Inverse Identification of Viscoelastic Material Properties using an Error in Constitutive Equations Approach

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ABSTRACT:

KEY WORDS: Inverse problems; Error in Constitutive Equations; Viscoelasticity.

1 INTRODUCTION

It is well known that the mechanical properties of soft biological tissue are closely related to pathology. Thus, the identification of viscoelastic material properties has shown significant promise for disease diagnosis. For instance, viscoelastic properties can significantly increase specificity in differentiating malignant and benign tumors [4]. Yet, the direct measurement of viscoelastic material properties in-vivo is very difficult, if not impossible. However, indirect measurements in the form of solutions to inverse problems have been promising.

In this work, we present an inverse problem methodology based on an error in constitutive equations (ECE) for the identification of viscoelastic properties from dynamic tests. The basic premise in the ECE approach is that, given an over-determined set of boundary or internal data (e.g. displacements and tractions), and a set of kinematically admissible displacements and statically admissible stresses, a cost functional is defined based on the error in the constitutive equations that connect these sets of stresses and strains. This cost functional has the important property of being zero for the exact constitutive equations and strictly positive otherwise. For example, ECE-based identification strategies for transient and materially nonlinear situations have been recently proposed in [2], while other aspects of ECE are surveyed in [1]. For viscoelasticity, we will present an ECE approach for frequency domain formulations.

2 FORMULATION

2.1 The Forward Problem

The variational form of the forward steady-state dynamics problem can be stated as find $\mathbf{u} \in U$ such that

$$a(\mathbf{u},\mathbf{v}) = \ell(\mathbf{v}) \;\forall\; \mathbf{v} \in V \tag{1}$$

where

$$a(\mathbf{u},\mathbf{v}) = \int_\Omega \nabla \mathbf{v}^* : \sigma \; d\Omega - \rho\omega^2 \int_\Omega \mathbf{v}^* \cdot \mathbf{u} \; d\Omega \tag{2}$$

$$\ell(\mathbf{v}) = \int_{\Gamma_t} \mathbf{v}^* \cdot \mathbf{t} \; d\Gamma_t, \tag{3}$$

In the above equations, the test function space V and the trial solution space U are defined as

$$V = \{\mathbf{v} : \mathbf{v} \,|\mathbf{v} \in \; H^1(\Omega), \mathbf{v} = 0 \text{ on } \Gamma_u\} \tag{4}$$

$$U = \{\mathbf{u} \colon \mathbf{u} \;|\; u_i \in H^1(\Omega), \mathbf{u} = \mathbf{u}_0 \text{ on } \Gamma_u\}. \tag{5}$$

The asterisk denotes complex conjugate and bold quantities are used to represent vectors and second-order tensors. The space $H^1(\Omega)$ is defined as the collection of functions that along with their first derivatives are square integrable. In the above equations, Ω represents the interior of a body whose boundary is $\Gamma = \Gamma_u \cup \Gamma_t$, Γ_t is the portion of the boundary where external tractions are specified, Γ_u is the portion of the boundary where displacements are specified, ω denotes angular frequency, σ is the stress tensor, ρ is the mass density (assumed constant in this work), $\mathbf{u}$ is the displacement field, and $\mathbf{t}$ denotes tractions.

The solution to the variational problem defined in Eq. (1) was approximated in this work using the finite element method. The details for the discretization of the problem can be found in conventional finite element textbooks and are not shown herein for the sake of brevity.

2.2 The Error in Constitutive Equations Approach

The inverse viscoelasticity problem can be described as, given a set of displacement fields $\{\mathbf{u}_i^m\}_{i=1}^n$, corresponding to frequencies $\{\omega_i\}_{i=1}^n$, find the complex moduli G and K as functions frequency. The part of the domain where displacements are measured is denoted as $\Omega_m \subseteq \overline{\Omega} = \Omega \cup \Gamma$.

The basic premise in the ECE approach is to define a cost functional based on the error in the constitutive equations that connect a set of kinematically admissible displacements and a set of dynamically admissible stresses. The inverse problem is solved by finding material properties along with admissible displacement and stress fields such that the ECE functional is minimized. The ECE functional used in this work is defined as

$$J(\sigma_N, \mathbf{u}_D, K, G) = \frac{1}{2}\int_\Omega \|\sigma_N - 2G\mathbf{E_d}(\mathbf{u_D}) - Ke_u\mathbf{I}\|^2 d\Omega \quad (6)$$

where $e_u = \mathbf{E}(\mathbf{u_D})_{kk}$ is the volumetric strain, $\mathbf{E_d}(\mathbf{u_D}) = \mathbf{E}(\mathbf{u_D}) - \frac{1}{3}e_u\mathbf{I}$ is the deviatoric strain tensor, $\mathbf{E}(\mathbf{u_D})$ is the strain tensor, and $\mathbf{I}$ is the second-order identity tensor. The subscript N in the stress field and D in the strain field are used to highlight the fact that these fields are constructed from different forward problems as explained below. Since the fields for different frequencies are independent of each other, we can concentrate on the derivations of the basic equations for a single frequency.

