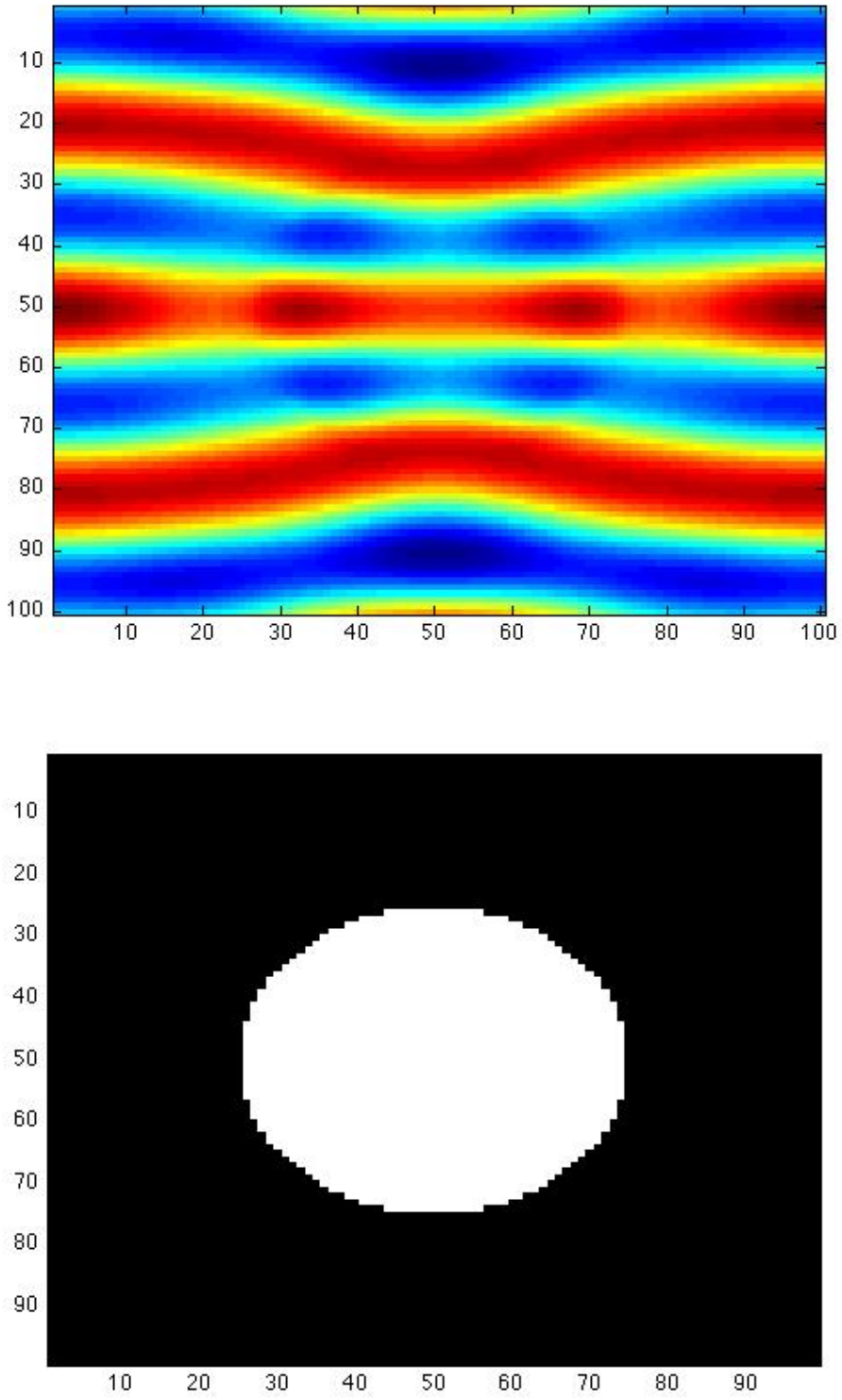

Figure 8.1. Circular Scatterer

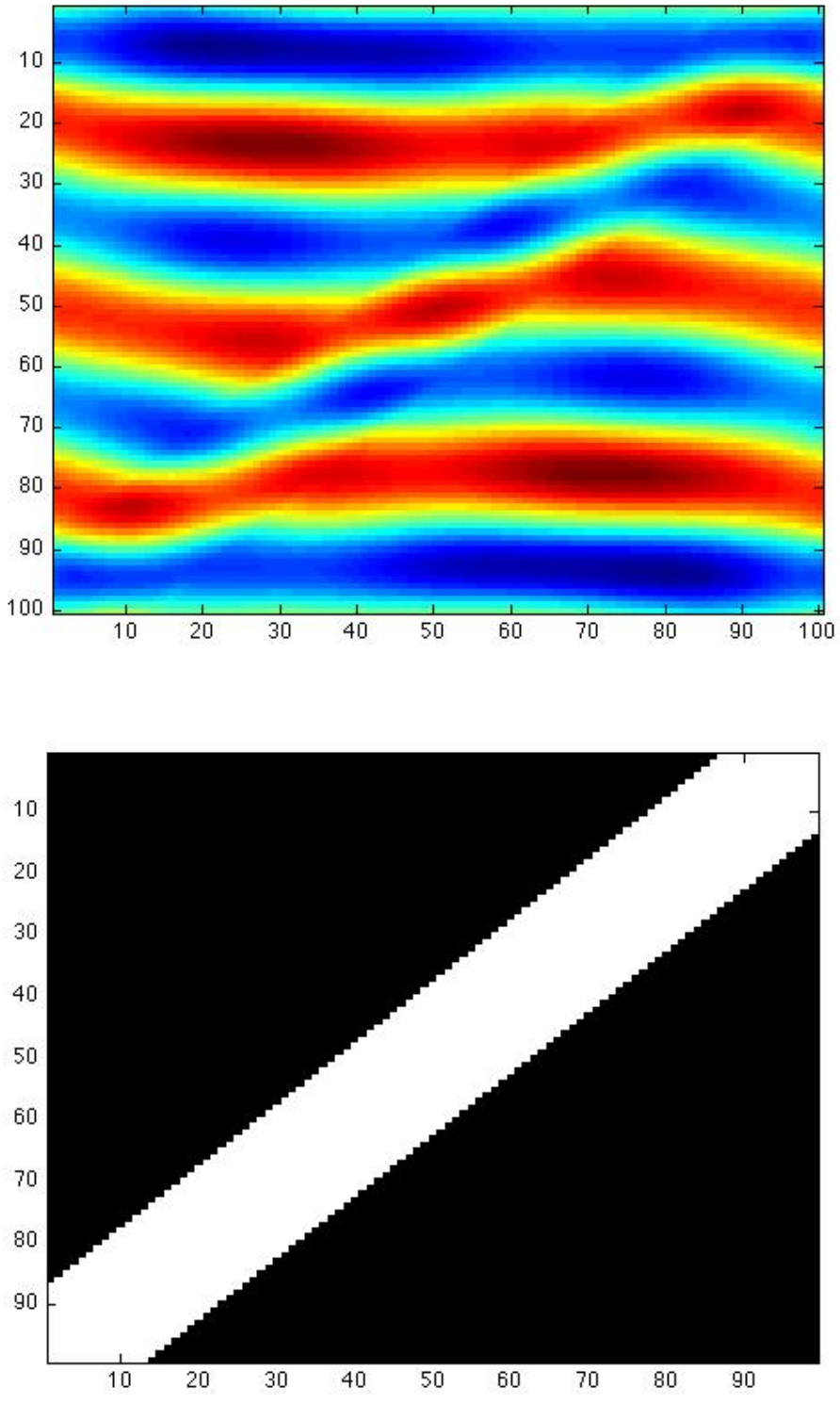

Figure 8.2. Bar Scatterer

CHAPTER 9

A VARIATIONAL INVERSE PROBLEM FOR THE COMPLEX HELMHOLTZ EQUATION

In this chapter we study the inverse problem of determining the density and the bulk modulus of a material from boundary measurements of pressure and velocity. This problem is very closely related to the electrical impedance tomography (EIT) problem, so we start there.

9.1 Background on the EIT Problem

Here we give a short introduction to the problem of electrical impedance tomography. We will follow the presentation in [7].

As we have seen in the background material, the electrical response of a material depends heavily on the electrical conductivity σ and the electrical permittivity ε. In a conducting material, the conductivity is large and current flows easily through the material. In a dielectric, the permittivity is large, and only alternating current is able to flow.

The complex admittivity function

$$\gamma(x, \omega) = \sigma(x) + i\omega\varepsilon(x)$$

combines the materials response to both the conductivity and the permittivity. The inverse of the admittivity is called the impedance, and it measures the ratio between the electric field and the current at the point x. Suppose that the material in question occupies a domain $\Omega \subset \mathbb{R}^d$, and that simultaneous measurements of the direct or alternating currents and voltages on $\partial\Omega$ are available to us through experiments. Then

the electrical impedance tomography problem is the inverse problem of determining the impedance from these boundary measurements of current and potential.

Since different materials have different electrical properties, impedance tomography can be used to determine the internal structure of objects. Impedance tomography has application in the fields of medicine, geophysics, and environmental sciences. Some medical applications of impedance tomography are the detection of pulmonary emboli, monitoring of apnea, monitoring of heart function and blood flow, and breast cancer detection (see the references in [7]).

The approximation to the Maxwell's equations that is often used in the model to which impedance tomography is applied is

$$\nabla \times H(x,\omega) = \gamma(x,\omega)E(x,\omega),\ \nabla \times E(x,\omega) = 0.$$

We can then define an electric potential φ and current density j such that

$$E(x,\omega) = -\nabla\varphi(x,\omega),\ j(x,\omega) = \gamma(x,\omega)E(x,\omega).$$

Combining these, we have Ohm's law

$$j(x,\omega) = -\gamma(x,\omega)\nabla\varphi(x,\omega).$$

Many of the results in impedance tomography assume that the material is isotropic, i.e., that γ is a bounded, scalar valued function in $L^\infty(\bar{\Omega})$.

The vector field j must be divergence free, so Ohm's law implies the partial differential equation

$$\nabla \cdot (\gamma(x,\omega)\nabla\varphi(x,\omega)) = 0 \text{ in } \Omega, \tag{9.1}$$

which can be solved with either Dirichlet boundary conditions

