Surrogate models for manufactured materials with random imperfections

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Abstract

Manufactured materials usually contain random imperfections due to the fabrication process, e.g., the 3D-printing, casting, etc. In this work, we present a new flexible class of digital surrogate models which imitate the manufactured material respecting the statistical features of random imperfections. The surrogate model is constructed as the level-set of a linear combination of the intensity field representing the topological shape and the Gaussian perturbation representing the imperfections. The mathematical design parameters of the model are related to physical ones and thus easy to comprehend. The calibration of the model parameters is performed using progressive batching sub-sampled quasi-Newton minimization, using a designed distance measure between synthetic samples and the data. Then, owing to a fast sampling algorithm, we have access to an arbitrary number of synthetic samples that can be used in Monte Carlo type methods for uncertainty quantification of the material response. In particular, we illustrate the method with a surrogate model for an imperfect octet-truss lattice cell, which plays an important role in additive manufacturing. We also discuss potential model extensions.

Keywords: Additive manufacturing, Surrogate model, Statistical properties/methods, Stochastic optimization

1. Introduction

In structural design, the shape and architecture of manufactured materials are usually optimized assuming perfect, defect-free geometries. However, the as-manufactured material may differ from the as-designed one, in particular, owing to defects induced by the manufacturing process. A typical example is the structures manufactured using 3D-printing technologies. Moreover, the material response of as-manufactured materials may be quite sensitive to the process-induced imperfections; see [1, 2, 3, 4, 5]. More robust material design requires that imperfections be taken into account [6]. Since the imperfections are random in nature, the characterization of the properties of manufactured materials is performed using statistical methods. Therefore, given that the number of real as-manufactured samples is limited, a common strategy is the development of a so-called digital twin – a mathematical model of a surrogate material given by a random field reproducing the topological shape and imitating statistical properties of the target real-world material. The philosophy is to introduce a flexible class of potential surrogate materials characterized by several design parameters that need to be tuned. Then, the numerical model can be employed in uncertainty quantification (UQ), a branch of computational science dealing with the statistics of physical models with uncertainties, where random fields typically enter as simulation inputs [7].

Machine learning is a popular and powerful approach for the construction of surrogate models; see, e.g., [8, 9, 10, 11]. However, it is usually used as a closed black box tool. The created model depends on a large number of not interpretable parameters and requires a large amount of training data. In order to simplify the method, we focus on cases where the topological shape of the structure is a priori known, and the uncertainties include only the process-induced imperfections. Therefore, only a few geometrically interpretable parameters are sufficient to describe the model in this situation.

In this work, we represent the material as a random phase field. Considering a class of surrogate material models characterized by several design parameters, we look for a projection of the target material onto this class by minimizing the distance between vectors of statistical descriptors associated with surrogate samples and the data, respectively.

We discuss a unified form of surrogate models for two-phase heterogeneous materials which present deterministic topological shapes but subject to uncertain imperfections. We formulate the surrogate phase field via the level-set method; see, e.g., [12, 13, 14, 15, 16, 17]. The introduced level-set function (called intensity) is a random field given by a combination of the known topological structure and a random perturbation field representing the imperfections. Then, we address several examples of the model construction for reproducing particular two-phase structure types such as pores, beams, cracks, lattices, etc.

We demonstrate the use of the proposed model for a 3D-
printed octet-truss lattice. First, we calibrate the model such that it reproduces statistical properties of several manufactured material samples obtained from RX-Tomography measurements. To this end, we formulate and solve a stochastic optimization problem to find the model design parameters minimizing a specific misfit measure between the synthetic samples and the data. In order to avoid oversampling, a progressive batching strategy is applied, when an appropriate number of samples is estimated at each iteration and is adaptively updated using a specific test; see [18, 19, 20, 21, 22]. Such efficient stochastic programming methods are important for large-scale decision-making problems, especially in engineering design, where oversampling is significantly costly. The implementation also benefits from algorithmic differentiation for learning the model parameters.

Once the surrogate model is calibrated, we use it to generate synthetic samples in the crude Monte Carlo method to quantify the uncertainties in the linear elastic response. We treat the material properties, such as homogenized bulk and shear moduli, computed on one material sample, as random variables, and we estimate their probability distribution.

