A MODIFIED ERROR IN CONSTITUTIVE EQUATION APPROACH FOR VISCOELASTICITY IMAGING WITH INTERIOR DATA

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This thesis presents the formulation and implementation details of a method based on the modified error in constitutive equation to address the viscoelasticity imaging problem in situations in which information on boundary conditions is unknown. In the viscoelasticity imaging problem, the goal is to produce images of the viscoelastic properties of a material from displacements measured in its interior. These measured displacements are always corrupted with noise, which poses a challenge to methods designed to solve such problems. Moreover, in practical applications such as biomedical imaging, where the material of interest is tissue, the magnitude and spatial distribution of the excitation used to generate the displacements that are measured are not exactly known. This is a challenge to optimization-based methods for the imaging problem, as the lack of boundary conditions leads to ill-posed forward problems. The method developed here overcomes this challenge and at the same time handles noisy and incomplete displacement data.

This thesis is divided into two chapters. The first chapter, which is an adaptation of a journal article that has been submitted for publication, presents the method and relevant derivations. Results from numerical experiments are also included in this chapter. The second chapter details the implementation of the method in the DinamicaE simulation suite, developed by the Computational Mechanics and Inverse Problems Group led by Professor Wilkins Aquino. The
DinamicaE simulation suite is the result of over four years of development effort, which is still ongoing. Development of a large component of this software has been one of the author’s main contributions as a Ph.D. student. DinamicaE is a massively parallel research code that solves problems in steady-state dynamics, acoustics, and acoustic-structure interaction. Moreover, the software also solves imaging problems in these domains. One of the main goals of DinamicaE is to assess the feasibility of algorithms such as the one presented in this thesis to solve problems of interest in the field of biomedical imaging, which seeks to provide early diagnosis for many physical illnesses. Its modular design, which is made possible by the features offered by the C++ programming language, allows for simple implementations of the algorithm presented in this thesis and many more.
Manuel was born and raised in Santo Domingo, Dominican Republic. Curious to see the rest of the world, he took a first step in this direction by pursuing undergraduate studies at Utah State University, where in May 2009 he completed majors in civil engineering and mathematics. He then enrolled in the graduate program of the School of Civil and Environmental Engineering at Cornell University, where he began to work towards a Ph.D. in August 2009. After two-and-a-half years of living in gorgeous Ithaca, NY, he moved to bullish Durham, NC, where he continued to work on his degree until its completion. Manuel’s interests include playing multiple sports, Latin dancing, traveling, spending time with friends, and daydreaming.
To my Mom and Dad.

“Lo que hace más importante a tu rosa es el tiempo que tú has perdido con ella.”

– Antoine de Saint-Exupéry
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CHAPTER 1
A MODIFIED ERROR IN CONSTITUTIVE EQUATION APPROACH FOR
FREQUENCY-DOMAIN VISCOELASTICITY IMAGING USING
INTERIOR DATA

Abstract

This chapter presents a method for the identification of linearly viscoelastic material parameters in the context of steady-state dynamics using interior data. In this method, the inverse problem of viscoelasticity imaging is solved by minimizing an objective which includes the modified error in constitutive equation (MECE) functional and is subject to the conservation of linear momentum without the need to introduce any knowledge of external excitations or boundary conditions. The MECE functional measures the discrepancy in the constitutive equations that connect kinematically admissible strains and dynamically admissible stresses; in addition to this, it also incorporates the measurement data in a quadratic penalty term. Regularization is achieved through a penalty parameter in combination with the discrepancy principle due to Morozov. Numerical results demonstrate the robust performance of the method in situations where the available measurement data is incomplete and corrupted by noise of varying levels.
1.1 Introduction

Inverse characterization of viscoelastic properties is of high relevance in many areas of science, engineering, and medicine. In particular, in the medical field, it is well-known that viscoelastic properties are correlated to tissue pathology [27]. This observation has spurred the development of elastography or elasticity imaging techniques, in which the goal is to identify the elastic or viscoelastic properties of tissue non-invasively (see [12, 24, 21, 13, 23] for reviews). Other applications abound, including the nondestructive evaluation of structural systems such as buildings, bridges, and aircraft components.

In this work, we are concerned with finding viscoelastic material properties using noisy interior data in domains where traction and/or displacement conditions are unknown or uncertain. This problem is highly relevant in elasticity imaging, where displacement or velocity fields are obtained using ultrasound or MRI and the magnitude and nature of the excitation sources are highly uncertain. Different techniques have been developed that address this problem, including algebraic direct inversion [20, 27, 22] and the Adjoint Weighted Equations (AWE) methods [2, 30]. These techniques have the advantage of being non-iterative, but need derivatives of the data, making them very sensitive to noise. Optimization approaches [9, 19, 11, 6, 1], which have the advantage of handling sparse and imperfect data, have received limited or no attention for problems with interior data in which the boundary conditions are unknown due to the complication that the forward problem is ill-posed when no boundary conditions are specified.

Our goal in this work is to develop a method for reconstructing viscoelastic
properties from interior, imperfect data using iterative optimization algorithms. To this end, we exploit the concept of the modified error in constitutive equation (MECE) [16, 11, 4]. The MECE functional combines the error in constitutive equation (ECE) [17], which measures the discrepancy in the constitutive equations that connect kinematically admissible strains and dynamically admissible stresses, and a quadratic error term that incorporates the measurement data. MECE-based approaches have found applications in model updating with vibrational data [16, 5], time-domain formulations [3, 11], and large scale identification problems in both elastodynamics [4] and coupled acoustic-structure systems [29]. One of the main features of the approach proposed here is that the MECE formulation leads to systems that are invertible even in the absence of conventional Neumann and Dirichlet conditions, which addresses some of the limitations found in other optimization-based formulations. In addition, we extend previous ideas regarding the solution strategy for the minimization problem to the realms of viscoelasticity, where positivity requirements are enforced using inequality constraints.

The rest of this chapter is organized as follows. Section 1.2 describes the steady-state viscoelasticity problem and the inverse problem of interest. The details of the derivation are then presented in Section 1.3. Other details specific to the method presented in this work are addressed in Section 1.4. Section 1.5 is devoted to a series of numerical examples designed to showcase the capabilities of the method, and finally, concluding remarks are offered in Section 1.6.
1.2 Problem Setting

**Governing equations of motion** Let a solid viscoelastic body occupy a bounded and connected domain \( \Omega \subset \mathbb{R}^d \) \((1 \leq d \leq 3)\) with boundary \( \Gamma \). The time-harmonic motion of this body is governed by the balance equations

\[
\nabla \cdot \sigma + b = -\rho \omega^2 u \quad \text{in} \ \Omega, \tag{1.1a}
\]

\[
\sigma \cdot n_s = t \quad \text{on} \ \Gamma_N, \tag{1.1b}
\]

where \( u \) is the displacement field, \( \omega \) represents the specified angular frequency, \( \rho \) denotes the known mass density, \( b \) is a given body force density, \( \sigma \) represents the stress tensor, \( t \) and \( \Gamma_N \subseteq \Gamma \) are the given surface force density (traction) and its support, respectively, and \( n_s \) is the outward unit vector normal to \( \Gamma \); the kinematic equations

\[
u = 0 \quad \text{on} \ \Gamma_D, \tag{1.2a}
\]

\[
\epsilon[u] = \frac{1}{2}(\nabla u + \nabla u^T) \quad \text{in} \ \Omega, \tag{1.2b}
\]

where \( \epsilon[u] \) denotes the linearized strain tensor associated with \( u \) and \( \Gamma_D \subseteq \Gamma \) is the portion of the boundary where the displacement is known; and the (linear viscoelastic) constitutive relation

\[
\sigma = \mathbf{C} : \epsilon[u] \quad \text{in} \ \Omega, \tag{1.3}
\]

where \( \mathbf{C} \) is the fourth-order, complex-valued viscoelasticity tensor field. Equation (1.2a) specifies a boundary condition that is homogeneous, which is assumed in this work for the sake of simplicity and without loss of generality; the case of a nonhomogeneous boundary condition can be treated with minor modifications.
The boundary sets \( \Gamma_N \) and \( \Gamma_D \) are only required to not overlap (i.e., \( \Gamma_N \cap \Gamma_D = \emptyset \)) and do not necessarily have to form a cover of \( \Gamma \) (i.e., \( \Gamma_N \cup \Gamma_D \subseteq \Gamma \)). When they do not form a cover, equations (1.1a)-(1.3) admit a solution which is not unique. A unique solution exists only when \( \Gamma_N \cup \Gamma_D = \Gamma \). We allow this generality regarding the boundary sets for the sake of the upcoming formulation, in which the lack of boundary conditions specified on the entirety of the boundary does not pose an issue.

**Weak formulation** We denote the \( L^2(\Omega) \) inner product of square-integrable second-order tensor fields \( \mathbf{a} \) and \( \mathbf{b} \) with \( \langle \mathbf{a}, \mathbf{b} \rangle \):

\[
\langle \mathbf{a}, \mathbf{b} \rangle := \int_{\Omega} \mathbf{a} : \mathbf{b} \, dV = \int_{\Omega} a_{ij} b_{ij} \, dV,
\]

where the overline denotes complex conjugation and indicial notation is used (with repeated indices implying summation). The inner product of vector and scalar fields follow the same notation. A similar notation is used for the inner product of fields defined over a surface; e.g.,

\[
\langle \mathbf{a}, \mathbf{b} \rangle_{\Gamma} := \int_{\Gamma} \mathbf{a} : \mathbf{b} \, dS.
\]

The weak formulation of the balance equations (1.1a) and (1.1b) then reads

\[
\langle \sigma, \mathcal{E}(\mathbf{v}) \rangle - \omega^2 \langle \rho \mathbf{u}, \mathbf{v} \rangle - \langle \mathbf{b}, \mathbf{v} \rangle_{\Gamma(\Gamma_N \cup \Gamma_D)} = \mathcal{F}(\mathbf{v}), \quad \forall \mathbf{v} \in \mathcal{W}, \tag{1.4}
\]

with the test function space \( \mathcal{W} \) defined as \( \mathcal{W} := \{ \mathbf{w} : \mathbf{w} \in H^1(\Omega; \mathbb{R}^d), \mathbf{w} = 0 \text{ on } \Gamma_D \} \) and where the linear functional

\[
\mathcal{F}(\mathbf{w}) = \langle \mathbf{b}, \mathbf{w} \rangle + \langle t, \mathbf{w} \rangle_{\Gamma_N} \tag{1.5}
\]

embraces the known excitations in \( \Omega \) and on \( \Gamma_N \). We remark that \( \rho \in L^\infty(\Omega) \) is assumed to be bounded below by a positive constant. Moreover, the space of
dynamically admissible stresses is defined as

\[ S(u) := \{ \sigma : \sigma \in L^2(\Omega; \mathbb{R}^{3,3}_{\text{sym}}), \text{ eqn. (1.4) holds} \}. \] (1.6)

Likewise, we define the space \( Z \) of admissible viscoelasticity tensor fields as

\[ Z = \{ \mathcal{C} \in L^\infty(\Omega; Q) | \epsilon : \text{Re} [\mathcal{C}(x)]: \epsilon > c_0 \epsilon : \epsilon, \epsilon : \text{Im} [\mathcal{C}(x)]: \epsilon \geq 0 \ \forall x \in \Omega \text{ and } \epsilon \in \mathbb{R}^{3,3}_{\text{sym}}, \epsilon \neq 0 \}, \]

where \( Q \) denotes the 21-dimensional vector space of fourth-order tensors \( \mathcal{C} \) with major and minor symmetries (i.e., \( C_{ijkl} = C_{klij} = C_{jilk} \)) and \( c_0 \) is some fixed positive constant. \( \text{Re} [\cdot] \) and \( \text{Im} [\cdot] \) denote the real and imaginary parts, respectively, of a complex-valued quantity.