$$\varphi(x,\omega) = V(x,\omega) \text{ on } \partial\Omega \tag{9.2}$$

or Neumann conditions

$$\gamma(x,\omega)\nabla\varphi(x,\omega)\cdot n(x) = \gamma\frac{\partial\varphi}{\partial n} = I(x,\omega) \text{ on } \partial\Omega, \tag{9.3}$$

where $I(x,\omega)$ must satisfy

$$\int_{\partial\Omega} I(x,\omega)\ dS = 0$$

and $n(x)$ is the unit outward normal vector to Ω. While the solving of the PDE (9.1) with the Dirichlet boundary conditions determines φ uniquely, doing so with the Neuman conditions does so only up to an additive constant. This constant can be fixed by requiring

$$\int_{\partial\Omega} \varphi(x,\omega)\ dS = \int_{\partial\Omega} V(x,\omega)\ dS = 0.$$

The equation (9.1), when solved with boundary conditions, gives a method for determining j and φ when $\gamma(x,\omega)$ is a known function. This is the forward problem. As mentioned above, the inverse problem is to determine γ from knowledge of j and φ on the boundary $\partial\Omega$.

The Dirichlet and Neumann conditions satisfied on the boundary $\partial\Omega$ by a given solution φ to (9.1) are related by the Dirichlet to Neumann map $\Lambda_\gamma : H^{\frac{1}{2}}(\partial\Omega) \to H^{-\frac{1}{2}}(\partial\Omega)$ defined by

$$\Lambda_\gamma V(x,\omega) = \gamma(x,\omega)\frac{\partial\varphi(x,\omega)}{\partial n},$$

where φ satisfies (9.1) and (9.2).

Suppose we are given two solutions φ and ψ to (9.1) with Dirichlet boundary data $V(x,\omega)$ and $W(x,\omega)$, respectively. We define an inner product by

$$\langle f, g\rangle = \int_{\partial\Omega} f^*(x)g(x)\ dS,$$

where $*$ denotes complex conjugation. We then have

$$\langle W, \Lambda_\gamma V\rangle = \int_{\partial\Omega} W^*\gamma\frac{\partial\varphi}{\partial n}\ dS = \int_\Omega \gamma\nabla\varphi\cdot\nabla\psi^*\ dx$$

and

$$\langle \Lambda_\gamma W, V\rangle = \int_{\partial\Omega} V\gamma^*\frac{\partial\psi^*}{\partial n}\ dS = \int_\Omega \gamma^*\nabla\varphi\cdot\nabla\psi\ dx.$$

Note that if $V = W$, then $\langle V, \Lambda_\gamma V\rangle = 0$ if and only if $\nabla\varphi = 0$ a.e. in Ω, so the Dirichlet to Neumann map has the nontrivial nullspace $N(\Lambda_\gamma) = \{V \in H^{\frac{1}{2}}(\partial\Omega) : V \text{ is constant}\}$. In the static case $\omega = 0$, we have $\gamma(x,\omega) = \sigma(x)$, and so $\Lambda_\gamma = \Lambda_\sigma$ is self adjoint. It is also positive definite, since

$$\langle V, \Lambda_\sigma V\rangle = \min_{u|_{\partial\Omega}=V} \int_\Omega \sigma(x)|\nabla u(x)|^2\ dx.$$

Similar arguments show that the Neumann to Dirichlet map Λ_σ^{-1} is also self-adjoint and positive definite with variational formulation

$$\langle I, \Lambda_\sigma^{-1} I \rangle = \min_{\substack{\nabla \cdot j = 0 \\ -j \cdot n|_{\partial\Omega} = I}} \int_\Omega \frac{1}{\sigma(x)} |j(x)|^2 \, dx.$$

In practice, it is more advisable to work with the Neumann to Dirichlet map rather than the Dirichlet to Neumann map, since it is smoothing and gives better results with noisy data. However, both maps contain the same information, and often the Dirichlet to Neumann map is used for convenience.

