Topography optimization under microscale uncertainty using stochastic gradients

Subhayan De¹ · Kurt Maute² · Alireza Doostan²

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Abstract
This paper considers the design of structures made of engineered materials, accounting for uncertainty in material properties. We present a topology optimization approach that optimizes the structural shape and topology at the macroscale assuming design-independent uncertain microstructures. The structural geometry at the macroscale is described by an explicit level set approach, and the macroscopic structural response is predicted by the eXtended Finite Element Method (XFEM). We describe the microscopic layout by either an analytic geometric model with uncertain parameters or a level-cut from a Gaussian random field. The macroscale properties of the microstructured material are predicted by homogenization. Considering the large number of possible microscale configurations, one of the main challenges of solving such topology optimization problems is the computational cost of estimating the statistical moments of the cost and constraint functions and their gradients with respect to the design variables. Methods for predicting these moments, such as Monte Carlo sampling, and Taylor series and polynomial chaos expansions often require a large number of random samples resulting in an impractical computation. To reduce this cost, we propose an approach wherein, at every design iteration, we only use a small number of microstructure configurations to generate an independent, stochastic approximation of the gradients. These gradients are then used either with a gradient descent algorithm, namely Adaptive Moment (Adam), or the globally convergent method of moving asymptotes (GCMMA). Three numerical examples from structural mechanics are used to show that the proposed approach provides a computationally efficient way for macroscale topology optimization in the presence of microstructural uncertainty and enables the designers to consider a new class of problems that are out of reach today with conventional tools.

Keywords Topology optimization · Microscale uncertainty · Stochastic gradients

1 Introduction

The ubiquitous presence of uncertainty in geometry, material properties, and loading conditions of a structure must be considered in the design process in order to achieve a robust and reliable performance. Most commonly, in reliability-based design optimization, a probabilistic failure criterion estimated by first- or second-order Taylor series expansion (Haldar and Mahadevan 2000) is considered through a design constraint (Bae and Wang 2002; Maute and Frangopol 2003; Kharmanda et al. 2004; Jung and Cho 2004; Moon et al. 2004; Kim et al. 2006; Mogami et al. 2006; Eom et al. 2011). On the other hand, in design optimization under uncertainty, the effect of uncertainty is taken into account by optimizing the mean value of the structural performance (Beyer and Sendhoff 2007; De et al. 2017; Diwekar 2020). Often a contribution from the variability of the performance is added to the objective to generate designs that are less
sensitive to uncertainty (Alvarez and Carrasco 2005; Conti et al. 2009; Guest and Igusa 2008; Chen et al. 2010; Chen and Chen 2011; Asadpour et al. 2011; Tootkaboni et al. 2012; Maute 2014; Keshavarzzadeh et al. 2017; De et al. 2020a).

Topology optimization (TO) considers how one or more materials can be optimally placed within a design domain to achieve a desired mechanical performance while satisfying design constraints. TO has found applications in several fields, such as structural mechanics, fluid flow, optics, and acoustics. The readers are referred to Sigmund and Maute (2013), Deaton and Grandhi (2014), and references therein for details. In most of these applications, the structure is designed exclusively at the macroscale, assuming homogeneous materials (Bendsoe and Kikuchi 1988; Suzuki and Kikuchi 1991; Diaz and Bendsoe 1992; Xia and Breitkopf 2017). However, an increasing number of studies consider the use of heterogeneous materials, i.e., materials with spatially varying properties, such as engineered composites. The design of these heterogeneous materials at the microscale was performed, for example, in Sigmund (1994, 1995), Lipton and Stuebner (2007), Noël and Duysinx (2017), Collet et al. (2018), and Chatterjee et al. (2021) to achieve prescribed effective properties at the macroscale. An overview of the design of layered microstructure is given in Eschenauer and Olhoff (2001). Concurrent multiscale TO (Bendsoe and Kikuchi 1988; Xia 2016; Xia and Breitkopf 2017) seeks to optimize the structure at the macro as well as in the microscale [see references in Xia and Breitkopf (2017) for a comprehensive list]. In Rodrigues et al. (2002) and Coelho et al. (2008), a hierarchical approach is used, where a microstructure is designed for each element in the finite element mesh, which is then used to estimate the macroscale objective. Schury et al. (2012) employed free material optimization method that designs the stiffness tensor values for each finite element with appropriate constraints from the microscale problem. Xia and Breitkopf (2014) solved the concurrent design problem at macro and for every element in the finite element mesh in the microscale by using computational homogenization that estimates the macroscale responses due to microscale inhomogeneity. Sivapuram et al. (2016) considered the microstructure to remain the same inside a sub-region in the structure and used linearization to decompose the concurrent design problem. The connection between different adjacent microstructures was addressed in Du et al. (2018).

These highly optimized structures are, however, sensitive to defects (Pasini and Guest 2019), which can be introduced at the microscale during manufacturing. For example, melting based additive manufacturing, can affect the pore and grain sizes (Beuth and Klingbeil 2001; Aboulkhair et al. 2014; Parry et al. 2016). This, in turn, affects the structural properties in the macroscale (Liu and Shin 2019) and limits the application of TO Dong et al. (2017), Marmarelis and Ghanem (2020). Hence, the design optimization process needs to incorporate the effects of these random defects at the microscale in order to produce robust structures.

In this paper, we describe the variability in geometry at the microscale and impurities in the constituent materials of the microstructure using uncertainties characterized by known probability distributions. Hence, the TO design problem at the macroscale needs to address the uncertainties in geometry and material properties of the microstructure. In gradient-based approaches for solving the resulting TO problem, the evaluation of a large number of objective, constraints, and their gradients for many possible microstructure configurations may be needed using a standard Monte Carlo approach if variances of the gradients are large. As the number of possible microstructure scenarios combining many realizations of the microstructure can be extremely large, the optimization process becomes computationally burdensome. To quantify the uncertainty, polynomial chaos expansion and its sparse variation (Ghanem and Spanos 2003; Doostan et al. 2007; Blatman and Sudret 2008; Doostan and Owhadi 2011) can be used to construct surrogate models of the performance, but the number of expansion coefficients and hence the number of objective, constraints, and gradient evaluations rapidly increases as the stochastic dimension of the problem increases. Perturbation methods, such as Taylor series expansion, with respect to the uncertain parameters can be used efficiently to estimate many gradients, but the expansion accuracy deteriorates for nonlinear objectives and constraints.

To alleviate the computational burden of gradient-based approaches to solve TO under microscale uncertainty, we herein propose a method based on stochastic estimates of these quantities. We construct stochastic approximations of the objective, constraints, and gradients, using only a handful of random configurations of the microstructure generated independently at every design optimization iteration. To solve the optimization problem, these stochastic estimates are then used with Adam, a popular variant of the stochastic gradient descent, and globally convergent method of moving asymptotes (GCMMA). To the best of our knowledge, this is the first approach that can address TO of structures in the presence of high-dimensional microstructure uncertainty. We illustrate the efficacy of the proposed approach using two- and three-dimensional structures with two types for microstructural materials: (a) randomly dispersed inclusions
in host matrix and (b) chopped fiber composites. The microstructural properties, such as the shape, size, and distribution of the inclusions, elastic moduli of the fiber and matrix, as well as the orientation of the fibers, are assumed uncertain and design independent. The results from these numerical examples show that the proposed approach produces an average design that has computational cost only a small factor larger the cost of the corresponding deterministic TO.

The rest of the paper is organized as follows: In the next section, we define the TO problem under microscale uncertainty and briefly discuss the level set method used to describe the geometry of the structure at the macroscale. The subsequent section discusses the use of stochastic gradients with random microstructures and homogenization techniques to solve the TO problem. We illustrate the proposed approach using three numerical examples in Sect. 4 before concluding the paper with a discussion on the future directions of this approach.

2 Optimization problem

In this paper, we seek to optimize the structural shape and topology at the macroscale. The structure is made of a composite material whose effective properties are stochastic due to uncertainty at the microscale. We assume spatially varying uncertainty in geometry and material properties. Figure 1 shows a schematic of the problem, where the macrostructure is optimized over a design domain \( \Omega \). Dirichlet boundary condition \( u = u \) is applied at the boundary \( \Gamma_u \), and Neumann boundary condition \( t = t \) is applied at the boundary \( \Gamma_t \). The figure also shows one realization of the representative volume element (RVE) of the microstructure at macroscopic point A. In this section, we formulate the optimization problem and then discuss the analysis model used to solve this problem.