**Measurements** In addition to the fundamental equations (1.1a)-(1.3), we assume that the steady-state displacements are measured for the angular frequency \( \omega \). More explicitly, we assume availability for the specified frequency \( \omega \) of (a) measured displacements \( \tilde{d} \) in \( \Omega_m \subset \Omega \) or (b) measured displacements \( \tilde{u} \) on \( \Gamma_u \subset \Gamma \), i.e.:

\[ u = \tilde{d} \text{ in } \Omega_m, \quad u = \tilde{u} \text{ on } \Gamma_u, \] (1.7)

where \( \Omega_m \) and \( \Gamma_u \) are not both simultaneously empty. Moreover, the measurement surface \( \Gamma_u \) is assumed to satisfy \( \Gamma_D \cap \Gamma_u = \emptyset \), which follows from the fact that a displacement measurement \( \tilde{u} \) is not needed on the part of the boundary where one knows the true displacement exactly.

**Remark 1** Even though (1.7) expresses an equality between the experimentally-measured displacements \( \tilde{d} \) and \( \tilde{u} \) and the model displacement \( u \), this equality will be relaxed in the upcoming formulation, and \( u \) will be required to approximate (and not necessarily equal) \( \tilde{d} \) and \( \til\til{u} \) due to the noisy nature of experimental measurements.
Inverse Problem  The inverse problem addressed in this work consists of the following: reconstruct the viscoelasticity tensor field $C \in \mathcal{Z}$ that satisfies the governing equations of motion (1.1a)-(1.3) and that is consistent with the measurement of the steady-state response of the solid for a known angular frequency $\omega$.

$L^2$ minimization  A common way to solve the inverse problem described above relies on finding the material parameters that minimize the mean squared error between the measured and computed responses [19, 10]. We refer to this method as $L^2$ minimization, which uses the error functional defined by

$$J(u, C) := \frac{1}{2} \left[ \langle u - \tilde{u}, u - \tilde{u} \rangle_{\Omega_m} + \langle u - \tilde{u}, u - \tilde{u} \rangle_{\Gamma_u} \right] + R(C),$$  \hspace{1cm} (1.8)

where $R$ is a non-negative regularization functional. Thus, the $L^2$ minimization method finds the solution to the inverse problem as

$$(u^*, C^*) := \arg \min_{u, C} J(u, C) \quad \text{subject to Eqs.}(1.1a) - (1.3),$$  \hspace{1cm} (1.9)

which is typically solved using Newton or quasi-Newton methods. Such methods require the computation of the gradient of $J(u, C)$, which usually relies on solving a variational problem such as (1.4) (see [19] for details). This problem is ill-posed, however, when $\Gamma_N$ and $\Gamma_D$ do not form a cover of $\Gamma$.

1.3 Modified error in constitutive equation (MECE) approach to viscoelasticity imaging using interior data

Following the approach presented in [4, 29], the inverse problem addressed in this work is formulated as an optimization problem in which the unknown con-
stitutive tensor is estimated by minimizing an objective function that consists of two error terms: 1) an ECE functional [17] that has been adapted for viscoelastic materials and that measures the discrepancy in the constitutive equation that connects kinematically admissible strains and dynamically admissible stresses and 2) a quadratic error term that quantifies the mismatch between the predicted (or model) displacements and the measured ones. Thus, the objective function, hereafter referred to as the viscoelasticity MECE functional, used in this work is

$$\Lambda(u, \sigma; C) := U(u, \sigma; C) + \frac{\kappa}{2} \left[ \langle u - \tilde{d}, u - \tilde{d} \rangle_{\Omega_m} + \langle u - \tilde{u}, u - \tilde{u} \rangle_{\Gamma_u} \right],$$  \hspace{1cm} (1.10)$$

where

$$U(u, \sigma; C) := \frac{1}{2} \int_{\Omega} (\sigma - C : \varepsilon[u]) : P^{-1} : (\sigma - C : \varepsilon[u]) \, dV$$ \hspace{1cm} (1.11)$$

is the ECE functional that has been adapted for viscoelastic materials; \( P \) is a fourth-order tensor that is symmetric, positive-definite, and real-valued; and \( \kappa \) is a positive weight parameter that adjusts the relative contribution of the different summands to \( \Lambda \) in (1.10). Further discussion of \( P \) and \( \kappa \) (e.g., how to select them) is deferred to Section 1.4.

The version of \( \Lambda \) used in [4, 29] differs from the one shown in (1.10) in the following way: \( P^{-1} \) in (1.11) is substituted with \( C^{-1} \). Since this work is concerned with viscoelastic materials, while [4, 29] address elastic materials only, this substitution is required because \( C \) is not positive-definite for viscoelastic materials in general and fails to yield \( U \) with the following desirable properties:

$$U(u, \sigma; C) \geq 0 \quad \forall \, C \in \mathcal{Z},$$ \hspace{1cm} (1.12)$$

$$U(u, \sigma; C) = 0 \quad \iff \sigma = C : \varepsilon[u].$$ \hspace{1cm} (1.13)$$

These properties are preserved, nevertheless, with the use of \( P^{-1} \) in \( U \). Thus, for a given triplet \((u, \sigma, C) \in \mathcal{W} \times S(u) \times \mathcal{Z}\) (see Weak formulation in Section 1.2
for the definition of these sets), $\Lambda(u, \sigma; \mathcal{C})$ provides a quantitative measure of the compatibility of these variables with (1) the available measurements $\tilde{d}$ and $\tilde{u}$ and (2) the constitutive equation. Since lower values of $\Lambda$ suggest better compatibility, the solution to the inverse problem of viscoelasticity imaging using a generalized ECE approach is given by

$$ (u^*, \sigma^*, \mathcal{C}^*) := \arg \min_{u \in \mathcal{W}, \sigma \in \mathcal{S}(u), \mathcal{C} \in \mathcal{Z}} \Lambda(u, \sigma; \mathcal{C}). \quad (1.14) $$

Notice that (1.14) defines a PDE-constrained optimization problem. A common approach to solve (1.14) is to use an alternating minimization strategy [11, 4, 29]. This iterative approach defines the transition from the current iterate $(u, \sigma, \mathcal{C})^n$ to the next iterate $(u, \sigma, \mathcal{C})^{n+1}$ through two successive and complementary partial minimizations of $\Lambda(u, \sigma; \mathcal{C})$. The first of these minimizations,

$$ (u^{n+1}, \sigma^{n+1}) := \arg \min_{u \in \mathcal{U}, \sigma \in \mathcal{S}(u)} \Lambda(u, \sigma; \mathcal{C}^n), \quad (1.15) $$

updates the mechanical fields $u$ and $\sigma$ and imposes the balance of linear momentum, without the need to introduce any knowledge of external excitations or boundary conditions as a constraint, while the second minimization pertains to the update of the material parameter $\mathcal{C}$:

$$ \mathcal{C}^{n+1} := \arg \min_{\mathcal{C} \in \mathcal{Z}} \Lambda(u^{n+1}, \sigma^{n+1}; \mathcal{C}). \quad (1.16) $$

### 1.3.1 Updating the Mechanical Fields

The minimization defined in (1.15) is itself a PDE-constrained optimization problem. In order to solve this optimization subproblem, we derive the optimality conditions using a Lagrange multiplier approach. This requires defining
the Lagrangian \( \mathcal{L} : \mathcal{W} \times \mathcal{W} \times \mathcal{S}(u) \times \mathcal{Z} \rightarrow \mathbb{R} \) as

\[
\mathcal{L}(u, w, \sigma; C) := \Lambda(u, \sigma; C) + \text{Re} \left( \langle \sigma \cdot n_s, w \rangle_{\Gamma(N \cup D)} \right) + \langle \sigma, \epsilon[w] \rangle + \omega^2 \langle \rho u, w \rangle + F(w),
\]

(1.17)

where \( \text{Re}(\cdot) \) denotes the real part of a complex quantity. Notice that \( w \in \mathcal{W} \) plays the role of the Lagrange multiplier and that the term \( \langle \sigma \cdot n_s, w \rangle_{\Gamma(N \cup D)} \) in (1.17) is crucial for the case in which \( \Gamma_N \cup \Gamma_D \neq \Gamma \) (i.e., boundary conditions are not known over the entire boundary).

In order to derive the optimality conditions, the gradient of \( \mathcal{L} \) with respect to \( u, w, \) and \( \sigma \) needs to be computed. In order to compute the different gradients of \( \mathcal{L} \), we make use of the Gâteaux derivative. The Gâteaux derivative of a functional \( F(g) \) with respect to \( g \) in the direction \( \delta g \) is defined as

\[
F'_g(\delta g) := \left. \frac{d}{d\epsilon} F(g + \epsilon \delta g) \right|_{\epsilon=0}.
\]

The quantity \( F'_g \) represents the gradient of \( F \) with respect to \( g \). Thus, with this definition, the Gâteaux derivative of \( \mathcal{L} \) with respect to \( \sigma \) in the direction \( \delta \sigma \in \mathcal{S}(u) \) is

\[
\mathcal{L}'_{\sigma}(\delta \sigma) = \text{Re} \left( \langle \delta \sigma, \mathcal{P}^{-1} : \sigma \rangle - \langle \delta \sigma, \mathcal{C} : \epsilon[u] \rangle - \langle \delta \sigma \cdot n_s, w \rangle_{\Gamma(N \cup D)} \right) + \langle \delta \sigma, \epsilon[w] \rangle = \text{Re} \left( \langle \delta \sigma, \mathcal{P}^{-1} : (\sigma - \mathcal{C} : \epsilon[u]) \rangle - \epsilon[w] \right) + \langle \delta \sigma \cdot n_s, w \rangle_{\Gamma(N \cup D)}. \quad (1.18)
\]

Since \( \mathcal{L}'_{\sigma}(\delta \sigma) = 0 \ \forall \delta \sigma \in \mathcal{S}(u) \), we obtain from (1.18)

\[
w = 0 \quad \text{on} \ \Gamma \setminus (\Gamma_N \cup \Gamma_D), \quad (1.19)
\]

\[
\sigma = \mathcal{C} : \epsilon[u] + \mathcal{P} : \epsilon[w] \quad \text{in} \ \Omega. \quad (1.20)
\]

Notice that (1.19) implies that \( w \in \mathcal{W}_0 \subseteq \mathcal{W} \), where \( \mathcal{W}_0 := \{w : w \in \mathcal{W}, w = 0 \ \text{on} \ \Gamma \setminus (\Gamma_N \cup \Gamma_D)\} \).
Proceeding in a similar manner, the Gâteaux derivative of $L$ with respect to $u$ in the direction $\delta u \in W$ is
\[
L_u'(\delta u) = \text{Re}\left(\langle (C: \epsilon[u] - \sigma) : P^{-1} : \mathcal{C}, \epsilon[\delta u] \rangle + \kappa \left(\langle u - \bar{d}, \delta u \rangle_{\Omega_m} + \langle u - \bar{u}, \delta u \rangle_{\Gamma_u} \right) + \omega^2 \langle \rho \delta u, w \rangle \right) \quad (1.21)
\]
After substituting (1.20) into (1.21) and noticing that $L_u'(\delta u) = 0$ $\forall \delta u \in W$, we arrive at
\[
\langle C: \epsilon[w], \epsilon[\delta u] \rangle - \omega^2 \langle \rho w, \delta u \rangle = \kappa \left(\langle u - \bar{d}, \delta u \rangle_{\Omega_m} + \langle u - \bar{u}, \delta u \rangle_{\Gamma_u} \right) \quad \forall \delta u \in W. \quad (1.22)
\]
Following the same steps for the Lagrange multiplier $w$ and using (1.20) yields
\[
\langle C: \epsilon[u] + P : \epsilon[w], \epsilon[\delta w] \rangle - \omega^2 \langle \rho u, \delta w \rangle = F(\delta w) \quad \forall \delta w \in W_0. \quad (1.23)
\]
Notice that $\langle \sigma \cdot n_s, \delta w \rangle_{\Gamma \setminus (\Gamma_N \cup \Gamma_D)}$ vanishes because $\delta w \in W_0$, i.e. $\delta w = 0$ on $\Gamma \setminus (\Gamma_N \cup \Gamma_D)$.