The results in this section can be easily generalized to the variational principles of Chapter 4, as will be seen in the sequel.

9.2 The Essential to Natural Map

In the previous chapter, we introduced the Dirichlet to Neumann map Λ_σ, which maps the boundary values of a solution φ to the boundary value problem

$$\begin{cases} -\nabla \cdot \sigma \nabla \varphi = 0 & \text{in } \Gamma \\ \varphi = V & \text{on } \partial\Gamma \end{cases}$$

to the corresponding Neumann values, or more precisely,

$$\Lambda_\sigma V = \sigma \frac{\partial \varphi}{\partial n}.$$

We can think of the map Λ_σ as mapping the boundary values of the primary variable φ to those of the dual variable $j \cdot n$. These dual variables are related by the constitutive relation $j = \sigma \nabla u$. By analogy with this idea, we seek to define a map that relates the boundary values of the variables on the two sides of the constitutive relation for the complex Helmholtz equation,

$$\begin{pmatrix} \mathcal{G}'' \\ \mathcal{F}'' \end{pmatrix} = \mathcal{L} \begin{pmatrix} \mathcal{F}' \\ -\mathcal{G}' \end{pmatrix}.$$

Therefore, if (P', v'') are the corresponding parts of a solution to the essential boundary value problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P' = P_0' & \text{on } \partial\Gamma \\ v'' \cdot n = v_0'' \cdot n & \text{on } \partial\Gamma \end{cases},$$

we define the "essential to natural" map $\Lambda_{\mathcal{L}}$ by

$$\Lambda_{\mathcal{L}}(P_0', v_0'' \cdot n) = (-P'', v' \cdot n),$$

where, as usual, P'' is the imaginary part of the pressure and v' is the real part of the complex velocity. It is then straightforward to show that the map $\Lambda_{\mathcal{L}}$ shares the same properties as Λ_σ. If we define an inner product by

$$\langle r, U \cdot n; s, T \cdot n \rangle = \omega \int_{\partial\Gamma} [rT \cdot n + U \cdot ns]\, dS,$$

and if p is a solution to

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla p - \dfrac{\omega^2}{\kappa} p = 0 & \text{in } \Gamma \\ p' = p_0' & \text{on } \partial\Gamma \\ V'' \cdot n = V_0'' \cdot n & \text{on } \partial\Gamma \end{cases},$$

where $V = -i/\omega \nabla p$, then

$$\begin{aligned} \langle P_0', v_0'' \cdot n; \Lambda_{\mathcal{L}}(p_0', V_0'' \cdot n) \rangle &= \omega \int_{\partial\Gamma} [P_0' V_0' \cdot n - v_0'' \cdot n p_0'']\, dS \\ &= \omega \int_\Gamma [\nabla \cdot (P'V') - \nabla \cdot (p''v'')]\, dx \\ &= \omega \int_\Gamma [\nabla P' \cdot V' + P' \nabla \cdot V' - \nabla p'' \cdot v'' - p'' \nabla \cdot v'']\, dx \\ &= \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \begin{pmatrix} \omega V' \\ \nabla p'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \begin{pmatrix} \nabla V' \\ \omega p'' \end{pmatrix} \right] dx \\ &= \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla p' \\ -\omega \nabla V'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega p' \\ -\nabla \cdot V'' \end{pmatrix} \right] dx, \end{aligned}$$

and a similar calculation shows that

$$\begin{aligned} &\langle \Lambda_{\mathcal{L}}(P_0', v_0'' \cdot n); p_0', V_0'' \rangle \\ &= \int_\Gamma \left[\begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla p' \\ -\omega \nabla V'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega p' \\ -\nabla \cdot V'' \cdot n \end{pmatrix} \right] dx \end{aligned}$$

as well, so $\Lambda_{\mathcal{L}}$ is self-adjoint. Also, if $P_0' = P_0'$ and $v_0'' = V_0''$, then by the positivity of the quadratic form on the right-hand side above, we have that $\langle \Lambda_{\mathcal{L}}(P_0', v_0'' \cdot n); P_0', v_0'' \rangle \geq 0$. However, $\Lambda_{\mathcal{L}}$ has a trivial null space because of its dependence on the P variable and not only its gradient.

9.3 Formulation of the Inverse Problem

The inverse problem for the complex Helmholtz equation is exactly analogous to the electrical impedance tomography problem described in Chapter 9.1: given full knowledge of the essential to natural map $\Lambda_{\mathcal{L}}$, we wish to determine $\mathcal{L}$ inside the body Γ.

Here is a general outline of the idea behind the method. Suppose we are give the boundary data for one experiment performed on the object whose coefficients (ρ and κ) we want to identify. For example, for fixed frequency ω, the a fixed pressure P_0 is applied on the boundary and the corresponding velocity v_0 is measured on the boundary. Then the solution (P', v'') to the boundary value problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla P - \dfrac{\omega^2}{\kappa} P = 0 & \text{in } \Gamma \\ P' = P'_0 & \text{on } \partial\Gamma \\ v'' \cdot n = v''_0 \cdot n & \text{on } \partial\Gamma \end{cases}$$

and the $(\tilde{P}', \tilde{v}'')$ from the solution to the problem

$$\begin{cases} -\nabla \cdot \rho^{-1} \nabla \tilde{P} - \dfrac{\omega^2}{\kappa} \tilde{P} = 0 & \text{in } \Gamma \\ \tilde{P}'' = \tilde{P}''_0 & \text{on } \partial\Gamma \\ \tilde{v}' \cdot n = \tilde{v}'_0 \cdot n & \text{on } \partial\Gamma \end{cases}$$

are the same. In other words, if we have the correct ρ and κ, then

$$0 = \|P' - \tilde{P}'\|^2_{L^2(\Gamma)} + \|v'' - \tilde{v}''\|^2_{L^2(\Gamma, \mathbb{R}^d)},$$

where (P', v'') and $(\tilde{P}', \tilde{v}'')$ are as defined above. Our goal, then, is to minimize the right-hand side of the line above with respect to ρ and κ, subject to the constraints that (P', v'') be a solution to the Helmholtz equation with the essential boundary data, and $(\tilde{P}', \tilde{v}'')$ be a solution to Helmholtz equation with the natural boundary data.

A classical approach to this minimization problem would be to calculate a gradients of the functional with respect to ρ and κ. In doing so, one would have to compute the solution to an adjoint problem with roughly the same form as the two boundary value problems above. While this is a perfectly good approach, the goal of

our method is to improve upon it by essentially doing both the minimization and the solving of the PDEs simultaneously.