2.1 Problem formulation

In macroscale optimization of structures under microscale uncertainty, the design optimization is performed at the macroscale while accounting for uncertainties in the microstructures. The cost function \( f(\theta; \xi) : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R} \) and the constraint \( g(\theta; \xi) : \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}^n \) depend on the macroscale optimization variables \( \theta \in \mathbb{R}^n \) as well as on the random variables \( \xi \in \mathbb{R}^n \) with known probability distributions associated with the microstructure uncertainty.

Accordingly, the design optimization problem under uncertainty using average values of the cost function and constraints can be defined as

\[
\min_{\theta} R(\theta) := \mathbb{E}_\xi[f(\theta; \xi)] \\
\text{subject to } C_i(\theta) := \mathbb{E}_\xi[g(\theta; \xi)] \leq 0, \quad i = 1, \ldots, n_g.
\]

(1)

where \( \mathbb{E}_\xi[\cdot] \) denotes the expectation of its argument with respect to the probability distribution of \( \xi \); \( R(\theta) \) is the objective and known as the expected risk; and \( C(\theta) \) is the expected constraint violation. A contribution from the variance or standard deviation can also be added to the objective. For example, see De et al. (2020a) for a detailed discussion on including a variance component in the objective of topology optimization problems. In the next subsection, we briefly discuss the model used to describe the geometry of the structure and estimate the sensitivity of the design with respect to the optimization variables.

2.2 Geometry and analysis model

In this paper, we describe the geometry of the structures at the macroscale using a level set method following specifically the approach of Villanueva and Maute (2014) and Sharma et al. (2017). Considering a two-phase problem, the level set field \( \phi(x) \) decomposes the design domain \( \Omega_D \) into two distinct subdomains \( \Omega_I \) and \( \Omega_H \) as follows

\[
x \in \begin{cases} 
\Omega_I & \forall \phi(x) < 0; \\
\Omega_H & \forall \phi(x) > 0; \\
\Gamma_{I,H} & \forall \phi(x) = 0,
\end{cases}
\]

(2)

where \( x \) denotes the spatial coordinates and \( \Gamma_{I,H} \) represents the interface between \( \Omega_I \) and \( \Omega_H \) as shown in Fig. 2. In this paper, the level set design field, \( \phi(x) \), is discretized by

\[
\phi(x) = \sum_{i=1}^{N_s} \phi_i N_i(x),
\]

(3)
where $N_s(x)$ are bilinear or trilinear shape functions in 2D and 3D, respectively, and $N_n$ is the total number of nodes in the finite element mesh. Following Kreissl and Maute (2012), we use a linear filter for the nodal level set values as follows

$$\tilde{\phi}_i = \frac{\sum_{j=1}^{N_{rf}} w_{ij} \phi_j}{\sum_{j=1}^{N_{rf}} w_{ij}},$$

where $N_{rf}$ is the number of nodes within the filter radius $r_f$; the weights are defined as $w_{ij} = \max(0, r_f - |x_i - x_j|)$; and $\phi_j$ is the level set function value at node $i$ before filtering. These unfiltered nodal level set values, $\phi_i$, are used as the design parameters. This approach allows for solving the optimization problem with the help of mathematical programming methods.

We use the eXtended Finite Element Method (XFEM) to discretize the governing equations and use a generalized Heaviside enrichment strategy to approximate the displacement field in the solid domain. We use the unsymmetric

Nitsche’s method to weakly implement the Dirichlet boundary conditions (Nitsche 1971; Burman and Hansbo 2012). The XFEM formulation is stabilized by the face-oriented ghost penalty method (Burman and Hansbo 2014; Schott et al. 2015) to avoid ill-conditioning arising from small intersections of elements. Structural springs are also added to the disconnected solid subdomains to prevent rigid body motion (Geiss et al. 2019). The shape sensitivities of the cost function $f(\theta, \xi)$ and the constraints $g_j(\theta, \xi)$, $i = 1, \ldots, n_g$, with respect to the optimization variables, are computed by the adjoint method as detailed in Sharma et al. (2017). We use these gradients to determine the search direction during the optimization process, as described in the next section.

### 3 Use of stochastic gradients

In the standard Monte Carlo approach, $R(\theta)$ and $C(\theta)$ in (1), and their gradients with respect to the design optimization variables $\theta$ are estimated using $N_s$, e.g., $N_s \sim \mathcal{O}(1)$, evaluations of the structural response for a given vector of optimization variables $\theta$ as follows

$$\hat{R}(\theta) = \frac{1}{N_s} \sum_{i=1}^{N_s} f(\theta; \xi_i);$$

$$\hat{C}_j(\theta) = \frac{1}{N_s} \sum_{i=1}^{N_s} g_j(\theta; \xi_i); \quad j = 1, \ldots, n_g;$$

$$\nabla \hat{R}(\theta) = \frac{1}{N_s} \sum_{i=1}^{N_s} \nabla f(\theta; \xi_i);$$

$$\nabla \hat{C}_j(\theta) = \frac{1}{N_s} \sum_{i=1}^{N_s} \nabla g_j(\theta; \xi_i); \quad j = 1, \ldots, n_g.$$  

(5)

Here, a hat notation is used for an estimate of a quantity. We do not explicitly state the dependence of these estimates on $\xi$. Note that, in general, to achieve a small estimation error, $N_s$ needs to be large, leading to a high computational cost. Motivated by the success of the stochastic gradient descent method and its different variants for solving nonlinear non-convex optimization problems, e.g., in deep learning and macroscale topology optimization (De et al. 2020a, b; Li and Zhang 2020), we propose a stochastic gradient-based approach to alleviate the computational burden of topology optimization under microscale uncertainty. In this approach, instead of calculating the objective, constraints, and their gradients for large number of microstructures realizations at every integration point, a small number of random samples $n_s \ll N_s$, e.g., $n_s \sim \mathcal{O}(1)$, are randomly chosen to give small-sample unbiased estimates of the mean values in (5) as
\[ \hat{R}^{(n_s)}(\theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} f(\theta; \xi_i); \]
\[ \hat{C}^{(n_s)}_j(\theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} g_j(\theta; \xi_i); \quad j = 1, \ldots, n_g; \]
\[ \hat{V}R^{(n_s)}(\theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} \nabla f(\theta; \xi_i); \]
\[ \hat{V}C^{(n_s)}_j(\theta) = \frac{1}{n_s} \sum_{i=1}^{n_s} \nabla g_j(\theta; \xi_i); \quad j = 1, \ldots, n_g; \]

where the superscript \((n_s)\) is used to specify that the approximation uses \(n_s \ll N_s\) number of random samples. Note that at every iteration different \(n_s\) number of independent and identically distributed random samples are used to evaluate \((6)\). These coarse approximations of objective, constraints, and their design sensitivities are used in optimization algorithms, which are described next. In particular, following (De et al. 2020a), two algorithms are investigated in this paper, namely the Globally Convergent Method of Moving Asymptotes (GCMMA) (Svanberg 2002) popular in TO, and Adaptive Moment (Adam) (Kingma and Ba 2014), a variant of the stochastic gradient descent algorithm.