The structure of the paper is as follows. In Section 2, we formulate the general problem and introduce the notation. In Section 3, we formulate the surrogate material model and discuss several examples of the structure. In Section 4, we focus on a particular example, the octet-truss lattice, to demonstrate the calibration of the surrogate model and its application. To this end, we formulate a distance measure between synthetic samples and the data, and proceed with optimization of the model parameters. The technical details of the sub-sampled quasi-Newton minimization algorithm are given in Appendix A. Once the surrogate model is calibrated, we use it to generate synthetic samples in a crude Monte Carlo method to quantify the uncertainties in the linear elastic response. Finally, we discuss possible model extensions and perspectives in Section 5.

2. Preliminaries

Let $\Omega = [0, 1]^3$ be the 3-dimensional unit cube with periodic boundaries associated with a representative volume element (RVE) of the architected material. We consider a two-phase (binary) material, defined by the phase field

$$\varphi(x) = \begin{cases} 0, & \text{if } x \in \Omega_1, \\ 1, & \text{if } x \in \Omega_2, \end{cases}$$

where the domain $\Omega_1$ corresponds to the phase one and $\Omega_2 = \Omega \setminus \Omega_1$ to the phase two. Owing to uncertainties in the manufacturing process, the phase field $\varphi$ is a random field. That is, for each $x \in \Omega$, the value $\varphi(x)$ is a random value correlated with all other points in $\Omega$. Thus, a digital 3D image representation of the phase field $\varphi$ is given by a multivariate random vector.

We shall consider a series of particular realizations of the material distribution expressed by the phase field $\varphi(x; \omega)$, where $\omega$ is a sample indicator. For simplicity, we will also write $\varphi(\omega) := \varphi(\cdot; \omega)$. In particular, in our numerical experiments, we associate $\omega$ with the seed of the pseudorandom number generator. We also denote the mean value by $\mathbb{E}_\omega[f(\varphi(\omega))]$ for any given functional $f$.

Let us further denote by $\varphi_*$ the phase field characterizing the real manufactured material, which we will call the target material. In practice, this distribution is unknown, and only a small number of samples $X_i = \varphi_*(\omega_i)$, $i = 1 \ldots N_{\text{data}}$, is accessible (e.g., as CT scans).

Our purpose is to construct a surrogate mathematical model (so-called digital twin) which allows the generation of synthetic samples with small computational cost and have statistical properties similar to the target material $\varphi_*$. Let us define a surrogate material model $M_\theta$ as a parametrized family of random phase fields $\varphi_\theta = \varphi(\theta)$, where $\theta$ is the vector of design parameters. Then, our digital twin is understood as a projection of $\varphi_*$ onto the set $M_\theta$. That is, we want to find the optimal design parameters minimizing some distance measure between the distributions $\varphi_\theta$ and $\varphi_*$, formulated in terms of specific statistical descriptors. However, given only a set of samples of $\varphi_*$, we can minimize only the distance between the random field $\varphi(\theta)$ and the data set $X = \{X_1, \ldots\}$ of available realizations. In particular, we consider an objective function $J(\theta) := \mathbb{E}_\omega[J(\varphi(\theta, \omega), X)]$, where $J(\varphi(\theta, \omega), X)$ denotes the distance from a particular surrogate sample $\omega$ to the data set $X$. A choice of such distance measure will be further discussed in details in Section 4.1, where we formulate the corresponding stochastic optimization problem. A visual diagram of the calibration process of the surrogate material model is given in Figure 1.

In this way, extracting statistical information from the morphology of the given samples of the architected material, we construct a random field, which captures the principal geometric features and imitates the statistical properties of the target material samples. Then, employing a fast sampling procedure, we have access to an arbitrary number of synthetic samples that can be used for computational purposes, in particular, in Monte Carlo methods, for uncertainty quantification of the material response, quantities of interest, etc..

