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An efficient PDE-constrained stochastic inverse algorithm for probabilistic geotechnical site characterization using geophysical measurements

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ABSTRACT

This paper develops an efficient, PDE-constrained stochastic inverse analysis methodology to probabilistically estimate site-specific elastic parameters of soil from sparse geophysical test measurements by accounting for the uncertain spatial variability of soil deposits and any measurement uncertainty associated with the geophysical experiment. Hypothesizing the soil parameters at any site to be three-dimensional, heterogeneous, anisotropic random fields, the methodology first probabilistically simulates the geophysical experiment using the finite element method in conjunction with a stochastic collocation approach to compute statistical measures of a quantity of interest such as the soil displacement or acceleration throughout the soil domain. To this end, the random fields are discretized into finite number of random variables by utilizing a Gaussian mixture model that allows for mimicking the soil formation process. The parameters of the random fields are initially assumed based on the generic data available in the literature for the geological soil type. The stochastic collocation approach utilizes a recently developed non-product quadrature method, conjugate unscented transformation, to accurately estimate the statistical moments corresponding to the model response variables in a computationally efficient manner. The methodology, then, employs a minimum variance framework to fuse the finite element model output with sparse real measurements to update the initially assumed soil statistical parameters. The methodology is illustrated through numerical geophysical experiments at a fictitious geotechnical site and is verified with three very different true profiles of the soil modulus. Moreover, a probabilistic sensitivity analysis is carried out by varying the number and locations of sensors. It is observed that by judiciously selecting the sensor locations, following a set of information maps, obtained by exploiting the equations of the minimum variance scheme, more information may be extracted from any geophysical experiments, leading to less uncertain estimates of the soil parameters.

1. Introduction

Site characterization represents one of the most important components of the design process of any civil infrastructure objects. Nonetheless, site characterization is currently treated as an intuitive process based on engineering judgment. Soil deposits are typically very heterogeneous with presence of non-uniform layers and lenses within layers. However, conventional site characterization practice of sampling at a few locations (based on intuition) in a soil deposit to infer spatially variable soil parameters for the entire site inherently suffers from uncertainty due to limited data. Even any statistical analysis like the Kriging [\[31,16\]](#page--1-0) or random field modeling [\[55,54\]](#page--1-1) of soil parameters with this limited information results in bias in the analysis.

Geophysical approach, which is increasingly being used to perform geotechnical site characterization, offers a better alternative as not only geophysical tests yield larger volume of data but also geophysical measurements (waveforms) contain more information on the spatial variability of any soil deposit as waveforms' characteristics change as they travel through layers and lenses. However, geophysical measurements are traditionally analyzed with simplifying assumptions so that the inversion process remains tractable. For example, the widely used spectral analysis of surface waves (SASW) assumes any soil deposit to be horizontally layered and ground waves to consist only of Rayleigh waves and thereby neglects effects of other types of surface as well as body waves [\[43\]](#page--1-2). In recent years, with advancement of mathematical machineries and availability of faster computers, partial differential equation (PDE) constrained, three-dimensional, full waveform inversions of geophysical measurements have also been successfully attempted (see, for example, Refs. [\[26,21\]](#page--1-3)). They not only account for all types of waves in a soil continuum for more accurate estimation of soil

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parameters but also overcome the issue of limited data to a certain extent by integrating measurements with PDE-driven model predictions. However, such inversion processes, due to their deterministic nature, fail to account for the uncertain spatial variability of soil parameters and any measurement uncertainty associated with the geophysical experiments.

This paper presents a methodology to perform PDE-constrained stochastic full waveform inversions of geophysical measurements in probabilistically estimating three-dimensional profiles of the elastic parameters of any soil deposit by accounting for uncertain spatial variability and measurement uncertainty as well as uncertainty due to limited data. The methodology hypothesizes the elastic soil parameters to be three-dimensional, heterogeneous, anisotropic random fields and probabilistically simulates the geophysical experiment to compute statistical moments associated with a quantity of interest (QOI) such as the soil displacement or acceleration. It then integrates the forward model output with sparse real measurements using a minimum variance framework to update the parameters of the random fields.

The fusion of observation data with numerical simulation within a probabilistic framework is not a new concept. It had its birth with the development of Kalman filter [\[27\]](#page--1-4). Though computationally expensive, with the availability of faster computers, it is increasingly being used for stochastic inverse analysis in many fields of science and engineering, including geophysics [\[23,56,9,14,52,53,12,18,37,57,62,25,51,20,57,42,15,](#page--1-5) [46,19\]](#page--1-5). However, the main novelty of this paper lies, in addition to first time application of such technique in full 3D geotechnical site characterization, in efficient probabilistic solution of the uncertain forward problem. The uncertain forward problem involves numerical simulation of the geophysical experiment with the soil elastic parameters modeled as three-dimensional random fields to compute statistics of the QOI at any geotechnical site.

