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Stochastic reduced order models for inverse problems under uncertainty

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Abstract

This work presents a novel methodology for solving inverse problems under uncertainty using stochastic reduced order models (SROMs). Given statistical information about an observed state variable in a system, unknown parameters are estimated probabilistically through the solution of a model-constrained, stochastic optimization problem. The point of departure and crux of the proposed framework is the representation of a random quantity using a SROM - a low dimensional, discrete approximation to a continuous random element that permits efficient and non-intrusive stochastic computations. Characterizing the uncertainties with SROMs transforms the stochastic optimization problem into a deterministic one. The non-intrusive nature of SROMs facilitates efficient gradient computations for random vector unknowns and relies entirely on calls to existing deterministic solvers. Furthermore, the method is naturally extended to handle multiple sources of uncertainty in cases where state variable data, system parameters, and boundary conditions are all considered random.

The new and widely-applicable SROM framework is formulated for a general stochastic optimization problem in terms of an abstract objective function and constraining model. For demonstration purposes, however, we study its performance in the specific case of inverse identification of random material parameters in elastodynamics. We demonstrate the ability to efficiently recover random shear moduli given material displacement statistics as input data. We also show that the approach remains effective for the case where the loading in the problem is random as well.

Keywords

Stochastic inverse problems; stochastic optimization; stochastic reduced order models; uncertainty quantification; material identification

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1. Introduction

Inverse problems arise in a range of important engineering applications including elasticity imaging, source identification, and damage detection. Generally speaking, one is provided data regarding the observed or measured state of a system and then uses this information to estimate some unknown parameters of interest. A common approach is to pose the inverse problem as a constrained optimization problem. In this optimization problem, the solution is obtained by minimizing a relevant objective function involving the state data and parameters subject to the condition that a governing boundary value problem be satisfied.

Uncertainty is ubiquitous in forward and inverse problems (boundary conditions, geometry, material properties, measured data, etc.). While explicitly incorporating these uncertainties in the solution framework provides robustness to fluctuations in input data and rigorous quantification of solution uncertainty, it generally comes at the expense of complex implementations and substantial computational cost. This work focusses on a practical and efficient approach to solving inverse problems under uncertainty.

Existing methods to treat inverse problems with uncertainty can be broadly classified into two categories: the Bayesian inference approach and the newer stochastic optimization approach. In the former, the posterior probability distribution of the unknown/design parameters given a realization of the state variable is first formulated using Bayes' theorem. This conditional distribution combines the information from the input data through the likelihood function with any *a priori* knowledge of the unknowns using a user-specified prior distribution. The posterior distribution is then sampled using Markov Chain Monte Carlo (MCMC) algorithms in order to estimate the statistics of the unknown parameters. While this approach has achieved success in a number of applications [17, 24, 19, 18], a well-known drawback of the approach is computational cost (since every MCMC sample generally requires a deterministic simulation) and the sensitivity of the resulting solutions to the prior distribution model chosen.

This paper considers a stochastic optimization approach for inverse problems. Here, the point of departure from Bayesian inference is immediate - the input data for the inverse problem is the statistics of the system state rather than a single deterministic realization. An objective function is formulated in terms of the given state variable statistics and then the unknown parameters are estimated probabilistically as the random variables that minimize this objective function. The random state and parameters of the system in consideration are related through a governing stochastic model, which therefore constrains the optimization problem. For tractability, this stochastic optimization problem is generally translated into a deterministic one through a suitable parameterization of the random quantities. From here, conventional deterministic optimization algorithms can be applied to estimate the unknown parameters of the probabilistic models used.

The stochastic optimization approach was first proposed in [21], where the framework was applied to solve a stochastic inverse heat conduction problem. Here, an unknown, random heat flux was estimated given the probability distribution function (PDF) of the temperature at discrete points in a conducting solid. The system uncertainties were represented using

generalized polynomial chaos expansions (GPCE) [26, 28] and a conjugate gradient approach was used to solve the optimization problem constrained by the forward stochastic heat conduction problem. The spectral stochastic finite element method (SSFEM) [5] was employed to solve all subproblems during the optimization algorithm (evaluating the forward problem, calculating gradients), requiring extensive modification of the existing deterministic solver and limiting the overall scalability of the approach.

To overcome these shortcomings associated with reliance on the SSFEM, the work was later extended in [4] by representing uncertainty with a sparse grid collocation approach for the stochastic inverse heat conduction problem. The non-intrusive nature of stochastic collocation [1, 27] yielded a decoupled framework for stochastic optimization that can be readily parallelized (and is hence scalable) and relies solely on calls to deterministic simulators and optimization software. An adaptive sparse-grid approach was later proposed in [16] in an effort to use as few collocation points and hence model evaluations as possible for stochastic optimization problems. The approach was combined with a trust-region algorithm to efficiently solve PDE-constrained optimization under uncertainty. In the latter work, only the data in the PDEs was considered random, while the design variables were taken to be deterministic.

The point of departure from existing work and the crux of the method proposed here is the representation of a random quantity using a stochastic reduced order model (SROM). A SROM is a low-dimensional, discrete approximation to a continuous random element comprised of a finite and generally small number of samples with varying probability. Such a representation allows for non-intrusive and efficient stochastic computations in terms of only this small set of defining samples and probabilities. The SROM concept was originally proposed in [7] and then further refined in [25]. The application of SROMs has thus far exclusively focused on propagating uncertainty in forward models, including the determination of effective conductivities for random microstructures [8], the estimation of linear dynamic system states [9, 10], and the quantification of uncertainty in intergranular corrosion rates [23]. The primary strengths of SROMs, as shown in these papers, are their ability to represent an underlying random quantity with low-dimensionality and to subsequently solve uncertainty propagation problems in a fraction of the computational time required by traditional Monte Carlo simulation.

This work represents the first application of SROMs for uncertainty quantification in inverse problems by introducing a novel approach for stochastic optimization with model constraints based on this concept. The framework represents a practical approach with the following strengths: 1) it relies entirely on calls to existing deterministic solvers and standard optimization software, 2) it is easily parallelized and scalable, and 3) it is readily extended to handle multiple sources of uncertainty. Additionally, in contrast with existing stochastic collocation-based methods that discretize the entire probability space equally, SROMs naturally give higher weight to important areas of the probability space. This property yields low-dimensional approximations and thus relatively few calls to deterministic models.

The SROM-based inverse problem approach presented here is formulated for a general stochastic optimization problem in terms of an abstract objective function and model

constraint. The transformation of the constrained optimization problem from stochastic to deterministic using SROMs is developed in these abstract terms and followed by a general derivation of gradients. In order to study the performance of the method, we then show the adaptation of the formulation to the specific case of inverse identification of random material parameters in elastodynamics. We demonstrate the ability to efficiently recover random shear moduli given material displacement statistics as input data. We also show that the approach remains effective for the case where the loading in the problem can only be characterized probabilistically.

The article is organized as follows. In Section 2, we provide the necessary background for this study, introducing SROMs and describing their traditional use for propagating uncertainty in stochastic systems. Then, Section 3 describes the proposed SROM-based inverse problem approach, providing the formulation for general stochastic optimization problems and subsequently, in section 4, the application of the method for inverse material identification in elastodynamics. Section 5 presents three numerical examples, demonstrating the effectiveness of the proposed method for cases of multiple sources of uncertainty, limited/sparse input data, and problems with multiple unknown, random parameters. We finally conclude in Section 6 with a summary of this work.

2. Background

2.1. General stochastic model setting

Consider an operator $\mathcal{M}$: an deterministic $\mathcal{M}: \mathcal{U} \times \mathcal{V} \rightarrow \mathcal{Z}$ where $\mathcal{U}, \mathcal{V}$ and $\mathcal{Z}$ are some appropriate function spaces. We first introduce abstract model of the form

$$\mathcal{M}(s, x) = 0, \quad s \in \mathcal{U}, x \in \mathcal{V} \quad (1)$$

For instance, Eq. (1) commonly represents a system of partial differential equations with appropriate boundary and initial conditions. In our work, we will refer to s as the state variable, while x is referred to as the input (or control) variable. For instance, in an elastodynamics problem (as the one considered later in this work), s can represent a displacement field, while x can represent material properties.

Numerical methods (e.g. finite element method, finite volume method, etc.) are commonly used to obtain approximate solutions to Eq. (1). After discretization with a suitable numerical technique, a system of algebraic equations is obtained, which can be represented as

$$\mathbf{M}(s, x) = 0, \quad s \in \mathbf{U} \subset \mathbb{R}^n, \quad x \in \mathbf{V} \subset \mathbb{R}^d \quad (2)$$

We will assume that for each $x \in \mathbf{V}$ there is a unique solution $s(x) \in \mathbf{U}$ such that

$$\mathbf{M}(s(x), x) = 0 \quad (3)$$

That is, we assume that the forward problem is well-posed. Also, we will also assume that $\mathbf{M}$ is continuously differentiable with respect to $(x, s) \in \mathbf{V} \times \mathbf{U}$ and that the Jacobian $\frac{\partial \mathbf{M}}{\partial x}$ has a

bounded inverse everywhere. Then, from the Implicit Function Theorem [13], $s(\mathbf{x})$ is continuously differentiable. Notice that these assumptions are not very restrictive as they are commonly realized in many practical models.

We will be concerned with stochastic states and controls denoted as $\mathbf{S}$ and $\mathbf{X}$, respectively. These are interpreted, in general, as random elements (e.g. scalars or vectors). Let $(\Omega, \mathcal{F}, P)$ and $(\Psi, \mathcal{G})$ denote a probability space and a measurable space, respectively. Here, Ω is the sample space, $\mathcal{F} \subseteq 2^\Omega$ is the δ -algebra (event space), and $P: \mathcal{F} \rightarrow [0, 1]$ is the probability measure. A function $Y: \Omega \mapsto \Psi$ is a random element if it is measurable from $(\Omega, \mathcal{F})$ to $(\Psi, \mathcal{G})$, that is, if $Y^{-1}(H) = \{\omega: Y(\omega) \in H\} \in \mathcal{F}$, $\forall H \in \mathcal{G}$ [6]. In our discussion, we assume $\Psi = \mathbb{R}^d$ and $\mathcal{G} = \mathcal{B}(\mathbb{R}^d)$ is the Borel δ -algebra on $\mathbb{R}^d$ and so $Y: \Omega \mapsto \mathbb{R}^d$ is a d -dimensional random vector.

Using $\mathbf{X}$ and $\mathbf{S}$ in (2), we obtain a system of stochastic algebraic equations described as

$$\mathbf{M}(\mathbf{S}, \mathbf{X}) = \mathbf{0}, \quad \mathbf{S} \in \mathcal{S} \subset \mathbb{R}^n, \quad \mathbf{X} \in \mathcal{X} \subset \mathbb{R}^d \quad (4)$$

We note that models depending on random fields can be described by the general form (4) after appropriate parameterization or discretization. As we will see in the next section, one of the main features of SROMs is the ability to propagate uncertainty in a non-intrusive fashion. Performing stochastic computations of the general form (4) using SROMs requires the construction of an accurate probabilistic representation of $\mathbf{X}$ and then a method to propagate uncertainty to estimate the statistics $\mathbf{S}$. The next section briefly describes these procedures after first introducing and defining SROMs.

