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Identification of Stiffness Coefficients in Resonant Ultrasound Spectroscopy Experiment Using Particle Swarm Optimization

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***Abstract*—Resonant ultrasound spectroscopy (RUS) is an experimental method for measuring the full elastic tensor of a small solid sample from the free resonant frequencies. One important step of the method is to adjust the stiffness coefficients in a model to minimize the difference between computed and measured frequencies. This inverse problem is traditionally solved with the Levenberg-Marquardt (LM) minimization algorithm. The convergence rate and accuracy of the method depend on the initial guess of the elastic tensor that should be relatively close to the sought solution in order to reach the global minimum (as opposed to a local one). To overcome this limitation, we introduce in this paper the particle swarm optimization (PSO) algorithm for its potential in finding a nearly global solution without the need for an accurate initial guess for the model parameters.**

Keywords—resonant ultrasound spectroscopy, particle swarm optimization, Bayesian formulation, stiffness coefficients

I. INTRODUCTION

Resonant Ultrasound Spectroscopy (RUS) is an experimental method for identifying material properties of an elastic object by exciting the resonant frequencies of the object. The material properties including density, dimensions, and more often the elastic moduli are determined by solving an inverse problem. Using a model (forward problem) to calculate the natural frequencies, the stiffness coefficients are adjusted to minimize the difference between computed and measured frequencies [1,2].

A least-squares optimization criterion with a gradient-based optimization, such as Levenberg-Marquardt method, is historically used to solve such inverse problem [1-3]. The relative closed initial guessing elastic properties to real results are essential in the algorithm, which often converges to a wrong solution even lead to divergence without appropriate initial settings [4]. A Bayesian-based method can take into account the experience of the operator, reduce the uncertainty of the estimation of stiffness coefficients and be insensitive to the initial guessing values [5]. The sampling method based on Markov chain Monto Carlo (MCMC) is often utilized to estimate variables in such Bayesian-based RUS [4-6]. However, in practice, MCMC is computationally expensive for the calculations of the forward problem. And the nonlinearity of the problem can cause the occurrence of multiple peaks of the posterior probability density function (pdf), which can result in errors in estimating the stiffness coefficients by using the mean of the distribution. It is necessary to estimate the peak of maximum posterior probability density of the stiffness coefficients correctly.

In this work, a RUS formulation based on particle swarm optimization (PSO), an evolutionary population-based method to solve global optimization problems [7], is proposed to find the peak of the maximum posterior probability density of the stiffness coefficients. The approach allows a fast estimation of the elastic properties of the sample within a large solution space. And the effectiveness of the method was verified by data simulated numerically for a transversally isotropic enamel material.

II. EXPERIMENTAL METHODS

A. The Forward Problem

Energy minimization technique with Rayleigh-Ritz method is widely used to calculate resonant frequencies of a parallelepiped specimen given the shape, dimension, mass and stiffness coefficients of the sample [1-6]. The brief form of the method can be expressed as follows:

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$$(2\pi f)^2 \boldsymbol{Ma} = \boldsymbol{Ka} \quad (1)$$

where f is a resonant frequency, $\boldsymbol{a}$ is the corresponding resonant mode, $\boldsymbol{M}$ and $\boldsymbol{K}$ are called the mass and stiffness matrices, respectively. In what follows, for convenience, the solution of the forward problem is expressed as $\boldsymbol{f}_{cal}$.

B. Bayesian Formulation of RUS

The Bayesian technique is a popular strategy in inverse problem theory. It allows evaluating the posterior probability distribution $p(\boldsymbol{C} \mid \boldsymbol{f})$ of the model parameters (here, the coefficients of the stiffness tensor $\boldsymbol{C}$), given several observation data $\boldsymbol{f}$ (the measured natural frequencies) and some prior information $p(\boldsymbol{C})$ on $\boldsymbol{C}$ [8]. For RUS, the following formulation can be established [4]:

$$p(\boldsymbol{C} \mid \boldsymbol{f}) = \frac{p(\boldsymbol{C})p(\boldsymbol{f} \mid \boldsymbol{C})}{p(\boldsymbol{f})} \quad (2)$$

Where the likelihood function $p(\boldsymbol{C} \mid f)$ describing the relation between the parameters and the observed resonant frequencies (with their uncertainties) is represented by a multivariate Gaussian distribution [4]. And in this work, the prior probability in the space of the stiffness coefficients $\boldsymbol{C}$ is a multivariate logarithmic Gaussian distribution with mean value $\log \boldsymbol{C}_0$ and covariance matrix Σ , which can be constructed from data available in literature.