3. Surrogate material model

A common strategy to define a synthetic phase field is the level-set method (gray-scale thresholding), where the phases are defined as level-sets of some continuous intensity field (gray-scale). That is, we define the phase field as

$$\varphi(x; \theta, \omega) = \begin{cases} 0, & \text{if } u(x; \theta, \omega) < 0, \\ 1, & \text{otherwise}, \end{cases}$$

$x \in \Omega$, where the random intensity field $u$ is parametrized with $\theta$ and $\omega$ is a sample indicator.

Our purpose is to construct the field which combines both a deterministic topological shape and uncertain imperfections. An example of such combination can be found, for example, in [17], where the intensity is considered as a Gaussian random field with the mean non-constant in $\Omega$. In the current work, we consider a generalized hybrid model, where the intensity field is given by a linear combination of two intensities:

$$u(x; \theta, \omega) = (1 - \alpha) \cdot u_1(x; \theta, \omega) + \alpha \cdot u_2(x; \theta, \omega).$$
Here, $u_1$ defines the topological support, and $u_2$ is a random perturbation representing the imperfections. Note that the topological support $u_1$ can also exhibit uncertainties and that $u_1$ and $u_2$ are statistically independent. The parameter $\alpha \in [0; 1]$ defines the perturbation level, controlling the contribution of each logical support $u_1$ and $u_2$. The perturbation representing the imperfections. Note that the topological support $u_1$ is already scaled with $\alpha$.

### 3.1. Perturbation field. Gaussian model

We define the intensity perturbation $u_2$ as a centered Gaussian random field with a given covariance function $C(x, y) := \mathbb{E}[u_2(x)u_2(y)]$. As $u_2$ is already scaled with $\alpha$, we can assume without loss of generality that it has unit marginal variance $C(x, x) = 1$ for all $x$. Moreover, we assume that the random field $u_2$ is statistically homogeneous (stationary), that is, the covariance function is of the form $C(x, y) = C(x - y)$.

A stationary Gaussian random field $u_2$ can be formally written as a convolution; see [23]:

$$u_2(x) = C_1 * u(x),$$  \hspace{1cm} (3)

$x \in \Omega$, where $\ast$ denotes the convolution product in $\mathbb{R}^3$, and $\eta$ denotes the white Gaussian noise in $\mathbb{R}^3$ [24, 25]. The convolution kernel $C_1$ is the square root of the the covariance operator in the sense that $C_1 \cdot C_1 = C$.

The covariance function defines how the values $u_2(x)$ are correlated at distinct points $x$. We will consider herein a stationary covariance function of the form

$$C(x - y) = M_\nu \left( \frac{\sqrt{2\nu}}{\ell} ||x - y|| \right).$$  \hspace{1cm} (4)

where $||\cdot||$ stands for the Euclidean norm, and $M_\nu(x)$ is the normalized Matérn kernel [26, 27]:

$$M_\nu(x) = \frac{x^\nu K_\nu(x)}{2^{\nu-1} \Gamma(\nu)}.$$  \hspace{1cm} (5)

Here, $\Gamma(x)$ and $K_\nu(x)$ denote the Euler Gamma function and the modified Bessel function of the second kind [28, 29], respectively. The covariance function is parametrized using two parameters: regularity $\nu > 0$ and correlation length $\ell > 0$, which thus make part of the design parameters vector of the surrogate model. The Matérn covariance is widely used in statistics [27, 30], geostatistics [31] and machine learning [32]. It represents a large class of covariance kernels, varying from the exponential ($\nu = 0.5$) to the squared-exponential ($\nu \to \infty$). In particular, the parameter $\nu$ controls the regularity of the function at zero: from weak singularity to infinite smoothness. The regularity of the kernel at the origin is directly related to the smoothness of the level-set of the corresponding Gaussian field. However, because of the voxelized nature of the digital samples, the accuracy of the parameter $\nu$ is limited by the resolution of the image. Moreover, as shown in [17], when fitting the data to a Matérn model, there arises a manifold of near-optimal pairs ($\nu, \ell$); see also [33]. This makes the identification of a unique regularity $\nu$ and correlation length $\ell$ problematic.