### 3.1 Stochastic gradient descent (SGD) method

In the standard SGD method (Bottou et al. 2018), a single realization of \(\xi\) is used at every optimization iteration to estimate the gradients in \((6)\). Here, a straightforward extension of the standard SGD method using a small batch of \(n_s \geq 1\) random samples to estimate the gradients in \((6)\) is used in the numerical examples, which reduces the variance of the gradients used in each iteration resulting in a faster convergence. This version is known as the mini-batch gradient descent (Ruder 2016; Bottou et al. 2018). The parameters are updated at \(k\)th iteration as follows

\[ h_k = \hat{V}R^{(n_s)}(\theta_k) + \sum_{j=1}^{n_g} \kappa_j \hat{V}C^{(n_s)}_j(\theta_k); \]
\[ \theta_{k+1} = \theta_k - \eta h_k, \]

where \(\eta\) is the step size, also known as the learning rate; \(\kappa_j, j = 1, \ldots, n_g\) are positive hyperparameters to enforce the constraints. As SGD methods are restricted to unconstrained problem, we use a penalty formulation to account for the inequality constraints in \((1)\) and define \(C^{+}_j(\theta)\) as

\[ C^{+}_j(\theta) = E_\xi \left[ \left( g_j^+(\theta; \xi) \right)^2 \right]; \quad j = 1, \ldots, n_g. \]

where \(g_j^+(\theta; \xi) = 0\) for \(g_j(\theta; \xi) \leq 0\) and \(g_j^+(\theta; \xi) = g_j(\theta; \xi)\) otherwise. The computational cost of SGD is small compared to that of standard Monte Carlo methods. However, the convergence of the standard SGD method can be slow since the descent is only achieved in expectation (i.e., the expectation of the stochastic gradients is the same as the gradients of objective and constraints in \((5)\)).

Recently, several variants of the standard SGD method with improved convergence have been proposed for training of neural networks (Ruder 2016). In this paper, one such variant, namely, the Adaptive Moment (Adam) (Kingma and Ba 2014) is used in the numerical examples. This algorithm seeks to reduce the variability in \(h\) over the iterations by accumulating historical gradient and squared gradient information using two exponential decay rates, \(\beta_m\) and \(\beta_v\). At \(k\)th iteration, the gradients are updated as follows

\[ m_k = \beta_m m_{k-1} + (1 - \beta_m) \hat{h}_k; \]
\[ v_{k,j} = \beta_v v_{k-1,j} + (1 - \beta_v) \hat{h}_{k,j}^2, \quad j = 1, \ldots, n_g. \]

We use \(\beta_m = 0.9\) and \(\beta_v = 0.999\) herein as suggested in Kingma and Ba (2014). An initialization bias correction is applied to \(m_k\) and \(v_{k,j}\) as follows

\[ \hat{m}_k = \frac{m_k}{1 - \beta_m^k}; \]
\[ \hat{v}_{k,j} = \frac{v_{k,j}}{1 - \beta_v^k}, \quad j = 1, \ldots, n_g. \]

Using these quantities, the parameters are updated as

\[ \theta_{k+1,j} = \theta_{k,j} - \eta \frac{\hat{m}_{k,j}}{\sqrt{\hat{v}_{k,j}} + \epsilon}, \quad j = 1, 2, \ldots, n_g. \]

Algorithm 1 summarizes these steps.

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### Algorithm 1: Adam (Kingma and Ba, 2014)

Given \(\eta, \beta_m, \beta_v, \) and \(\epsilon.\)

Initialize \(\theta_1.\)

Initialize \(m = 0.\)

Initialize \(v = 0.\)

for \(k = 1, 2, \ldots, \) do

Compute \(h_k := h(\theta_k).\)

Set \(m \leftarrow \beta_m m + (1 - \beta_m) h_k.\) [see Eqn. (9)]

Set \(v_{j} \leftarrow \beta_v v_{j} + (1 - \beta_v) h_{k,j}^2, \quad j = 1, 2, \ldots, n_g.\) [see Eqn. (9)]

Set \(m \leftarrow m/(1 - \beta_m^k).\) [see Eqn. (10)]

Set \(v \leftarrow v/(1 - \beta_v^k).\) [see Eqn. (10)]

Set \(\theta_{k+1,j} \leftarrow \theta_{k,j} - \frac{\eta m_{k,j}}{\sqrt{v_{k,j}} + \epsilon}, \quad j = 1, 2, \ldots, n_g.\) [see Eqn. (11)]

end for
3.2 Globally convergent method of moving asymptotes (GCMMA) with stochastic gradients

We also study GCMMA (Svanberg 2002) with stochastic gradients in this paper. In this algorithm, conservative approximations of the objective and constraint functions around the current design are used to formulate \( n_o \) decoupled convex subproblems, which are solved by a primal-dual solution strategy. This algorithm gained popularity in solving TO problems with a large number of design parameters as the subproblems are separable, i.e., the primal problem can be decomposed in \( n \) single-variable problems. In this paper, we use GCMMA with no inner iteration and shape sensitivities are computed using the adjoint method (Sharma et al. 2017).

3.3 Generation of random microstructures

At every iteration of the algorithms described above, we use \( n_s \) number of microstructural combinations per iteration. Each of these combinations assign randomly generated microstructures to each element in the finite element discretization of the structure. Note that, in general, the microstructure at each integration point inside an element can be considered different. However, in this study, we assume the microstructures at all integration points inside an element are the same. While these random microstructures can be generated during the optimization process, in this paper, we generate \( N_s \) number of microstructures and perform homogenization before the optimization process. Next, we randomly assign these microstructures in each element during the optimization. Another way to assign the microstructures is to assign them using spatial correlation. However, this is only an extension of the currently used random assignment. Also, with random assignment, the microstructure properties can vary significantly in the neighboring elements compared to the correlated assignment. A detailed study on the effect of spatial correlation of the microstructures on the designed structure at the macro scale is left as a future exercise. In this subsection, we describe how these random microstructures are generated and utilized in the numerical examples in Sect. 4.

We investigate two types of microstructures—chopped fiber composite and randomly distributed two-phase material. In the chopped fiber composite, short fibers are suspended in a matrix as shown in Fig. 3a. These fibers are parameterized using the aspect ratio \( l/d \), in-plane angle \( \theta_i \), and out-of-plane angle \( \theta_o \); \( l \) and \( d \) are length and diameter of the fiber, respectively (see Fig. 3b). These geometric parameters of the fiber, as well as the elastic moduli of the fiber and matrix, are assumed uncertain with known probability distributions as specified in Sect. 4.

The second class of microstructures, two-phase material with a stiff phase and a compliant phase, is generated following the procedure in Roberts and Teubner (1995). A \( T \)-periodic zero-mean Gaussian random field is considered as follows

\[
\psi(\mathbf{r}) = \sum_{l=-N}^{N} \sum_{m=-N}^{N} \sum_{n=-N}^{N} c_{l,m,n} e^{i \mathbf{r} \cdot \mathbf{F}_{l,m,n}},
\]

where \( \mathbf{r} \) is the position vector; \( \mathbb{E}[\psi(\mathbf{r})] = 0; i = \sqrt{-1} \); and the vector \( \mathbf{f}_{l,m,n} = \frac{2\pi}{T} (l\mathbf{e}_x + m\mathbf{e}_y + n\mathbf{e}_z) \) with \( \mathbf{e}_x, \mathbf{e}_y, \) and \( \mathbf{e}_z \) being the unit vectors along \( x, y, \) and \( z \) directions, respectively. Here, a cube with \( 2N \times 2N \times 2N \) resolution is used.

Fig. 3 A schematic of the chopped fiber composite that consists of multiple short fibers suspended in a matrix is shown in (a). The uncertain geometric parameters of these fibers, namely the length \( l \), diameter \( d \), in-plane angle \( \theta_i \), and out-of-plane angle \( \theta_o \), are shown in (b).
the corresponding spectral density are, respectively, given by

\begin{align}
\mathbb{E}\left[a_{l,m,n}^2\right] &= \mathbb{E}\left[b_{l,m,n}^2\right] = \frac{1}{2} S_{\psi\psi,K}(f_{l,m,n}) \left(\frac{2\pi}{T}\right)^3.
\end{align}

(13)

Here, \(S_{\psi\psi,K}(f)\) is the spectral density of the random field \(\psi(\mathbf{r})\) at \(f\) (i.e., Fourier transform of the correlation function of \(\psi(\mathbf{r})\) at \(f\)) truncated at \(f_{l,m,n} \geq K\), which is related to the non-truncated spectral density \(S_{\psi\psi}(f)\) of the random field as follows

\begin{align}
S_{\psi\psi,K}(f) &= \frac{S_{\psi\psi}(f)}{\int_0^K 4\pi f^2 S_{\psi\psi}(f) df}.
\end{align}

(14)

We assume the correlation function of the random field and the corresponding spectral density are, respectively, given by

\begin{align}
\mathbb{E}[\psi(\mathbf{r}_1)\psi(\mathbf{r}_2)] &= e^{-\|\mathbf{r}_1 - \mathbf{r}_2\|^2_2};

S_{\psi\psi}(f) &= \frac{e^{-f^2/4}}{(4\pi)^{3/2}}.
\end{align}

(15)

where \(\| \cdot \|_2\) denotes the \(\ell_2\)-norm of its argument. Using (13), realizations of \(a_{l,m,n}\) and \(b_{l,m,n}\) are generated first, which are then used to generate realizations of the Gaussian random field \(\psi(\mathbf{r})\). Once we generate the random field, we perform a level-cut at zero using the Heaviside function assigning \(\psi(\mathbf{r}) > 0\) to the stiff phase (red) and \(\psi(\mathbf{r}) \leq 0\) to the compliant phase (blue), which gives a three-dimensional RVE of the microstructure as shown in Fig. 4 for \(T = 4\pi\) and \(K = 25\). For two-dimensional problems, we use a slice through the 3D RVE at the left end (see Fig. 4c).