For a given $\mathcal{C}^n \in \mathcal{Z}$ at the $n$th iteration of the alternating directions scheme, the mechanical field update thus corresponds to solving the following coupled variational problems: find $(u, w)^{n+1} \in W \times W_0$ such that
\[
\langle \mathcal{C} : \epsilon[w^{n+1}], \epsilon[\delta u] \rangle - \omega^2 \langle \rho w^{n+1}, \delta u \rangle - \kappa A(u^{n+1}, \delta u) = - \kappa A_m(\delta u) \quad \forall \delta u \in W,
\]
\[
\langle P : \epsilon[w^{n+1}], \epsilon[\delta w] \rangle + \langle \mathcal{C}^n : \epsilon[u^{n+1}], \epsilon[\delta w] \rangle - \omega^2 \langle \rho u^{n+1}, \delta w \rangle = F(\delta w) \quad \forall \delta w \in W_0, \quad (1.24)
\]
where
\[
A(u^{n+1}, \delta u) := \langle u^{n+1}, \delta u \rangle_{\Omega_m} + \langle u^{n+1}, \delta u \rangle_{\Gamma_u} \quad (1.25)
\]
and
\[
A_m(\delta u) := \langle \bar{d}, \delta u \rangle_{\Omega_m} + \langle \bar{u}, \delta u \rangle_{\Gamma_u}. \quad (1.26)
\]
After solving (1.24) for $u^{n+1}$ and $w^{n+1}$, the stress $\sigma^{n+1}$ can be computed using (1.20).

### 1.3.2 Updating the Material Properties

After computing the updated mechanical fields $u^{n+1}$ and $w^{n+1}$, the next step in the alternating directions scheme is to solve (1.16). This inequality constrained optimization problem is referred to as the material update step. Given the nature of the constraints imposed by $Z$ on the admissible viscoelasticity tensor fields, the approach used here to compute the material update $C^{n+1}$ consists of the following two substeps.

1. **Proposal substep:** A proposed material update $\tilde{C}^{n+1}$ is computed by enforcing the first-order necessary optimality condition $L'_C(\delta C) = 0 \forall \delta C \in Z$.

2. **Correction substep:** If the proposed material update $\tilde{C}^{n+1}$ is not admissible (i.e., $\tilde{C}^{n+1} \notin Z$), then the actual material update $C^{n+1}$ is taken as an admissible viscoelasticity field which approximates $\tilde{C}^{n+1}$. Otherwise, $C^{n+1}$ is set to $\tilde{C}^{n+1}$.

**Proposal substep** Enforcing the condition $L'_C(\delta C) = 0 \forall \delta C \in Z$, one obtains the rule for $\tilde{C}^{n+1}$ as

$$\forall \delta C \in Z, \left\langle \left(\tilde{C}^{n+1} : \epsilon[u^{n+1}] - \sigma^{n+1}\right), \mathcal{P}^{-1} : \epsilon[w^{n+1}], \delta C \right\rangle = 0. \quad (1.27)$$

We will focus on isotropic materials for the rest of this chapter. Thus, $C$ has the form

$$C = \left( B - \frac{2}{3} G \right) (I \otimes I) + 2GZ \quad (1.28)$$
with $B$ and $G$ denoting (spatially-dependent) bulk and shear complex moduli, respectively. $I$ and $\mathcal{I}$ are the second- and fourth-order identity tensors, respectively.

The tensor $\mathcal{P}$ is assumed to have the same major and minor symmetries as $\mathcal{C}$. Hence, $\mathcal{P}$ can be represented as

$$\mathcal{P} = \left( B_p - \frac{2}{3} G_p \right) (I \otimes I) + 2 G_p \mathcal{I} \quad (1.29)$$

where $G_p$ and $B_p$ are real, positive constants to be explicitly defined in Section 1.4.1.

The formulae for the proposed update are obtained by first decoupling the stress and strain tensors into deviatoric and volumetric components; i.e.,

$$\sigma = \sigma_{dev} + qI, \quad \epsilon[u] = \epsilon_{dev}[u] + \frac{1}{3} \epsilon_u I,$$

where $\sigma_{dev}$ and $\epsilon_{dev}$ are the deviatoric stress and strain tensors, respectively, $q = \frac{1}{3} \text{tr}(\sigma)$ is the mean stress, and $\epsilon_u = \text{tr}(\epsilon[u])$ is the volumetric strain. Then, combining (1.27), (1.28) and (1.29), yields

$$\left\langle \frac{1}{2G_p} \left( 2G^{n+1}_{\text{dev}} \epsilon_{\text{dev}}[u^{n+1}] - \sigma^{n+1}_{\text{dev}} \right) : \epsilon_{\text{dev}}[\tilde{u}^{n+1}], \delta G \right\rangle +$$

$$\left\langle \frac{\epsilon_u^{n+1}}{B_p} \left( \tilde{B}^{n+1} \epsilon_u^{n+1} - q^{n+1} \right), \delta B \right\rangle = 0 \quad \forall \delta G, \delta B, \quad (1.30)$$

From (1.30), it now follows that the pointwise rule for the proposed bulk modulus update is

$$\tilde{B}^{n+1} = \frac{q^{n+1}}{\epsilon_u^{n+1}} = \frac{\text{tr}(\sigma^{n+1})}{3 \text{tr}(\epsilon[u^{n+1}])), \quad (1.31)$$

while the pointwise rule for the proposed shear modulus update is

$$\tilde{G}^{n+1} = \frac{\sigma^{n+1}_{\text{dev}} : \epsilon_{\text{dev}}[\tilde{u}^{n+1}]}{2 \epsilon_{\text{dev}}[u^{n+1}] : \epsilon_{\text{dev}}[\tilde{u}^{n+1}]), \quad (1.32)$$
The formulae just shown for the proposed material update can be easily extended to the case in which these moduli are known to be constant over some region $D \subseteq \Omega$. In this case, both the numerator and denominator of (1.31) and (1.32) carry an implicit integration over $D$; i.e.,

$$
\tilde{B}^{n+1} = \frac{\int_D \text{tr}(\sigma^{n+1}) \, dV}{3 \int_D \text{tr}(\epsilon[\mathbf{u}^{n+1}]) \, dV},
$$

$$
\tilde{G}^{n+1} = \frac{\langle \sigma^{n+1}_{\text{dev}}, \epsilon_{\text{dev}}[\mathbf{u}^{n+1}] \rangle_D}{2 \langle \epsilon_{\text{dev}}[\mathbf{u}^{n+1}], \epsilon_{\text{dev}}[\mathbf{u}^{n+1}] \rangle_D}.
$$

(1.33a) (1.33b)

**Correction substep**  The proposed material update computed through (1.31) and (1.32) may not satisfy the inequality constraints imposed by $Z$ [7]. Thus, for the purpose of this work, the actual bulk update $B^{n+1}$ and shear update $G^{n+1}$ are taken to be

$$
h(B^{n+1}) := \begin{cases} 
h(\tilde{B}^{n+1}) & : h(B_{\text{low}}) \leq h(\tilde{B}^{n+1}) \leq h(B_{\text{up}}) \\
h(\theta B^n + (1 - \theta) B_{\text{low}}) & : h(\tilde{B}^{n+1}) < h(B_{\text{low}}) \\
h(\theta B^n + (1 - \theta) B_{\text{up}}) & : h(\tilde{B}^{n+1}) > h(B_{\text{up}}) \
\end{cases},
$$

(1.34)

$$
h(G^{n+1}) := \begin{cases} 
h(\tilde{G}^{n+1}) & : h(G_{\text{low}}) \leq h(\tilde{G}^{n+1}) \leq h(G_{\text{up}}) \\
h(\theta G^n + (1 - \theta) G_{\text{low}}) & : h(\tilde{G}^{n+1}) < h(G_{\text{low}}) \\
h(\theta G^n + (1 - \theta) G_{\text{up}}) & : h(\tilde{G}^{n+1}) > h(G_{\text{up}}) \
\end{cases},
$$

(1.35)

where the function $h(\cdot)$ can be substituted with the $\text{Re}(\cdot)$ or $\text{Im}(\cdot)$ functions and $\theta \in [0, 1)$ is a user-defined parameter ($\theta = 0.5$ for the examples shown in Section 1.5). The complex numbers $B_{\text{low}}$ and $B_{\text{up}}$ serve as lower and upper bounds, respectively, for the bulk modulus; similarly, $G_{\text{low}}$ and $G_{\text{up}}$ serve as lower and upper bounds, respectively, for the shear modulus. These bounds, which are prescribed a priori, act as box constraints on the real and imaginary parts of the moduli. Whenever the real (imaginary) part of the proposed update falls outside of the allowable interval, it is replaced with a weighted average of the real (imaginary) part of the previous estimate and the bound being violated.
The approach presented here to compute the material update can be made equivalent to the gradient projection method by replacing the correction sub-step with a subspace minimization (see [18, p. 488] for details), but in practice, approximate methods such as the correction substep presented herein are used to address the subspace minimization problem.

### 1.3.3 Discretization

The finite element method was used in this work to approximate the solution of the governing variational problems. Using standard Voigt notation, the trial and test functions and their derivatives are expressed as

\[
\begin{align*}
\mathbf{u}^h &= [N] \{u\}, & \delta \mathbf{u}^h &= [N] \{\delta u\}, & \mathbf{\epsilon}[\mathbf{u}^h] &= [B] \{u\}, \\
\mathbf{w}^h &= [N] \{w\}, & \delta \mathbf{w}^h &= [N] \{\delta w\}, & \mathbf{\epsilon}[\mathbf{w}^h] &= [B] \{w\},
\end{align*}
\]

where \([N]\) and \([B]\) represent matrices of finite element shape functions and their derivatives with respect to spatial coordinates, respectively. Moreover, the viscoelasticity field \(C\) is discretized using piecewise constant basis functions (i.e., the material properties are assumed to remain constant in an element but can vary from one element to the next).

After substituting the above approximations into (1.24) and applying the standard finite element method, the discrete coupled system of equations is obtained as

\[
\begin{bmatrix}
[T] & [K] - \omega^2 [M] \\
([K] - \omega^2 [M])^H & -\kappa [D]
\end{bmatrix}
\begin{bmatrix}
\{w\} \\
\{u\}
\end{bmatrix} =
\begin{bmatrix}
\{F\} \\
-\kappa \{R\}
\end{bmatrix}.
\]

Notice that the superscript notation used to denote an iteration within the alternating directions scheme has been dropped for the sake of clarity. The matrices
and vectors in the above block system of equations are defined as follows.

\[ [K] := \sum_{\text{elements}} \int_{\Omega^e} [B]^T [C] [B] \, dV \quad (1.37a) \]

\[ [T] := \sum_{\text{elements}} \int_{\Omega^e} [B]^T [P] [B] \, dV \quad (1.37b) \]

\[ [M] := \sum_{\text{elements}} \int_{\Omega^e} \rho [N]^T [N] \, dV \quad (1.37c) \]

\[ [D] := \sum_{\text{elements}} \int_{\Omega^e_m} [N]^T [N] \, dV + \sum_{\text{elements}} \int_{\Gamma_u} [N]^T [N] \, dS \quad (1.37d) \]

\[ \{F\} := \sum_{\text{elements}} \int_{\Omega^e_N} [N]^T \mathbf{t} \, dS + \sum_{\text{elements}} \int_{\Omega^e} [N]^T \mathbf{b} \, dV \quad (1.37e) \]

\[ \{R\} := \sum_{\text{elements}} \int_{\Omega^e_m} [N]^T \mathbf{d} \, dV + \sum_{\text{elements}} \int_{\Gamma_u} [N]^T \mathbf{u} \, dS \quad (1.37f) \]

\([C]\) and \([P]\) denote the appropriate matrix representations of the fourth-order tensors \(\mathcal{C}\) and \(\mathcal{P}\), respectively. Moreover, notice that the coefficient matrix in (1.36) is a Hermitian matrix. The measured displacements \(\mathbf{\tilde{d}}\) and \(\mathbf{\tilde{u}}\) in (1.37f) are assumed to be a continuous field over the part \(\Omega_m\) of the domain and \(\Gamma_u\) of the boundary. However, the case in which the measurement data is not continuous and available only at a finite number of locations (i.e., sparse data) can be easily taken into consideration. In this case, measurement locations can be made to coincide with finite element nodes, and \([D]\) in (1.36) is then replaced by a diagonal Boolean matrix \([Q]\) with entries being nonzero only for the global degrees of freedom (dofs) where measurements were taken. In addition, \(\{R\}\) becomes a vector whose entries are the measured displacements at the different dofs. For this work, the system (1.36) was solved using the parallel, direct linear solver PARDISO [25, 26], which provides efficient solutions to such systems.