To achieve this, we explicitly enforce the constraints that the boundary value problems above be satisfied by adding the corresponding minimization functionals to the objective. More precisely, we seek now to minimize

$$J(\rho,\kappa,P',v'',\tilde{P}',\tilde{v}'') = \|\psi_0'+P'-\tilde{P}'\|^2_{L^2(\Gamma)}+\|\phi_0''+v''-\tilde{v}''\|^2_{L^2(\Gamma,\mathbb{R}^d)}+\beta_1 Y(\psi_0'+P',\phi_0''+v'')$$
$$+\beta_2\left(Y(\tilde{P}',\tilde{v}'')+2\omega\int_\Gamma\left[\nabla\tilde{P}'\cdot\phi_0'+\tilde{P}'\nabla\cdot\phi_0'+\nabla\psi_0''\cdot\tilde{v}''+\psi_0''\nabla\cdot\tilde{v}''\right]dx\right)$$

over $\rho\in L^\infty(\Gamma)$ with positive imaginary part, $\kappa\in L^\infty(\Gamma)$ with negative imaginary part, $P'\in H_0^1(\Gamma)$, $v''\in H_0(\mathrm{div},\Gamma)$, $\tilde{P}'\in H^1(\Gamma)$, and $\tilde{v}''\in H(\mathrm{div},\Gamma)$. Here $\psi_0\in H^1(\Gamma)$ and $\phi_0\in H(\mathrm{div},\Gamma)$ are fixed functions such that $\psi_0=P_0$ and $\phi_0\cdot n=v_0\cdot n$ on $\partial\Gamma$. Note that for the purposes of the minimization, each of the variables upon which J depends is considered independent from all the others. As a consequence, there are no longer any adjoint problems to be solved, but there are many more terms in the objective functional, each requiring the calculation of a gradient.

In order to keep track of the gradients that need to be calculated, we split J into several constituent functionals, namely

$$J_1(P',\tilde{P}') = \int_\Gamma(\psi_0'+P'-\tilde{P}')^2\,dx,$$
$$J_2(v'',\tilde{v}'') = \int_\Gamma(\phi_0''+v''-\tilde{v}'')^2\,dx,$$
$$J_3(r',q,P',v'') = \int_\Gamma\begin{pmatrix}\nabla\psi_0'+\nabla P'\\ -\omega(\phi_0''+v'')\end{pmatrix}\cdot\mathcal{R}\begin{pmatrix}\nabla\psi_0'+\nabla P'\\ -\omega(\phi_0''+v'')\end{pmatrix}dx,$$
$$J_4(k',\mu,P',v'') = \int_\Gamma\begin{pmatrix}\omega(\psi_0'+P')\\ -\nabla\cdot\phi_0''-\nabla\cdot v''\end{pmatrix}\cdot\mathcal{K}\begin{pmatrix}\omega(\psi_0'+P')\\ -\nabla\cdot\phi_0''-\nabla\cdot v''\end{pmatrix}dx,$$
$$J_5(r',q,\tilde{P}',\tilde{v}'') = \int_\Gamma\begin{pmatrix}\nabla\tilde{P}'\\ -\omega\tilde{v}''\end{pmatrix}\cdot\mathcal{R}\begin{pmatrix}\nabla\tilde{P}'\\ -\omega\tilde{v}''\end{pmatrix}dx,$$
$$J_6(k',\mu,\tilde{P}',\tilde{v}'') = \int_\Gamma\begin{pmatrix}\omega\tilde{P}'\\ -\nabla\cdot\tilde{v}''\end{pmatrix}\cdot\mathcal{K}\begin{pmatrix}\omega\tilde{P}'\\ -\nabla\cdot\tilde{v}''\end{pmatrix}dx,$$
$$J_7(\tilde{P}',\tilde{v}'') = 2\omega\int_\Gamma\left[\nabla\tilde{P}'\cdot\phi_0'+\psi_0''\nabla\cdot\tilde{v}''\right]dx$$

and

$$J_8(\tilde{P}', \tilde{v}'') = 2\omega \int_\Gamma \left[\tilde{P}' \nabla \cdot \phi_0' + \nabla \psi_0'' \cdot \tilde{v}'' \right] \, dx,$$

where $q = (r'')^{-1}$ and $\mu = (k'')^{-1}$.

In order to find the gradient of a function $L(s)$ with respect to the variable s, we calculate

$$\lim_{t \to 0} \frac{1}{t} \left(L(s + t\delta s) - L(s) \right),$$

and manipulate the result into an integral of the form

$$\int_\Gamma L_s \delta s \, dx.$$

The function L_s is the gradient of the function L with respect to the variable s in $L^2(\Gamma)$. We follow the pattern of this computation for each of the functions $J_1, \ldots, J_8$. For J_1, we find that

$$J_{1,P'} = 2(\psi_0' + P' - \tilde{P}') \text{ and } J_{1,\tilde{P}'} = -2(\psi_0' + P' - \tilde{P}').$$

Similarly, the gradients of J_2 are

$$J_{2,v''} = 2(\varphi_0'' + v'' - \tilde{v}'') \text{ and } J_{2,\tilde{v}''} = -2(\varphi_0'' + v'' - \tilde{v}'').$$

For J_3, we have

$$J_{3,r'} = \begin{pmatrix} \nabla \psi_0' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix} \cdot \mathcal{R}_{r'} \begin{pmatrix} \nabla \psi_0' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix}$$

and

$$J_{3,q} = \begin{pmatrix} \nabla \psi_0' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix} \cdot \mathcal{R}_q \begin{pmatrix} \nabla \psi_0'' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix},$$

where

$$\mathcal{R}_{r'} = \begin{pmatrix} 2r'q & q \\ q & 0 \end{pmatrix} \text{ and } \mathcal{R}_q = \begin{pmatrix} -q^{-2} + (r')^2 & r' \\ r' & I \end{pmatrix}.$$

Note that we are assuming that ρ is isotropic. Also,

$$J_{3,\nabla P'} = \begin{pmatrix} \nabla \psi_0' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \mathbf{1} \\ 0 \end{pmatrix} \text{ and } J_{3,v''} = \begin{pmatrix} \nabla \psi_0' + \nabla P' \\ -\omega(\phi_0'' + v'') \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} 0 \\ \mathbf{1} \end{pmatrix},$$

where $\mathbf{1}$ denotes a vector function whose components are the constant function 1. Similarly, the gradients of J_4 are

$$J_{4,k'} = \begin{pmatrix} \omega(\psi_0'' + P') \\ -\nabla \cdot \phi_0'' - \nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K}_{k'} \begin{pmatrix} \omega(\psi_0' + P') \\ -\nabla \cdot \phi_0'' - \nabla \cdot v'' \end{pmatrix},$$

$$J_{4,\mu} = \begin{pmatrix} \omega(\psi_0' + P') \\ -\nabla\cdot\phi_0'' - \nabla\cdot v'' \end{pmatrix} \cdot \mathcal{K}_\mu \begin{pmatrix} \omega(\psi_0' + P') \\ -\nabla\cdot\phi_0'' - \nabla\cdot v'' \end{pmatrix},$$

$$J_{4,P'} = \begin{pmatrix} \omega(\psi_0' + P') \\ -\nabla\cdot\phi_0'' - \nabla\cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \text{ and } J_{4,\nabla\cdot v''} = \begin{pmatrix} \omega(\psi_0' + P') \\ -\nabla\cdot\phi_0'' - \nabla\cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} 0 \\ 1 \end{pmatrix},$$

where

$$\mathcal{K}_{k'} = \begin{pmatrix} 2k'\mu & \mu \\ \mu & 0 \end{pmatrix} \text{ and } \mathcal{K}_\mu = \begin{pmatrix} -\mu^{-2} + (k')^2 & k' \\ k' & 1 \end{pmatrix}.$$

The gradients for J_5 and J_6 are the same as those calculated for J_3 and J_4 with the replacements $P' \to \tilde{P}'$ and $v'' \to \tilde{v}''$, and with $\psi_0' = 0$ and $\phi_0'' = 0$.