Remark 1. Notice that in the stochastic case, continuity of the operator $\mathbf{M}$ on its arguments is interpreted in the almost sure sense. That is, if we have a sequence $\{\mathbf{X}_n\} \xrightarrow{a.s.} \mathbf{X}$, continuity, for instance, at $\mathbf{X}$ implies

$$\lim_{n \rightarrow \infty} \mathbf{M}(\mathbf{S}(\omega), \mathbf{X}_n(\omega)) = \mathbf{M}(\mathbf{S}(\omega)) \quad \text{for almost all } \omega \text{ (i.e. } \omega \in \Omega \setminus N, P(N) = 0). \quad (5)$$

Also, differentiability is interpreted similarly.

2.2. SROM definition

Stochastic reduced order models (SROMs) provide a low-dimensional, discrete approximation of a given random quantity and have been used in several past works [8, 9, 23] to facilitate efficient stochastic computations. A SROM $\tilde{\mathbf{X}}$ for a random vector $\mathbf{X}$ is a simple random element with a finite set of samples $\{\tilde{\mathbf{x}}^{(1)}, \dots, \tilde{\mathbf{x}}^{(m)}\}$ and corresponding probabilities $(p^{(1)}, \dots, p^{(m)})$ such that $p^{(k)} \geq 0 \quad \forall k$ and $\sum_{k=1}^m p^{(k)} = 1$, that is close to $\mathbf{X}$ in a statistical sense [8]. Hence, the SROM $\tilde{\mathbf{X}}$ is completely defined by the model size m and sample-probability pairs $\{\tilde{\mathbf{x}}^{(k)}, p^{(k)}\}_{k=1}^m$ and effectively provides a discrete-valued approximation to a given continuous random quantity $\mathbf{X}$.

When SROMs are used for uncertainty propagation in forward models, it is assumed that the statistics of $\mathbf{X}$ are known a priori. For example, one is provided with the following expressions for its marginal distributions, moments of order q , and correlation matrix

$$F_i(x_i) := P(X_i \leq x_i) \quad (6)$$

$$\mu_i(q) := E[X_i^q] \quad (7)$$

$$\mathbf{r} := E[\mathbf{X}\mathbf{X}^T] \quad (8)$$

Then, once the SROM parameters $(\{\tilde{\mathbf{x}}\} \text{ and } \mathbf{p})$ are specified, the corresponding expressions for its statistics are given by

$$\tilde{F}_i(x_i) := \sum_{k=1}^m p^{(k)} 1(\tilde{\mathbf{x}}_i^{(k)} \leq x_i) \quad (9)$$

$$\tilde{\mu}_i(q) := \sum_{k=1}^m p^{(k)} (\tilde{\mathbf{x}}_i^{(k)})^q \quad (10)$$

$$\tilde{r}(i, j) := \sum_{k=1}^m p^{(k)} \tilde{\mathbf{x}}_i^{(k)} \tilde{\mathbf{x}}_j^{(k)} \quad (11)$$

where $1(\cdot)$ is the indicator function. Note that by design, the SROM is constructed such that $\tilde{\mathbf{X}}$ provides a satisfactory discrete approximation to $\mathbf{X}$, and so Equations (9)-(11) provide estimates of the true statistics in (6)-(8). The details of this construction is provided in the following section.

2.3. SROM construction for forward problems

In order to solve stochastic problems of the general form (4), which we will refer to as the “forward problem”, we first describe how to construct a SROM of $\mathbf{X}$ given knowledge of its statistics. An optimal reduced order representation of a random input can be obtained by selecting the SROM parameters such that the statistics of $\tilde{\mathbf{X}}$ ((9)-(11)) best approximate those of $\mathbf{X}$ ((6)-(8)). In practice, this is done by solving an optimization problem with objective function measuring the discrepancies between SROM and target marginal distributions, marginal moments up to order q^{-1} , and correlation matrices as

$$e_1(\{\tilde{\mathbf{x}}\}, \mathbf{p}) := \frac{1}{2} \sum_{i=1}^d \int_{I_i} (\tilde{F}_i(x_i) - F_i(x_i))^2 dx_i \quad (12)$$

$$e_2(\{\tilde{\mathbf{x}}\}, \mathbf{p}) := \frac{1}{2} \sum_{i=1}^d \sum_{q=1}^{\tilde{q}} \left(\frac{\tilde{\mu}_i(q) - \mu_i(q)}{\mu_i(q)} \right)^2 \quad (13)$$

$$e_1(\{\tilde{\mathbf{x}}\}, \mathbf{p}) := \frac{1}{2} \sum_{i,j=1; j>i=1}^d \left(\frac{\tilde{r}(i,j) - r(i,j)}{r(i,j)} \right)^2, \quad (14)$$

respectively, where I_i denotes the support of F_i . The optimization problem for selecting the defining SROM parameters is then formally stated as

$$\begin{aligned} \tilde{\mathbf{X}} &:= \underset{\{\tilde{\mathbf{x}}\}, \mathbf{p}}{\operatorname{argmin}} \left(\sum_{i=1}^3 \alpha_i e_i(\{\tilde{\mathbf{x}}\}, \mathbf{p}) \right) \\ \text{s.t. } &\sum_{k=1}^m p^{(k)} = 1 \quad \text{and} \quad p^{(k)} \geq 0, \quad k=1, \dots, m, \end{aligned} \quad (15)$$

where $\{\alpha_i \geq 0\}_{i=1}^3$ are weighting factors controlling the relative contribution of each error term to the cost functional. It is important to mention that the model size m can be selected a priori based on computational cost considerations, or through adaptive schemes. For this work, we will use the former approach (i.e. fixed model size “m”) and adaptive schemes will be pursued in future work. Details on the solution of (15) can be found in [25] and are omitted here for brevity.

Remark 2. It was shown in [7] that the statistics of the SROM $\tilde{\mathbf{X}}$ converge to those of the target random variable $\mathbf{X}$ with increasing model size, i.e. $e_i \rightarrow 0 \quad \forall i$ as $m \rightarrow \infty$. As m increases indefinitely, the samples of SROM become equally likely for the following two reasons. First, samples used by the Monte Carlo method are equally likely. Second, Monte Carlo estimates of moments, correlations, and distributions approach the actual moments, correlation, and distributions as the sample size increases indefinitely. Therefore, the objective function used to construct the SROM (see (15)) goes to zero as $m \rightarrow \infty$. Accordingly, as $m \rightarrow \infty$, the samples of the SROM become equally likely so as to minimize the objective function.

2.4. Propagating uncertainty with SROMs

After a SROM is generated for the random input $\mathbf{X}$ of a system, the uncertainty in the state $\mathbf{S}$ can be estimated non-intrusively in a manner analogous to Monte Carlo methods. This is done by simply solving for the state samples from

$$\mathbf{M}(\tilde{s}^{(k)}, \tilde{\mathbf{x}}^{(k)}) = 0, \quad k=1, \dots, m \quad (16)$$

The resulting state samples $\{\tilde{s}\}$ along with the original input SROM probabilities $\mathbf{p}$ define a SROM $\tilde{\mathbf{S}}$ of new $\mathbf{S}$. Now, we can $\tilde{\mathbf{S}}$ to estimate the statistics of the state using expressions analogous to (9)-(11). For example, the marginal distributions and moments of $\mathbf{S}$ can be approximated as

$$P(S_i \leq s_i) \approx P(\tilde{S}_i \leq s_i) := \sum_{k=1}^m p^{(k)} 1(\tilde{s}_i^{(k)} \leq s_i) \quad (17)$$

$$E[S_i^q] \approx E[\tilde{S}_i^q] := \sum_{k=1}^m p^{(k)} (\tilde{s}_i^{(k)})^q \quad (18)$$

Viewing the above procedure for propagating uncertainty with SROMs, it is evident that the method shares the same benefits of Monte Carlo simulation in its generality and non-intrusiveness. However, the SROMs are designed to better represent the underlying random quantity through the optimization problem in Equation (29), and therefore generally require far fewer samples and model evaluations to obtain a solution. Indeed, SROMs have been shown in numerous previous studies to significantly reduce computational cost over Monte Carlo simulation, while maintaining accuracy [25, 23].

2.4.1. Comments on Convergence of SROMs—We now provide some observations on the convergence of SROMs. To this end, convergence is interpreted in the sense of statistics unless otherwise noted. let $\mathbf{M}_h(\mathbf{S}_h, \mathbf{X}_h) = 0$ correspond to a model discretization and the subindex h represent a discretization level. Notice that the operator is also assumed to vary with discretization (e.g. because of numerical integration). Let $\tilde{S}_h(m)$ be a SROM of order m associated with a model with discretization level h . Furthermore, let S be the solution to the stochastic infinite dimensional problem $M(S, X) = 0$. The following proposition describes conditions that guarantee $\tilde{S}_h(m) \rightarrow S$.

Proposition 1. A sequence of SROM solutions parametrized by h and m (i.e. $\tilde{S}_h(m)$) converges to the solution of the infinite dimensional problem S , i.e. $\tilde{S}_h \rightarrow S$ as $m \rightarrow \infty$ $h \rightarrow 0$ if the following two conditions hold.

1. $X_h \rightarrow X$ and $S_h(m) \rightarrow S_h$ as $m \rightarrow \infty$ for any discretization level h .
2. $X_h \xrightarrow{a.s.} X$ and $S_h \xrightarrow{a.s.} S$. That is, $\mathbf{S}_h(\Omega) \rightarrow \mathbf{S}(\Omega)$ and $\mathbf{X}_h(\Omega) \rightarrow \mathbf{X}(\Omega)$ for almost all Ω .

Proof. Let $e(X, Y)$ define an error metric measuring distance in statistics between two random elements. Then, the error between a SROM solution and the solution of the infinite dimensional problem is bounded as $e(\tilde{S}_h(m), S) \leq e(\tilde{S}_h(m), S_h) + e(S, S_h)$, using the triangle inequality. Now, using Conditions 1 and 2 above, we get $e(\tilde{S}_h(m), S) \rightarrow 0$ as $h \rightarrow 0$ and $m \rightarrow \infty$.

The first condition states that for any discretization level, a SROM finds a limit, which is the solution of the stochastic algebraic system of equations associated with a given h . The proof to this statement can be found in, for instance, [7]. The second condition is realized in many practical models and we note that almost sure convergence implies convergence in statistics. This latter condition is interpreted as a requirement that any numerical method used produces convergent sequences upon discretization for almost all samples.

2.5. Multiple sources of uncertainty with SROMs—An additional strength of the SROM approach to stochastic computations detailed in this section is that it can be naturally

extended to handle problems with multiple sources of uncertainty. Consider the case where, in addition to the parameters $\mathbf{X}$, the state of a system $\mathbf{S}$ also depends on a separate and independent source of randomness represented by the random element Φ . This could occur, for example, when the variability in the state of a system is influenced by both internal randomness (material properties, geometry, etc.) as well as uncertainty from external sources (boundary conditions, loads, fluxes, etc.) In this case, the abstract system model in Equation (4) takes the form

$$\mathbf{M}(\mathbf{S}, \mathbf{X}; \Theta) = 0 \quad (19)$$

Note here that we could very well encapsulate all random parameters as $\mathbf{Y} := [\mathbf{X} \ \Phi]^T$. However, this explicit separation will be helpful in the inverse problem setting where $\mathbf{X}$ is considered unknown, while Φ is given.