The goal is to find the fields, $\sigma_N, \mathbf{u}_D, G$, and K that minimize the ECE functional (6) under the constraints that the stresses are dynamically admissible and the strains are kinematically admissible. The dynamically admissible set is composed of stresses that satisfy the variational form of the equations of motion and is defined formally as

$$\hat{S} = \Big\{\sigma_N : \sigma_N \in L_2(\Omega),\ \int_\Omega \left(\nabla\mathbf{v}^* : \sigma_N - \rho\omega^2\mathbf{v}^*\cdot\mathbf{u_N}\right) d\Omega - \int_{\Gamma_t}\mathbf{v}^*\cdot(\sigma_N\mathbf{n_s})\, d\Gamma_t = 0\ \forall\mathbf{v}\in V\Big\} \quad (7)$$

The variable $\mathbf{u}_N$ appearing in the above equations is an auxiliary displacement needed to define a well-posed forward problem from which a dynamically admissible stress field is obtained.

The kinematically admissible set is composed of displacement fields that are in the appropriate functional space as required by the variational problem and satisfy Dirichlet conditions and the measurements. That is,

$$\hat{U} = \{\mathbf{u}_D\colon \mathbf{u}_D \in H^1(\Omega),\ \mathbf{u}_D = \mathbf{u}_0 \text{ on } \Gamma_u,\ \mathbf{u}_D = \mathbf{u}^m \text{ in } \Omega^m\} \quad (8)$$

An alternating directions approach, as decribed in [1], was used in the present work for the identification of the complex moduli. The approach consists in breaking the optimization process into two steps. In the first step, given a current best guess for the complex relaxation moduli, (G,K), we find a dynamically admissible stress field and a kinematically admissible displacement field by solving two forward problems for each frequency. Then, fixing these admissible fields, a new update for the complex moduli is obtained by minimizing the ECE functional (6).

2.3 Obtaining the Admissible Fields

A dynamically admissible stress field that is consistent with the most current guess of the material properties can be obtained by solving the following variational problem. Find $\mathbf{u}_N \in U$ such that

$$a(\mathbf{u}_N, \mathbf{v}) - \ell(\mathbf{v}) = 0\ \forall\ \mathbf{v}\in V \quad (9)$$

which is essentially the same as the forward problem given in (1) with the stress tensor defined as

$$\sigma_N = 2G\mathbf{E_d}(\mathbf{u_N}) + Ke_{u_N}\mathbf{I} \quad (10)$$

We refer to the above forward problem as the Neumann problem and, hence, denote fields associated with it with a subscript N.

The kinematically admissible field is found analogously by solving the following problem. Find $\mathbf{u}_D \in \hat{U}$ such that

$$a(\mathbf{u}_D, \mathbf{v}) - \ell(\mathbf{v}) = 0\ \forall\ \mathbf{v}\in V \quad (11)$$

We refer to the above problem as the Dirichlet problem and denote fields associated with it with a subscript D. It is important to point out that the main difference between the variational problem in (9) and the one given in (11) is that the latter enforces the measurement field $\mathbf{u}^m$ as part of the Dirichlet or essential boundary conditions. In other words, its solution belongs to $\hat{U}$ instead of U.

2.4 Moduli updating

In the alternating directions approach, once the admissible fields σ_N and $\mathbf{u}_D$ are obtained, a new estimate of the complex moduli G and K can be obtained by minimizing the ECE functional with σ_N and $\mathbf{u}_D$ fixed. First, we define the functional

$$\hat{J}(G,K) = J(\sigma_N(G,K), \mathbf{E}(\mathbf{u}; \mathbf{G}, \mathbf{K}), \mathbf{G}, \mathbf{K}) \quad (12)$$