The gradients of J_7 are

$$J_{7,\nabla\tilde{P}'} = 2\omega\phi_0' \text{ and } J_{7,\nabla\cdot\tilde{v}''} = 2\omega\psi_0'',$$

and the gradients of J_8 are

$$J_{8,\tilde{P}'} = 2\omega\nabla\cdot\phi_0' \text{ and } J_{8,\tilde{v}''} = 2\omega\nabla\psi_0''.$$

With these formulas for the gradients of $J_1, \ldots, J_8$ in hand, we can implement a gradient descent algorithm to find the minimizing coefficients r', q, k', and μ of a material configuration having the essential-natural pair $(P_0', v_0''\cdot n) \to (P_0'', v_0'\cdot n)$. We should certainly expect better results when more information from the real to imaginary map is included in the problem, so in practice we minimize

$$\sum_{j=1}^{M} J(\rho, \kappa, P_j', v_j'', \tilde{P}_j', \tilde{v}_j''), \tag{9.4}$$

with corresponding auxiliary functions ψ_{0j} and ϕ_{0j} satisfying the boundary data from the jth experiment.

9.4 Numerical Implementation

In the numerical algorithm, we will assume that the domain Γ is the unit square $(0,1)^2$, upon which we impose an $N\times N$ computational grid. In order to implement the gradient descent algorithm as outlined, we keep track of each the variables P', v'', $\tilde{P}'$, and $\tilde{v}''$ by using the finite element expansions for these functions that was introduced above. The material coefficients ρ and κ are represented by $(N-1)\times(N-1)$ matrices containing the values of the material coefficients at the centers of the grid squares.

9.4.1 Calculation of the Gradients

Although the gradient descent algorithm is mostly straightforward, there are a few points to be aware of:

1. Whenever the gradient of one of the constituent functionals $J_1, \ldots, J_8$ is calculated with respect to P', the result is a function defined on all of Γ, which is represented discretely by possibly nonzero values at all of the nodes in the $N \times N$ grid. However, the function P' is assumed to be an element of $H_0^1(\Gamma)$. Therefore, when we add the gradient of a functional to P', we add only the values from the $(N-2) \times (N-2)$ interior grid.

2. Just as in the last item, when a gradient is calculated with respect to v'', it is important to remember that v'' is assumed to have zero normal component, i.e., $v'' \in H_0(\mathrm{div}, \Gamma)$. In order to preserve this requirement, we add only the $N-2$ interior columns of the computed gradient to the first component of v'' and the $N-2$ interior rows of the computed gradient to the second component of v''.

3. Some of the gradients calculated in the last section were taken with respect to $\nabla P'$ or $\nabla \tilde{P}'$ ($J_{3,\nabla P'}$, $J_{5,\nabla \tilde{P}'}$, and $J_{7,\nabla P'}$) instead of with respect to P' or $\tilde{P}'$. In effect, this tells us how we should change $\nabla P'$ or $\nabla \tilde{P}'$ in order to minimize the objective functional. Since the variable which is changed and stored is P' or $\tilde{P}'$, we must find a function g such that (for example)

$$\nabla g = J_{3,\nabla P'} \text{ in } \Gamma.$$

If we think of this as a minimization

$$\inf_{g \in H_0^1(\Gamma)} \|\nabla g - J_{3,\nabla P'}\|^2_{L^2(\Gamma),\mathbb{R}^2)},$$

then the Euler-Lagrange equation is

$$\int_\Gamma \nabla g \cdot \nabla s \; dx = \int_\Gamma J_{3,\nabla P'} \cdot \nabla s \; dx.$$

Numerically, we solve this problem by using the bilinear elements used previously to represent the P' variable. Then the coefficients in the expansion of g

provide the values on the nodes of the grid, and a multiple of this is what is added to P' in the gradient descent.

4. Similarly, when the gradient above is calculated with respect to the variable $\nabla \cdot v''$ or $\nabla \cdot \tilde{v}''$, then we seek a vector field G which is a solution to the problem (for example)

$$\inf_{G \in H_0(\mathrm{div},\Gamma)} \|\nabla \cdot G - J_{4,\nabla \cdot v''}\|^2_{L^2(\Gamma)},$$

which has Euler-Lagrange equation

$$\int_\Gamma \nabla \cdot G \nabla \cdot q \; dx = \int_\Gamma J_{4,\nabla \cdot v''} \nabla q \; dx.$$

Again, this problem is discretized as in the finite element method previously described and solved for the gradient with respect to v'', a multiple of which is then added to v''.

5. A slight difficulty is introduced in the fact that the functions are represented on an $N \times N$ grid, while the material coefficients are represented on an $(N-1) \times (N-1)$ grid. In many cases, (for example $J_{3,v''}$), it is necessary to add and multiply functions represented on both these grids. For this purpose, we introduce the following rules:

   To restrict a function represented on the $N \times N$ to the $(N-1) \times (N-1)$ grid, we assume that the nodal values are the coefficients in the expansion of that function in the bilinear finite element basis. We then calculate the values of the function at the centers of the grid squares, which results in a representation on the $(N-1) \times (N-1)$ grid.

   To take a function from the $(N-1) \times (N-1)$ grid to the $N \times N$ grid, we define it's value at each node to be the average of the values at the centers of the surrounding grid squares.

6. Each time one of the material coefficients is updated, care must be taken to maintain the sign of the imaginary part. For this reason we use a "projected gradient" step in these cases. When a gradient step is indicated that would

violate the coercivity conditions on ρ or κ, the imaginary part is scaled back so that this does not happen. In practice, one would hope to have some bounds on the imaginary parts of the constituent materials in the object being imaged to use in the implementation of the projection.

By implementing the steps outlined above, we arrive at the following algorithm for the gradient descent method.

Given M pairs of experimental boundary data ψ_{0j} and ϕ_{0j}, fix initial values for P_j', v_j'', $\tilde{P}_j'$, $\tilde{v}_j''$, r', q, k', and μ.