The procedure for solving Equation (19) using SROMs is consistent with the approach described previously with the caveat of treating the additional random element Φ . The

SROMs $\tilde{\mathbf{X}} := \{\tilde{\mathbf{x}}^{(i)}, p_x^{(i)}\}_{i=1}^{m_x}$ and $\tilde{\Theta} := \{\tilde{\theta}^{(j)}, p_\theta^{(j)}\}_{j=1}^{m_\theta}$ must be formed in this case for both $\mathbf{X}$ and Φ by solving the optimization problem in Equation (15) given the probabilistic description of each variable. In this case, the SROM approximation $\tilde{\mathbf{S}}$ to the system state $\mathbf{S}$ is generated by evaluating the model $m_x \times m_\Phi$ times as

$$\mathbf{M}(\tilde{\mathbf{s}}^{(k)}, \tilde{\mathbf{x}}^{(i)}; \tilde{\theta}^{(j)}) = 0, \quad \text{for } i=1, \dots, m_x, \quad j=1, \dots, m_\theta \quad (20)$$

$$k = (j-1) \times m_x + i \quad (21)$$

Here, the probabilities associated with the SROM $\tilde{\mathbf{S}}$ are given by

$$p_s^{(k)} = p_x^{(i)} \times p_\theta^{(j)} \quad (22)$$

Using the SROM defined by these samples and probabilities, the statistics of $\mathbf{S}$ can again be approximated using the expressions in (17) and (18). This concept generalizes in the same manner to more than two (independent) random inputs.

3. Stochastic inverse problem approach

In this section, we introduce a novel framework for solving inverse problems under uncertainty using SROMs. We define the inverse problem as a stochastic, constrained optimization problem, and transform it into a deterministic counterpart by introducing a SROM approximation of random elements. We subsequently layout the fundamental steps involved in gradient-based optimization involving SROMS. Finally, we comment on the extension of the approach to the case of optimization and inverse problems in the presence of multiple uncertainties.

Here, given statistics of the observed state of a system, represented as $\mathbf{S}_m$, we seek to determine random elements $\mathbf{X}$ and $\mathbf{S}$ that best approximate, in a statistical sense, the

observed quantities. Furthermore, we require that these random elements satisfy the model problem (4). Contrast this with the problem of uncertainty propagation in forward models, as described in the previous section using SROMs, where the situation is reversed (i.e. we are given statistics of $\mathbf{X}$ and use $\mathbf{M}$ to compute the statistics of $\mathbf{S}$ directly). We will denote the objective function to be minimized as $\mathcal{J}(\mathbf{S}, \mathbf{X})$ where $\mathcal{J}: \mathbb{R}^n \times \mathbb{R}^d \rightarrow \mathbb{R}$. In the present context of inverse problems, we can define this objective function in the general form

$$\mathcal{J}(\mathbf{S}, \mathbf{X}) := \mathcal{Y}(\mathbf{S}, \mathbf{S}_m) + \mathcal{R}(\mathbf{X}, \mathbf{X}_0) \quad (23)$$

where the operators $\mathcal{Y}(\cdot, \cdot)$, and $\mathcal{R}(\cdot, \cdot)$ metrics distances random For elements. For this work, we will limit our discussion to metrics that define distances between random elements in the sense of statistics. The operator $\mathcal{R}(\cdot, \cdot)$ and the random variable $\mathbf{X}_0$ describe a priori knowledge about the statistics of the control variable $\mathbf{X}$. Concrete forms of these metrics will be given in subsequent sections in the context of a specific application. Notice that, by definition, the objective function is deterministic.

With this notation adopted, we can pose the general form of the constrained stochastic optimization problem as follows

$$\begin{aligned} \min_{\mathbf{S} \in \mathcal{S}, \mathbf{X} \in \mathcal{X}} \mathcal{J}(\mathbf{S}, \mathbf{X}) \\ \text{such that } \mathbf{M}(\mathbf{S}, \mathbf{X}) = \mathbf{0} \end{aligned} \quad (24)$$

We would like to point out that our proposed approach using SROMS is general and J could also represent an objective in the context of an optimal control or design problem. Likewise, the context of any of these problems can span a wide range of systems as no specific form has been assumed for the model $\mathbf{M}$.

3.1. The SROM approach to stochastic optimization

We choose a “Discretize-Optimize” approach [11, 12] where we will work with a SROM in the optimization problem. Existing approaches for stochastic optimization usually adopt spectral representations of $\mathbf{X}$ and $\mathbf{S}$ [4]. In contrast, we use SROM approximations, $\tilde{\mathbf{X}}$ and $\tilde{\mathbf{S}}$, of these quantities. In accordance with the previous section, the state and control random elements can now be expressed in terms of m control samples $\{\tilde{\mathbf{x}}\}$, the resulting state samples $\{\tilde{\mathbf{s}}\}$, and the vector of probabilities $\mathbf{P} \in \mathbb{R}^m$, corresponding to each sample pair. For notational convenience, we will interpret the SROM samples as the block vectors

$$\{\tilde{\mathbf{x}}\} := \left\{ \begin{array}{c} \tilde{\mathbf{x}}^{(1)} \\ \vdots \\ \tilde{\mathbf{x}}^{(m)} \end{array} \right\} \in \mathbb{R}^D; \quad \{\tilde{\mathbf{s}}\} := \left\{ \begin{array}{c} \tilde{\mathbf{s}}^{(1)} \\ \vdots \\ \tilde{\mathbf{s}}^{(m)} \end{array} \right\} \in \mathbb{R}^N, \quad (25)$$

where $D = d \times m$ and $N = n \times m$.

Likewise, the model constraints using the SROM approximation are given by

$$\tilde{\mathbf{M}} := \mathbf{M}(\tilde{\mathbf{S}}, \tilde{\mathbf{X}}) = \begin{Bmatrix} \mathbf{M}(\tilde{s}^{(1)}, \tilde{\mathbf{x}}^{(1)}) \\ \vdots \\ \mathbf{M}(\tilde{s}^{(m)}, \tilde{\mathbf{x}}^{(m)}) \end{Bmatrix} = \mathbf{0} \in \mathbb{R}^N \quad (26)$$

where we have converted the governing stochastic constraint equations into m sets of decoupled, deterministic constraint equations. We point out that our objective of satisfying $\mathbf{M}(\mathbf{S}, \mathbf{X}) = \mathbf{0}$ almost surely is approximately achieved by enforcing (26).

By introducing the SROM approximations of the random state and parameter vectors, we can now effectively define a deterministic constrained optimization problem. First, the objective function can be expressed in terms of the SROMs as

$$\mathcal{J}(\mathbf{S}, \mathbf{X}) \approx \mathcal{J}(\tilde{\mathbf{S}}, \tilde{\mathbf{X}}) = \mathcal{J}(\{\tilde{s}\}, \{\tilde{\mathbf{x}}\}, \mathbf{p}) \quad (27)$$

Recall from Section 2.1 that we can take a sample of the state $\tilde{s}^{(k)}$ to be an implicit function of the control sample $\tilde{\mathbf{x}}^{(k)}$ by the properties of the operator $\mathbf{M}$. Hence, we can express the objective function only in terms of the control variables and probabilities as

$$\hat{\mathcal{J}}(\{\tilde{\mathbf{x}}\}, \mathbf{p}) := \mathcal{J}(\{\tilde{s}(\{\tilde{\mathbf{x}}\})\}, \{\tilde{\mathbf{x}}\}, \mathbf{p}) \quad (28)$$

We can now define the SROM solution to the stochastic optimization problem as

$$\tilde{\mathbf{X}}^* := \underset{\{\tilde{\mathbf{x}}\} \in \mathcal{Q}, \mathbf{p} \in \mathcal{P}}{\operatorname{argmin}} \hat{\mathcal{J}}(\{\tilde{\mathbf{x}}\}, \mathbf{p}) \quad (29)$$

where $\mathcal{P}$ is the feasible set of SROM probabilities

$$\mathcal{P} := \left\{ \mathbf{p} \mid \mathbf{p} \in \mathbb{R}^m, \sum_{i=1}^m p^{(i)} = 1 \quad \text{and} \quad p^{(i)} \geq 0, \quad \forall i \right\} \quad (30)$$

and $\mathcal{Q}$ is the feasible set of samples, which could, for example, reflect specified inequality constraints on $\{\tilde{\mathbf{x}}\}$

$$\mathcal{Q} := \left\{ \{\tilde{\mathbf{x}}\} \mid \{\tilde{\mathbf{x}}\} \in \mathbb{R}^D, \{\tilde{\mathbf{x}}\}_{\min} \leq \{\tilde{\mathbf{x}}\} \leq \{\tilde{\mathbf{x}}\}_{\max} \right\} \quad (31)$$

In the remaining formulation, however, we shall focus on the model constraints (26) and forego the treatment of the more straightforward equality and inequality constraints on $p^{(i)}$ and $\{\tilde{\mathbf{x}}\}$ for the sake of simplicity.

Remark 3. The above formulation is commonly referred to as a reduced-space approach in the PDE-constrained optimization literature [3].

3.2. Solution strategy for the SROM-based optimization problem

We now focus on the details of the solution to the deterministic SROM-based optimization problem defined in (29). For the sake of brevity and simplicity, we will limit the treatment to gradient-based optimization algorithms that require only the computation of the objective function $\hat{\mathcal{J}}$ and its gradient (e.g. nonlinear conjugate gradient, quasi-Newton methods, etc.). Along these lines, we now provide an efficient approach for computing the gradient using an adjoint approach and then summarize the full procedure for implementing the SROM optimization framework.

3.2.1. Gradient derivations—Here, we illustrate an adjoint approach based on a Lagrangian [14] for deriving the gradient of the objective function $\hat{\mathcal{J}}$ with respect to the unknown SROM parameters $\{\tilde{\mathbf{x}}\}$ and $\mathbf{p}$. For this purpose, we assume $\hat{\mathcal{J}}$ to be differentiable with respect to both $\{\tilde{\mathbf{x}}\}$ and $\mathbf{p}$. We focus primarily on obtaining an expression for the gradient $\nabla_{\{\tilde{\mathbf{x}}\}} \hat{\mathcal{J}}$, which is significantly more involved due to presence of the model constraint (Eq. (26)). We begin by first introducing the Lagrangian function

$$\mathcal{L}(\{\tilde{\mathbf{x}}\}, \mathbf{p}, \{\tilde{\mathbf{w}}\}) := \hat{\mathcal{J}}(\{\tilde{\mathbf{x}}\}, \mathbf{p}) + \{\tilde{\mathbf{w}}\}^T \tilde{\mathbf{M}} \quad (32)$$

where $\{\tilde{\mathbf{w}}\} \in \mathbb{R}^N$ is the the adjoint variable vector. Note that if we consider state samples $\{\tilde{\mathbf{s}}\}$ that are generated via Equation (26), we have $\mathcal{L}(\{\tilde{\mathbf{x}}\}, \mathbf{p}, \{\tilde{\mathbf{w}}\}) = \hat{\mathcal{J}}(\{\tilde{\mathbf{x}}\}, \mathbf{p})$ since $\tilde{\mathbf{M}}=0$ is satisfied for all choices of $\{\tilde{\mathbf{w}}\}$. Therefore, the gradient of the objective function with respect to the unknown SROM samples can be expressed as

$$\hat{\mathcal{J}}_{\{\tilde{\mathbf{x}}\}} = \mathcal{L}_{\{\tilde{\mathbf{x}}\}} \quad (33)$$

where we have adopted the shorthand notation $\hat{\mathcal{J}}_{\{\tilde{\mathbf{x}}\}} := \frac{\partial \hat{\mathcal{J}}}{\partial \{\tilde{\mathbf{x}}\}}$ for derivatives.