C. Estimation of Stiffness Coefficients

To determine the stiffness coefficients based on the posterior probability distribution (as in (2)), an intuitive strategy is to run a Monte Carlo sampling to estimate the overall distribution of the model space [6]. However, this is a computationally expensive and time-consuming method. In most cases, it is not necessary to obtain the complete probability distribution. In practice, it is sufficient to find the peak of the posterior probability density (values of C_{ij}) and to assess the vicinity of the peak (errors of C_{ij}). We propose to apply the particle swarm optimization (PSO) algorithm to the optimization of RUS so that the stiffness coefficients can still be calculated successfully when the initial guessed values are far from the actual ones. And the uncertainty estimates could be easily established according to the Laplace approximation [8].

PSO, first proposed by Kennedy and Eberhart in 1995, is a population-based stochastic optimization technique to find the global optimum of the problem [7]. A PSO algorithm works on a group (also referred to as the swarm) of potential solutions (referred to as the particles) to a problem that can be expressed in terms of an objective function for which extremum must be found in the search space. The optimal solution of the problem can be found by iteratively exchanging information between particles. A modified version of PSO with gradient operator and mutation operator, proposed by Hu et *al*. [9], was introduced to RUS. A slightly difference in this work is that the gradient operator was added to all particles to speed up the convergence of the algorithm.

D. Numerical Experiment

The approach was applied to data simulated numerically for a transversally isotropic enamel material, with known stiffness coefficients C_{ij}^{real} derived from our early work [10]. Step one, we calculated the resonant frequencies $\boldsymbol{f}_{init} = \left[f_1, f_2 \ldots f_i \ldots f_n\right]$ by Rayleigh-Ritz method, where f_i is the *i*th resonant frequency. Step two, an experimental frequencies set $\boldsymbol{f}_{exp} \sim N\left(\boldsymbol{f}_{init}^{-}, \left(0.005\boldsymbol{f}_{init}^{-}\right)^2\right)$ was simulated by randomly deleting several resonant frequencies from $\boldsymbol{f}_{init}$ to simulate missing frequencies in a typical RUS experiment, and adding a 0.5% noise to the remaining resonant frequencies $\boldsymbol{f}_{init}^{-}$. Step three, assuming that the stiffness coefficients C_{ij}^{real} are unknown and the PSO method was used to find the optimal C_{ij}^{cal} from minimization of the difference between $\boldsymbol{f}_{cal}$ and $\boldsymbol{f}_{exp}$. The second and third steps were repeated one hundred times to evaluate the errors of C_{ij}^{cal} from the root-mean-square of $\left(C_{ij}^{cal} - C_{ij}^{real}\right) / C_{ij}^{real}$. The search space defined by the upper and lower bounds of the model stiffness coefficients is twice larger than that selected when using conventional RUS setting.

All errors of stiffness coefficients resulting from frequency imprecision were found to be less than 5%, with 1.03% for C_{11} , 1.37% for C_{33} , 2.27% for C_{12} , 4.17% for C_{13} , and 0.77% for C_{44} , respectively.

III. Discussion

RUS is an accepted technique for the accurate estimation of elastic properties in many fields. In this paper, the PSO algorithm was successfully applied for the first time to RUS data numerically simulated for an enamel material, providing estimates of stiffness coefficients that were in good agreement with reference values.

One key step of the RUS is to adjust stiffness coefficients to minimize the difference between calculated and experimental frequencies resulting in an inverse problem. In order to solve the inverse problem consisting in the estimation of the anisotropic elastic properties of the material from the list of resonant frequencies, Bayesian modeling and particle swarm optimization (PSO) were combined to formulate a feasible algorithm which provided several advantages:

(1) Identification of a global minimum (as opposed to a local one) without the need for the initial guessed set of model parameters to be close to the sought solution.

(2) Rapid convergence rate in contrast to MCMC sampling method.

(3) Intrinsic uncertainty estimates of the probabilistic model on stiffness coefficients.

And future work should address the application of real specimens for further verification of the feasibility of the method.

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