Fix a step length $\tau > 0$

For $n = 1, 2, \ldots$

Calculate the gradients

$$J_{1,P_j'},\ J_{1,\tilde{P}_j'},\ J_{2,v_j''},\ J_{2,\tilde{v}_j''},\ J_{3,r'},\ J_{3,q},\ J_{3,\nabla P_j'},\ J_{3,v_j''},\ J_{4,k'},\ J_{4,\mu},\ J_{4,P_j'},\ J_{4,\nabla\cdot v_j''},\ J_{5,r'},$$

$$J_{5,q},\ J_{5,\nabla\tilde{P}_j'},\ J_{5,\tilde{v}''},\ J_{6,k'},\ J_{6,\mu},\ J_{6,\tilde{P}_j'},\ J_{6,\nabla\cdot\tilde{v}_j''},\ J_{7,\nabla\tilde{P}_j'},\ J_{7,\nabla\cdot\tilde{v}_j''},\ J_{8,\nabla\tilde{P}_j'},\ J_{8,\tilde{v}_j''}.$$

As in remarks 3 and 4 above, calculate

$$J_{3,P_j'},\ J_{4,v_j''},\ J_{5,\tilde{P}_j'},\ J_{6,\tilde{v}_j''},\ J_{7,\tilde{P}'},\ J_{7,\tilde{v}_j''}$$

by solving the corresponding system of equations.

Take a gradient step:

$$P_j' = P_j' - \tau(J_{1,P_j'} + \beta_1(J_{3,P_j'} + J_{4,P_j'}))$$

$$v_j'' = v_j'' - \tau(J_{2,v_j''} + \beta_1(J_{3,v_j''} + J_{4,v_j''}))$$

$$\tilde{P}_j' = \tilde{P}_j' - \tau(J_{1,\tilde{P}_j'} + \beta_2(J_{5,\tilde{P}_j'} + J_{6,\tilde{P}_j'} + J_{7,\tilde{P}_j'} + J_{8,\tilde{P}_j'}))$$

$$\tilde{v}_j'' = \tilde{v}_j'' - \tau(J_{2,\tilde{v}_j''} + \beta_2(J_{5,\tilde{v}_j''} + J_{6,\tilde{v}_j''} + J_{7,\tilde{v}_j''} + J_{8,\tilde{v}_j''}))$$

$$r' = r' - \tau\sum_{j=1}^{M}(\beta_1 J_{3,r'}(r', q, P_j', v_j'') + \beta_2 J_{5,r'}(r', q, \tilde{P}_j', \tilde{v}_j''))$$

$$q = q - \tau\sum_{j=1}^{M}(\beta_1 J_{3,q}(r', q, P_j', v_j'') + \beta_2 J_{5,q}(r', q, \tilde{P}_j', \tilde{v}_j''))$$

$$k' = k' - \tau \sum_{j=1}^{M} (\beta_1 J_{4,k'}(k', \mu, P_j', v_j'') + \beta_2 J_{6,k'}(k', \mu, \tilde{P}_j', \tilde{v}_j''))$$

$$\mu = \mu - \tau \sum_{j=1}^{M} (\beta_1 J_{4,\mu}(k', \mu, P_j', v_j'') + \beta_2 J_{6,\mu}(k', \mu, \tilde{P}_j', \tilde{v}_j''))$$

If necessary, project the material coefficients back to maintain coercivity

end

Set

$$\rho = \frac{-r' + \frac{1}{q} i}{(r')^2 + \frac{1}{q^2}},$$

$$\kappa = \frac{k' - \frac{1}{\mu} i}{(k')^2 + \frac{1}{\mu^2}}.$$

9.4.2 Regularization

In order to overcome the ill-posedness of the parameter estimation problem as outlined above, we add a regularization terms to the objective functional that we seek to minimize. Since the ultimate goal of the inverse problem is to determine the material coefficients ρ and κ, these are the variables that we seek to regularize. We add our regularization terms to the functional in (9.4) to obtain

$$\sum_{j=1}^{M} J(\rho, \kappa, P_j', v_j'', \tilde{P}_j', \tilde{v}_j'') + \beta_3 J_9(r', q, k', \mu),$$

where

$$J_9(r', q, k', \mu) = \|r'\|^2_{L^2(\Gamma)} + \|q\|^2_{L^2(\Gamma)} + \|k'\|^2_{L^2(\Gamma)} + \|\mu\|^2_{L^2(\Gamma)}.$$

Straightforward calculation shows that

$$J_{9,r'} = 2r', \;\; J_{9,q} = 2q, \;\; J_{9,k'} = 2k', \;\; \text{and } J_{9,\mu} = 2\mu.$$

The gradient descent steps for the material parameter variables r', q, k', and μ then become

$$r' = r' - \tau \left(\sum_{j=1}^{M} (\beta_1 J_{3,r'}(r', q, P_j', v_j'') + \beta_2 J_{5,r'}(r', q, \tilde{P}_j', \tilde{v}_j'')) + \beta_3 J_{9,r'} \right)$$

$$q = q - \tau \left(\sum_{j=1}^{M} (\beta_1 J_{3,q}(r', q, P'_j, v''_j) + \beta_2 J_{5,q}(r', q, \tilde{P}'_j, \tilde{v}''_j)) + \beta_3 J_{9,q} \right)$$

$$k' = k' - \tau \left(\sum_{j=1}^{M} (\beta_1 J_{4,k'}(k', \mu, P'_j, v''_j) + \beta_2 J_{6,k'}(k', \mu, \tilde{P}'_j, \tilde{v}''_j)) + \beta_3 J_{9,k'} \right)$$

$$\mu = \mu - \tau \left(\sum_{j=1}^{M} (\beta_1 J_{4,\mu}(k', \mu, P'_j, v''_j) + \beta_2 J_{6,\mu}(k', \mu, \tilde{P}'_j, \tilde{v}''_j)) + \beta_3 J_{9,\mu} \right)$$

We expect adding regularization to the method to result in improved numerical results. For a discussion of the existence and uniqueness of a solution to the inverse problem in the real (stationary) case, see [28]. Despite the small differences between this problem and the one treated in the reference, at the very lease we can say that at each successive iteration the numerical solution is being improved as an approximation to a true solution.

CHAPTER 10

BOUNDS ON THE ESSENTIAL TO NATURAL MAP

Our focus in the last chapter was to develop a method for determining the material parameters ρ and κ from knowledge of the real to imaginary map $\Lambda_{\mathcal{L}}$, as detailed in Section 9.2. However, rather than taking the effort to solve for ρ and κ completely, often one desires to have bounds on the observed behavior of the material in question. For these purposes, we present several elementary upper bounds on the quadratic form for the essential to natural map made possible by the minimization nature of the variational principles of Milton, Seppecher, and Bouchitté and the natural boundary value problem formulation due to Milton and Willis.