Using Equation (32) and the fact that the samples $\{\tilde{\mathbf{s}}\}$ are viewed as implicit functions of $\{\tilde{\mathbf{x}}\}$, we have

$$\begin{aligned} \mathcal{L}_{\{\tilde{\mathbf{x}}\}} &= \left[\{\tilde{\mathbf{s}}\}_{\{\tilde{\mathbf{x}}\}} \right]^T \mathcal{J}_{\{\tilde{\mathbf{s}}\}} + \mathcal{J}_{\{\tilde{\mathbf{x}}\}} + \left[\{\tilde{\mathbf{s}}\}_{\{\tilde{\mathbf{x}}\}} \right]^T \left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{s}}\}} \right]^T \{\tilde{\mathbf{w}}\} + \left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{x}}\}} \right]^T \{\tilde{\mathbf{w}}\} \\ &= \mathcal{J}_{\{\tilde{\mathbf{x}}\}} + \left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{x}}\}} \right]^T \{\tilde{\mathbf{w}}\} + \left[\{\tilde{\mathbf{s}}\}_{\{\tilde{\mathbf{x}}\}} \right]^T \left(\left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{s}}\}} \right]^T \{\tilde{\mathbf{w}}\} + \mathcal{J}_{\{\tilde{\mathbf{x}}\}} \right) \end{aligned} \quad (34)$$

We can then eliminate the third term by choosing the adjoint variables such that they satisfy

$$\left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{s}}\}} \right]^T \{\tilde{\mathbf{w}}\} = - \mathcal{J}_{\{\tilde{\mathbf{s}}\}} \quad (35)$$

where $\left[\tilde{\mathbf{M}}_{\{\tilde{\mathbf{s}}\}} \right]$ is the Jacobian of the discretized state equations. Here, we can leverage the non-intrusive nature of the SROM approximation to greatly simplify the solution of (35).

Adopting the shorthand notation $\tilde{M}^{(i)} := M(\tilde{s}^{(i)}, \tilde{\mathbf{x}}^{(i)})$, we note that

$$\left[\tilde{\mathbf{M}}_{\tilde{s}^{(j)}}^{(i)} \right] = [\mathbf{0}], \quad \text{for } i \neq j, \quad (36)$$

and so the problem decouples into m independent systems of equations as

$$\left[\tilde{\mathbf{M}}_{\tilde{s}^{(k)}}^{(k)} \right]^T \tilde{\mathbf{w}}^{(k)} = -\mathcal{J}_{\tilde{s}^{(k)}}, \quad \text{for } k=1, \dots, m \quad (37)$$

Finally, using this set of adjoint variables that satisfy (37), we can express the gradient in (33) as

$$\hat{\mathcal{J}}_{\tilde{\mathbf{x}}} := \begin{Bmatrix} \hat{\mathcal{J}}_{\tilde{\mathbf{x}}^{(1)}} \\ \vdots \\ \hat{\mathcal{J}}_{\tilde{\mathbf{x}}^{(m)}} \end{Bmatrix} = \begin{Bmatrix} \mathcal{J}_{\tilde{\mathbf{x}}^{(1)}} + \left[\tilde{\mathbf{M}}_{\tilde{\mathbf{x}}^{(1)}}^{(1)} \right]^T \tilde{\mathbf{w}}^{(1)} \\ \vdots \\ \mathcal{J}_{\tilde{\mathbf{x}}^{(m)}} + \left[\tilde{\mathbf{M}}_{\tilde{\mathbf{x}}^{(m)}}^{(m)} \right]^T \tilde{\mathbf{w}}^{(m)} \end{Bmatrix} \quad (38)$$

where we have again decoupled the expression using the fact that

$$\left[\tilde{\mathbf{M}}_{\tilde{\mathbf{x}}^{(j)}}^{(i)} \right] = [\mathbf{0}], \quad \text{for } i \neq j \quad (39)$$

With regard to the gradient with respect to the SROM probabilities $\hat{\mathcal{J}}_{\mathbf{p}}$, since these parameters do not appear in the model constraints explicitly, we have

$$\hat{\mathcal{J}}_{\mathbf{p}} = \mathcal{L}_{\mathbf{p}} = \mathcal{J}_{\mathbf{p}} \quad (40)$$

Note that in general this expression will be easily obtained due to the simple linear relations of the SROM statistics (9) - (11) with respect to $\mathbf{p}$.

3.2.2. Implementation summary—Here, we briefly summarize the procedure for computing the objective function and gradient for the optimization problem defined in Equation (29), so that it can be readily solved using gradient-based optimization software. Given a set of SROM parameters $\{\tilde{\mathbf{x}}\}$ and $\mathbf{p}$, the following steps are to be carried out to supply $\hat{\mathcal{J}}$ and $\nabla_{\{\tilde{\mathbf{x}}\}} \hat{\mathcal{J}}$ to the optimization algorithm used:

1. Solve m decoupled, forward problems (Equation (26)) for the state samples $\{\tilde{s}\}$.
2. Solve m decoupled, adjoint problems (Equation (37)) for the adjoint variables $\{\tilde{\mathbf{w}}\}$.
3. Evaluate the objective function $\hat{\mathcal{J}}(\{\tilde{\mathbf{x}}\}, \mathbf{p})$.
4. Evaluate the gradients $\hat{\mathcal{J}}_{\{\tilde{\mathbf{x}}\}}$ and $\hat{\mathcal{J}}_{\mathbf{p}}$ using Equations (38) and (40), respectively.

It is clear from this procedure that computing the objective function and gradient at each iteration requires $2m$ deterministic model solves. However, it should be emphasized that since the solves are decoupled, they can be easily parallelized to improve scalability. Furthermore, a primary strength of the proposed method is that the number of deterministic solves remains constant regardless of the dimension d of the unknown parameters $\mathbf{X}$. A

detailed discussion of optimization algorithms can be found in [22] and is outside the scope of this study. We also note that the Hessian (or the operation of a Hessian on a vector) could be derived along similar lines to the above approach in order to utilize second-order optimization algorithms

3.3. Optimization under multiple uncertainties

In this section, we briefly describe the generalization of the proposed SROM framework for stochastic optimization problems with multiple sources of uncertainty. Similar to Section 2.5, we consider an additional and independent (known) source of uncertainty in the parameters Θ , so that the governing model takes the form (19). We assume that the SROM

$\tilde{\Theta} := \{\tilde{\theta}^{(j)}, p_{\theta}^{(j)}\}_{j=1}^{m_{\theta}}$ has been formed online to represent Θ prior to the solution of the stochastic optimization problem.

As was the case for propagating uncertainty in forward models with multiple (independent) sources of randomness, the SROM approach to stochastic optimization is similarly straightforward. The introduction of the random parameters Θ does not directly affect the objective function (27), but it does result in the following modified form of the discretized constraint equations

$$M(S, X; \Theta) = 0 \quad (41)$$

Using the SROM approximations $\tilde{X}$ and $\tilde{\Theta}$ the approach to propagating uncertainties given in Equation (20), the associated set of deterministic constraint equations is now given by

$$M(\tilde{S}, \tilde{X}; \tilde{\Theta}) = M(\{\tilde{s}\}, \tilde{x}; \{\tilde{\theta}\}) := \left\{ \begin{array}{c} M(\tilde{s}^{(1)}, \tilde{x}^{(1)}; \tilde{\theta}^{(1)}) \\ \vdots \\ M(\tilde{s}^{(k)}, \tilde{x}^{(i)}; \tilde{\theta}^{(j)}) \\ \vdots \\ M(\tilde{s}^{(m_s)}, \tilde{x}^{(m_x)}; \tilde{\theta}^{(m_{\theta})}) \end{array} \right\} = 0 \in \mathbb{R}^{\hat{N}} \quad (42)$$

Here, $\hat{N} = n \times m_x \times m_{\theta}$ and we have assumed the indexing scheme from Equation (21). It follows that one of the main changes to the optimization formulation is the need to solve the $m_x \times m_{\theta}$ forward problems in (42) to obtain the state samples $\{\tilde{s}\} \in \mathbb{R}^{\hat{N}}$, as opposed to the m_x problems in (26).

Computing the gradient with respect to the SROM samples in Equation (33) for the case of multiple uncertainties still benefits from the decoupled nature of the SROM approach. To illustrate this, we adopt the shorthand notation for a given forward problem instance

$$\tilde{M}^{(i,j)} = M(\tilde{s}^{(k)}, \tilde{x}^{(i)}; \tilde{\theta}^{(j)}) \quad (43)$$

where Equation (21) is again implied for the index k . Then, it is clear that the following simplifications (analogous to (36) and (39)) apply when taking derivatives with respect to the model equations

$$\tilde{\mathbf{M}}_{\mathbf{s}^{(k)}}^{(i,j)} = [\mathbf{0}], \quad \text{for } k \neq (i-1) \times m_x + j \quad (44)$$

$$\tilde{\mathbf{M}}_{\mathbf{x}^{(k)}}^{(i,j)} = [\mathbf{0}], \quad \text{for } k \neq j \quad (45)$$

The first expression implies a similar decoupling of the full adjoint problem in Equation (35) to a series of independent solutions of Equation (37). Note that in this case one must perform $m_x \times m_\theta$ solves for the adjoint variables $\{\tilde{\mathbf{w}}\} \in \mathbb{R}^{\hat{N}}$. Finally, we must update each component of the gradient vector in (38) as follows

$$\hat{\mathcal{J}}_{\tilde{\mathbf{x}}^{(i)}} = \mathcal{J}_{\tilde{\mathbf{x}}^{(i)}} + \sum_{j=1}^{m_\theta} [\tilde{\mathbf{M}}_{\tilde{\mathbf{x}}^{(i)}}^{(i,j)}]^T \tilde{\mathbf{w}}^{(j)} \quad (46)$$

where (45) has been enforced to simplify the expression.

In summary, the SROM-based optimization framework can be straightforwardly extended to handle multiple sources of uncertainty. One must simply update the gradient expression according to (46) and cope with an increased computational cost in proportion to the size of the SROM used to model Θ . While in this case it requires $2(m_x \times m_\phi)$ model evaluations to compute the gradient at each optimization iteration, the solves remain decoupled from one another and hence easily parallelized.

4. Application

In this section, we introduce the problem of random material identification in elastodynamics and demonstrate the use of the SROM optimization approach in this setting. We begin by formulating the elastodynamics forward problem in both continuous and discrete forms and then describe the associated inverse problem of recovering random shear moduli given displacement statistics as input data. Finally, we illustrate how the general stochastic optimization framework using SROMs described in the previous section can be adapted to solve this stochastic inverse problem.