We now explore the invertibility of the coefficient matrix in (1.36). Let \([A] = [K] - \omega^2 [M]\) and assume that \(\Gamma_N \neq \Gamma\) (i.e., not all of the boundary \(\Gamma\) has a natural
boundary condition such as (1.1b)). Notice that the latter condition makes \([T]\) positive definite and, hence, invertible. Let \(\{u\}\) and \(\{w\}\) be elements of the kernel of the coefficient matrix in (1.36). We then have

\[
[T]\{w\} + [A]\{u\} = \{0\} \\
[A]^H\{w\} - \kappa[D]\{u\} = \{0\}.
\]  

(1.38)

(1.39)

We can see from the above equations that the kernel of the coefficient matrix is trivial (i.e., \(\{u\} = \{w\} = \{0\}\)) only if

\[
\operatorname{Ker}([A]^H[T]^{-1}[A]) \cap \operatorname{Ker}([D]) = \{0\},
\]  

(1.40)

where \(\operatorname{Ker}(\cdot)\) denotes the kernel of a matrix. Notice that since \([T]\) is positive definite, Condition (1.40) reduces to \(\operatorname{Ker}([A]) \cap \operatorname{Ker}([D]) = \{0\}\). It is important to point out that we do not consider the case in which \(\Gamma_N = \Gamma\) because it is of little relevance for interior data problems.

We would like to emphasize that Condition (1.40) calls for a careful design of experiments in order to obtain an invertible coupled system. For instance, we will consider in Section 1.5 problems in which boundary conditions are absent over the entire boundary. In this case, a measured displacement field over the whole domain (i.e. full-field data) is assumed to be available. This measurement condition produces a positive definite-observation matrix \([D]\) (i.e., \(\operatorname{Ker}([D]) = \{0\}\)) and the coupled system is guaranteed to be invertible as per (1.40).
1.4 The Scaling Tensor \( P \) and the Penalty Term \( \kappa \)

This section discusses the details concerning the scaling tensor \( P \) and the weight parameter \( \kappa \) first introduced in (1.10). These quantities were defined in the preceding formulation, but the particular choices used for this work will now be presented.

1.4.1 Choosing \( P \)

As mentioned in Section 1.3, \( P \) is a real-valued, symmetric, positive definite, and fourth-order tensor, which results in a matrix representation \([P]\) (as found in (1.37b)) with the same properties (i.e., real, symmetric, and positive definite). In this work, \( P \) is taken to be some conical combination (i.e., a linear combination in which the coefficients are all positive) of the real and imaginary parts of the initial value assigned to \( C \) in the first iteration of the alternating directions scheme (i.e., \( C_{\text{init}} \)). Notice that this choice makes \( P \) constant with respect to the viscoelastic tensor \( C \) and satisfies the properties required for \( P \). Moreover, this particular choice of \( P \) results in a matrix \([T]\), as defined in (1.37b), that is the same conical combination of the real and imaginary parts of the initial stiffness matrix, denoted from here on as \([K]_{\text{init}} \) and defined by (1.37a) with \([C]\) replaced by \([C_{\text{init}}]\). Various options for the conical combination that defines \( P \) were explored for this work, and the algorithm was found to be robust in this aspect. The arbitrary choice of equally weighting the real and imaginary parts of \([K]_{\text{init}} \) with a coefficient of 1 was made for all results reported later. Moreover, we have taken \( P \) to be independent of, or constant with respect to, the viscoelastic constitutive tensor \( C \), a condition that can be relaxed and will be the subject of
future work.

1.4.2 Choosing $\kappa$

The parameter $\kappa$ in (1.10) weights the relative importance between minimizing the ECE term and matching the experimental data and thus affects the quality of the reconstruction of $C$. The parameter $\kappa$, as it affects the smoothness of $C$, acts in this sense as a regularizer. However, the role of $\kappa$ is, as discussed in [29], reciprocal to that of a conventional Tikhonov regularization parameter.

As a first step, the following form for $\kappa$, originally proposed in [4], is used as

$$
\kappa := \alpha A,
$$

(1.41)

$$
A := \int_{\Omega} \epsilon[u_{\text{init}}] : \mathbf{P} : \epsilon[u_{\text{init}}] \, dV,
$$

(1.42)

where $\alpha \in \mathbb{R}^+$ is a dimensionless weighting parameter and $u_{\text{init}}$ is the solution to a dynamics problem described by equations (1.1a)-(1.3) with the initial guess $C = C_{\text{init}}$. In the case of unknown boundaries, it is necessary to prescribe some fictitious Neumann and/or Dirichlet conditions in order to obtain a solution. The arbitrariness of these boundary conditions does not affect the generality of the method as the solution is used as a means to scale the parameter $\kappa$. Notice that (1.41) makes the different terms in $\Lambda$ (1.10) dimensionally consistent, with every term having units of energy.

The next step is to appropriately choose the weighting parameter $\alpha$. This parameter is critical because high values of $\alpha$ will result in low values of the displacement-misfit functionals in (1.10), which is undesirable in the case of noisy data. Moreover, low values of $\alpha$ will result in high values of the
displacement-misfit functionals, which is undesirable due to the potential loss of important information contained in the measurements and the over-smoothing of the solution to the inverse problem.

The selection of $\alpha$ in this work is based on the discrepancy principle of Morozov [8, 15], a well-established approach which assumes the level of noise $\delta$ in the measurement data to be known \textit{a priori}. This principle dictates that the parameter $\alpha$ should be chosen to be the smallest positive number such that the final discrepancy between the computed and measured system response is at the noise level. Thus, if $u_\alpha$ denotes the displacement field obtained as a solution to the optimality system (1.14) for some $\alpha$, the discrepancy principle states that $\alpha$ should be chosen such that

$$
\frac{1}{\delta^2} \left| \frac{\langle u_\alpha - \tilde{d}, u_\alpha - \tilde{d} \rangle_{\Omega_m} + \langle u_\alpha - \tilde{u}, u_\alpha - \tilde{u} \rangle_{\Gamma_u}}{\langle \tilde{d}, \tilde{d} \rangle_{\Omega_m} + \langle \tilde{u}, \tilde{u} \rangle_{\Gamma_u}} - \delta^2 \right| \leq \epsilon_m,
$$

(1.43)

where $\epsilon_m$ is a specified tolerance. A simple bisection method was implemented to find $\alpha$ according to (1.43). This requires solving at each step of the bisection method the optimization problem (1.14) (using, for instance, the alternating directions scheme described earlier). A tolerance $\epsilon_m = O(10^{-2})$ was found to be adequate for the examples of Section 1.5. Lower error tolerances did not yield any noticeable differences in the solution.

### 1.5 Numerical Experiments

This section is devoted to a series of numerical experiments, all inspired by the field of biomedical imaging, that are intended to showcase the capabilities of the methodology explained earlier. In particular, the examples demonstrate that the approach proposed in this chapter produces adequate reconstructions of the
complex-valued bulk and shear moduli of viscoelastic materials in situations in which information on the boundary conditions is absent. In Example 1, we consider a two-dimensional problem where the shear and bulk moduli fields are estimated using noisy two-dimensional displacement data with boundary conditions both known and unknown. Example 2 uses the same setup as Example 1, but the reconstruction of the shear and bulk moduli fields is done in a window of the problem domain. In Example 3, we image the shear and bulk moduli fields in a three-dimensional domain using a full displacement field. We also remark that the frequencies in the examples presented herein were chosen so as to maintain low wavenumbers in the domain. This choice was made without loss of generality and in the interest of avoiding excessively fine meshes.

Synthetic measurement data was generated for all the examples by performing a finite element simulation with the known material parameters and then interpolating and corrupting with random noise, in this order, the simulated displacements. Denoting the simulated displacement at a node $i$ as $\hat{u}_i$, the corresponding noisy measurement $\tilde{u}_i$ is given as

$$\tilde{u}_i = \hat{u}_i (1 + \delta r_i),$$

where $r_i$ is a normal random variable with zero mean and unit variance and the parameter $\delta$ is a prescribed relative noise level. In our examples, we use $\delta = 0.01$ and 0.05. Although this noise model does not incorporate spatial correlation, it is still adequate to illustrate the capabilities of the MECE method, since numerical tests (not reported herein) reveal that the MECE method produces results for spatially correlated noise which are similar to the results presented in this chapter.

Additionally, the relative $L^1$ and $L^2$ errors of the reconstructed moduli are
reported for some of the examples. For this purpose, we denote the relative $L^1$ errors by

$$
e^G_{L^1} := \frac{\int_\Omega |G - G^\text{ref}| \, dV}{\int_\Omega |G^\text{ref}| \, dV},$$  \hspace{1cm} (1.45)

$$
e^B_{L^1} := \frac{\int_\Omega |B - B^\text{ref}| \, dV}{\int_\Omega |B^\text{ref}| \, dV},$$  \hspace{1cm} (1.46)

where $G$ and $B$ denote the reconstructed shear and bulk moduli, respectively, $\Omega$ is the domain of the inverse problem (i.e., the finite element mesh used for the inverse problem), and $G^\text{ref}$ and $B^\text{ref}$ are the true shear and bulk moduli, respectively, in $\Omega$. $G^\text{ref}$ and $B^\text{ref}$ were obtained by projecting and interpolating the moduli fields from the finite element mesh used to generate synthetic data unto the mesh used for the inverse problem. Likewise, the relative $L^2$ errors are given by

$$
e^G_{L^2} := \left[ \frac{\int_\Omega |G - G^\text{ref}|^2 \, dV}{\int_\Omega |G^\text{ref}|^2 \, dV} \right]^{\frac{1}{2}},$$  \hspace{1cm} (1.47)

$$
e^B_{L^2} := \left[ \frac{\int_\Omega |B - B^\text{ref}|^2 \, dV}{\int_\Omega |B^\text{ref}|^2 \, dV} \right]^{\frac{1}{2}}.$$  \hspace{1cm} (1.48)

For this work, the alternating directions scheme was stopped and deemed to have converged when the relative change in the functional (1.10) between two successive iterations dropped below 0.1% for Examples 1 and 2 and 1% for Example 3. A higher tolerance was selected for Example 3 to avoid excessively long computation times. As pointed out in [29], this criterion was confirmed to be adequate for the examples presented herein as it was verified (from extensive numerical testing) that the relative change in the mechanical fields and moduli was negligible for these levels of change in the functional.
Figure 1.1: Diagram of the problem domain in Examples 1, 2, and 3

1.5.1 Example 1: 2D reconstruction with 2D data

This example shows the ability of the methodology explained earlier to image the shear and bulk moduli fields of viscoelastic materials with the use of noisy two-dimensional displacement data. The results shown here were produced using two different scenarios. The first scenario assumes complete knowledge of the boundary conditions (i.e., $\Gamma_D \cup \Gamma_N = \Gamma$), while the other assumes no knowledge of the boundary conditions (i.e., $\Gamma_D = \Gamma_N = \emptyset$). Figure 1.1 shows a schematic of the domain used in this example. It consists of a square background with an elliptical inclusion. Each side of the square is 4 cm, and the ellipse has a major radius, respectively minor radius, of $8\sqrt{2}$ mm, respectively $5\sqrt{2}$ mm. Moreover, the major radius of the ellipse has an orientation of $45^\circ$ with respect to the $x$–axis. A plane strain condition was assumed in this example.