10.1 Simple Bounds from the Minimum Principle

If (P', v'') is a minimizer of the natural boundary condition function (5.2), then

$$\begin{aligned} Y(P', v'') &= \int_\Gamma \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \mathcal{R} \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \mathcal{K} \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \, dx \\ &= \int_\Gamma \begin{pmatrix} \nabla P' \\ -\omega v'' \end{pmatrix} \cdot \begin{pmatrix} -\omega v' \\ \nabla P'' \end{pmatrix} + \begin{pmatrix} \omega P' \\ -\nabla \cdot v'' \end{pmatrix} \cdot \begin{pmatrix} -\nabla \cdot v' \\ \omega P'' \end{pmatrix} \, dx \\ &= \int_\Gamma \left[-\omega \nabla P' \cdot v' - \omega \nabla P'' \cdot v'' - \omega P' \nabla \cdot v' - \omega P'' \nabla \cdot v'' \right] \, dx \\ &= -\omega \int_\Gamma \left[\nabla \cdot (P' v') + \nabla \cdot (P'' v'') \right] \, dx = -\omega \int_{\partial\Gamma} \left[P' v' \cdot n + P'' v'' \cdot n \right] \, dS. \end{aligned}$$

Therefore, the value of the natural boundary condition functional at this minimizer is

$$\tilde{Y}(P', v'') = Y(P', v'') + 2\omega \int_{\partial\Gamma} \left[P' v' \cdot n + v'' \cdot n P'' \right] dS = \omega \int_{\partial\Gamma} \left[P' v' \cdot n + P'' v'' \cdot n \right] \, dx$$

Since $\tilde{Y}(P', v'') \leq \tilde{Y}(s, T)$ for any choice of test functions $s \in H^1(\Gamma)$ and $T \in H(\mathrm{div}, \Gamma)$, we have

$$\omega \int_{\partial\Gamma} [(P' - 2s)v' \cdot n + P''(v'' - 2T) \cdot n] \ dS \leq Y(s, T).$$

This bound is potentially useful because the test functions are not assumed to satisfy any particular boundary condition.

We first take test functions of the form

$$s = c \cdot x, \ T = Bx,$$

for a fixed constant vector c and fixed constant matrix B. These assumptions imply that

$$\nabla s = c, \ \nabla \cdot T = \mathrm{tr}(B),$$

and then the inequality above implies that

$$\begin{aligned} &\omega \int_{\partial\Gamma} [(P' - 2c \cdot x)v' \cdot n + P''(v'' - 2Bx) \cdot n] \ dS \\ &\leq \int_{\Gamma} \big[c \cdot \mathcal{R}_{11} c - 2\omega c \cdot \mathcal{R}_{12} Bx + \omega^2 Bx \cdot \mathcal{R}_{22} Bx \\ &+\omega^2 (c \cdot x)^2 \mathcal{K}_{11} - 2\omega (c \cdot x)\mathrm{tr}(B)\mathcal{K}_{12} + (\mathrm{tr}(B))^2 \mathcal{K}_{22}\big] \ dx \end{aligned}$$

An even more simple inequality comes from using test functions $s = 0, \ T = q$ for a constant vector q. The inequality then becomes

$$\omega \int_{\partial\Gamma} [P'v' \cdot n + P''(v'' - 2q) \cdot n] \ dS \leq \int_{\Gamma} \omega^2 q \cdot \mathcal{R}_{22} q \ dx.$$

This inequality could be useful for a two component medium in deriving bounds on the volume fractions: if $\Gamma = \Gamma_1 \cup \Gamma_2$ with material 1 occupying Γ_1 and material 2 occupying Γ_2, then

$$\omega \int_{\partial\Gamma} [P'v' \cdot n + P''(v'' - 2q) \cdot n] \ dS \leq |\Gamma_1| \omega^2 \mathcal{R}_{22}^{(1)} |q|^2 + |\Gamma_2| \omega^2 \mathcal{R}_{22}^{(2)} |q|^2,$$

where $\mathcal{R}_{22}^{(1)}$ is the value of $(r'')^{-1}$ for the first material, and $\mathcal{R}_{22}^{(2)}$ is the value for the second. If the value of the quadratic form for the real to imaginary map between $(P', v'' \cdot n)$ and $(P'', v' \cdot n)$ is known, then we can solve the inequality above to obtain a bound on the volume fractions of the component materials.

CHAPTER 11

CONCLUSION

The variational principles for the complex Helmholtz equation provided by Milton, Seppecher, and Bouchitté, which build upon the work done for the complex conductivity equation done by Cherkaev and Gibiansky, allow us to extend the sophisticated mathematical framework and machinery developed for the solution of minimization problems to the complex Helmholtz equation. As was mentioned at the outset, many problems can be posed in terms of minimization, and by using these variational principles, we are able to solve problems where the state equation is Helmholtz equation, which has traditionally been viewed as only a stationary problem. In particular, the availability of a minimization variational principle leads directly to a finite element numerical method, which gives rise to a system of equations with a symmetric positive definite coefficient matrix. This system can then be solved efficiently using relatively simple iterative methods, such as the preconditioned conjugate gradient method outlined above. With straightforward modifications, several different boundary conditions can be handled, including the usual Dirichlet, Neumann and even Robin conditions.

Having a minimization variational principle is also advantageous for any type of optimization problem, and as we demonstrated above, the the inverse problem of determining ρ and κ from boundary measurements can be formulated as an optimization, where the variables are constrained to be solutions to the complex Helmholtz equation. This constraint can then be incorporated into the objective functional that we seek to minimize by adding a constant multiple of the correct minimization functional. This avoids the computational effort required to solve adjoint problems, since all of the variables can then be considered as independent of one another.

Another obvious advantage to having a minimization variational principle is that bounds are easily derived. Herein we have demonstrated simple bounds on the quadratic form for the essential to natural map. Such bounds can be useful in the context of electrical impedance tomography, for they may be used as constraints for the material coefficients. The effectiveness of incorporating extra constraints in an inversion method for the tomography problem is demonstrated in [8].

11.1 Future Work

The work presented herein demonstrates only a few of the possible applications of minimization variational principles. The following are some areas of potential future research in which I plan to engage.

11.1.1 Transmission Boundary Conditions

I would like to extend the numerical methods that I have already developed for the Dirichlet, Neumann, and Robin problems to more exotic boundary conditions, such as transmission conditions [22]. Although these boundary conditions are similar in form to the Robin boundary conditions already covered, they differ in that there is a nonlocal operator involved. The challenge is to discover the best way to implement the finite element method for this boundary condition while retaining the minimization nature of the variational principle.

11.1.2 Regularity

Another future project will be to derive a regularity result for minimizers of the variational principles. It is of course possible to get regularity results using standard regularity theory, but since these variational principles have as minimizers fields from both sides of the original constitutive relation, it would be useful (especially in light of the convergence result for the numerical methods) to have a regularity theory that treats the solutions in a natural way.

11.1.3 PDE Constrained Optimization

There is much current interest in metamaterials and the ways in which they can be constructed. One way to view the design of such materials is by thinking of them

as a PDE constrained optimization problem for the effective material coefficients. By formulating the problem in this way, designs can be found that exhibit the effective properties of a specified metatmaterial. Another possible application of PDE constrained optimization that uses these variational principles is to attempt to cloak an object by determining the non-homogeneous term that will make the fields the same as if the object were not present.