### 3.4 Homogenization methods

Homogenization methods are used to estimate the effective material properties at the macroscale considering the microstructural layout. In the following, we consider a finite element setting, where the weak form of the governing equations is integrated at the macroscale.

For linear elastic problems, the material constitutive relation at the macroscale position \(\mathbf{x}\) is given by

\[ \mathbf{\bar{\sigma}}(\mathbf{x}) = \mathbf{C}_{\text{hom}} : \mathbf{\bar{e}}(\mathbf{x}), \]

(16)

where \(\mathbf{\bar{\sigma}}(\cdot)\) is the macroscopic stress tensor; \(\mathbf{\bar{e}}(\cdot)\) is the macroscopic strain tensor; and \(\mathbf{C}_{\text{hom}}\) is the fourth order homogenized constitutive tensor. The Mori-Tanaka homogenization method (Mori and Tanaka 1973; Benveniste 1987) is used in this paper for chopped fiber composite and is discussed next. For random two-phase materials, we use a first-order
computational homogenization method, which is also briefly discussed in this section.

3.4.1 Mori-Tanaka method

The Mori-Tanaka method (Mori and Tanaka 1973; Benveniste 1987), a mean-field homogenization method based on Eshelby’s inclusion problem (Eshelby 1957), estimates the effective elasticity tensor for a fiber-reinforced composite material by (Benveniste 1987; Zaoui 2002; Böhm 2004; Tran et al. 2018; Budarapu et al. 2019)

\[ C_{\text{hom}} = C_f + v_f \langle (C_m - C_f) : A \rangle : (1 - v_f) I + v_f \langle A \rangle \] \tag{17}

Here, \( v_f \) is the fiber volume fraction of the composite material; \( C_m \) and \( C_f \) are fourth order elasticity tensors of the matrix and fiber, respectively; \( I \) is the fourth order identity matrix; \( A \) is the strain concentration tensor that relates the strain \( e_f \) in the fiber with the strain \( e_m \) in the matrix as \( e_f = A : e_m \); and \( \langle \cdot \rangle \) denotes the average over all fiber orientations. The stress concentration tensor \( A \) is computed by

\[ A = [I + S : C_m^{-1} : (C_f - C_m)]^{-1}, \] \tag{18}

where \( S \) is the fourth order Eshelby’s tensor (Eshelby 1957).

3.4.2 Computational homogenization method

This approach assumes separation of scales and periodicity of the microstructure (Xia 2016; Xia and Breitkopf 2017). The homogenized stress tensor and the macroscopic constitutive tensor are computed from the solutions of a boundary value problem defined over a representative volume element for different boundary conditions. Consider one such integration point with macroscale position \( x \) and microscale position \( y \). In this approach, the macroscopic stress \( \bar{\sigma}(x) \) is related to the microscale stress \( \sigma(x, x') \) over the RVE domain \( \Omega_{mi} \) as follows

\[ \bar{\sigma}(x) = \langle \sigma(x, x') \rangle = \frac{1}{|\Omega_{mi}|} \int_{\Omega_{mi}} \sigma(x, x') \, dx', \] \tag{19}

where \( \langle \cdot \rangle \) denotes the volume average over the RVE domain. The microscale stress \( \sigma(x, x') \) is estimated from the boundary value problem associated with the RVE with a constraint on the macroscopic strain \( \bar{\epsilon}(x) \) given by

\[ \bar{\epsilon}(x) = \langle \epsilon(x, x') \rangle = \frac{1}{|\Omega_{mi}|} \int_{\Omega_{mi}} \epsilon(x, x') \, dx', \] \tag{20}

where \( \epsilon(x, x') \) is the microscale strain. To define the RVE boundary value problem that needs to be solved for each of these microstructures, let us consider the first-order local displacement field \( u(x, x') \) and the strain field \( e(x, x') \) as, Michel et al. (1999), Xia and Breitkopf (2014),

\[ u(x, x') = \bar{u}(x) \cdot x' + u^*(x'); \] \tag{21}

\[ e(x, x') = \bar{\epsilon}(x) + e^*(x'), \]

where \( u^*(x') \) is periodic up to a rigid body motion and \( e^*(x') \) with \( (e^*(x')) = 0 \) is due to the periodic displacement field \( u^*(x') \). The local stress field \( \sigma(x, x') \) is periodic as well, and the boundary value problem at the microscale becomes

\[ \sigma(x, x') = C(x') : (\bar{\epsilon}(x) + e^*(x')); \] \tag{22}

\[ \text{div}(\sigma(x, x')) = 0 \text{ in } \Omega_{mi}; \]

\[ u^*(x') \text{ is periodic; } \]

\[ \sigma(x, x') \cdot n \text{ is anti-periodic. } \]

Here, each of the phases in the microstructure is assumed linear elastic with constitutive tensor \( C(x') \); \( \text{div}(\cdot) \) denotes the divergence of its vector argument; the anti-periodicity imposes the condition that \( \sigma(x, x') \cdot n \) has opposite values at the opposite boundaries of \( \Omega_{mi} \), which is due to the periodicity of \( \sigma(x, x') \) and the unit normal vector \( n \) being opposite on the opposite boundaries. The implementation of the periodicity in (21) in the finite element approach is performed by specifying \( \bar{\epsilon}(x) \) and applying nodal displacement constraints (Michel et al. 1999; Xia and Breitkopf 2014). Once the problem in (22) is solved for all six independent components of the strain, (16) can be used to estimate the homogenized constitutive tensor.

Figure 5 depicts a schematic showing that in the presence of uncertainty in the microscale, many realizations of the random microstructure at an integration point in an element are needed to estimate the macroscale average stress tensor for a given macroscopic strain state. Instead, in the proposed stochastic gradient-based approach, for every element in the finite element mesh, we consider one random realization of the uncertain microstructure to generate a microstructure layout configuration. A small number, \( n_i \sim O(1) \), of these microstructure layouts are then used at every iteration of the optimization process resulting in a computational cost that is only a few times larger than the cost of the corresponding deterministic optimization.
In this section, we use three numerical examples to illustrate the utility of stochastic gradients in designing the macrostructure under microscale uncertainty. The first two examples consider the design of a two- and a three-dimensional beam, respectively. In the third example, we design a bracket to support a payload box. The geometry of the structures in these examples are described using the level set method and the governing equations are discretized using the XFEM approach as described in Sect. 2.2. The common parameters used during analysis of these examples are listed in Table 1.