The frequency used in this example was 100 Hz, and the mass density of both the background and the inclusion was 1,000 $\text{kg/m}^3$. Moreover, the bulk
The moduli of the background and the inclusion were 50 kPa and 200 kPa, respectively; the bulk modulus was assumed to be purely elastic as is the case in many practical applications. Likewise, the shear modulus of the background and the inclusion was taken as $5 + 2.5i$ kPa and $20 + 10i$ kPa, respectively, where $i = \sqrt{-1}$. Thus, the material properties of the inclusion were four times those of the background. The boundary conditions used to generate the measurement data can also be appreciated in Figure 1.1. The bottom was fixed, while traction loads were applied to all other sides. The tractions were as follows: $t_1 = [0 - 5]$ kPa, $t_2 = [-5 5]$ kPa, and $t_3 = [5 - 5]$ kPa. Moreover, the measurement data was generated by performing a finite element simulation using a mesh with about 22,000 linear quadrilateral (Q4) elements, interpolating the resulting displacements to the inverse problem mesh with about 15,600 Q4 elements, and adding random noise as described earlier. The inverse problem mesh did not account for the geometry of the inclusion. Moreover, the noise levels considered for this particular example were $\delta = 0.01$ and 0.05.

The initial guess for the moduli in the alternating directions algorithm described earlier was the corresponding values of the background. Thus, the initial guess for the bulk modulus was 50 kPa, while the initial guess for the shear modulus was $5 + 2.5i$ kPa. Figure 1.2 shows the reconstruction results for the real part of the bulk modulus. As it can be appreciated, the value of the background was correctly identified in all cases. Moreover, the shape of the inclusion was also accurately recovered, but its value, however, varies according to the noise in the data and the presence or absence of boundary conditions. For instance, the value of the inclusion corresponding to the reconstructions done with 1%-noise data is closer to the true value of the inclusion than those corresponding to the 5%-noise data, which is expected. Moreover, the unknown
boundaries reconstructions show a degradation in accuracy when compared to their known boundaries counterpart, but this degradation is not significant. Indeed, the presence of a stiff inclusion can be identified in all images in Figure 1.2.

The imaging results for the real and imaginary parts of the shear modulus are shown in Figures 1.3 and 1.4, respectively. Trends similar to the results for the real part of the bulk modulus can again be observed in these figures. We also notice that the reconstruction of the imaginary part of the shear modulus appears to be less accurate than the reconstruction of the other quantities, as it can be appreciated from the images. This can be explained by the sensitivity of the imaginary part of the shear modulus on the measured data, since different reconstructions (not reported herein) were obtained using data generated with different loading conditions.

Tables 1.1 and 1.2 show the values of the weighting parameter $\alpha$ selected according to Morozov’s Principle (see Section 1.4.2) for the results corresponding to the scenarios with known and unknown boundary conditions, respectively. These tables also report the relative $L^1$ and $L^2$ errors in the reconstructed moduli as defined in (1.45)–(1.48). For comparison purposes, the inverse problem was also solved using an initial guess for the moduli in the alternating directions scheme that corresponds to an elastic material (i.e., the real part of the true background moduli), and the corresponding values for $\alpha$ and the relative errors in the reconstructed moduli were also reported in Tables 1.1 and 1.2. As it can be appreciated in these tables, the value of $\alpha$ decreased with increasing noise level – which is indeed expected because the noisier the measurement data, the less strictly it should be enforced. Additionally, the $\alpha$ values corresponding to
Figure 1.2: Real Part of Bulk Modulus for Example 1. Units: kPa, mm
Figure 1.3: Real Part of Shear Modulus for Example 1. Units: kPa, mm
Figure 1.4: Imaginary Part of Shear Modulus for Example 1. Units: kPa, mm
the elastic initial guess are lower by a few orders of magnitude than those corresponding to the initial guess of the background moduli. This is a direct result of the choice of normalization used for this work, which is presented in (1.41) and (1.42). More specifically, an elastic initial guess yields $u_{\text{init}}$, which often has a larger magnitude than the one obtained using a viscous initial guess (holding the real part constant), since $u_{\text{init}}$ in the latter case is attenuated by damping. Hence, $u_{\text{init}}$ with a larger magnitude leads to a higher value of $A$, which is compensated with a lower value for $\alpha$ in order to satisfy Morozov’s Principle.

Table 1.1: Algorithm diagnostics for Ex. 1 results with known boundary conditions.

<table>
<thead>
<tr>
<th>Initial Guess</th>
<th>Noise Level</th>
<th>$\alpha$</th>
<th>$e^B_{L1}$</th>
<th>$e^B_{L2}$</th>
<th>$e^G_{L1}$</th>
<th>$e^G_{L2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background</td>
<td>1%</td>
<td>0.20</td>
<td>0.15</td>
<td>0.23</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>5%</td>
<td>0.14</td>
<td>0.28</td>
<td>0.36</td>
<td>0.25</td>
<td>0.24</td>
</tr>
<tr>
<td>Real Part of Background</td>
<td>1%</td>
<td>6.6 x 10^-5</td>
<td>0.16</td>
<td>0.22</td>
<td>0.15</td>
<td>0.15</td>
</tr>
<tr>
<td></td>
<td>5%</td>
<td>4.9 x 10^-5</td>
<td>0.27</td>
<td>0.33</td>
<td>0.26</td>
<td>0.25</td>
</tr>
</tbody>
</table>

Table 1.2: Algorithm diagnostics for Ex. 1 results with unknown boundary conditions.

<table>
<thead>
<tr>
<th>Initial Guess</th>
<th>Noise Level</th>
<th>$\alpha$</th>
<th>$e^B_{L1}$</th>
<th>$e^B_{L2}$</th>
<th>$e^G_{L1}$</th>
<th>$e^G_{L2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Background</td>
<td>1%</td>
<td>0.30</td>
<td>0.29</td>
<td>0.30</td>
<td>0.32</td>
<td>0.29</td>
</tr>
<tr>
<td></td>
<td>5%</td>
<td>0.10</td>
<td>0.45</td>
<td>0.48</td>
<td>0.40</td>
<td>0.39</td>
</tr>
<tr>
<td>Real Part of Background</td>
<td>1%</td>
<td>8.9 x 10^-5</td>
<td>0.27</td>
<td>0.29</td>
<td>0.34</td>
<td>0.29</td>
</tr>
<tr>
<td></td>
<td>5%</td>
<td>2.7 x 10^-5</td>
<td>0.41</td>
<td>0.46</td>
<td>0.47</td>
<td>0.42</td>
</tr>
</tbody>
</table>

It is important to point out that the $L^1$ and $L^2$ errors presented in Tables 1.1 and 1.2 may provide a misleading sense of the accuracy of the reconstructed
moduli. For instance, small errors in the shape or location of the reconstructed inclusion could lead to relatively high $L^1$ and $L^2$ errors, but as it can be appreciated in Figures 1.2–1.4, these high errors are not truly representative of the visual quality of the reconstructions. The $L^1$ and $L^2$ errors presented in Tables 1.1 and 1.2, however, are useful for making relative comparisons between the different reconstructions. For example, the errors in the reconstructed moduli increase with greater noise levels in the measured displacement data, which is indeed expected. Moreover, the nature of the initial guess (i.e., elastic vs. viscoelastic) does not seem to have a significant impact on the final reconstruction of the moduli. In other words, the algorithm exhibits robustness with respect to the initial guess. Finally, the reconstructions obtained with unknown boundary conditions are accompanied by $L^1$ and $L^2$ errors in the moduli that are higher than those for the reconstructions obtained with known boundary conditions, which is expected due to the loss of boundary information in the former case.

1.5.2 Example 2: 2D reconstruction with window

This example highlights the ability of the approach proposed in this chapter to perform reconstructions of the shear and bulk moduli fields in a subdomain, or window, of the original problem domain. The current example also shows the effects of using different initial guesses for the viscoelastic parameters required by the alternating directions scheme. For this purpose, the problem setup used for this example was very similar to the one used for Example 1. In particular, every detail except the domain and mesh used for the inverse problem (i.e., the domain and mesh for which the measured data is available) was the same as in Example 1. The domain used for the inverse problem was in fact a subdomain
of the one shown in Figure 1.1 and consisted of a square window with sides of 28 mm in length and whose center coincided with the center of the larger domain. This window covered 49% of the area of the larger domain and was uniformly meshed with 6,400 linear quadrilateral (Q4) elements. Additionally, a noise level of $\delta = 0.01$ and different initial guesses for the viscoelastic moduli were considered.

Figures 1.5, 1.6, and 1.7 show the reconstructions, all performed without any knowledge of boundary conditions. Each figure shows the true solution of the inverse problem along with the window in which the reconstructions were performed. In addition, these figures show the reconstructions obtained with different initial guesses for the alternating directions algorithm. The initial guesses considered are as follows: 1) $B_{\text{init}} = 50$ kPa and $G_{\text{init}} = 5$ kPa, which correspond to the real part of the background moduli; 2) $B_{\text{init}} = 50$ kPa and $G_{\text{init}} = 5 + 2.5i$ kPa, which correspond to the true background moduli; 3) $B_{\text{init}} = 50$ kPa and $G_{\text{init}} = 5 + 4.5i$ kPa; and 4) $B_{\text{init}} = 50$ kPa and $G_{\text{init}} = 10 + 3i$ kPa. Thus, each initial guess represents a different level of damping in the shear modulus.

As it can be seen in Figure 1.5, the different initial guesses did not have a significant effect on the reconstruction of the real part of the bulk modulus. This is indeed expected because the bulk modulus of the initial guess was the same for all cases. Moreover, these reconstructions correctly identified the value of the background modulus, but underestimated the value of the inclusion modulus. This is also seen in Figure 1.6 to be the case for the real part of the shear, whose estimated value is nevertheless more accurate. In addition, an initial guess of $B_{\text{init}} = 50$ kPa and $G_{\text{init}} = 10 + 3i$ kPa resulted in a reconstruction of the real part of the background shear modulus with a higher error than the other reconstruc-
tions, which seems to be a reflection of the large discrepancy between the real part of the shear modulus of the initial guess and the corresponding true value for the background. Finally, all reconstructions of the real part of both the shear and bulk moduli correctly identified the shape of the inclusion.

The reconstruction of the imaginary part of the shear modulus, shown in Figure 1.7, was the most affected by the different initial guesses considered. We observed that the quality of the reconstruction of the inclusion improved as the value of the imaginary part of the shear modulus taken as initial guess increased. Indeed, the shape and estimated value of the imaginary part of the inclusion shear modulus seem most accurate in the reconstruction obtained with an initial guess of \( B_{\text{init}} = 50 \text{ kPa} \) and \( G_{\text{init}} = 5 + 4.5i \text{ kPa} \). This trend appears to be reversed, however, for the reconstruction of the imaginary part of the background shear modulus. Additionally, the use of a window led to a degradation in the quality of the reconstructions. It is conjectured that this degradation is due to less displacement data being taken into consideration in a window sub-domain.