REFERENCES

[1] D.N. Arnold, *Mixed finite element methods for elliptic problems*, Comput. Methods Appl. Mech. Engrg. **82** (1990), 281–300.

[2] A.Wexler, B. Fry, and M. Neumann, *Impedance-computed tomography algorithm and system*, Appl. Opt. **24** (1985), 3985–3992.

[3] O. Axelsson and V. A. Barker, *Finite element solution of boundary value problems, theory and computation*, SIAM, Philidelphia, PA, 2001.

[4] G. Bao, G.W. Wei, and S. Zhao, *Numerical solution of the Helmholtz equation with high wavenumbers*, Int. J. Numer. Meth. Engng. **59** (2004), 389–408.

[5] J.G. Berryman, *Convexity properties of inverse problems with variational constraints*, J. Franklin Institute **328** (1991), 1–13.

[6] J.G. Berryman and R.V. Kohn, *Variational constraints for electrical impedance tomography*, Phys. Rev. Lett. **65** (1990), 325–328.

[7] L. Borcea, *Electrical impedance tomography*, Inverse Problems **18** (2002), R99–R136.

[8] ———, *Variationally constrained solution of electrical impedance tomography*, Inverse Problems **19** (2003), 1159–1184.

[9] L. Borcea, J.G. Berryman, and G.C. Papanicolau, *High contrast impedance tomography*, Inverse Problems **12** (1996), 935–958.

[10] A. Borzi and V. Schulz, *Multigrid methods for PDE optimization*, SIAM Review **51** (2009), 361–395.

[11] H. Brezis, *Analyse functionelle*, Dunod, Paris, France, 1983.

[12] F. Brezzi and M. Fortin, *Mixed and hybrid finite element methods*, Springer-Verlag, New York, NY, 1991.

[13] O.P. Bruno and F. Reitich, *Solution of a boundary value problem for Helmholtz equation via variation of the boundary into the complex domain*, Proc. R. Soc. A **122** (1992), 317–340.

[14] O. Cessenat and B. Despres, *Application of an ultra weak variational formulation of elliptic PDEs to the two-dimensional Helmholtz problem*, SIAM J. Num. Anal. **35** (1998), 255–299.

[15] A.V. Cherkaev, *Variational methods for structural optimization*, Springer, New York, NY, 2000.

[16] A.V. Cherkaev and L.V. Gibiansky, *Variational principles for complex conductivity, viscoelasticity, and similar problems in media with complex moduli*, Journal of Mathematical Physics **35** (1994), 127–145.

[17] B. Dacorogna, *Direct methods in the calculus of variations*, Springer-Verlag, New York, NY, 1989.

[18] J. Demmel, *The condition number of equivalence transformations that block diagonalize matrix pencils*, SIAM J. Num. Anal. **20** (1983), 599–610.

[19] ———, *Applied numerical linear algebra*, SIAM, Philidelphia, PA, 1997.

[20] D.C. Dobson, *Convergence of a reconstruction method for the inverse conductivity problem*, SIAM J. Appl. Math **52** (1992), 442–458.

[21] ———, *Estimates on resolution and stabilization for the linearized inverse conductivity problem*, Inverse Problems **8** (1992), 71–81.

[22] ———, *Optimal design of periodic antireflective structures for the Helmholtz equation*, European Journal of Applied Mathematics **4** (1993), 321–340.

[23] Y.A. Erlangga, C. Vuik, and C.W. Oosterlee, *On a class of preconditioners for solving the Helmholtz equation.*, Appl. Num. Math. **50** (2004), 409–425.

[24] L.C. Evans, *Partial differential equations*, American Mathematical Society, Providence, RI, 1998.

[25] K. Golden and G. Papanicolau, *Bounds on effective parameters of heterogeneous media by analytic continuation*, Commun. Math. Phys. **90** (1983), 473–491.

[26] Y.A. Gryazin, M.V. Kilbanov, and T.R. Lucas, *Two numerical methods for an inverse problem for the 2-D Helmholtz equation*, J. Comp. Phys. **184** (2003), 122–148.

[27] C.-H. Guo, *Incomplete block factorization preconditioning for linear systems arising in the numerical solution of the Helmholtz equation*, Appl. Num. Math. **19** (1996), 495–508.

[28] F. Gylys-Colwell, *An inverse problem for the Helmholtz equation*, Inverse Problems **12** (1996), 139–156.

[29] G.R. Hadley, *A complex Jacobi iterative method for the indefinite Helmholtz equation*, J. Comp. Phys. **203** (2005), 358–370.

[30] I. Harari, M. Slavutin, and E. Turkel, *Analytical and numerical studies of a finite element PML for the Helmholtz equation*, J. Comput. Acoust. **8** (2000), 212–137.

[31] J.D. Jackson, *Classical electrodynamics*, Wiley, Hoboken, NJ, 1999.

[32] R. Kechroud, A. Soulaimani, Y. Saad, and S. Gowda, *Preconditioning techniques for the solution of the Helmholtz equation by the finite element method*, Math. Comput. Simulat. **65** (2004), 303–321.

[33] R.V. Kohn and A. McKenney, *Numerical implementation of a variational method for electrical impedance tomography*, Inverse Problems **6** (1990), 389–414.

[34] R.V. Kohn and M. Vogelius, *Determining conductivity by boundary measurements*, Commun. Pure Appl. Math. **37** (1984), 113–123.

[35] D. Lahaye, H. De Gersem, S. Vanderwalle, and K. Hameyer, *Algebraic multigrid for complex symmetric systems*, IEEE Trans. Magn. **36** (2000), 1535–1538.

[36] G.W. Milton, *The theory of composities*, Cambridge University Press, Cambridge, UK, 2002.

[37] G.W. Milton, P. Seppecher, and G. Bouchitté, *Minimization variational principles for acoustics, elastodynamics, and electromagnetism in lossy inhomogeneous bodies at fixed frequency*, Proc. R. Soc. A **465** (2009), 367–396.

[38] G.W. Milton and J.R. Willis, *Minimum variational principles for time-harmonic waves in a dissipative medium and associated variational principles of Hashin-Shtrikman type*, Proc. Roy. Soc. Lond. to appear.

[39] ———, *On modifications of Newton's second law and linear continuum elastodynamics*, Proc. R. Soc. A **463** (2007), 855–880.

[40] P. Monk, *Finite element methods for Maxwell's equations*, Clarendon Press, Oxford, UK, 2003.

[41] W. Rudin, *Real and complex analysis*, McGraw-Hill, Boston, MA, 1987.

[42] C. Vogel, *Computational methods for inverse problems*, SIAM, Philidelphia, PA, 2002.

[43] Z. Wang and S.F. Wu, *Helmholtz equation-least-squares method for reconstructing the acoustic pressure field*, J. Acoust. Soc. Am. **102** (1997), 2020–2032.