During optimization, \( N_m \) number of microstructure layouts are constructed by assigning randomly each element in the mesh a microstructure realization from a set of \( N_m \) microstructures generated before the start of the optimization as discussed in Sect. 3.3. This random assignment of microstructure follows discrete uniform distribution. In this paper, we use \( N_m = 200 \), but this can be increased further with only an increase in the cost of the homogenization step. We note that the reason we consider \( N_m = 200 \) microstructures is to replicate a practical scenario where the microstructure samples are obtained from, say CT, images and that these images, instead of a built probabilistic model, are driving the design.
4.1 Example 1: design of a two-dimensional beam

4.1.1 Problem description

We first consider a two-dimensional simply supported beam subjected to a point load at the midspan (Fig. 6). At the macroscale, the shape and topology of the beam is optimized to minimize the strain energy subject to a 40% mass constraint. Using symmetry, only one-half of the domain is used for optimization. The optimization problem is defined as follows

\[
\min_{\theta} R(\theta) = \frac{\mathbb{E}_i [\Psi'(\theta; \xi_i)]}{\Psi_0} + w_{\text{per}} P_{\text{per}}(\theta) + w_{\text{reg}} P_{\text{reg}}(\theta);
\]

subject to \( C(\theta) = g(\theta) = \int_{\Omega} p(\theta) \, dx \int_{\Omega} \, dx - \gamma_{\text{req}} \leq 0, \)

where \( \Psi'(\theta; \xi) \) is the strain energy of the structure; \( w_{\text{per}} \) is the weight for the strain energy in the objective; \( \Psi_0 \) is the initial strain energy of the structure; and \( \Omega \) denotes design domain in the macroscale. The two penalty terms, \( P_{\text{per}} \) and \( P_{\text{reg}} \), are defined following (Barrera et al. 2020) as

\[
P_{\text{per}} = \frac{\int_{I_{\text{max}}(\theta)} \, dA}{\int_{\Gamma} \, dA}; \quad P_{\text{reg}} = w_{\phi} \frac{\int_{\Omega} (\phi(x; \theta) - \bar{\phi}(x; \theta))^2 \, dx}{\int_{\Omega} (\bar{\phi}_{\text{max}} - \bar{\phi}_{\text{min}})^2 \, dx} + w_{\varphi} \int_{\Omega} |\nabla \phi(x; \theta) - \nabla \bar{\phi}(x; \theta)|^2 \, dx + w_{\psi} \int_{\Omega} \bar{\phi}(x; \theta) \, dx.
\]

where \( I_{\text{max}}(\theta) \) denotes the boundary between the structure and void in the design domain \( \Omega; \Gamma \) is the boundary of the design domain \( \Omega; A \) denotes the surface area; \( \bar{\phi}(x; \theta) \) is a signed distance field truncated at \( \bar{\phi}_{\text{min}} \) and \( \bar{\phi}_{\text{max}} \); and the parameters \( w_{\phi} \) and \( w_{\varphi} \) are set at \( 1/\int_{\Gamma} \, dA \) (see Barrera et al. 2020 for details). Note that we add the perimeter penalty to avoid the emergence of any geometric features with irregular shapes and add the level set regularization penalty to avoid any spurious oscillations in the level set field \( \phi(x; \theta) \). The weights for the strain energy term and the penalty terms are set at \( w_{\psi} = 0.9, w_{\text{per}} = 0.025 \), and \( w_{\text{reg}} = 0.5 \), respectively. In the constraint, we use \( \gamma_{\text{req}} = 0.40 \), which is enforced with a penalty parameter \( \kappa = 1000 \) in Adam as described in Sect. 3.1.

We describe the geometry of the structure at the macroscale using a level set and use XFEM for the solution of governing equations (see Sect. 2.2). The finite element mesh of the half-domain has a total of \( 120 \times 40 \) bilinear elements. The initial geometry of the structure is shown in Fig. 8a, where we add 18 holes in the global x-direction for each of the 6 rows in the global y-direction of the half-domain. The level set field with these 18 holes is generated as \( \phi(x) = \max_i \{ \phi_i \}_{i=1}^{18} \), where

\[
\phi_i = 1 - (\frac{x_{\text{hole}}}{r_{\text{hole}}})^{10} + (\frac{y_{\text{hole}}}{r_{\text{hole}}})^{10}.
\]

Here, \( (x_{\text{hole}}, y_{\text{hole}}) \) is the local coordinate of the hole, and we use \( r_{\text{hole}} = 1/15 \). Note that a positive level set value represents void. We summarize the specifications used in this example in Table 2.

4.1.2 Microstructure scenarios

In this example, each of the elements in the finite element mesh is assumed to have any microstructure from the 200 possible scenarios. Hence, the microstructure in each element of the finite element mesh can be thought of as a uniformly distributed discrete random variable with 200 possible realizations. These realizations are generated using the Gaussian random field model described in Sect. 3.3. We use the finite element method to compute the first-order homogenized constitutive tensor for each of these random microstructures discretized in \( 100 \times 100 \) mesh with bilinear elements. Note that each of the two-dimensional microstructures requires three linear finite element analyses to estimate three independent components of the strain and the homogenized constitutive tensor \( C_{\text{hom}} \).

We study the design problem under two cases distinguished by the anisotropy in the two-phase microstructures. These cases and the corresponding observations are discussed below. In each of these cases, we approximate the objective, constraints, and their design sensitivities with four configurations of the microstructure layout per optimization iteration. In every configuration, each of the elements in the mesh is randomly assigned a microstructure from the 200 possible instances. Note that with a larger number of microstructural configurations per iteration, the gradient estimation will be more accurate, but the computational cost will increase significantly. On the other hand, with a small number of microstructure layout configurations per iteration, the convergence will be slower. Hence, based on preliminary tests, \( n_s = 4 \) is selected in this example to keep the cost small while the optimization process converges within a reasonable number of iterations. For a detailed discussion on the choice of \( n_s \), see De et al. (2020a).

Case Ia In this case, we generate 200 random microstructures using \( T = 4\pi \) and \( K = 25 \) in (12) to give \( N = 50 \), which results in a finely dispersed distribution of the two phases. We set the ratio of the elastic moduli of the phases to \( E_1/E_2 = 10 \), where \( E_i \) is the elastic modulus of the stiff
| Category                          | Parameter                                      | Value  |
|----------------------------------|------------------------------------------------|--------|
| Problem formulation              | Weight for strain energy, $w_p$                | 0.90   |
|                                  | Weight for perimeter penalty, $w_{per}$        | 0.025  |
|                                  | Weight for regularization penalty, $w_{reg}$   | 0.50   |
|                                  | Point load, $P$                                | 1.00   |
|                                  | Mass constraint, $y_{eq}$                      | 0.40   |
| Mesh (half-domain)               | Length, $L/2$                                  | 3.0    |
|                                  | Height, $L/6$                                  | 1.0    |
|                                  | Discretization                                 | $120 \times 40$ |
| Case Ia                          | Microstructure                                |        |
|                                  | Period, $T$                                    | $4\pi$ |
|                                  | Max. wavenumber, $K$                           | 25     |
|                                  | Elastic modulus (red phase), $E_1$             | 10.0   |
|                                  | Elastic modulus (blue phase), $E_2$            | 1.0    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.05   |
| Case Ib                          | Microstructure                                |        |
|                                  | Period, $T$                                    | $4\pi$ |
|                                  | Max. wavenumber, $K$                           | 25     |
|                                  | Elastic modulus (red phase), $E_1$             | 10.0   |
|                                  | Elastic modulus (blue phase), $E_2$            | 0.1    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.05   |
| Case Ic                          | Microstructure                                |        |
|                                  | Period, $T$                                    | $4\pi$ |
|                                  | Max. wavenumber, $K$                           | 25     |
|                                  | Elastic modulus (red phase), $E_1$             | 100.0  |
|                                  | Elastic modulus (blue phase), $E_2$            | 0.1    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.05   |
| Case Id                          | Microstructure                                |        |
|                                  | Period, $T$                                    | $4\pi$ |
|                                  | Max. wavenumber, $K$                           | 25     |
|                                  | Elastic modulus (red phase), $E_1$             | 100.0  |
|                                  | Elastic modulus (blue phase), $E_2$            | 0.1    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.05   |
| Case IIa                         | Microstructure                                |        |
|                                  | Period, $T$                                    | $2\pi$ |
|                                  | Max. wavenumber, $K$                           | 50     |
|                                  | Elastic modulus (red phase), $E_1$             | 10.0   |
|                                  | Elastic modulus (blue phase), $E_2$            | 1.0    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.025  |
| Case IIb                         | Microstructure                                |        |
|                                  | Period, $T$                                    | $2\pi$ |
|                                  | Max. wavenumber, $K$                           | 50     |
|                                  | Elastic modulus (red phase), $E_1$             | 10.0   |
|                                  | Elastic modulus (blue phase), $E_2$            | 0.1    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.025  |
| Case IIc                         | Microstructure                                |        |
|                                  | Period, $T$                                    | $2\pi$ |
|                                  | Max. wavenumber, $K$                           | 50     |
|                                  | Elastic modulus (red phase), $E_1$             | 100.0  |
|                                  | Elastic modulus (blue phase), $E_2$            | 0.1    |
|                                  | Poisson’s ratio (both phases), $\nu_1$, $\nu_2$| 0.3    |
| Optimization                     | Step size, $\eta$                             | 0.05   |

Table 2: Summary of specifications used to formulate and solve the optimization problem in Example I.
(red) phase and $E_2$ is the elastic modulus of the compliant (blue) phase. The fine dispersion and the chosen ratio of elastic moduli lead to a moderate level of anisotropy. Four such microstructures are shown in Fig. 7a.