Table 1.3 shows the value for \( \alpha \) obtained according to Morozov’s Principle and the relative \( L^1 \) and \( L^2 \) errors in the reconstructed moduli for the different initial guesses considered. As it can be seen, the errors in the reconstructed moduli do not vary significantly from one initial guess to the next, which confirms the robustness of the algorithm in this sense, but these errors are, in general, slightly greater than their counterparts in Example 1, which is evidence of the small degradation in the quality of the reconstructions obtained with the use of a window. Moreover, as was the case with Example 1, the value for \( \alpha \) corresponding to the elastic initial guess is lower than the corresponding values for
Figure 1.5: \( \text{Re}(B) \) for Example 2. Background is \( B_{\text{BACK}} = 50 \) and \( G_{\text{BACK}} = 5 + 2.5i \). Units: kPa, mm
Figure 1.6: Re(G) for Example 2. Background is $B_{\text{BACK}} = 50$ and $G_{\text{BACK}} = 5 + 2.5i$. Units: kPa, mm
Figure 1.7: Im(G) for Example 2. Background is $B_{\text{BACK}} = 50$ and $G_{\text{BACK}} = 5 + 2.5i$. Units: kPa, mm
the other initial guesses.

Table 1.3: Algorithm diagnostics for Ex. 2 results with **unknown boundary conditions**.

<table>
<thead>
<tr>
<th>Initial Guess</th>
<th>(\alpha)</th>
<th>(e_{L1}^B)</th>
<th>(e_{L2}^B)</th>
<th>(e_{L1}^G)</th>
<th>(e_{L2}^G)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(B = 50, \text{kPa}; G = 5, \text{kPa})</td>
<td>0.05</td>
<td>0.55</td>
<td>0.45</td>
<td>0.53</td>
<td>0.41</td>
</tr>
<tr>
<td>(B = 50, \text{kPa}; G = 5 + 2.5i, \text{kPa})</td>
<td>0.43</td>
<td>0.58</td>
<td>0.47</td>
<td>0.51</td>
<td>0.40</td>
</tr>
<tr>
<td>(B = 50, \text{kPa}; G = 5 + 4.5i, \text{kPa})</td>
<td>0.61</td>
<td>0.57</td>
<td>0.46</td>
<td>0.60</td>
<td>0.44</td>
</tr>
<tr>
<td>(B = 50, \text{kPa}; G = 10 + 3i, \text{kPa})</td>
<td>0.43</td>
<td>0.58</td>
<td>0.48</td>
<td>0.65</td>
<td>0.47</td>
</tr>
</tbody>
</table>

**1.5.3 Example 3: 2D reconstruction with 1D data**

This example is inspired by the field of ultrasound imaging. In such situations, the displacement data collected is unidirectional, specifically along the axis of the ultrasound transducer. Thus, we show how the unknown boundaries scenario can be used for the purpose of estimating the complex-valued shear modulus field using noisy unidirectional data. The domain used is the same as in Example 1 (where a more detailed description can be found) and is shown in Figure 1.1. For this example, moreover, a frequency of 300 Hz was used, and the mass density was again set to 1,000 kg/m\(^3\). The bulk modulus of both the background and inclusion was fixed to 2.2 GPa, while the shear modulus of the background and the inclusion was set to \(5 + 1i\) kPa and \(20 + 5i\) kPa, respectively. These properties rendered the material nearly-incompressible, and thus, the mean-dilatation approach [14] was used to handle such phenomenon.

The boundary conditions used to generate the synthetic displacement data
can be appreciated in Figure 1.1; these were chosen to produce a displacement field dominated by one direction due to the limitations of ultrasound. In this case, \( t_2 = t_3 = 0 \), and \( t_1 = [5 + 0.5i, 0] \) kPa. Additionally, the bottom, instead of being fixed, simulated an absorbing boundary (i.e., the domain was semi-infinite). Moreover, the mesh used for the finite element simulation to produce the raw (i.e., before interpolating and adding noise) displacements had around 22,000 linear quadrilateral (Q4) elements, and the one used for the inverse problem, onto which the raw displacements were interpolated, had about 15,600 Q4 elements. In addition, random noise, in this case with a level \( \delta = 0.01 \), was added to the displacements after interpolation to produce the measurement data.

For this example, the bulk modulus was assumed to be known and thus was not imaged (i.e., reconstructed). This selection was done to mimic the fact that soft biological tissue is nearly incompressible. Moreover, the initial guess for the shear modulus in the alternating directions algorithm was taken to be the real part of the background, 5 kPa. We also remark that since the available measurement data for the inverse problem was unidirectional (i.e., in the direction of the \( x \)–axis in Figure 1.1), we had to estimate the displacements in the missing direction, which corresponds to the \( y \)–axis, in order to obtain meaningful reconstructions for the unknown boundaries scenario. The vertical displacements were estimated in this case to be exactly zero, which is a reasonable assumption given the setup of the problem (i.e., the boundary conditions used to generate the measurement data produced displacements in the vertical direction which were about one order of magnitude smaller than displacements in the horizontal direction). Such a setup is quite common in experimental settings such as shear wave elasticity imaging [28, 13, 23], for instance. However, due to esti-
mating the displacement data in the missing direction, the true level of noise in the measurement data was unknown, and as a result, Morozov’s principle was not applicable to select the weighting parameter $\alpha$. In this scenario, the error balance approach introduced in [29] was used. This criterion seeks to adjust $\alpha$ so as to strike a balance between the minimization of the different components of the viscoelasticity MECE functional, hoping to achieve a satisfactory tradeoff between over-smoothing the inverse problem solution (over-emphasis on ECE minimization) and over-fitting the data (over-emphasis on data discrepancy minimization). Using this selection criterion, the weighting parameter was determined to be $\alpha = 106$. Moreover, 15 iterations of the alternating directions algorithm were sufficient to achieve convergence – a lower number of iterations required in this case due to the higher value of $\alpha$.

Figure 1.8 shows the results obtained for the unknown boundaries scenario. We first notice that the inverse problem domain has been truncated, and the height of the truncated square is 31 mm. The top 9 mm of the original domain were discarded for the inverse problem because the displacement data was not dominated by one direction in this region, and as a result, our assumption broke down, introducing a significant error. We highlight the fact that the ability to truncate the domain in this manner is a salient feature of the approach presented in this chapter.

As it can be appreciated in Figure 1.8, the reconstruction of the real part of the shear modulus clearly shows the inclusion (i.e., the shape and value of the inclusion were correctly recovered). Moreover, this reconstruction also correctly identified the value of the background. The reconstruction of the imaginary part of the shear modulus, however, is not as accurate as its real counterpart. As in
Examples 1 and 2, reconstructing the imaginary part of the shear modulus was harder than reconstructing its real counterpart, but for this example, the error introduced by estimating the displacements in the missing direction may be quite large and make a meaningful pointwise reconstruction of the imaginary part of the shear modulus impossible.

Nevertheless, if the reconstruction is done assuming known geometries (i.e., the mesh for the inverse problem includes the elliptical inclusion, and both the
background and inclusion are each assumed to be homogeneous), the values of
the imaginary part of the shear modulus are correctly identified. Such a recon-
struction may be done once the shape of the inclusion is identified (as seen in the
pointwise reconstruction of the real part of the shear modulus in Figure 1.8(b)).
In this case, the imaginary part of the shear modulus of the background and the
inclusion were estimated to be 1.14 kPa and 3.42 kPa, respectively. Likewise,
the real part of the shear modulus of the background and the inclusion were
estimated to be 4.7 kPa and 17.4 kPa, respectively. Moreover, the weighting pa-
rameter used for this reconstruction was $\alpha = 502$, and a total of five iterations
of the alternating directions scheme were necessary to achieve convergence.

1.5.4 Example 4: 3D reconstruction with 3D data

This example is designed to showcase the ability of the algorithm discussed ear-
lier to scale to more general three-dimensional situations. The reconstructions
performed for this example were done for the unknown boundaries scenario
and using noisy displacement data. The domain, which is shown in Figure 1.9,
consists of an elliptic cylinder inclusion whose center coincides with the center
of a cube with an edge length of 4 cm. The elliptic cylinder has a height of 2 cm,
a major radius of 11.3 mm, and a minor radius of 7 mm. Moreover, the cylinder
has been rotated 45° in the $xy$-plane.

The frequency used in this example was 50 Hz, and the mass density of both
the background and the inclusion is 1,000 kg/m$^3$. Moreover, the bulk modu-
lus of the background and the inclusion were taken as 100 kPa and 300 kPa,
respectively. Likewise, the shear modulus of the background and the inclusion
were $20 + 2i$ kPa and $60 + 8i$ kPa, respectively. The boundary conditions used to generate the measurement data consisted of compression and shearing loads on every face of the cube except the bottom face, which was fixed. Moreover, the measurement data was generated by performing a finite element simulation using a mesh with about 60,000 quadratic tetrahedral elements, interpolating the resulting displacements to the inverse problem mesh with about 15,600 linear hexahedral elements, and adding random noise as described earlier. The noise level considered for this particular example was $\delta = 0.01$.

The initial guess for the moduli in the alternating directions algorithm described earlier corresponds to the background. Thus, the initial guess for the bulk modulus was 100 kPa, while the initial guess for the shear modulus was $20 + 2i$ kPa. Figure 1.10 shows threshold plots for all reconstructed values of the moduli. These plots show the cube background and the inclusion with corresponding elements from the mesh shaded in for reference purposes. Additionally, Figure 1.11 shows cuts parallel to the cube faces, going through the center of the domain. As it can be observed in these figures, the algorithm was
able to correctly identify the location and shape of the inclusion as well as the value of the background’s moduli. The reconstructed values of the inclusion, nevertheless, underestimate in all instances the true values. Indeed, the reconstructed maximum value in the domain is less than the corresponding value of the modulus of the inclusion in all cases. We observed consistently during our numerical investigations that accuracy was lost in reconstructions obtained without any knowledge of boundary conditions when compared to the same reconstructions obtained with application of the boundary conditions. It may be possible to improve the accuracy of the results obtained with unknown boundary conditions by enriching the measured data using multiple experiments. The authors are presently investigating this possibility.
Figure 1.11: Reconstructed moduli for Example 4 in planes through center of domain: \( xy \)-plane (left column), \( yz \)-plane (middle column), and \( xz \)-plane (right column). Units: kPa
Table 1.4 shows the value of the weighting parameter $\alpha$, selected according to Morozov’s Principle, and the relative $L^1$ and $L^2$ errors in the reconstructed moduli in the scenario with unknown boundary conditions and, for comparison purposes, in the scenario with known boundary conditions. As it can be appreciated, the lack of knowledge of boundary conditions yields reconstructions that are less accurate than those obtained using knowledge of the boundary conditions, but the former reconstructions, as demonstrated by Figures 1.10 and 1.11, are still meaningful and useful for biomedical imaging purposes.