4.1. The forward elastodynamics problem

We now present the governing equations for the forward steady-state elastodynamics problem. We will assume small strains and deformations in a material governed by an isotropic elastic model. Furthermore, we shall neglect damping effects in the system and consider real-valued quantities only for simplicity. To begin, we consider the stochastic steady-state elastodynamics boundary-value problem given in strong-form as

$$\nabla \cdot \Sigma = -\rho \gamma^2 \mathcal{U} \quad \text{in } \mathcal{D} \quad (47)$$

$$\Sigma = 2G\mathcal{E}_d[\mathcal{U}] + b \operatorname{tr}(\mathcal{E}[\mathcal{U}])\mathbf{I} \quad \text{in } \mathcal{D} \quad (48)$$

$$\mathcal{E}[\mathcal{U}] = \frac{1}{2}(\nabla \mathcal{U} + \nabla \mathcal{U}^T) \quad \text{in } \mathcal{D} \quad (49)$$

$$\mathcal{U} = 0 \quad \text{on } \Gamma_u \quad (50)$$

$$\Sigma \cdot \mathbf{n} = \boldsymbol{\tau} \quad \text{on } \Gamma_t \quad (51)$$

where D is the physical domain, Σ is the stress tensor, σ is the mass density, γ is the angular frequency, $\mathbf{U}$ is the displacement field, and $\boldsymbol{\tau}$ is an applied traction. Γ_u and Γ_t represent the portion of the boundary with a specified displacement and traction, respectively, and $\mathbf{n}$ is the outward normal along Γ_t . Moreover, G and b are the shear and bulk modulus, respectively, $\operatorname{tr}(\cdot)$ is the trace of a second-order tensor, $\mathbf{I}$ is the identity tensor, and

$\mathcal{E}_d := \mathcal{E} - \frac{1}{3}\operatorname{tr}(\mathcal{E}[\mathcal{U}])\mathbf{I}$ is the deviatoric part of the strain tensor.

For our study, the shear modulus is assumed to be the primary source of randomness in the system, while the other stochastic variables (displacement, stress, strain) are considered random through their dependence on the shear modulus. The remaining material parameters (bulk modulus, density) will be taken to be deterministic and constant for simplicity.

Furthermore, we consider a domain partitioned into d distinct regions $\{\mathcal{D}_i\}_{i=1}^d$, each with a different shear modulus represented by the components of the vector $G \in \mathbb{R}^d$. In the spirit of the general formulation in the previous section, the shear moduli represent the parameters of interest (denoted as $\mathbf{X}$ in our general formulation), while the displacements are the state variables (denoted as $\mathbf{S}$ in the general formulation). Hence, we can represent the governing elastodynamics equations (47) - (51) as the abstract model

$$\mathcal{M}(\mathcal{U}, G) = 0 \quad (52)$$

implying that, given a specified shear moduli G , we can obtain a corresponding displacement $\mathbf{U}$ through the model $\mathcal{M}$.

To apply the SROM stochastic optimization approach developed previously, we will work with a discrete form of the model in (52). Here, we use the finite element method (FEM) for the discretization, but note that in general other methods (finite difference, spectral methods, etc.) could be used. Using the FEM, we assume a solution of the form

$$\mathcal{U}^h = [N] \mathbf{U} \quad (53)$$

where $[N]$ is a matrix of FEM basis functions and $\mathbf{U} \in \mathbb{R}^n$ is a vector of displacement values at the nodes of a numerical grid. Using this discrete approximation and a variational form of the governing equations (47) - (51) we can obtain the following algebraic system of equations

$$\mathbf{M}(\mathbf{U}, \mathbf{G}) := [\mathbf{A}(\mathbf{G})] \mathbf{U} - \mathbf{f} = \mathbf{0} \quad (54)$$

where

$$[\mathbf{A}(\mathbf{G})] := [\mathbf{K}(\mathbf{G})] - \gamma^2 [\mathbf{M}] \quad (55)$$

and the stiffness matrix $[\mathbf{K}]$, mass matrix $[\mathbf{M}]$, and force vector $\mathbf{f}$ are given by

$$[\mathbf{M}] := \sum_e \int_{\mathcal{D}_e} \rho [\mathbf{N}]^T [\mathbf{N}] d\mathcal{D} \quad (56)$$

$$\begin{aligned} [\mathbf{K}(\mathbf{G})] &:= \sum_{i=1}^d G_i \left(\sum_{e \in \mathcal{D}_i} \int_{\mathcal{D}_i^e} [\mathbf{B}]^T [\mathbf{D}_s] [\mathbf{B}] d\mathcal{D} \right) + b \sum_e \int_{\mathcal{D}_e} [\mathbf{B}]^T [\mathbf{D}_v] [\mathbf{B}] d\mathcal{D} \\ &= \sum_{i=1}^d G_i [\mathbf{H}_i] + b [\mathbf{J}] \end{aligned} \quad (57)$$

$$\mathbf{f} := \sum_e \int_{\Gamma_e^c} [\mathbf{N}]^T \boldsymbol{\tau} \, d\mathbf{S} \quad (58)$$

Here, $[\mathbf{B}]$ is a matrix containing the derivatives of the FEM basis functions and $[\mathbf{D}_s]$ and $[\mathbf{D}_v]$ are matrices that separate the deviatoric and volumetric components of the stiffness matrix, respectively. Note that here we have used the discrete material assumption to view the shear portion of the stiffness matrix as a sum of separate contributions from each material, with $e \in \mathcal{D}_i$ signifying a sum over the particular elements that fall within the part of the domain corresponding to material i . For the sake of brevity, we omit the derivations of the weak form other FEM details and simply refer the reader to [15, 2].

4.2. The stochastic elastodynamics inverse problem

The inverse problem associated with the elastodynamics forward problem consists in estimating the statistics of the unknown shear moduli G given information about an observed stochastic displacement vector $V \in \mathbb{R}^n$. Specifically, we assume that we are provided moments for V as

$$\langle V_i^r \rangle = \mathbb{E} [V_i^r], \quad r = 1, \dots, \bar{r}, \quad i \in \mathcal{I}_m, \quad (59)$$

Here, $\mathcal{I}_m$ represents the set of degrees of freedom in the domain where moment data is available. Furthermore, let $E^r \in \mathbb{R}^n$ denote the vector of differences between the r^{th} moment of V and the computed displacement U . The components of E^r are given as

$$E_i^r := \begin{cases} \langle V_i^r \rangle - \langle V_i^r \rangle & \text{if } i \in \mathcal{I}_m \\ 0, & \text{otherwise} \end{cases} \quad (60)$$

In the sequel, we will use the notation $\|E^r(U)\|_2^2 := \sum_i |E_i^r|^2$. We can now define an objective function, analogously to that for the abstract formulation (see 23), as

$$\mathcal{J}(\mathbf{U}, \mathbf{G}) = \frac{1}{2} \sum_{r=1}^{\bar{r}} C_r \|\mathbf{E}^r(\mathbf{U})\|_2^2 + \mathcal{R}(\mathbf{G}, \mathbf{G}_0) \quad (61)$$

where

$$C_r = \left(\sum_{i \in \mathcal{I}_m} \|\langle V_i^r \rangle\|^2 \right)^{-1} \quad (62)$$

are normalization constants and $\mathcal{R}(\cdot, \cdot)$ is an operator that can be used to specify *a priori* knowledge on the statistics of $\mathbf{G}$ as introduced in (23). The examples presented later assume that there is no *a priori* knowledge on the statistics of $\mathbf{G}$, and hence the operator $\mathcal{R}(\cdot, \cdot)$ will be omitted from hereon.

In the same fashion as the abstract problem in (24), the random material identification problem can now be posed as the following stochastic optimization problem

$$\begin{aligned} & \underset{\mathbf{U}, \mathbf{G}}{\operatorname{argmin}} \mathcal{J}(\mathbf{U}, \mathbf{G}) \\ & \text{such that } \mathbf{M}(\mathbf{U}, \mathbf{G}) := [\mathbf{A}(\mathbf{G})]\mathbf{U} - \mathbf{f} = \mathbf{0} \end{aligned} \quad (63)$$

Note that the only dependence of J on $\mathbf{G}$ in this case is implicitly through $\mathbf{U}$, but this need not be the case in general. With the stochastic elastodynamics inverse problem assuming this form, the SROM optimization approach can be readily applied to estimate the statistics of $\mathbf{G}$. The details of this are provided in the following section.

4.3. SROMs for the inverse elastodynamics problem

We now illustrate how the proposed SROM-based optimization framework described in Section 3 can be used to solve the stochastic elastodynamics inverse problem (63). As described, we first introduce an SROM approximation $\tilde{\mathbf{G}}$ to the unknown shear moduli vector $\mathbf{G}$ and corresponding displacement SROM $\tilde{\mathbf{U}}$. The uncertainty in the stochastic inverse problem can now be expressed in terms of the SROM parameters $\{\tilde{\mathbf{g}}\} \in \mathbb{R}^D$, $\{\tilde{\mathbf{u}}\} \in \mathbb{R}^N$, and $\mathbf{p} \in \mathbb{R}^m$, where, again, $D = d \times m$ and $N = \times m$ are the dimensions of the SROM sample vectors.

Along the lines of Section 3.1, we use $\tilde{\mathbf{G}}$ and $\tilde{\mathbf{U}}$ to transform the optimization problem in (63) from stochastic to deterministic. First, the objective function is rewritten in terms of the SROM shear moduli parameters as

$$\hat{\mathcal{J}}(\{\tilde{\mathbf{g}}\}, \mathbf{p}) := \mathcal{J}(\{\tilde{\mathbf{u}}(\tilde{\mathbf{g}})\}, \mathbf{p}) = \frac{1}{2} \sum_{r=1}^{\bar{r}} C_r \|\mathbf{E}^r(\{\tilde{\mathbf{u}}(\tilde{\mathbf{g}})\})\|_2^2 \quad (64)$$

where the displacement moments $\langle \tilde{\mathbf{U}}^r \rangle$ that appear in $\mathbf{E}^r$ (60) can be straightforwardly computed using the SROM moment estimate in Equation (18). Next, in a manner analogous

to (26), the stochastic elastodynamics model constraint (54) can be decoupled using the SROMs as

$$\tilde{\mathbf{M}}^{(i)} := \mathbf{M}(\tilde{\mathbf{u}}^{(i)}, \tilde{\mathbf{g}}^{(i)}) = \left[\mathbf{A}(\tilde{\mathbf{g}}^{(i)}) \right] \tilde{\mathbf{u}}^{(i)} - \mathbf{f} = \mathbf{0}, \quad i=1, \dots, m \quad (65)$$

Now, similar to (29), we can search for the SROM solution $\tilde{\mathbf{G}}^*$ to the original stochastic inverse problem in (63) as

$$\tilde{\mathbf{G}}^* := \underset{\{\tilde{\mathbf{g}}\} \in \mathcal{G}, \mathbf{p} \in \mathcal{P}}{\operatorname{argmin}} \hat{\mathcal{J}}(\{\tilde{\mathbf{g}}\}, \mathbf{p}) \quad (66)$$

where $\mathcal{P}$ is defined in (30) and $\mathcal{G}$ is the set of shear moduli vectors with positive components

$$\mathcal{G} = \left\{ \{\tilde{\mathbf{g}}\} \mid \{\tilde{\mathbf{g}}\} \in \mathbb{R}^D, \quad 0 < \{\tilde{\mathbf{g}}\} \right\} \quad (67)$$

We now focus on obtaining expressions for the gradients of the objective function with respect to the unknown SROM parameters $\{\tilde{\mathbf{g}}\}$ and $\mathbf{p}$ as in (33) and (40). The latter, $\hat{\mathcal{J}}_{\mathbf{p}}$, is easily obtained by examining the derivative with respect to one component of the probability vector $p^{(k)}$ as follows

$$\begin{aligned} \hat{J}_{p^{(k)}} &= \frac{1}{2} \sum_r C_r \sum_i \left(\frac{\partial |E_i^r|^2}{\partial \langle \tilde{U}_r^i \rangle} \right) \left(\frac{\partial \langle \tilde{U}_r^i \rangle}{\partial p^{(k)}} \right) \\ &= \sum_r C_r \sum_i E_i^r \left(\tilde{u}_i^{(k)} \right)^r \end{aligned} \quad (68)$$

where we have used a straightforward application of the chain rule and the simple linear dependence of the SROM moments (18) on $\mathbf{p}$.