We use GCMMA and Adam with a step size $\eta = 0.05$. Figure 8 shows the initial and optimized designs and objectives obtained from Adam and GCMMA. The color shading in the structure corresponds to the ratio $C_{1111}/C_{2222}$ of the first two diagonal elements of the constitutive matrix. This ratio represents the level of anisotropy of the two-phase composite. In this case, the final designs from Adam and GCMMA both achieve similar objectives, but the convergence of GCMMA is faster. To confirm the accuracy of estimating the expected values for the objective and constraint of the proposed approach, the final design from GCMMA is further evaluated for 1000 random configurations of the microstructure layout, a reasonably large number. The objective value from these 1000 random configurations is shown with a (yellow) square in Fig. 8d, which coincides with the (red) dashed curve for GCMMA at the end of the optimization verifying the convergence of the proposed stochastic gradient-based approach using only four such configurations per iteration. Figure 8e, however, shows that the coefficient of variation of the objective (i.e., the ratio of the standard deviation to the mean of the objective) is small in this case.

**Case Ib** To increase the level of material anisotropy, we set the ratio $E_1/E_2 = 100$, but keep $T$ and $K$ the same as in Case Ia. Figure 9 shows the designs and objectives

![Figure 7](https://example.com/figure7.png)

**Fig. 7** Four random microstructures from each of the two cases studied with Example 1. Note that we select $K$ such that $N = 50$, which results in the same number of terms in (12) and the same finite element discretization during the first-order computational homogenization for both of these cases. (a,b)
obtained from Adam and GCMMA with a step size $\eta = 0.05$. The color shading shows that in this case the variation in $C_{1111}/C_{2222}$ is much larger compared to Case Ia with $E_1/E_2 = 10$. As a result, the final designs obtained from Adam and GCMMA both have more bars. The initial convergence of Adam is faster during the initial stages of the optimization. However, the final designs from Adam and GCMMA both have similar objective values at the end of
the optimization. We further evaluate the final design from GCMMA by using 1000 random configurations of the microstructure layout. The (yellow) square in Fig. 9c shows that it coincides with the objective values at the end of the optimization. Figure 9d shows that the coefficient of variation of the objective is increased to $\sim 3\%$ in this case.
Case Ic To further increase the level of material anisotropy, we set the ratio \( \frac{E_1}{E_2} = 1000 \), but keep \( T \) and \( K \) the same as in Case Ia. Interestingly, in this case, with increased variation in the homogenized material properties, GCMMA diverges and fails to produce a meaningful design. Note that similar observation was made by the authors in De et al. (2020a), where GCMMA failed for a problem with large uncertainty in the gradients. Figure 10 shows the design and objective obtained from Adam with a step size \( \eta = 0.05 \). In this case, the variation in \( \frac{C_{1111}}{C_{2222}} \) is much larger compared to the previous two cases. As a result, the final design obtained from Adam has more bars. We further evaluate the final design from Adam by using 1000 random configurations of the microstructure layout. The (green) circle in Fig. 10b shows that it coincides with the objective values at the end of the optimization. Figure 10c shows that the coefficient of variation of objective has increased to \( \sim 6\% \) in this case.

Case Id Next, we keep the ratio \( \frac{E_1}{E_2} = 1000 \) with \( T \) and \( K \) the same as in Case Ia, but we include a contribution of the variance of the strain energy \( \frac{\varepsilon^2}{2} \) to the objective following Beyer and Sendhoff (2007) and De et al. (2020a). Hence, in this case, the optimization problem in (23) is replaced by the following

\[
\begin{align*}
\min_{\theta} \quad R(\theta) &= w_0 \frac{\mathbb{E}_\xi [\Psi(\theta; \xi)]}{\psi_0^0} + w_{\text{per}} P_{\text{per}}(\theta) + w_{\text{reg}} P_{\text{reg}}(\theta) \\
&+ \lambda \frac{w^2}{\psi_0^0} \text{Var}_\xi(\Psi(\theta; \xi)) ;
\end{align*}
\]

subject to \( C(\theta) = g(\theta) = \frac{\int_{\Omega} \rho(\theta) \, dx}{\int_{\Omega} \, dx} - \gamma_{\text{req}} \leq 0 \),

(26)

where \( \text{Var}_\xi(\cdot) \) denotes the variance of its argument with respect to the probability distribution of \( \xi \) and we add a contribution from the variance with a factor \( \lambda = 10.0 \). Similar to Case Ic, with increased variation in the homogenized
material properties, GCMMA diverges and fails to produce a meaningful design. Figure 11a shows the design obtained from Adam with less but mostly thicker bars to address the addition of a variance component in the objective. In this case, the reduction of the variance \( \text{Var}(\psi(\theta; \xi)) \) is 18.20% when compared to Case Ic, where the final designs are evaluated using 1000 random microstructure layouts. Figure 11b and c show the reduction of objective and variance during the optimization.

**Case IIa** In this case, we generate 200 random microstructures using \( T = 2\pi \) and \( K = 50 \) in (12) to give \( N = 50 \). The ratio of elastic moduli of the two phases is set as \( E_1/E_2 = 10 \). Figure 7b depicts four such microstructures, which shows that in this case the dispersion of the two phases is coarser than Case Ia. Adam and GCMMA with a step size \( \eta = 0.025 \) are used for the optimization. Figure 12 shows designs and objectives obtained from Adam and GCMMA for this case. As in Case Ia, final designs from Adam and GCMMA both achieve similar objectives, and again the convergence of GCMMA is faster. The final design from GCMMA, when evaluated for 1000 random configurations of the microstructure layout, produces an objective, shown with a (yellow) square in Fig. 12c, that coincides with the (red) dashed curve for GCMMA. Figure 12d shows that the coefficient of variation of the objective remains at \( \sim 2.5\% \) in this case.

**Case IIb** Next, we use \( E_1/E_2 = 100 \) with \( T \) and \( K \) same as in Case IIa to further increase the level of anisotropy. Figure 13 shows the designs and objectives obtained from Adam and GCMMA with step size \( \eta = 0.025 \). Compared to Cases I and IIa, here the level of anisotropy is larger as can be seen from the \( C_{1111}/C_{2222} \) ratios. To account for the increased anisotropy, the final designs obtained from Adam and GCMMA both have more bars. Figure 13c, however,
Fig. 12 Comparison of the designs obtained from Adam (a) and GCMMA (b) for Case IIa of Example 1 using $E_1/E_2 = 10$. The color shading of the elements in (a) and (b) corresponds to the ratio $C_{1111}/C_{2222}$ for one random microstructure layout. The evolution and coefficient of variation of the objectives are shown in (c) and (d), respectively, in addition to the objective of the final design from GCMMA evaluated with 1000 random microstructure scenarios shown with a yellow square in (e). Color figure online

shows that the final design from GCMMA has a slightly higher objective value compared to the Adam design. When evaluated with 1000 random configurations of the microstructure layout, the objective value of the GCMMA design is similar to the (red) dashed curve at the right end. Similarly, the (green) circle for the Adam design coincides with the (blue) solid line at the end of the optimization when evaluated with 1000 random samples. Figure 13d shows that the coefficient of variation of the objective is increased to $\sim 6\%$ in this case.