In fact, it is the efficient solution algorithm of the uncertain forward problem that makes this large scale stochastic inverse analysis computationally manageable. A geophysical experiment, in essence, is propagation of waves through soils which is governed by the equilibrium, strain compatibility, and constitutive equations. In a deterministic setting, the governing equations of wave propagation are commonly solved numerically using the finite element method. However, difficulty arises when the soil parameters are modeled as random fields and one needs to probabilistically solve the governing equations. Traditional Monte Carlo (MC) approach [\[41\]](#page--1-6) is very inefficient (and probably intractable) for large scale probabilistic dynamic problems in a finite element setting due to its slow convergence. Among alternative approaches, the intrusive stochastic Galerkin and non-intrusive stochastic collocation approaches are more common. Intrusive stochastic Galerkin approaches [\[17,22,29,39,58,61\]](#page--1-7) usually represent all the uncertain parameters of a model using some type of finite series expansions (e.g., the Taylor series expansion, the polynomial chaos expansion, etc.) and then employ a Galerkin technique to minimize the errors of finite representation which result in a system of coupled (deterministic) equations. Non-intrusive stochastic collocation approaches [\[10,38,59,62\],](#page--1-8) on the other hand, can be viewed as a MC type sampling technique, with the exception that, instead of at random, the sampling points are selected following some kind of numerical quadrature schemes which are used to estimate the statistical moments of the solution variable. A major advantage of the non-intrusive stochastic collocation approaches is that they do not require any modifications to the underlying deterministic (finite element) code; the collocation scheme just acts as a wrapper on the deterministic code. However, the main challenge with the stochastic collocation approaches is the selection of the quadrature scheme, especially for three-dimensional problems.

Traditional Gaussian quadrature methods that rely on the tensor product of one-dimensional quadrature points to yield multi-dimensional quadrature points suffer from the curse of dimensionality and become computationally very inefficient. Sparse grid quadratures (e.g., Smolyak quadrature [\[48\]\)](#page--1-9), on the other hand, take the sparse product

of one-dimensional quadrature rules and thus have fewer points than the equivalent Gaussian quadrature rules, but at the cost of introducing negative weights [\[50\].](#page--1-10) There also exists unscented transformation (UT) method [\[50\]](#page--1-10) that yields a linear growth of points with dimensions. However, it is exact only to degree 2 and hence, cannot be used to evaluate higher order moments. This paper uses recently developed conjugate unscented transformation (CUT; $[1,2]$) method – an extension of the conventional UT method that satisfies additional higher order moment constraints – to efficiently and accurately evaluate the statistical moments of the solution variables within a stochastic collocation scheme. Moreover, this paper utilizes a Gaussian mixture method, instead of the conventional Kosambi-Karhunen-Loève (KKL) theorem [\[30,28,33\]](#page--1-12), to discretize the soil parameter random fields in order to avoid repeated – equal to the number of collocation points – use of the computationally expensive KKL-eigenanalysis.

The salient features of the adaptive Gaussian mixture method and the CUT-based stochastic collocation approach in generating high-fidelity, probabilistic ensembles of waveform analysis models of any geophysical experiment and of the stochastic inverse methodology in integrating waveform model ensembles with sparse sensor measurements, are highlighted through numerical geophysical experiments at a fictitious geotechnical site. The numerical examples assume only the Young's modulus of soil to be uncertain and unknown, while the Poisson's ratio and density of soil to be deterministic and known. Moreover, this paper does not use experimental data as the real measurements. Instead, one of the realizations of the soil modulus random field is considered as the true profile of the soil modulus and a geophysical experiment is numerically simulated using that profile to generate acceleration time histories at the sensor locations. Gaussian white noise that mimics sensor measurement uncertainty is then added to each of the generated acceleration time histories and the resulting acceleration time histories are considered as "real" measurements. The inverse analysis algorithm is verified with three very different realizations of the soil modulus as the true profile – a very heterogeneous realization with a softer middle region; a more uniform, horizontally layered realization; and a randomly weighted average of several realizations. The inverse analysis results are presented in terms of threedimensional profiles of the mean and standard deviation of soil modulus as well as its correlation structure. Furthermore, towards the goal of reducing uncertainty in the estimated soil modulus, a sensitivity analysis is also performed by varying the number and locations of sensors.

2. The PDE-constrained stochastic inverse algorithm

The PDE-constrained stochastic inverse algorithm may be viewed to be comprised of two interrelated modules, namely the forward problem module and the inverse problem module (see [Fig. 1\)](#page--1-13). The forward problem module will produce statistics of simulated geophysical measurements that will be integrated with sparse real measurements in the inverse problem module using a minimum variance framework. In the following, these modules are discussed in detail.

2.1. The forward problem module

The objective of this module is to formulate a high-fidelity model of any geophysical experiment and to develop a strategy to probabilistically solve the model so that the model predictions can be used to compensate for sparse real measurements in the inverse problem module. A geophysical experiment may be modeled using the governing equations of a three-dimensional elastic solid, which in the Cartesian coordinate system, are given as:

$$
\frac{\partial \sigma_{ij}}{\partial x_j} + b_i = \rho \ddot{u}_i \qquad \text{(equilibrium equation)} \tag{1}
$$

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