Next, we derive the gradient with respect to the SROM shear moduli samples, $\hat{\mathcal{J}}_{\{\tilde{\mathbf{g}}\}}$, following the formulation in Section 3.2.1. We must first define the right-hand side and coefficient matrix of the adjoint problems (37). The right-hand side, $\hat{\mathcal{J}}_{\tilde{\mathbf{u}}^{(k)}}$, can be defined component-wise as

$$\begin{aligned} \hat{\mathcal{J}}_{\tilde{u}_j^{(k)}} &= \frac{1}{2} \sum_r C_r \sum_i \left(\frac{\partial |E_i^r|^2}{\partial \langle \tilde{U}_i^r \rangle} \right) \left(\frac{\partial \langle \tilde{U}_i^r \rangle}{\partial \tilde{u}_j^{(k)}} \right) \\ &= \sum_r C_r \left(E_j^r \right) \left(p^{(k)} \right)^r \left(\tilde{u}_j^{(k)} \right)^{(r-1)} \end{aligned} \quad (69)$$

To obtain the coefficient matrix for the adjoint problem, the derivative of the discretized model constraints (Eq. (65)) with respect to a particular SROM displacement sample is simply

$$\left[\tilde{\mathbf{M}}_{\tilde{\mathbf{u}}^{(k)}}^{(k)} \right] = \left[\mathbf{A}(\tilde{\mathbf{g}}^{(k)}) \right] \quad (70)$$

Furthermore, it is straightforward to see from Equations (55)-(57) that $[A] = [A]^T$ is symmetric. Hence, for the elastodynamics inverse problem we consider, the adjoint problems in (37) are given by

$$\left[A \left(\tilde{\mathbf{g}}^{(k)} \right) \right] \tilde{\mathbf{w}}^{(k)} = - \mathcal{J}_{\tilde{\mathbf{u}}^{(k)}}, \quad \text{for } k=1, \dots, m \quad (71)$$

where the coefficient matrix remains unchanged between the forward and adjoint problems.

With the adjoint variables obtained via (71), we need only the final expression for the gradient vector $\hat{\mathcal{J}}_{\tilde{\mathbf{g}}^{(k)}}$ in (38). Since the objective function in (64) has no explicit dependence on the unknown SROM parameters $\{\tilde{\mathbf{g}}\}$, the first term in the gradient vanishes ($\hat{\mathcal{J}}_{\tilde{\mathbf{g}}^{(k)}} = 0, \quad \forall k$) and we just need to define $\tilde{M}_{\tilde{\mathbf{g}}^{(k)}}^{(k)}$. Using Equations (65) and (57) and considering the expression component-wise for clarity, we have

$$\begin{aligned} \tilde{M}_{\tilde{\mathbf{g}}_i^{(k)}}^{(k)} &= \left[\frac{\partial A \left(\tilde{\mathbf{g}}^{(k)} \right)}{\partial \tilde{\mathbf{g}}_i^{(k)}} \right] \tilde{\mathbf{u}}^{(k)} = \left[\frac{\partial K \left(\tilde{\mathbf{g}}^{(k)} \right)}{\partial \tilde{\mathbf{g}}_i^{(k)}} \right] \hat{\mathbf{u}}^{(k)} \quad (72) \\ &= [H_i] \tilde{\mathbf{u}}^{(k)} \quad (73) \end{aligned}$$

Therefore, we arrive at the following simple expression for a given component of the gradient $\hat{\mathcal{J}}_{\tilde{\mathbf{g}}^{(k)}}$

$$\hat{\mathcal{J}}_{\tilde{\mathbf{g}}_i^{(k)}} = \left(\tilde{\mathbf{u}}^{(k)} \right)^T [H_i]^T \left(\tilde{\mathbf{w}}^{(k)} \right). \quad (74)$$

4.4. A note on random loading

In order to test the SROM optimization framework with multiple uncertainties, we will consider the case where the applied traction τ is also random. Similar to the Equation (41), the discretized elastodynamics model in (54) now takes the form

$$\mathbf{M}(\mathbf{U}, \mathbf{G}; \tau) = [A(\mathbf{G})] \mathbf{U} - \mathbf{F}(\tau) = \mathbf{0} \quad (75)$$

due to the dependence of the force vector on τ in Equation (58). Likewise, after an SROM $\tilde{\tau}$ has been formed for the random load, the decoupled model constraints using the SROM approximations are given by

$$\tilde{M}^{(i,j)} = [A(\tilde{\mathbf{g}}^{(i)})] \tilde{\mathbf{u}}^{(k)} - \mathbf{f}(\tilde{\tau}^{(j)}) = \mathbf{0} \quad (76)$$

where the indexing scheme (21) is implied for index k . The remaining modifications to the formulation needed to treat the additional random load follow straightforwardly from the developments in Section 3.3.

5. Numerical examples

In this section, the proposed stochastic inverse problem framework is used in three numerical examples of random material identification in elastodynamics. In Example 1, the random shear modulus of a single homogeneous material is estimated using moment data of the displacement field throughout the domain. This problem is solved considering both a deterministic and random loading and serves as an illustration of the performance of the framework and the convergence of solutions with respect to SROM size. Example 2 considers a random material with an interior inclusion and uses only sparse input data (i.e. on the boundary) to estimate the statistics of the background and inclusion shear moduli. In Example 3, a five-dimensional random vector of shear moduli is estimated in a domain comprised of layered materials under a random loading.

The proposed SROM-based approach described in the previous section was implemented using the optimization toolbox in MATLAB [20]. The implementation is based on the `fmincon` function for constrained nonlinear optimization, which accepts the objective function (64) and gradients (Eq. (68) and (74)) to solve the optimization problem in (63). In all the examples presented herein, the ‘interior-point’ algorithm was used along with a L-BFGS [22] Hessian approximation.

5.1. Example 1: Homogeneous material

We consider a two-dimensional square domain with a single homogeneous material under plane strain conditions. We seek to recover the statistics of the random shear modulus using moments of an observed (full) displacement field as input data. We note that full field information is used in this case despite there being only one unknown for the sake of illustrating the properties of the method in a simple setting, while problems with sparse data and multiple unknowns are presented subsequently. The problem is first solved for the case where the loading is deterministic and then for the situation when it is random. The performance of the method is studied for varying SROM sizes in both the shear modulus and the random load.

A sketch of the problem domain for this example can be seen in Figure 1(a), where we take $G_b = G_i = G$, e.g. a homogeneous domain. We shall consider scaled and dimensionless quantities in this work for simplicity, where the domain is the unit square ($L = 1.0$). The density and bulk modulus are considered known and constant in the examples at $\rho = 1.0$ and $b = 8.33$, respectively. The domain is intentionally loaded at a low frequency of $f = 0.75$ to yield larger wavelengths and permit the use of relatively coarse computational grids for the solution of (54) with the FEM.

In this study, we choose to represent the random shear modulus using a scaled beta random variable. The beta distribution is a common and flexible choice for representing random variables with finite range. The shear modulus may then be expressed as

$$G = G_{min} + (G_{max} - G_{min}) X_B \quad (77)$$

where X_B is a standard beta random variable with probability density given by

$$f(x_B; \beta_1, \beta_2) = \frac{x_B^{\beta_1-1} (1-x_B)^{\beta_2-1}}{B(\beta_1, \beta_2)} \quad (78)$$

Here, $B(\beta_1, \beta_2)$ is the beta function. The mean and variance of X_B can be defined in terms of the parameters β_1 and β_2 as

$$\mathbb{E}[X_B] = \frac{\beta_1}{\beta_1 + \beta_2} \quad (79)$$

$$\text{Var}[X_B] = \frac{\beta_1 \beta_2}{(\beta_1 + \beta_2)(\beta_1 + \beta_2 + 1)} \quad (80)$$

Adopting this representation allows us to conveniently specify a target shear modulus in terms of the desired support ($G_{\min}$, $G_{\max}$) and mean and variance. From here, the parameters β_1 and β_2 are calculated from (79) and (80) and the resulting beta random variable is appropriately scaled using (77).

The displacement moment data (Eq. (59)) for this example was generated using Monte Carlo simulation. Here, 15,000 independent samples of the shear modulus were drawn and each used to compute a corresponding displacement sample by solving Eq. (54) with a uniform 15×15 grid. The first ten moments ($r = 10$) of the displacements were calculated from the Monte Carlo samples and then interpolated to a coarser 10×10 grid for the stochastic inverse problem. Both meshes were comprised of four-node, bilinear finite elements.

5.1.1. Deterministic load—The SROM approach was first used to solve the stochastic inverse problem in Eq. (63) when considering a deterministic loading of $\tau = 1.0$. The target shear modulus in this case has range $[G_{\min}, G_{\max}] = [4, 7]$ and a mean and variance of 5.0 and 0.25, respectively. The initial guess for the SROM $\tilde{G}$ in the optimization problem was taken as samples $\{G\}$ drawn from a uniform distribution in $[G_{\min} - 1, G_{\max} + 1]$ with equal probability $p_i = 1/m_G$, $\forall i$. The optimization algorithm was terminated based on a tolerance on the relative change in objective function between iterations, specified as 10^{-4} in this case. The problem was solved for SROM sizes m_G from 1 to 10.

First, we studied the behavior of the minimum value of the objective function (Eq. (64)) for increasing SROM size as shown in Figure 2(a). As expected, the minimum objective function value decreases with increasing SROM size. A SROM $\tilde{G}$ with more parameters should be capable of better approximating the statistics in G , and hence produce displacements $\tilde{U}$ that better match those given as input data. From Figure 2(a), it is seen that a relatively small number of samples and probabilities defining $\tilde{G}$ were able to produce a small discrepancy between computed and observed moments. Indeed, very little improvement in final objective function value is observed as the model size is increased from 3 to 6. We note that the large error for $m_G = 1$ is expected as in this case we are essentially approximating an unknown random quantity with a deterministic estimate (one sample $\tilde{G}_1$ with probability $p_1 = 1$). The number of iterations needed to obtain the minimum

objective function values in Figure 2(a) are shown in Table 1, where, as expected, we see it takes an increasing number of iterations for termination as the SROM size is increased.

In Figure 2(b), we study the accuracy of the SROM approximations for increasing model sizes. Here, the first eight moments are estimated from $\tilde{G}$ using Equation (18) and the resulting percent errors with respect to the true beta-distributed shear modulus are plotted for $m_G = 1, \dots, 6$. We observe a consistent decrease in moment error as the SROM size is increased. Here, the salient feature of SROM representations is clear, where it can be seen that very small model sizes yield accurate moment estimates. Indeed, $m_G = 6$ yields errors less than 1.0% for the first eight moments while SROMs with $m_G \geq 2$ produce estimates of the first two moments within 3.0% of the true values.