The Gaussian model admits an efficient sampling procedure by the spectral simulation method employing the Fast Fourier transform (FFT) algorithm on a regular grid; see [34, 35] and the references therein. Indeed, by the convolution theorem, the convolution product in (3) reduces under Fourier transformation to a point-wise product of two fields:

$$\hat{u}(k) = \hat{C}_1(k) \hat{\eta}(k),$$

where $k$ corresponds to the wavevector, $\hat{u}$ and $\hat{C}$ denote Fourier transforms of $u$ and $C$, respectively, and the Fourier transform $\hat{\eta}$ of the Gaussian noise is a complex Gaussian noise. The use of the FFT algorithm makes it possible to reduce the complexity of the generation of one sample from $O(N^2)$ for the direct convolution approximation to $O(N \log N)$, where $N$ corresponds to the number of voxels. The Fourier transform in $\mathbb{R}^d$ of the Matérn kernel is given explicitly by

$$\hat{C}(k) = \left| \hat{C}_1(k) \right|^2 =$$

$$= \left( \frac{2\pi^\frac{\nu}{2}}{\nu} \frac{\Gamma(\nu + \frac{d}{2})}{\Gamma(\nu)} \left( 1 + \frac{\ell^2}{2\nu ||k||^2} \right)^{-(\nu + \frac{d}{2})} \right),$$

see [36, Vol.II, section 8.13, formula (3)].

Remark 1. A remarkable feature of a Matérn kernel is that it
is associated with the Green’s function for the fractional differential equation of the form (up to a factor)

\[
(1 - \frac{c^2}{2\nu})^{(\nu+\frac{1}{2})/2} \quad u_2 = \eta,
\]

where \(\Delta\) is the Laplace operator; see [37] [38]. Thus, imposing boundary conditions and using variable coefficients, \(u_2\) can be extended to a more general non-stationary random field, see, e.g., [39] [40] [41]. Though it is important to mention these extension options, such models are beyond the scope of the current paper.

Example 1 (Gaussian level-set). Let \(\alpha = 0.5\), and let the structure term \(u_1\) be constant in \(\Omega\), i.e., \(u_1(x) \equiv \tau \in \mathbb{R}\) for \(x \in \Omega\). Then, the phase field \(\varphi\) is reduced to the threshold of a Gaussian random field with the mean \(\tau\) and covariance \(C(x, y)\), which corresponds to the common Gaussian level-set model; see, e.g., [42] [43] [44] [45] [46]. The resulting random field is statistically homogeneous and exhibits no particular topological shape.

In Figure 2, the sample (2a) presents a typical examples of the Gaussian level-set model, while the samples (2b) and (2c) illustrate its modified variants. In particular, the sample (2b) is obtained by introducing the anisotropic metric in (4), i.e., considering the norm \(\|A_k(\omega)(x - y)\|\) with the metric tensor \(A_k\) defined by a definite positive \(3 \times 3\) matrix. Its eigenvalues control the length scales in the directions defined by the corresponding eigenvectors, which leads to an anisotropic phase field. The sample (2c) is obtained by replacing \(u_2\) with \([u_2]\) (folded Gaussian distribution), which allows the connectivity properties of the two phases to be distinguished.

It is known that in the case of the Gaussian model, explicit closed-form formulas are available for statistical descriptors of the phase field \(\varphi\), such as the mean (expected volume fraction) \(\varphi\) and the two-point correlation function; see, e.g., [47] [48]. In particular, the expected volume fraction \(\varphi\) is uniquely defined by the mean of the Gaussian intensity \(\tau\). However, in the general case, explicit formulas for statistical moments are generally not available, and thus the statistics must be approximated numerically using, e.g., Monte Carlo methods.

Though stationary random fields are easy to sample, they cannot reproduce the topological features of the statistically inhomogeneous media, such as randomly oriented particles or beams, cracks, imperfect lattice, etc.