**Case IIc:** In the final case, we increase the level of material anisotropy by setting the ratio $E_1/E_2 = 1000$, but keep $T$ and $K$ the same as in Case IIa. Similar to Case Ic, with increased variation in the homogenized material properties, GCMMA diverges and fails to produce a meaningful design. Figure 14 shows the design and objective obtained from Adam with a step size $\eta = 0.05$. In this case, the variation in $C_{1111}/C_{2222}$ is largest compared to all other cases. As
a result, the final design obtained from Adam has the thickest bars. We further evaluate the final design from Adam by using 1000 random configurations of the microstructure layout. The (green) circle in Fig. 14b shows that it coincides with the objective values at the end of the optimization. Note that the coefficient of variation of objective has increased to ∼10% in this case as shown in (c) and (d), respectively, in addition to the objective of the final design from GCMMA evaluated with 1000 random microstructure scenarios shown with a yellow square in (c). Color figure online.

**Case IIId:** Next, we keep the ratio \( E_1/E_2 = 1000 \) with \( T \) and \( K \) the same as in Case IIc, but we include a contribution of the variance of the strain energy \( Y(\theta; \xi) \) to the objective following (Beyer and Sendhoff 2007) and (De et al. 2020a). Hence, in this case, the optimization problem in (23) is replaced by (26), where we add a contribution from the variance with a factor \( \lambda = 5.0 \). Similar to Case IIc, with increased variation in the homogenized material properties, GCMMA diverges and fails to produce a meaningful design. The design from Adam shown in Fig. 15a has less number of bars, but they are thicker to reduce the variance component in the design objective compared to the previous case. In this case, the reduction of the variance \( \text{Var}_\xi(Y(\theta; \xi)) \) is 18.37% when compared to Case IIc, where the final designs are evaluated using 1000 realizations of the microstructure layouts.
The reduction of objective and the variance component in the objective are shown in Fig. 15b and c, respectively. Note that the penalty approach used in Adam produces $C(\theta) \sim O(10^{-6})$ to $O(10^{-7})$ for all the cases in this example. However, GCMMA satisfies the mass constraint exactly in cases where it does not fail. Also, the final designs in all of these cases satisfy the constraint when evaluated using 1000 random configurations of the microstructure layout.

This example shows that, in the presence of microstructural uncertainty, the use of stochastic gradients effectively reduces the computational cost of topology optimization at the macroscale. The designs obtained for different levels of anisotropy and different ratios of the elastic moduli of the two phases in the microstructure, however, have different features. The designs obtained from Adam are different from GCMMA, but their objective values remain similar in most of the cases. However, with increased variation in the homogenized material properties, GCMMA fails to converge and produce a meaningful design. In the next two examples, we extend the proposed approach to design three-dimensional structures.

### 4.2 Example 2: design of a three-dimensional beam

#### 4.2.1 Problem formulation

In our second example, we consider the design of a beam with a line load at the midspan (see Fig. 16) subject to a 20% mass constraint. Assuming symmetry in the optimization variables, only one-fourth of the domain is used for
optimization. In this example, we define the optimization problem as follows

\[
\min_{\theta} \quad R(\theta) = \mathbb{E}_{\xi} \left[ w_p \frac{\mathcal{P}(\theta; \xi)}{\mathcal{P}_0} + w_m \frac{\mathcal{M}(\theta; \xi)}{\mathcal{M}_0} \right] \\
+ w_{\text{per}} P_{\text{per}}(\theta) + w_{\text{reg}} P_{\text{reg}}(\theta) ;
\]

subject to \( C(\theta) = g(\theta) = \frac{\int_{\Omega} \rho(\theta) \, dx}{\int_{\Omega} \, dx} - \gamma_{\text{req}} \leq 0 \),

where a term involving the total mass of the structure \( \mathcal{M}(\theta; \xi) \) is also added to objective with \( \mathcal{M}_0 = \int_{\Omega} \, dx \) and \( w_m = 1 \); and \( \gamma_{\text{req}} = 0.20 \) is used in the mass constraint. The two penalty terms are the same as in the previous example. For the weights \( w_p, w_{\text{per}}, \) and \( w_{\text{reg}} \), we also use the same values as in the previous example. We start the optimization from a structure with many square like holes as shown in Fig. 17a to facilitate hole seeding. In the initial design, we make 12 holes in the global \( x \)-direction for each of the 4 rows in the global \( y \)-direction, according to (25), and with \( r_{\text{hole}} = 0.09 \). These holes are then protruded in the global \( z \)
direction along the width. We summarize the specifications used in this example in Table 3 for convenient reproduction of the results presented herein.

4.2.2 Microstructure scenarios

The microstructure in the beam is assumed to be chopped fiber composite with uncertain properties listed in Table 4. We generate 200 realizations of the uncertain parameters of the microstructure from their respective uniform probability distributions as stated in Table 4. The homogenized constitutive properties are estimated using the Mori-Tanaka method described in Sect. 3.4.1. The finite element model of one-quarter of the domain has a total $72 \times 24 \times 12 = 20,736$ elements. For one realization of the random microstructure layout, we assign each element of the finite element mesh to one randomly selected microstructure out of 200 possible ones, similar to the previous example.

4.2.3 Optimization results

We use Adam and GCMMA with a step size $\eta = 0.1$ and penalty parameter $\kappa = 5 \times 10^4$ to implement the constraint and perform the optimization with four configurations of the microstructure layout per iteration for gradient calculations. Note that an assumption of symmetry holds here since every element in the finite element mesh is equally likely to have any of the 200 possible microstructures.

The optimized structures obtained from Adam and GCMMA are shown in Fig. 17b and c. Interestingly, Adam produces a design with two webs, but GCMMA produces a design with three webs. However, both of these designs use the same amount of mass. Figure 18 depicts the objective values for these two methods, where the Adam design with two webs can achieve a smaller objective when compared to a three-web design obtained using GCMMA. The objective of the final design from Adam is further verified with 1000 microstructural layout configurations and is shown in Fig. 18 with a yellow square. Note that both GCMMA and Adam satisfy the constraint. The ratio $\frac{C_{1111}}{C_{2222}}$ of the first two diagonal elements in the homogenized constitutive tensor $\mathbb{C}_{\text{hom}}$ for all the elements in the finite element model for one random layout of the microstructure for designs obtained from Adam and GCMMA shows the variability in material stiffness and anisotropy (see Fig. 19). As a result, the designs show a less smooth surface with kinks compared to a deterministic design. Further constraints can be added to produce smoother surfaces more amenable to 3D printing (Schmitt et al. 2016), but that is beyond the scope of the current paper as our focus here is on the optimization process itself.

The last two examples considered a common geometry used in the TO literature in two and three dimensions. The results show that the proposed approach is capable of producing average designs for two different types of random microstructures. In the next example, we use the stochastic gradient-based approach to design a bracket for supporting a payload box to show the usefulness of the proposed approach for more practical design exercises.
4.3 Example 3: design of a bracket

4.3.1 Problem formulation

In the third example, we consider a structure to support a payload box given a set of supports at the left and right ends as shown in Fig. 20. Note that the design domain is

Table 3  Summary of specifications used to formulate and solve the optimization problem in Example 2

| Category               | Parameter                              | Value |
|------------------------|----------------------------------------|-------|
| Problem formulation    | Weight for strain energy, $w_{sp}$      | 0.90  |
|                        | Weight for mass, $w_{m}$               | 1.00  |
|                        | Weight for perimeter penalty, $w_{per}$ | 0.025 |
|                        | Weight for regularization penalty, $w_{reg}$ | 0.50  |
|                        | Line load, $P$                         | 1.00  |
|                        | Mass constraint, $y_{reqd}$             | 0.20  |
| Mesh (quarter domain)  | Length, $L/2$                          | 3.0   |
|                        | Height, $L/6$                          | 1.0   |
|                        | Width, $L/12$                          | 0.5   |
|                        | Discretization                         | $72 \times 24 \times 12$ |
| Solution strategy      | No. of possible microstructures per elem. | 200   |
|                        | Random config. per iter., $n_s$        | 4     |
|                        | No. of optimization variables, $n_{\theta}$ | $3.04 \times 10^4$ |
|                        | Step size, $\eta$                      | 0.1   |
|                        | Penalty to implement $C(\Theta)$, $\kappa$ | $5 \times 10^4$ |