Finally, we use the obtained SROM $\tilde{G}$ to estimate the distribution of the random shear modulus using Equation (17). Figure 3(a) shows the resulting error in the SROM CDF estimates versus model size, as computed by

$$e_{CDF} = \frac{\int_{-\infty}^{+\infty} (\tilde{F}_G(g) - F_G(g))^2}{\int_{-\infty}^{+\infty} (F_G(g))^2 dg}, \quad (81)$$

while Figure 3(b) plots the actual CDF estimates versus the true distribution for three different SROM sizes. We observe a general decrease in error with increasing m_G in (a) and see the corresponding improvement in distribution resolution in (b) when increasing the SROM size from 2 to 4 and from 4 to 8. As seen in Figure 3(a), however, the decrease in CDF error is not monotonic in this case. This may be due to the fact that the samples from lower order SROMs are not kept in the higher order SROMs. Furthermore, another possibility is the existence of local minima and premature stopping of the optimization algorithm. Overall, however, the SROM CDF estimates provide satisfactory characterizations of the true underlying distribution given the discrete nature of the approximations and relatively low number of parameters.

5.1.2. Random load—We now demonstrate the ability of the SROM optimization framework to handle multiple sources of uncertainty by considering random loading. Here, τ was taken to be a gamma random variable with mean 1.5 and variance 0.25 that was shifted to take a minimum value of 0.5. In this case, the unknown shear was again beta-distributed, but with $[G_{\min}, G_{\max}] = [4, 8]$ and a mean and variance of 6.0 and 0.25, respectively. The displacement moment data for the problem was generated in the same fashion as 5.1.1 using Monte Carlo simulation from 15,000 randomly drawn samples of τ and G . We studied the performance of the method with varying SROM sizes for the load (m_τ) in addition to shear modulus (m_G).

The first step was to generate the SROM $\tilde{\tau}$ for the random load, which was done offline as a preprocessing step before the inverse problem solution. With the known expressions for the gamma random variable statistics, the SROM optimization problem in (29) for uncertainty propagation in forward models is solved to generate $\tilde{\tau}$ for a range of model sizes from 1 to 15. The distribution and moment error terms ((12) and (13)) are given equal weight in the objective function ($\alpha_1 = \alpha_2 = 1.0$). The convergence of the load SROM construction

problem with increasing SROM size m_τ is shown in Figure 4. It is clearly seen that with further refinement of the load SROM, we are able to closely approximate the statistics of the underlying random load. Note, however, that the computational cost of the inverse problem increases proportionally to the size of the SROM used. So, the smallest SROM representation yielding an acceptable error should be used in practice.

With the SROM $\tilde{\gamma}$ generated for the random load, the stochastic inverse problem (63) was solved to estimate the statistics of the shear modulus for different combinations of model sizes m_τ and m_G . The minimum objective function (64) values versus m_G are plotted for different load SROM sizes m_τ in Figure 5. As with the deterministic loading case, the decrease in objective function is most pronounced from $m_G = 1$ to $m_G = 2$ and appears relatively unchanged for larger model sizes for each m_τ . It is also seen that minimum value obtained by the objective function decreases as the load SROM size increases from $m_\tau = 3$ to $m_\tau = 8$. This is intuitive as an accurate characterization of the random load is a prerequisite to being able to obtain computed displacements that effectively approximate the true observed values. Since both SROM approximations $\tilde{\gamma}$ and $\tilde{G}$ contribute to the error

observed in displacement moments $\mathcal{J}(\{\tilde{G}\}, \mathbf{p})$, we can control and reduce the contribution of $\tilde{\gamma}$ to the error by increasing m_τ at added the expense of more function evaluations per optimization iteration.

Figure 6 illustrates the accuracy of the SROM approximations of shear modulus moments for this problem. Figure 6(a) shows the moment estimate errors for increasing m_G with $m_\tau = 8$ fixed, while (b) shows the errors for increasing m_τ with $m_G = 6$ fixed. In Figure 6(a), the moment errors are of similar magnitude for $m_G = 2, 4, 6$ and then decrease significantly for the larger models, where $m_G = 10$ yields moment estimates up to order eight within 5% of the true values. Similarly, we see in Figure 6(b) a general improvement in the moment estimates as the random load SROM $\tilde{\gamma}$ is refined.

We can observe in Figure 6(a) that $m_G = 6$ produced slightly higher errors than $m_G = 2, 4$. The reason for this behavior is that SROM samples were not retained from the lower order models as m_G was increased. That is, samples of $m_G = 2$ were not included in the samples of $m_G = 4, 6$. Hence, the optimization process can produce variability in the error such as those observed in this example. This behavior can be avoided by having a hierarchical construction in which samples from lower order SROMs are kept in the higher order ones. Indeed, if the SROM samples for $m_G = 2$ were retained as a subset of the SROM solution for $m_G = 4$ and so on, then a monotonic decrease in error would be observed. However, this approach was not pursued in this work.

In Figure 7, we view the accuracy of the SROM estimates of the shear modulus distribution function. Figure (a) plots the CDF error (Eq. 81) with increasing m_G for different load SROMs while (b) compares the SROM CDF approximation for different m_G to the true shear distribution with the load SROM size fixed at $m_\tau = 8$. Figure 7(a) provides a more comprehensive view of the trending accuracy in SROM approximations when increasing both m_G and m_τ where it is seen that there is a general decrease in CDF error when refining either of the models, $\tilde{G}$ or $\tilde{\gamma}$. The improved accuracy with increasing m_G is shown more

explicitly by comparing the three sample SROM CDFs in Figure 7(b). The discrete nature of the approximation is clearly improved with increased SROM parameters from $m_G = 2$ to $m_G = 8$.

5.1.3. Gaussian noise model—In this section, we briefly demonstrate an alternative means of generating input data for the stochastic inverse problem using a Gaussian noise model and show the resulting performance of the SROM approach. This is convenient, for example, when we have only one realization of the system state variable with an estimate of the noise inherent in the observation, rather than explicit information about its statistics. The Gaussian noise assumption allows straightforward calculation of an arbitrary number of state moments to use as input data for the SROM inverse problem framework.

To test this approach, rather than assuming an explicit distribution for the random shear modulus and generating synthetic moment data using Monte Carlo simulation, a deterministic forward problem was first solved with a constant shear modulus for the displacements $\hat{\mathbf{u}}$. Then, we assumed the following Gaussian noise model for the synthetic displacement data

$$V_j = \hat{u}_j (1 + \delta R_j) \quad (82)$$

where R_j is a standard normal random variable and δ is the prescribed noise level on the data. The r^{th} displacement moment was then computed according to

$$\mathbb{E} [V_j^r] = (\hat{u}_j^r) \mathbb{E} [(1 + \delta R_j)^r] \quad (83)$$

For this problem, the shear modulus was specified as $G = 5.0$ and displacement moments up to order eight were computed using (83) with other parameters remaining unchanged from the previous examples. The inverse problem was solved for 1%, 5%, 10%, and 15% noise levels (i.e. $\delta = 0.01, 0.05, 0.1, 0.15$) and for shear SROM sizes $m_G = 5$ and $m_G = 10$. Although the target shear modulus has been specified deterministically, we are interested in how the prescribed measurement errors in the input data translate into uncertainty in the solution estimates.

Figure 8 shows the SROM CDF estimate of the shear for the different noise levels with (a) $m_G = 5$ and (b) $m_G = 10$. Here, the true shear value, $G = 5.0$, is denoted with the vertical dashed line. Noting the way that the SROM CDF range grows with higher noise levels, it is clear that the SROM effectively captures the growing uncertainty in the shear estimate as the variability in the input data increases. With 1% noise, for example, the SROM CDF is nearly aligned with the vertical line representing the true solution, whereas for 15% noise the CDF takes a wider range from about 4.5 to 5.5. This trend is further verified in Table 2, which shows the mean and variance estimates for shear modulus for the different noise levels. The SROM estimate for the mean is seen to be extremely accurate for all noise levels, while the increasing variance at each level is an accurate reflection of the growing uncertainty in the input data.

5.2. Example 2: Material with inclusion using sparse data

In this example, we consider a two dimensional domain comprised of a square material inclusion embedded in a softer background material, where both shear moduli are considered random and unknown. The goal of the problem is to estimate the statistics of the unknown moduli using only sparse displacement data on the boundary of the domain, mimicking the scenario where only surface measurements are feasible. The accuracy of the SROM estimates is studied in full for the case where explicit distributions are assumed for the unknown shear moduli, and then briefly demonstrated for the case where the Gaussian noise model (82) is assumed.

The problem domain is seen in Figure 1(a) where the geometry is specified by $L = 1.0$ and $h = 0.33$. The distributions for the unknown shear moduli in the background and inclusion materials, G_b and G_i , respectively, were specified again using Equations (77) - (80) with parameters shown in Table 3. The load was applied deterministically as $\tau = 1.0$. The synthetic displacement moment data was again generated with 15,000 Monte Carlo samples, solving each forward problem on a 18×18 grid and interpolating onto a coarser 12×12 grid for the inverse problem. The first four ($r = 4$) moments were retained only along the boundary of the domain as input data for the problem.

The inverse problem was initially solved to estimate $\mathbf{G} = [G_b \ G_i]^T$ with SROM sizes $m_G = 1, \dots, 5$. The minimized objective function value for each size is shown in Figure 9(a) where we observe that the values decrease up to $m_G = 3$ before leveling off. Here, we will adopt the SROM $\tilde{\mathbf{G}}$ for $m_G = 4$ as the converged solution and proceed to illustrate the results for this case.

First, we view the errors in the first four moments for the background and inclusion shear modulus in Figure 9(b). We can see that using only boundary displacement information, we can approximate the first four moments of each modulus within 10% of the true values. It is interesting to notice that the mean estimates for the shear moduli are predicted within 0.20% and 2.00% for the background and inclusion modulus, respectively. It is also clear that the estimate for G_b is significantly more accurate than that of G_i . This is likely due to the use of only surface measurements, where there is less sensitivity of this data to the interior inclusion shear modulus as compared to the background modulus.

Next, we compare the SROM approximations of the shear moduli CDFs to the true distributions in 9(c). We observe that the range of the background material is well-resolved, while the spread of the inclusion material is underestimated, which again may be attributed to a lack of sensitivity to the boundary input data used. The impact of supplying additional moment data in the interior of the domain is shown in 9(d), where the SROM CDF errors are plotted as a function of m_G for the case of using only boundary data versus full field moment data. An increase in accuracy is observed with a more significant improvement for the inclusion material CDF estimates, as expected.

Lastly, this example was solved using the Gaussian noise model (82) for the input data. This version of the problem could represent an experimental set up in which the displacements are measured just once on the surface of the material being imaged, but we also have a

notion of the level of error associated with the measurement. The inverse problem was solved for 10% and 20% prescribed noise levels and the results are summarized in Table 4. Here, we show the SROM mean approximation with plus/minus two standard deviation intervals for $m_G = 4$. For both noise levels, we see that the mean estimates are very accurate with respect to the true values ($G_b = 4.0$ and $G_i = 8.0$). Also apparent is the increasing uncertainty in the SROM estimate with growing noise, a positive and expected behavior, as the standard deviation intervals in the plot become considerably larger from 10% to 20% noise.

5.3. Example 3: Layered materials with random force

This example demonstrates the effectiveness of the SROM optimization framework in problems with higher dimensional random unknowns as well as additional system uncertainties. Here, we seek to recover a five-dimensional random vector of shear moduli in a domain under random loading. In doing so, we illustrate the accuracy of the SROM approach for problems with higher dimensional random spaces. We also include results for the case when there is a practical limitation on the number of model evaluations possible, demonstrating the efficiency of the method in obtaining satisfactory moduli estimates with relatively low computational cost.