3.2. Topological support intensity

A very simple surrogate for a porous media can be obtained as a collection of particles of ideal shape, e.g., ellipsoids [49] [50]. Each such particle can be represented as level set of a cone in higher dimension [51]. This inspires us to introduce the intensity field for an arbitrary geometrical structure in (2) as a generalized cone given by the formula

\[
u_1(x; \omega) = \tau - \rho(x, \mathcal{G}(\omega)), \tag{5}
\]

where \(\rho(x, \mathcal{G})\) denotes the distance from the point \(x \in \Omega\) to a manifold \(\mathcal{G}\), which defines the geometrical structure; the parameter \(\tau\) corresponds to the characteristic size of the structure and plays the role of the threshold in the level set model (1). Thus, the phase field (1) with intensity (5) and \(\alpha = 0\), takes the value one in the points having a distance of at most \(\tau\) from the manifold \(\mathcal{G}\).

Example 2 (Collection of particles). An obvious example of structured material is a heterogeneous material with disjoint inclusions represented by collection of imperfect particles. Such structures can be constructed using the hybrid model (1) [1] [2] where the structure intensity \(u_1\) is given by the so-called maximum cones [51] – the maximum of the set of cones centered in randomly distributed points. Thus, it can be written in the form (5) with the associated support structure given by a collection of randomly distributed points, particles centers, \(\mathcal{G}(\omega) = \mathcal{G}_{\text{particles}}(\omega) = \{c_k(\omega), \quad k = 1, \ldots, N(\omega)\}\). Then, the distance to the manifold \(\mathcal{G}_{\text{particles}}\) is given by the maximum of the distances to each of the centers:

\[
\rho(x, \mathcal{G}_{\text{particles}}(\omega)) = \min_{k \leq N(\omega)} \|c_k(\omega)(x - c_k(\omega))\|_p.
\]

The particle shapes are defined by metric tensors \(A_k(\omega)\) and the norm type \(\|\cdot\|_p\). In particular, the values \(p = 1, p = 2\) or \(p = \infty\) correspond to the diamond, ellipsoid or rectangular shapes, respectively. For each particle \(k = 1, \ldots, N\), the eigenvectors and eigenvalues of the metric tensor \(A_k\) define the principal axes (particle orientation) and the corresponding length scales, respectively.

Figure 3 shows examples of imperfect inclusions with different eigen lengths. The particle orientation is random and obtained from three uniformly distributed Euler angles.

Example 3 (Cracks). A networks of cracks in the solids can also be represented in this framework. The support structure is the boundary of Voronoi tessellation, \(\mathcal{G}(\omega) = \mathcal{G}_{\text{Voronoi}}(\omega)\), associated with the set of random points \(\mathcal{G}_{\text{particles}}(\omega) = \{c_k(\omega), \quad k = 1, \ldots, N(\omega)\}\) from the previous example. In particular, we define the distance from a point \(x \in \Omega\) to the manifold \(\mathcal{G}_{\text{Voronoi}}\) by

\[
\rho(x, \mathcal{G}_{\text{Voronoi}}(\omega)) = \frac{1}{2} \left| \frac{a^2(x) - b^2(x)}{c(x)} \right|,
\]

where \(a\) and \(b\) are the distances from \(x\) to the two closest centers \(k_1\) and \(k_2\), i.e., two minimum distances of \(\rho(x, c_k) = \|x - c_k\|, \quad k = 1, \ldots, N\); and \(c\) is the distance between \(c_{k_1}\) and \(c_{k_2}\). An example of a surrogate solid with cracks is given in Figure 4a. Note that in this case, the parameter \(\tau\) in (5) corresponds to half of the mean crack opening size.

Example 4 (Gyroid). As another example, we consider a gyroid lattice [52], which is a popular architecture pattern in additive manufacturing. Although gyroid is defined by the equations involving elliptical integrals [53], its close approximation is given by level surface of a simple trigonometric expression [54]. This level-set function thus naturally defines our dis-
Figure 2: Examples of Gaussian level-set model (Example 1): (a) isotropic two-phase media; (b) anisotropic metric; (c) considering folded Gaussian distribution allows to distinguish connectivity of the phases.

Figure 3: Examples of the hybrid model with collection of random points as support structure (see Example 2): (a) isotropic metric (spherical particles); (b) anisotropic metric (disks); (c) anisotropic metric (beams). The surface imperfections are of level $\alpha = 0.01$ with covariance of regularity $\nu = 2$ and correlation length $\ell = 0.03$.