The values are in consistent units

Table 4  Uncertain parameters of the microstructure used in Example II

| Parameter                            | Lower limit | Upper limit |
|--------------------------------------|-------------|-------------|
| Elastic modulus of fiber, $E_f$      | 0.95        | 1.05        |
| Elastic modulus of matrix, $E_m$     | 0.0095      | 0.0105      |
| Aspect ratio, $ld$                   | 10          | 100         |
| In-plane angle, $\theta_i$          | 0°          | 180°        |
| Out-of-plane angle, $\theta_o$      | 0°          | 180°        |

These parameters are assumed uniformly distributed between a lower and an upper limit

Fig. 18  Comparison of the evolution of the objectives in Example II with a zoomed-in portion showing some oscillations at the end of the optimization due to the stochastic nature of gradients. The yellow square at the right end shows the objective from the final Adam design when evaluated using 1000 random microstructure layouts

(a) Adam design

(b) GCMMA design

Fig. 19  The color shading shows the ratio $C_{1111}/C_{2222}$ of the first two diagonal elements of the constitutive tensor $C_{hom}$ for the designed structure using Adam and GCMMA in Example 2 for one random layout of the microstructure. (a,b)
The structure is assumed to be made of Ti-6Al-4V alloy with impurities in it. The alloy has elastic modulus $E_{\text{Ti-6Al-4V}} = 1.138 \times 10^5$ MPa and Poisson's ratio $\nu_{\text{Ti-6Al-4V}} = 0.342$. The impurities in the material are assumed to have an elastic modulus $E_{\text{imp}} = 0.02E_{\text{Ti-6Al-4V}}$ and Poisson's ratio $\nu_{\text{imp}} = 0.3$. We generate 200 random microstructures with $T = 4\pi$ and $K = 25$ similar to shown in Fig. 4a (see Sect. 3.3). The first-order computational homogenization uses a discretization of $100 \times 100 \times 100$ and six linear analyses for each of these microstructures to estimate the homogenized constitutive tensor. For one layout of the microstructure configuration, we randomly assign each element in the finite element model one of the 200 possible microstructures. Hence, the stochastic dimension of this problem is extremely high. Instead, in our proposed approach, we only consider one random material layout per iteration and use a stochastic gradient-based approach.
4.3.3 Optimization results

Using Adam with a step size $\eta = 0.05$ and penalties $\kappa = [10^4, 10^4]^T$ to implement the constraints, we obtain the final design shown in Fig. 22b. When compared to a deterministic design using GCMMA with mean homogenized constitutive tensor estimated from 200 realizations of the random microstructure (see Fig. 22c), the Adam design under microstructural uncertainty produces a design with thicker members to address the variability in the material properties for different realizations of the microstructures over the design optimization iterations. In contrast, in the deterministic case, the material properties remain the same everywhere in the design domain throughout the design process. Note that the volumes of the deterministic and stochastic designs shown in Fig. 22c and b are 8.36 cm$^3$ and 31.09 cm$^3$, respectively. Figure 23 shows the progression of the objective during optimization. Note that the Adam algorithm satisfies the mass inequality constraint. The violation in the equality constraint to ensure connections at the bolts only is $O(10^{-6})$. In Fig. 24, we show the ratio of the first two diagonal elements of the constitutive tensor, illustrating the variability in the microstructural properties.

We also use GCMMA with the same step size as above, but GCMMA fails to converge in this example as it removes material from the design domain abruptly based on the stochastic gradients of the current optimization iteration. Smaller step sizes for GCMMA, on the other hand, slow down the convergence significantly. Similarly, increasing $n_v$ does not result in convergence within a reasonable computational budget for GCMMA. In one of our previous works (De et al. 2020a), we showed that GCMMA requires more accurate gradients to converge when the variance of the stochastic gradients is significantly large. As we are using only one random microstructure layout per iteration compared to four in the previous examples, GCMMA fails here.

5 Conclusions

Uncertainties in the microstructure of composite materials are frequently encountered across engineering applications. To design structures that are robust with respect to microstructural uncertainty, the mean performance needs to be estimated. Using standard gradient-based optimization methods requires accurate estimations of objectives, constraints, and their design sensitivities. Computing this information by the standard Monte Carlo methods may require a large number of samples increasing the computational cost. In this paper, to significantly reduce the computational cost, we presented an approach where only a handful ($\sim O(1)$) of the possible microstructural configurations selected randomly need to be considered per optimization iteration. This results in stochastic gradients, which we used with two algorithms,
namely Adam and GCMMA. The proposed approach, to the best of our knowledge, is the first to tackle such TO problems, as they are beyond the capabilities of current tools, which require a large computational budget. We illustrated this approach with a two-dimensional and two three-dimensional problems. These examples show the effectiveness of the proposed approach in reducing the computational cost of the optimization. Among the two algorithms, in the presence of large uncertainty, Adam outperforms GCMMA. Further, without an accurate estimation of the gradients, GCMMA is prone to diverge. Increasing the number of realizations of the uncertain parameters to get more accurate estimates of the gradients in GCMMA, however, results in an impossible computational budget. In the future, we plan to incorporate spatial correlation to generate random microstructures and additive manufacturing constraints into the proposed topology optimization process.

Fig. 22 We start the optimization from the initial design shown in (a) and Adam produces the final design shown in (b). The design shown in (c) is obtained from a deterministic design optimization with mean homogenized constitutive tensor estimated using 200 realizations of the random microstructure.

Fig. 23 Reduction of objective in Example 3 using Adam with a zoomed-in portion showing some oscillations at the end of the optimization due to the stochastic nature of gradients.

Fig. 24 The color shading shows the ratio $C_{1111}/C_{2222}$ of the first two diagonal elements of the constitutive tensor $\mathbb{C}_{\text{hom}}$ for the designed structure in Example 3 for one random layout of the microstructure.
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Declarations

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

Replication of results The stochastic gradient-based optimization algorithms used to generate results in Sect. 4 have been implemented in MATLAB and will be uploaded to the GitHub page https://github.com/CU-UQ/TOuU once the paper is published. The TO and XFEM calculations were performed using an in-house solver that is not at the stage of being publicly available. However, the MATLAB codes used in this study can interface with other TO and XFEM codes.

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Table 5 Summary of specifications used to formulate and solve the optimization problem in Example 3

| Category                      | Parameter                     | Value                        |
|-------------------------------|-------------------------------|------------------------------|
| Problem formulation           | Weight for strain energy, \( w_p \) | 0.05                         |
|                               | Weight for mass, \( w_m \)   | 50.0                         |
|                               | Weight for bolt connection penalty, \( w_{\phi} \) | \( 5 \times 10^4 \)         |
|                               | Weight for perimeter penalty, \( w_{per} \) | 0.10                         |
|                               | Weight for regularization penalty, \( w_{\text{reg}} \) | 1.00                         |
|                               | Uniform pressure on the payload | 120 MPa                     |
|                               | Mass constraint, \( r_{\text{equl}} \) | 0.30                         |
| Microstructure                | Period, \( T \)               | \( 4\pi \)                   |
|                               | Max. wavenumber, \( K \)     | 25                           |
|                               | Elastic modulus of Ti-6Al-4V alloy, \( E_{\text{Ti–6Al–4V}} \) | \( 1.138 \times 10^5 \) MPa  |
|                               | Elastic modulus of impurities, \( E_{\text{imp}} \) | \( 2.276 \times 10^3 \) MPa  |
|                               | Poisson’s ratio of Ti-6Al-4V alloy, \( \nu_{\text{Ti–6Al–4V}} \) | 0.342                        |
|                               | Poisson’s ratio of impurities, \( \nu_{\text{imp}} \) | 0.3                          |
|                               | Density of the impure alloy | 44.3 kg/m\(^3\)              |
| Solution strategy             | No. of possible microstructures per elem. | 200                          |
|                               | Random config. per iter., \( n_x \) | 1                           |
|                               | No. of optimization variables, \( n_{\theta} \) | \( 4.03 \times 10^5 \)       |
|                               | Step size, \( \eta \)         | 0.05                         |
|                               | Penalties to implement \( C_1(\theta) \) and \( C_2(\theta), \kappa \) | \([10^4, 10^4]^T\)        |

The values are in consistent units.
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