<table>
<thead>
<tr>
<th>Boundary Conditions</th>
<th>$\alpha$</th>
<th>$e^B_{L^1}$</th>
<th>$e^B_{L^2}$</th>
<th>$e^G_{L^1}$</th>
<th>$e^G_{L^2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Known</td>
<td>4.9</td>
<td>0.25</td>
<td>0.30</td>
<td>0.13</td>
<td>0.16</td>
</tr>
<tr>
<td>Unknown</td>
<td>2.7</td>
<td>0.38</td>
<td>0.40</td>
<td>0.31</td>
<td>0.35</td>
</tr>
</tbody>
</table>

### 1.6 Conclusions

We have developed and demonstrated the feasibility of an error in constitutive relationship methodology for the inverse identification of linearly viscoelastic material parameters using interior data. Our proposed approach would be particularly useful in the area of biomechanical imaging, where the goal is to produce images of the material parameters of a tissue from displacements measured in its interior and where accurate information on boundary conditions is not readily available. Thus, our contributions with this work include the ability to address viscoelasticity imaging problems through the use of a generalized error in constitutive equation functional and to handle, in a very natural way,
situations in which there is no knowledge on boundary conditions. In addition, the resulting optimality sub-system for the mechanical fields was shown to be invertible. Moreover, regularization of the inverse problem of viscoelasticity imaging is achieved using the discrepancy principle due to Morozov, which supposes that the relative noise level in the measurement data is known. The numerical experiments shown highlight the robust performance of the algorithm in characterizing the viscoelastic properties of a material in situations in which incomplete and noisy displacement data is available and, in addition, information on boundary conditions is unavailable. Finally, future directions of investigation include the following: 1) to validate the algorithm with real experimental data; 2) to extend the formulation to address imaging problems in which measured data from multiple experiments is available; 3) to determine the convergence properties of the alternating directions strategy; and 4) to devise regularization techniques to select the weighting parameter $\alpha$ in cases in which the noise level in the data is unknown.

1.7 Acknowledgments

This work was partially supported by NIH Grant # R01CA174723.
REFERENCES


2.1 Introduction

DinamicaE is a massively parallel finite element software package developed by the Computational Mechanics and Inverse Problems Group led by Professor Wilkins Aquino. Its development started in 2010, and efforts are ongoing to continue adding functionalities of interest. At the time of writing of this thesis, the DinamicaE simulation suite is able to perform finite element computations related to steady-state structural dynamics and acoustics, with the ability to handle nearly incompressible materials. Moreover, it has features to model infinite and semi-infinite domains through the implementation of absorbing boundary conditions and perfectly-matched layers (PML). In addition, DinamicaE has the ability to model problems in acoustic-structure interaction (ASI) with the added benefit of inheriting all the capabilities mentioned for each of the individual problem domains. A unique feature found in DinamicaE is the ability to solve large scale material identification problems in elasticity, viscoelasticity, and ASI.

DinamicaE has been developed in the C++ programming language with the help of Diffpack [4], a sophisticated collection of libraries that enables the numerical solution of partial differential equations through the finite element method. As such, DinamicaE (and Diffpack) takes advantage of the features offered by C++, which include object-oriented programming, abstract data types, templates, data encapsulation, and inheritance. This approach to developing numerics software has recently proven to be quite successful due to the ease of
maintaining and extending it [4].

The implementation of the MECE approach using finite elements will be explained throughout the rest of this thesis. We assume the availability of an implementation of a finite element solver and discuss how to extend it to include the MECE technique. An overview of the algorithm is first explained in the next section, while the subsequent section is devoted to details of the implementation. A brief overview of the assumed finite element solver functionalities is given, and the details of the implementation of the MECE approach are further explored. Finally, a crucial aspect of the MECE algorithm, the selection of the weighting parameter, is discussed, and some conclusions are offered afterwards.

2.2 Algorithm Details

The MECE algorithm is repeated here for convenience to the reader. Notice that the algorithm flow depends on whether the material is elastic or viscoelastic, which are the only kinds of material considered in this work. The reader is referred to [1] for details specific to the treatment of elastic materials in the context of the MECE algorithm. Moreover, it is assumed that the bulk and shear moduli are defined elementwise (i.e., they are both constant over each element in the mesh).
Data: Domain with mesh; harmonic frequency $\omega$; regularization parameter $\alpha$; initial guess $B_{\text{init}}$ and $G_{\text{init}}$; bounds $B_{\text{low}}, B_{\text{up}}, G_{\text{low}}, G_{\text{up}}$; measured displacement data

Result: Final estimates of $B$ and $G$, the displacement field $u$, and the Lagrange multiplier field $w$

/* Initialization */

Compute finite element traction vector $\{F\}_{\text{init}}$ from known (or assumed) loading;

Solve $([K]_{\text{init}} - \omega^2[M]) \{u\}_{\text{init}} = \{F\}_{\text{init}}$ for $\{u\}_{\text{init}}$;

if material is elastic then
  Set $A := \begin{bmatrix} u & {K}_{\text{init}}(u)_{\text{init}} \end{bmatrix}$;
else
  /* Material is viscoelastic */
  Set $[P] := \text{Re}([C]_{\text{init}}) + \text{Im}([C]_{\text{init}})$;
  Set $[T] := \text{Re}([K]_{\text{init}}) + \text{Im}([K]_{\text{init}})$;
  Set $A := \begin{bmatrix} u & {T}_{\text{init}}(u)_{\text{init}} \end{bmatrix}$;
end

Compute $\kappa$ according to

$$\kappa = A\alpha$$  \hspace{1cm} (2.1)

/* MECE iterations */

while not converged do
  Do: Mechanical fields update (see details in Algorithm 2)
  Do: Material update (see details in Algorithm 3)
end

Algorithm 1: MECE algorithm
Update [K] with latest values of \( B \) and \( G \);

if material is elastic then

Set \([T] := [K]\);

end

Solve

\[
\begin{bmatrix}
[T] & [K] - \omega^2 [M] \\
([K] - \omega^2 [M])^H & -\kappa [D]
\end{bmatrix}
\begin{bmatrix}
\{w\} \\
\{u\}
\end{bmatrix}
= 
\begin{bmatrix}
\{F\} \\
-\kappa \{u_m\}
\end{bmatrix}
\]

(2.2)

for \( \{u\} \) and \( \{w\} \);

**Algorithm 2**: MECE algorithm: Mechanical fields update
/* Material update */

for n := 1 to total number of mesh elements do

/* Proposal substep */
Set \( \{\epsilon\}_n^\text{elem} := [\hat{B}]^\text{elem} \{u\}_n^\text{elem} \);

if material is elastic then

Set \( \{\sigma\}_n^\text{elem} := [C]^\text{elem} [\hat{B}]^\text{elem} \{u\}_n^\text{elem} + \{w\}_n^\text{elem} \);
Set \( B_n^* := \frac{\langle \text{tr}(\{\sigma\}_n^\text{elem}), \text{tr}(\{\sigma\}_n^\text{elem}) \rangle_{1/2}}{3 \langle \text{tr}(\{\epsilon\}_n^\text{elem}), \text{tr}(\{\epsilon\}_n^\text{elem}) \rangle_{1/2}} \);
Set \( G_n^* := \frac{\langle \{\sigma\}_n^\text{dev}, \{\epsilon\}_n^\text{dev} \rangle_{1/2}}{\langle \{\epsilon\}_n^\text{dev}, \{\epsilon\}_n^\text{dev} \rangle_{1/2}} \);

else /* Material is viscoelastic */

Set \( \{\sigma\}_n^\text{elem} := [C]^\text{elem} [\hat{B}]^\text{elem} \{u\}_n^\text{elem} + [\mathcal{P}]^\text{elem} [\hat{B}]^\text{elem} \{w\}_n^\text{elem} \);
Set \( B_n^* := \frac{\int_{\Omega}^\text{elem} \text{tr}(\{\sigma\}_n^\text{elem}) \, dV}{3 \int_{\Omega}^\text{elem} \text{tr}(\{\epsilon\}_n^\text{elem}) \, dV} \);
Set \( G_n^* := \frac{\langle \{\sigma\}_n^\text{dev}, \{\epsilon\}_n^\text{dev} \rangle_{1/2}}{2 \langle \{\epsilon\}_n^\text{dev}, \{\epsilon\}_n^\text{dev} \rangle_{1/2}} \);

end

/* Correction substep for bulk modulus (analogous for shear modulus) */

/* \( h(\cdot) \) stands for Re(\cdot) and Im(\cdot). */

if \( h(B_n^*) < h(B_{\text{low}}) \) then

Set \( h(B_n) := h(\theta B_n + (1 - \theta) B_{\text{low}}) \);

else if \( h(B_n^*) > h(B_{\text{up}}) \) then

Set \( h(B_n) := h(\theta B_n + (1 - \theta) B_{\text{up}}) \);

else

Set \( h(B_n) := h(B_n^*) \);
end
end

Algorithm 3: MECE algorithm: Material update
Table 2.1 describes the different quantities that appeared in the MECE algorithm. For convenience, second-order tensor quantities such as stress and strain have been represented as vectors using Voigt notation. Additionally, angle brackets (i.e., $\langle \cdot, \cdot \rangle$) have been used to represent the $L^2$-inner product of two Voigt-notation vectors, and the trace function of such a vector is denoted with $\text{tr}(\cdot)$. We also remark that the function $h(\cdot)$ is used to denote the $\text{Re}(\cdot)$ function in the case of elastic materials and both the $\text{Re}(\cdot)$ and $\text{Im}(\cdot)$ functions in the case of viscoelastic materials. Finally, notice that the correction substep for the shear modulus has been omitted from the algorithm due to its similarity to the same substep for the bulk modulus.

### 2.3 Implementation

In this section, we explain how to exploit an existing finite element code and its associated functionalities in order to implement the MECE algorithm previously described. For this purpose, we reproduce the implementation of the algorithm done in the DinamicaE simulation suite.

#### 2.3.1 Existing Functionalities of a Finite Element Solver

Figure 2.1 shows the class structure of the existing finite element code (i.e., the structure assumed available to a developer) that is taken as the point of departure. In this figure, a solid line is used to represent direct inheritance between two classes, so for instance, $\text{IsoElastic}$ is assumed to be a child of the class $\text{Material}$. Moreover, a dashed line is used to indicate ownership, so for ex-
Table 2.1: Quantities found in MECE algorithm

<table>
<thead>
<tr>
<th>Variable</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$</td>
<td>normalization factor for regularization parameter</td>
</tr>
<tr>
<td>${F}$</td>
<td>finite element traction vector from known loading</td>
</tr>
<tr>
<td>${F}_{\text{init}}$</td>
<td>traction vector from known (or assumed) loading to compute $A$</td>
</tr>
<tr>
<td>$[K]_{\text{init}}$</td>
<td>stiffness matrix assembled with initial guess $B_{\text{init}}$ and $G_{\text{init}}$</td>
</tr>
<tr>
<td>$[M]$</td>
<td>mass matrix</td>
</tr>
<tr>
<td>${u}_{\text{init}}$</td>
<td>displacement vector used to compute $A$</td>
</tr>
<tr>
<td>${u_m}$</td>
<td>vector with measured displacements</td>
</tr>
<tr>
<td>$[C]_{\text{init}}$</td>
<td>matrix representation of constitutive tensor for initial guess</td>
</tr>
<tr>
<td>$B$</td>
<td>bulk modulus</td>
</tr>
<tr>
<td>$G$</td>
<td>shear modulus</td>
</tr>
<tr>
<td>$[K]$</td>
<td>stiffness matrix</td>
</tr>
<tr>
<td>$[D]$</td>
<td>measurement-location indicator matrix</td>
</tr>
<tr>
<td>${u}$</td>
<td>displacement vector</td>
</tr>
<tr>
<td>${w}$</td>
<td>Lagrange multiplier vector</td>
</tr>
<tr>
<td>${u}_{\text{elem}}^n$</td>
<td>element displacement vector for element $n$</td>
</tr>
<tr>
<td>${w}_{\text{elem}}^n$</td>
<td>element Lagrange multiplier vector for element $n$</td>
</tr>
<tr>
<td>$[\hat{B}]_{\text{elem}}^n$</td>
<td>element matrix with derivatives of finite element shape functions</td>
</tr>
<tr>
<td>$[C]_{\text{elem}}^n$</td>
<td>matrix representation of constitutive tensor for element $n$</td>
</tr>
<tr>
<td>${\sigma_{\text{dev}}}_{\text{elem}}^n$</td>
<td>deviatoric projection of ${\sigma}_{\text{elem}}^n$</td>
</tr>
<tr>
<td>${\epsilon_{\text{dev}}}_{\text{elem}}^n$</td>
<td>deviatoric projection of ${\epsilon}_{\text{elem}}^n$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>weighting parameter for correction substep</td>
</tr>
</tbody>
</table>
Figure 2.1: Class structure of existing finite element code

ample, ComplexSolidSS owns (i.e., has a pointer to) LinearSolver. The structure shown in Figure 2.1 has been assumed as such because it facilitates the implementation of the MECE algorithm discussed previously.