Figure 4: (a) Example of synthetic cracks network (Example 3) with the mean opening $2\tau = 0.02$ and imperfections of level $\alpha = 0.005$ with covariance of regularity $\nu = 2$ and correlation length $\ell = 0.03$; (b) Example of synthetic gyroid structure (Example 4) subject to surface imperfections of level $\alpha = 0.03$ with covariance of regularity $\nu = 2$ and correlation length $\ell = 0.015$, $\tau = 0.05$. 

(a) $\phi = 0.1, \nu = 2, \ell = 0.1$
(b) $\phi = 0.1, \nu = 2, \ell = 0.05$, lengthscales $[10, 1, 1]$
(c) $\phi = 0.1, \nu = 2, \ell = 0.1$, folded Gaussian intensity

(a) isotropic with $\tau = 0.08$
(b) lengthscales $[3, 1, 3]$ with $\tau = 0.05$
(c) lengthscales $[200, 1, 1]$ with $\tau = 0.05$
tance from a point \( x \in \Omega \) to the manifold \( \mathcal{G}_{\text{gyroid}} \):

\[
\rho(x, \mathcal{G}_{\text{gyroid}}) = [\sin(2\pi x) \cos(2\pi y) + \sin(2\pi x) \cos(2\pi z)]^2,
\]

where \( x = (x, y, z) \in \Omega \). Note that without loss of generality, the square can be replaced with the absolute value. Besides, the parameter \( \tau \) in (3) controls the thickness of the structure. An example of a surrogate gyroid structure is given in Figure 4b.

Example 5 (Octet-truss lattice). The octet-truss lattice structure (Figure 5a) is another popular architecture pattern in additive manufacturing. The connectivity of the struts in its unit cell is schematically depicted in Figure 5b. Owing to the cell symmetry, it is sufficient to construct a quarter (subcell) of the cell. The nodes of the subcell are given in local coordinates by

\[
[p_k, k = 1, \ldots, 4] = \{(0, 0, 0), (0, 1, 1), (1, 0, 1), (1, 1, 0)\}.
\]

Then, the manifold \( \mathcal{G}_{\text{lattice}} \) for the subcell is given by the set of the edges (struts):

\[
\{e_k = (e_{k,1}, e_{k,2}), k = 1, \ldots, 6\} =
(\{p_1, p_3\}, (p_1, p_2), (p_2, p_3), (p_3, p_4), (p_2, p_4), (p_1, p_4)).
\]

And, therefore, the distance to \( \mathcal{G}_{\text{lattice}} \) is defined as

\[
\rho(x, \mathcal{G}_{\text{lattice}}) = \min_{k \in 6} \rho(x, e_k),
\]

where \( \rho(x, e_k) \) is the distance from \( x \) to the edge \( e_k \) which is given by the formula

\[
\rho(x, e_k) := \left[ \frac{a^2 + b^2}{2} - \frac{c^2}{4} - \left( \frac{a^2 - b^2}{2c} \right)^2 \right]^{1/2},
\]

and \( a = \rho(x, e_{k,1}), b = \rho(x, e_{k,2}), c = \rho(e_{k,1}, e_{k,2}) \) are Euclidean distances between the points.

Figure 6 shows examples of the surrogate octet lattice cell with different values of the uncertainty level \( \alpha \) and the correlation length \( \ell \). The average strut radius is defined by the parameter \( \tau \) in (5). Notice that with a high imperfection level \( \alpha \), the struts may even lose their connectivity, which is an important case in risk-adverseness problems and in failure probability analysis.

4. Application example: Octet lattice

In this section, we demonstrate the calibration of a surrogate material model. To do this, we solve an optimization problem for finding the optimal design parameters of the model, minimizing the misfit between the synthetic model and the target material using a set of statistical/geometrical descriptors. Then, we proceed with an application of the surrogate material in stochastic homogenization. We use the calibrated model to generate an arbitrary number of synthetic samples within a Monte Carlo simulation for uncertainty quantification of the material effective properties. In what follows, for our numerical experiments, we focus on a particular structure: octet-truss lattice cell (see Example 5).