A diagram of the domain for this problem can be seen in Figure 1(b). Again, we considered a unit square domain ($L = 1.0$), but now comprised of five layers of material; all characterized by a different random shear modulus. The true shear modulus distributions for each material are given in Figure 10, where the defining parameters have been chosen as to create significant variability among the different moduli. The loading τ was random and consistent with that of Example 1 - gamma distributed with mean 1.5, variance of 0.25, and a minimum value of 0.5. Monte Carlo simulation was again used to generate the first four moments of the full displacement field for input data. The forward problem was solved on a 15×15 grid and interpolated to a 10×10 grid for the inverse problem. Here, 25,000 samples were used for the Monte Carlo estimates to ensure the moment accuracy given the added number of random variables.

5.3.1. Random shear moduli vector SROM estimates—The inverse problem was initially solved for $\tilde{G}$ with model sizes $m_G = 1, \dots, 5$ as well as varying load SROM sizes $m_\tau = 4, 6, 8$. The improvement of the SROM approximation with increasing size is demonstrated in Figure 11(a), showing the final minimized objective function (64) values as a function of m_G for the different m_τ values. It can be seen that the errors appear to stabilize for a shear SROM size $m_G = 3$ and a load SROM size $m_\tau = 8$. Therefore, we focus mainly on the SROM estimate $\tilde{G}$ formed from this combination of sizes in the following results.

The accuracy of the SROM shear moment estimates with $m_G = 3$ is demonstrated in Figure 11(b). Here, the average and maximum moment error across the five unknown shear moduli is shown for $m_\tau = 4, 6, 8$. Again, the improvement in overall solution quality as m_τ increases is clear in the plot, most notably with the maximum error in the fourth moment decreasing from 107.0% to just 14.3% for $m_\tau = 4$ and $m_\tau = 8$, respectively. For the solution deemed as converged from Figure 11(a) ($m_G = 3$ and $m_\tau = 8$), the moment estimates using $\tilde{G}$ are very

accurate. Indeed, the average moment error across the unknown moduli is under 9.0% for all four moments and is just 1.0% and 2.6% for the first and second moment, respectively. This accuracy is seen in more detail in Figure 12, which compares the SROM estimates of the first four moments to the true shear moduli moments for $m_G = 3$ and $m_\tau = 8$.

Remark 4. In practice, high-order moments (such as the ones used in the examples) may not be available or computable with reasonable accuracy. We would like to emphasize that the method can be used to extract information from any available data. In the end, the accuracy of any method will be limited by the information provided in the observed data.

5.3.2. Solutions with limited model evaluations—To demonstrate the computational efficiency of the SROM optimization approach, we now briefly show results for the case where there is a limit on the number of forward model evaluations allowed to obtain a solution. Note that the results shown thus far were generated by terminating the optimization algorithm according to a tolerance on the relative change in the objective function. Due to the simplicity of the elastodynamics forward model considered here, we could afford to choose a stringent stopping tolerance to guarantee the accuracy of the solutions. However, in many problems of practical importance, the number of calls to the deterministic simulator is limited by the complexity of the governing model (2). Hence, to mimic this scenario, we revisit this example where we instead terminate the optimization algorithm according to a prescribed maximum number of model evaluations.

From the formulation in Section 3.3, the total number of forward model evaluations to obtain an SROM optimization solution can be expressed as

$$\# \text{ model evaluations} = (2 \times m_G \times m_\tau) \times (\# \text{ objective function evaluations}) \quad (84)$$

assuming that the gradient computation is also carried out with each call to the objective function. Hence, given a prescribed number of allowed simulations, we can supply the optimization algorithm with the corresponding number of objective function evaluations at which to terminate using this relation. In this case, we solve the problem for $m_\tau = 8$, $m_G = 2$ and 3, and $\# \text{ model evaluations} = \{1000, 2000, 3000, 4000, 5000\}$.

First, we view the behavior of the minimum value of the objective function with limited model evaluations in Figure 13(a), where the markers on the curves represent approximately every 1000 forward solves, up to the maximum of 5000. For comparison, the same plot is shown from the results in the previous section in Figure 13(b), when the algorithm terminated according to a strict tolerance on the relative change in objective function. It is clear from the two plots that accurate solutions can be obtained with far fewer iterations and model evaluations than were carried out previously.

Also apparent in Figure 13(a) is that using $m_G = 2$ results in a lower objective function value as compared to $m_G = 3$ for the same number of model evaluations. The primary reason, as apparent from the relation in (84), is that a smaller model size requires fewer forward solves per iteration of the optimization algorithm and hence more iterations may be carried out for the same number of model evaluations. This is clear in Figure 13(a) as well, where for 5000 model evaluations, the optimization algorithm is able to proceed for 144 iterations for $m_G =$

2 and only 92 for $m_G = 3$. Note that the number of iterations need not correspond exactly with the number of objective function evaluations, as line search or trust region optimization algorithms [22] may require multiple calls to the objective function on a single iteration.

It is insightful to now view the errors in the shear moment estimates as a function of the number model evaluations. Figure 14 shows the average moment error across the five shear moduli versus number of model evaluations for a) $m_G = 2$ and b) $m_G = 3$. As was also apparent in Figure 13(a), the errors here for $m_G = 2$ are substantially lower than using $m_G = 3$ with the same number of model evaluations. For example, it can be seen that it takes 4000 deterministic model solves to reduce the average error in the first four moments under 20% with $m_G = 3$, while it takes just 2000 when $m_G = 2$. In each case, however, it takes relatively few solves to yield satisfactory results. When concerned with second moment accuracy, it takes just 3000 and 4000 solves to obtain estimates within 5% of the true values on average for $m_G = 2$ and $m_G = 3$, respectively.

In summary, this example illustrates one of the main strengths of the SROM optimization approach -the ability to yield accurate results in a computationally efficient manner (i.e. with limited calls to the deterministic model). Here, satisfactory solution estimates were obtained for a problem with a six-dimensional stochastic space with just 5000 or less forward solves. It is important to reemphasize the independence of the necessary model evaluations and potential scalability of the method with parallel processing. With access to a computing cluster, one can easily perform the SROM optimization framework on $m_G \times m_\tau$ processors and perform all necessary forward and adjoint solves in roughly the time it takes for two simulations.

6. Conclusion

In this study, we proposed a novel framework for inverse problems under uncertainty using stochastic reduced order models (SROMs). Viewing the inverse problem generally as a constrained stochastic optimization problem, the approach was formulated in terms of minimizing an abstract objective function with a stochastic model constraint. The non-intrusive nature of the SROM approximation transforms the constrained stochastic optimization problem into a deterministic one with decoupled, deterministic model constraints. In this way, the use of SROMs allows for a widely applicable method that relies solely on calls to existing deterministic forward solvers and standard optimization software. Furthermore, since the necessary forward model evaluations are completely independent from one another, the approach could be easily parallelized and hence scalable to large design and inverse problems. Finally, the SROM-based approach naturally handles problems with multiple sources of uncertainty.

We demonstrated the effectiveness of the proposed SROM inverse problem framework on the problem of random material identification in elastodynamics systems. We showed, through numerical examples, that the approach could accurately and efficiently estimate the statistics of random, unknown shear moduli in an elastic solid given moments of displacements as input data. Moreover, the method was shown to remain effective in the situation where there is only sparse input data available as well as cases where the loading in

the problem can only be characterized probabilistically. Lastly, the SROM approach was shown to be capable of satisfactorily estimating several random unknowns with relatively limited calls to the forward solver, in large part due to the low-dimensionality of the models.

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Figure 1.
Problem domains for the numerical examples.

Figure 2.

Behavior of the SROM shear modulus approximation in Example 1 with deterministic load.

(a) Minimized objective function (64) values versus SROM size. (b) The error in the SROM estimates of shear modulus moments for increasing SROM sizes.

Figure 3.

SROM shear distribution accuracy for Example 1 with deterministic loading. (a) The CDF error (Eq. (81)) versus SROM size. (b) Comparison of the SROM CDFs with the true shear distribution for different SROM sizes.

Figure 4. Convergence of the SROM construction problem (29) for forward uncertainty propagation with increasing SROM size when generating the SROM for the random load in Example 1.

Figure 5. Converged objective function (64) values for different shear and load SROM sizes for Example 1 with random loading.

Figure 6. SROM moment accuracy for Example 1 with random loading. a) Shear moment errors versus m_G for $m_\tau = 8$. b) Shear moment errors versus m_τ for $m_G = 4$.

Figure 7. SROM shear distribution accuracy for Example 1 with random loading. a) Shear CDF errors for different shear and load SROM sizes. b) CDF comparison for increasing m_G with $m_\tau = 8$.

Figure 8.

SROM CDF estimates for the shear distribution using the Gaussian noise model (82) with different noise levels for (a) $m_G = 5$ and (b) $m_G = 10$. The vertical, dashed line reflects the true shear modulus value, $G = 5.0$.

Figure 9.

Results for Example 2 with explicit unknown distributions for the shear moduli. (a) Behavior of the minimum objective function for increasing SROM size m_G . (b) The percent errors in the SROM moment estimates for the background and inclusion shear moduli with $m_G = 4$. (c) The SROM shear modulus CDFs for $m_G = 4$ compared to the true distributions. (d) A comparison of the SROM CDF errors when using only boundary input data versus full field data for increasing m_G .

Figure 10.
The true shear modulus distributions for Example 3.

Figure 11.

(a) Converged objective function values versus m_G for different m_τ . (b) The maximum and average percent error in the SROM moment estimates for $m_G = 3$ and different m_τ .

Figure 12.

Comparison of the SROM estimates for the first four moments versus the true values with $m_G = 3$ and $m_\tau = 8$.

Figure 13.

Behavior of the minimum value of the objective function when a) terminating the optimization algorithm according to a maximum number of model evaluations (Section 5.3.2) and b) terminating the algorithm with a strict tolerance on the relative change in objective function (Section 5.3.1). The markers appear on the curves for approximately every 1000 solves.

Figure 14.

The average percent error in the SROM moment estimates versus number of model evaluations for a) $m_G = 2$ and b) $m_G = 3$.

Table 1

The number of iterations taken to obtain the minimum objective function values in Figure 2(a).

m_G	Iterations
1	20
2	42
3	83
4	92
5	94
6	126

Table 2

SROM estimate for the mean and standard deviation for the true shear modulus $G = 5$ under the Gaussian noise assumption (82) for different levels of noise.

Noise	Mean	Variance
1%	4.991	0.001
5%	4.998	0.015
10%	5.019	0.061
15%	5.050	0.127

Table 3

The parameters describing the true shear moduli distributions for Example 2.

	$G_{\min}$	$G_{\max}$	$E[G]$	$\text{Var}[G]$
G_b	3.0	6.0	4.0	0.25
G_i	7.0	10.0	8.0	0.25

Table 4

The SROM mean approximations and minus/plus two standard deviation intervals in Example 2 with 10% and 20% noise. The SROM size is $m_G = 4$ and the target shear moduli values are $G_b = 4.0$ and $G_t = 8.0$.

		$E[G]$	$-/+ 2 \text{ STD}$
10% noise	G_b	4.02	(3.66, 4.38)
	G_t	7.88	(7.55, 8.22)
20% noise	G_b	4.09	(3.23, 4.96)
	G_t	7.82	(7.11, 8.53)