Then, a new update of the complex moduli is obtained as

$$(\check{G}, \check{K}) = \arg\min \hat{J}(G,K) \quad (13)$$

where $\check{G}$ and $\check{K}$ are our new updates of the complex moduli. In the case of the ECE functional (6), we can obtain analytical expressions for the updated moduli by setting the first variation of the functional to zero and solving for the new complex moduli. That is,

$$D_G\hat{J}\cdot\delta G = -2\Re\int_\Omega (\sigma_N - 2G\mathbf{E_d}(\mathbf{u_D})) : \mathbf{E}^*_\mathbf{d}(\mathbf{u}_D)\delta G^*\ d\Omega \quad (14)$$

$$D_K\hat{J}\cdot\delta K = -\Re\int_\Omega (\sigma_N - Ke_u\mathbf{I}) : \mathbf{I}e^*_u\delta K^*\ d\Omega \quad (15)$$

where $\Re$ denotes the real part of the complex number. Setting the above equations to zero leads to the following simple materials updating formulas

$$G = \frac{\int_\Omega \sigma_N : \mathbf{E}^*_\mathbf{d}(\mathbf{u_D})\ d\Omega}{\int_\Omega |\mathbf{E_d}(\mathbf{u_D})|^2 d\Omega} \quad (16)$$

$$K = \frac{\int_\Omega pe^*_u\ d\Omega}{\int_\Omega |e_u|^2 d\Omega} \quad (17)$$

It is important to notice that if the complex moduli are taken as piecewise constants in each element, the integrals in Equations (16) and (17) are then taken over the element domain. Hence, these simple updating formulas can be used for both homogeneous and heterogeneous materials.

2.5 The ECE Algorithm

The minimization of the ECE functional (6) can be carried out following this straightforward algorithm.

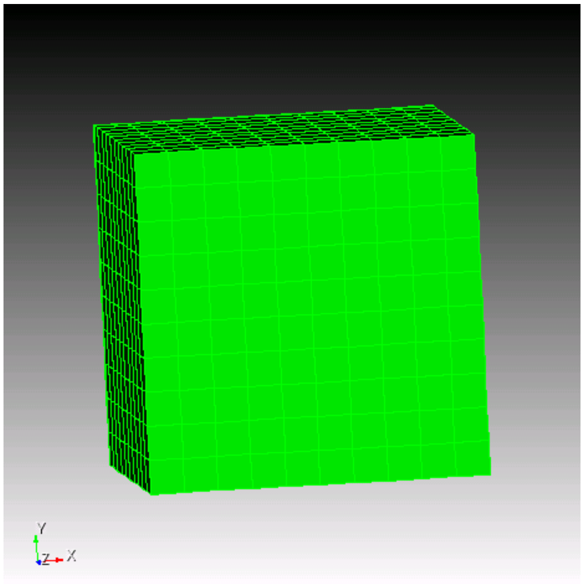

Figure 1. The geometry of the viscoelastic cube problem.

1. Set initial guesses for the complex moduli $\{G\}_{i=1}^{n}$ and $\{K\}_{i=1}^{n}$ corresponding to frequencies $\{\omega\}_{i=1}^{n}$
2. Do until a convergence criterion is reached
i. Obtain the dynamically admissible fields $\{\sigma_N\}_{i=1}^{n}$ by solving (9) for all frequencies.
ii. Obtain the kinematically admissible field $\{\mathbf{u_D}\}_{i=1}^{n}$ by solving (11) for all frequencies.
iii. Update the complex moduli $\{G\}_{i=1}^{n}$ and $\{K\}_{i=1}^{n}$ using (16) and (17), respectively, for all frequencies.

In this work, the algorithm was stopped after the ECE error (6) reached a certain tolerance or a predefined number of iterations was exceeded.

3 EXAMPLES AND RESULTS

In this section, we give numerical examples to demonstrate the capabilities described in the previous sections. The first example consists of cube made of a viscoelastic material. The real and imaginary parts of the complex moduli are sought, given a fixed boundary condition at the base and a pressure loading on the top of the plate. Figure 1 shows the geometry of the model. The measurements were generated by running the forward problem with known material properties, and then recording the three components of displacement at the nodes on the top surface only (where the pressure loading was applied). This data constituted the truth model that the inverse problem attempted to replicate.

Figures 2 and 3 show the comparison of the exact magnitude and $tan(\delta)$ for the shear modulus against those predicted by the inverse method. Excellent agreement is observed in the comparisons. Figures 4 and 5 show the same comparison for the bulk modulus. The agreement is not as good for the magnitude, but the $tan(\delta)$ comparisons are about as good as those for the shear modulus.