ComplexSolidSS handles tasks related to the finite element method such as preprocessing, assembly of the stiffness and mass matrices and the traction vector, solution of the resulting system of equations, and postprocessing. Even though there is a more complicated class structure surrounding ComplexSolidSS that distributes and decentralizes these tasks, only the classes most relevant to the implementation of the MECE algorithm have been shown for the sake of simplicity. For instance, the importance of explicitly showing the dependency of ComplexSolidSS on the class Material will become apparent later when the implementation of the MECE algorithm is discussed. For now, it is important to know that ComplexSolidSS gets from the class Material the constitutive matrix of each element of a material in the mesh in order to assemble the stiffness matrix. Moreover, depending on whether the material is elastic or viscoelastic, the constitutive matrix of the element is as-
Figure 2.2: Class structure of existing finite element code (in blue rectangles) and implementation of MECE algorithm (in green ovals)

The class `Material` serves as an interface between classes representing different material types and the main finite element simulator class `ComplexSolidSS`, which is an example of an efficient use of polymorphism allowing flexibility in DinamicaE. The other important class, `LinearSolver`, serves as an interface for `ComplexSolidSS` to communicate with a linear solver, which provides the solution to a linear system of equations upon request by `ComplexSolidSS`.

### 2.3.2 The MECE algorithm

Figure 2.2 shows the class structure of the MECE algorithm implementation. `SteadyStateMECE` is the driver class that administers the MECE iterations loop and is partly responsible for the initialization by storing the measured displacements in an internal data structure. The rest of the MECE algorithm initialization is completed by the class `SteadyStateBlockMECE`. This class takes advantage of the functionalities found in `ComplexSolidSS`, which is its parent, in order to compute $\kappa$ according to (2.1). Such functionalities include to set up...
and solve a system of equations that involves stiffness and mass matrices and a traction vector. SteadyStateBlockMECE is also responsible for the mechanical fields update, whereas the material update falls under the responsibility of the class InvMaterial.

Solving the Coupled System of Equations

Once the algorithm initialization is complete, the MECE iterations begin, and the first step here is the mechanical fields update. This step consists of solving the system of equations shown in (2.2), and the class SteadyStateBlockMECE is responsible for completing this step. This class relies on its parent class ComplexSolidSS to assemble the stiffness and mass matrices and the traction vector (in the case where boundary conditions are known). Moreover, SteadyStateBlockMECE assembles the matrix $[T]$ once the stiffness matrix is available, and it also assembles the measurement-location indicator matrix $[D]$ with the help of the measured displacements map. $[D]$ is a Boolean matrix with a nonzero entry (i.e., the entry is “1”) in the diagonal position corresponding to a degree of freedom where a displacement measurement was taken. Additionally, the class SteadyStateBlockMECE also assembles the vector with measured displacements.

Once all the individual blocks of the system (2.2) are assembled and ready, SteadyStateBlockMECE then puts together the coefficient matrix and the right-hand side of (2.2). Afterwards, this class enforces essential boundary conditions on the fields $u, w,$ or both through static condensation, a capability which is also provided by ComplexSolidSS. Now that the system of equations is ready to be solved, SteadyStateBlockMECE accesses LinearSolver.
in order to obtain a solution, and the latter class then stores the result in two different internal vectors for later use in the material update.

**Executing the Material Update**

Once the mechanical fields are updated, the next step is the material update. An important assumption behind the implementation of this latter step is that the material properties (i.e., the bulk and shear moduli) are assumed to be constant in one element. Hence, the material update step is done elementwise as is shown in the pseudocode for Algorithm 3. This can be easily modified, however, in order to accommodate situations in which the material properties are known to remain constant in a group of elements.

In order to initiate the material update step, SteadyStateMECE obtains the result from the previous step (i.e., the solution to the system (2.2)) and passes it to the class InvMaterial. This class is responsible for executing a loop over the total number of elements in the mesh, and once at the element level, the proposal and correction substeps take place. In the proposal substep, candidates for the bulk and shear moduli updates are computed according to the formulas shown in the pseudocode for Algorithm 3. If the element is identified as an elastic material, the class InvIsoElastic computes the candidates for the update, whereas the class InvIsoViscoElastic performs the corresponding computation for elements of a viscoelastic material. It is important to note that computing these candidates for the moduli update requires performing an integration over the element. This is easily achieved with the numerical integration functionality provided by Diffpack.
In the correction substep, the candidates computed by the previous proposal substep are checked to determine if they fall within some bounds specified a priori (i.e., the user of the MECE algorithm may know that the material properties of interest fall within some bounds). If the candidates satisfy these inequality constraints, they are taken as the update, whereas if they violate the constraints, the update is then computed as a weighted average between the current material property and the bound being violated. This correction is done for the real part of the bulk and shear moduli of elastic materials and for both the real and imaginary parts of the shear and bulk moduli of viscoelastic materials. Moreover, the weighted average is controlled by the parameter $\theta$ shown in the pseudocode for Algorithm 3; $\theta$ is currently set to 0.5 in the DinamicaE implementation of the correction substep.

Once the updates are finally computed, these are passed to \texttt{IsoElastic} or \texttt{IsoViscoElastic}, via the class \texttt{Material}, so that the material properties stored in these classes can be updated to their latest values, and this concludes the material update step of the MECE algorithm. It is important to notice the parallelism between the child classes of \texttt{Material} and those of \texttt{InvMaterial}. In this case, the flexibility of the C++ programming language allows developers to easily add the functionality to apply the MECE algorithm to other types of materials besides elastic and viscoelastic. For instance, if an orthotropic material is implemented as a child of \texttt{Material}, the corresponding class to compute the update in the MECE algorithm can be implemented as a child of the class \texttt{InvMaterial} once the corresponding update formulas have been derived.
Computing Errors

The MECE methodology naturally provides two quantities that are extremely useful in monitoring the progression of the algorithm iterations. These are the error in constitutive equation (ECE) and the displacement $L^2$-error. Suppose that the stress field $\sigma$, the displacement field $u$, and the constitutive tensor $C$ satisfy the partial differential equation of motion for steady-state dynamics (see [1] for more details) in $\Omega$. The ECE for elastic materials is defined as

$$U(u, \sigma; C) := \int_{\Omega} (\sigma - C: \varepsilon[u]) : C^{-1} : (\sigma - C: \varepsilon[u]) \, dV, \quad (2.3)$$

where $\varepsilon[\cdot]$ is the linearized strain operator, and the displacement $L^2$-error as

$$L(u) := \| u - u_m \|_{L^2(\Omega_m)}^2, \quad (2.4)$$

which is the square of the $L^2$-norm of the difference between $u$ and the measured displacements $u_m$. $\Omega_m$ is the subset of $\Omega$ on which $u_m$ is defined (i.e., where displacements were measured).

We first address the computation of the ECE. After the mechanical fields update step, the relationship

$$\sigma = C : (\varepsilon[u] + \varepsilon[w]) \quad (2.5)$$

holds true for elastic materials [1], where $w$ is the Lagrange multiplier field. After substituting (2.5) into (2.3) and simplifying, we obtain

$$U(w; C) = \int_{\Omega} \varepsilon[w] : C : \varepsilon[w] \, dV, \quad (2.6)$$

which is easily computed during the material update step by taking advantage of the already ongoing numerical integration. For viscoelastic materials, (2.6) becomes

$$U(w; C) = \int_{\Omega} \varepsilon[w] : P : \varepsilon[w] \, dV. \quad (2.7)$$
In practice, \( \Omega_m \) is a finite set, which is naturally associated with the counting measure, and hence, \( L(u) \) reduces to

\[
L(u) = (\{u\} - \{u_m\})^T (\{u\} - \{u_m\})
\]

(2.8)
because the displacement measurements are available at the discrete points part of \( \Omega_m \) which also coincide with finite element nodes. Moreover, this computation is simple to perform with the tools available in Diffpack.

The stopping criteria for the MECE algorithm iterations implemented in DynamicaE makes use of these two errors. The iterations are stopped once the relative change in \( U(w; C) + \kappa L(u) \) between two successive iterations drops below a certain user-defined tolerance. This stopping criteria has yielded successful results in numerical experiments.

### 2.4 Regularization Parameter Selection

As explained in Section 1.4.2, one of the most important aspects of the MECE algorithm involves the selection of the weighting parameter \( \alpha \), which controls how strongly the measured displacement data is enforced when computing a solution to the inverse problem. Although there is no optimal selection rule for the weighting parameter, the discrepancy principle due to Morozov [2, 3] is an intuitive approach that works well in practice (see Section 1.4.2 for details). If we let \( \{u_\alpha\} \) denote the solution to system (2.2) during the last MECE iteration (i.e., the displacement that is part of the MECE solution to the inverse problem) for a given value of \( \alpha \) and \( \delta \) denote the level of noise in the measurements, Morozov’s
discrepancy principle states that $\alpha$ should be chosen such that

$$
\frac{(\{u_\alpha\} - \{u_m\})^T (\{u_\alpha\} - \{u_m\})}{\{u_m\}^T \{u_m\}} = \delta^2
$$

(2.9)

When the level of noise $\delta$ is known, equation (2.9) is solved in DinamicaE with the bisection method. This method is implemented in the class SteadyStateMECE and calls the function that executes the MECE iterations whenever it requires a function evaluation.

In the event the level of noise in the measured data is unknown, a different rule is required to choose $\alpha$. One such rule, proposed in [6] and known as the error balance approach, states that the chosen value for $\alpha$ should minimize the sum $L^2_\alpha + U^2_\alpha$, where $L_\alpha$ and $U_\alpha$ are the displacement $L^2$-error and the ECE, respectively, at the end of the MECE iterations for a given value of $\alpha$. Analogous to the bisection method, a golden section search is implemented in the class SteadyStateMECE of DinamicaE in order to select $\alpha$ according to this rule.

One of the appealing aspects of DinamicaE is that it is fairly easy to implement other criteria to select $\alpha$ in order to compare their performance. Within the already discussed framework, a class that wraps around SteadyStateMECE can be designed in order to implement the different criteria and to call upon the latter to evaluate the required quantities whenever necessary. Moreover, optimization-based selection rules can be implemented along with well-known and available optimization algorithms such as BFGS [5] in order to leverage their performance.
2.5 Conclusion

The modified error in constitutive equation approach to solve inverse problems has shown great promise to tackle a wide range of imaging problems. Part of MECE’s success is due to its ability to use finite elements as the underlying modeling tool. Thus, with the versatility and generality of finite elements, MECE is able to address imaging problems that arise in numerous applications (e.g., from seismic inversion to biomedical imaging).

In addition, as it has been shown, MECE is relatively simple to implement in existing finite element codes, and more importantly, implementations in object-oriented languages are quite amenable to enhancements and adaptations. An example of this is the easy extension of MECE in DinamicaE to handle new material types (e.g., anisotropic or nonlinear). Moreover, the modular structure provided by an object-oriented implementation is another attractive aspect of MECE in DinamicaE, since the entire software package benefits from improvements to its different parts and pieces. For instance, the MECE algorithm in DinamicaE will inherit performance optimizations that are directly done to the linear solvers used in the software package, or benefit from a new and faster solver that is easy to interface with the existing framework due to its modularity.

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opment of DinamicaE.
REFERENCES