Figures 6 and 7 show the comparison of the exact magnitude and $tan(\delta)$ for the shear modulus against those predicted by the inverse method, inthe case that 5 percent noise is added to the measurement data. Excellent agreement is still observed in the

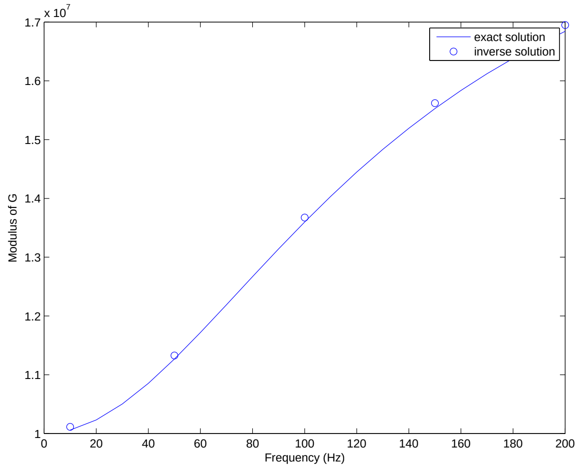

Figure 2. The magnitude of the shear modulus for the viscoelastic cube problem with zero noise.

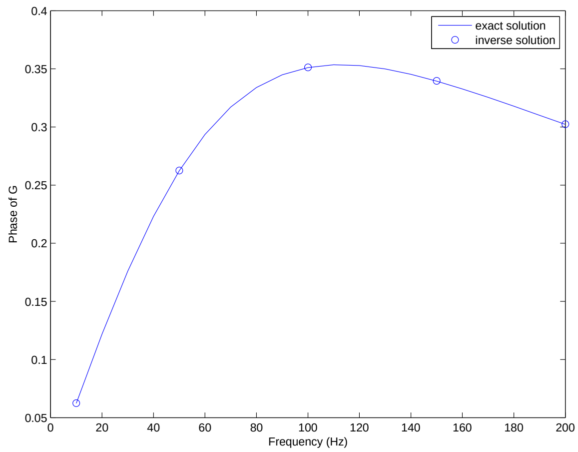

Figure 3. The $tan(\delta)$ of the shear modulus for the viscoelastic cube problem with zero noise.

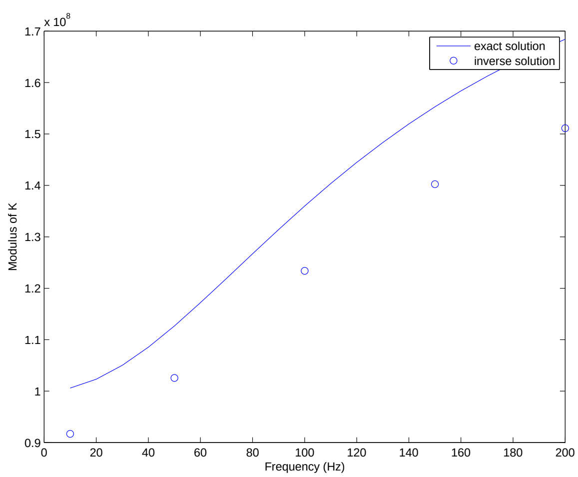

Figure 4. The magnitude of the bulk modulus for the viscoelastic cube problem with zero noise.

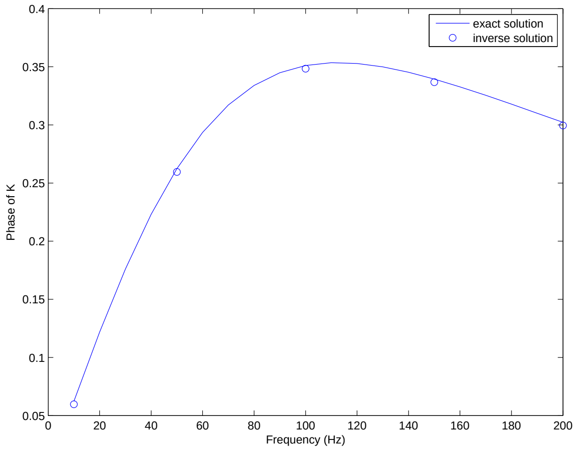

Figure 5. The $tan(\delta)$ of the bulk modulus for the viscoelastic cube problem with zero noise.

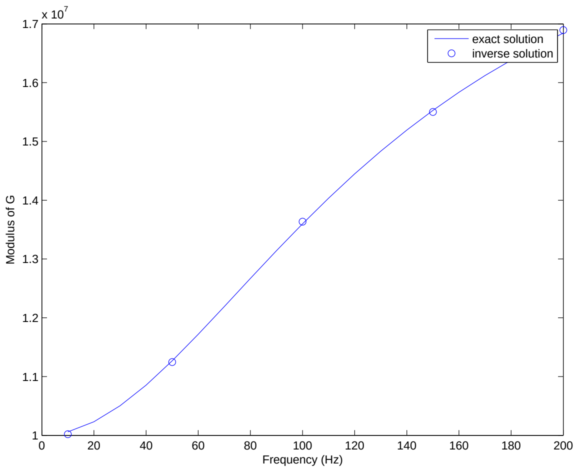

Figure 6. The magnitude of the shear modulus for the viscoelastic cube problem with 5 percent noise.

comparisons. Figures 8 and 9 show the same comparison for the bulk modulus, again with 5 percent noise in the measurements. The agreement is not as good for the magnitude, but the $tan(\delta)$ comparisons are about as good as those for the shear modulus. The introduction of noise does degrade the bulk modulus predictions compared with those with no noise.

4 CONCLUSIONS

In this paper, we presented an error in constitutive equations (ECE) approach for inverse identification of viscoelastic material properties. The standard cost functional in terms of the error in the measured data was augmented with an additional functional that measured the error in the constitutive equation. The formulation led to a forward problem and an adjoint problem, and an iterative outer loop that solved one forward problem and one adjoint problem at each iteration. An exact muduli updating procedure was also presented that eliminated the need for solving an optimization problem to determine the moduli. Finally, a numerical example was presented that demonstrated the capabilities of the method for

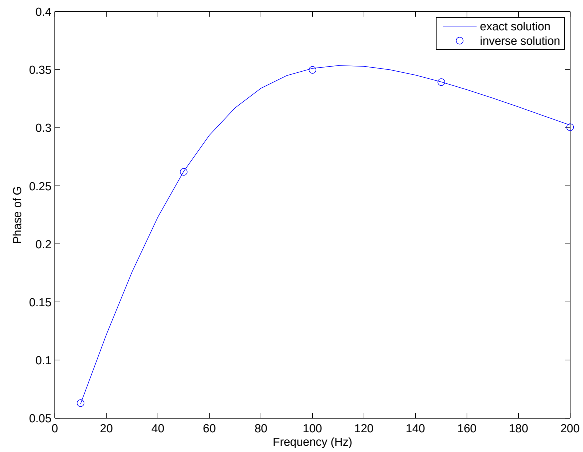

Figure 7. The $tan(\delta)$ of the shear modulus for the viscoelastic cube problem with 5 percent noise.

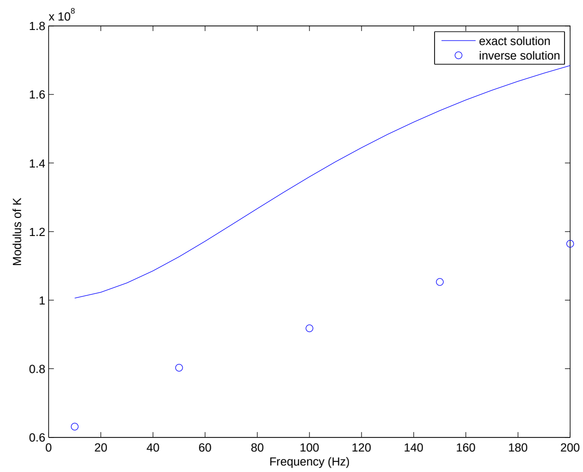

Figure 8. The magnitude of the bulk modulus for the viscoelastic cube problem with 5 percent noise.

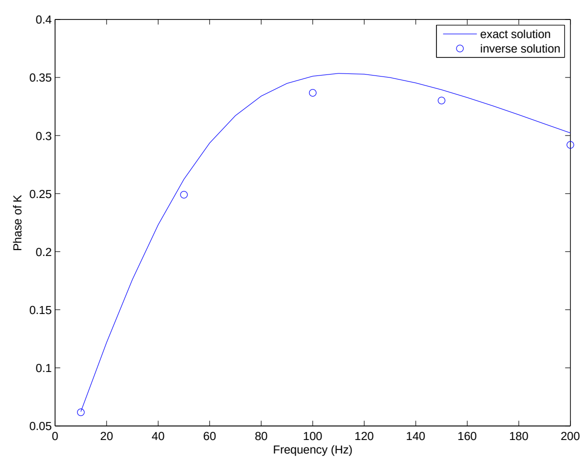

Figure 9. The $tan(\delta)$ of the bulk modulus for the viscoelastic cube problem with 5 percent noise.

resolving complex moduli and loss factors over a wide range of frequencies.

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