4.1. Calibration of the model parameters

We consider the following stochastic optimization problem:

\[
\min_{\theta} \mathbb{E}_\omega [J(\theta, \omega)],
\]

where by \( J \) we denote a distance measure between a surrogate sample \( \omega \) and the data. In order to define such a measure, we use a set of geometrical descriptors \( d_i \). The explicit choice of descriptors will be discussed below. Then, we define \( J \) as misfits between the corresponding descriptors:

\[
J(\theta, \omega) = \frac{1}{2} \sum_{i} \frac{||d_i(\varphi(\omega)) - d^*_i||^2}{||d^*_i||^2},
\]

where \( d^*_i \) are the target descriptors obtained from the data, and the norm is the \( L^2(\Omega) \)-norm.

The design parameters include here the average strut radius \( \tau > 0 \) and the imperfection level \( \alpha \in [0, 1] \) and the correlation length \( \ell > 0 \) of the surface imperfections. In order to avoid constrained optimization, we define the vector of design parameters as follows:

\[
\theta := [\log \tau, \tan\theta(2\pi - 1), -\log \ell].
\]

Remark 2. Note that in (1), the Heaviside unit step function is not differentiable. Thus, in the optimization process, we replace it with its smooth approximation:

\[
\varphi(x; \omega) = \sigma(u(x; \omega))
\]

with a smooth activation function approximating the unit step, e.g., \( \sigma(x) = (1 + \tanh(x/\epsilon))/2 \), where \( \epsilon \) is small. In particular, we use \( \epsilon = h^2 \), where \( h \) stands for the voxel size.

Let us now discuss the choice of the descriptors \( d_i \). We use the material volume fraction and its specific surface area as the two first geometrical descriptors. Specific surface area is the ratio of the surface area of the phase interface to the volume of the phase. For the regularized version of the two-phase material (8), we approximate the indicator function of the phase boundary with the absolute value of the gradient of the phase field. We will refer to it as the interface field \( |\nabla \varphi(x)| \). These descriptors are global and cannot catch the local structure of the
sample. To do this, we use the autocorrelation of the phase-field as another descriptor. For a statistically homogeneous random field, the field autocorrelation approximates the two-point correlation function. Here, though the perturbation field is considered to be homogeneous, the octet cell structure is not. Moreover, the structure size dominates the perturbation correlation length scale. That is, autocorrelation can provide information on the structure size, but it hardly detects the localized properties of the perturbation. In order to get information on the perturbation, we need to consider the geometric features of the material surface. To this end, we use the autocorrelation of the interface field as the fourth descriptor. Thus, in our numerical material surface. To this end, we use the autocorrelation of the perturbation, we need to consider the geometric features of the properties of the perturbation. In order to get information on the correlation length scale. That is, autocorrelation can provide information on the two-point correlation. Moreover, the structure size dominates the perturbation correlation length scale. That is, autocorrelation can provide information on the structure size, but it hardly detects the localized properties of the perturbation. To this end, we use the autocorrelation of the interface field as the fourth descriptor. Thus, in our numerical experiments, we use the following geometrical descriptor of a sampled phase field $\varphi$:

$$d_1(\varphi) = \int_{\Omega} \varphi(x) \, dx,$$

$$d_2(\varphi) = \int_{\Omega} |\nabla \varphi(x)| \, dx,$$

$$d_3(\varphi; r) = \int_{\Omega} [\varphi(x + r) - d_1(\varphi)] \cdot [\varphi(x) - d_1(\varphi)] \, dx,$$

$$d_4(\varphi; r) = \int_{\Omega} [\nabla \varphi(x + r) - d_2(\varphi)] \cdot [\nabla \varphi(x) - d_2(\varphi)] \, dx,$$

with the spacing $r \in \Omega$. Given an image of the real sample $X = \varphi_i(\omega)$, the target descriptors are defined as $d_j^* := d_j(X)$. In case of a batch of the target material samples $X = \{X_j = \varphi_i(\omega_j), \quad j = 1, \ldots, N_{\text{data}}\}$, the target descriptors can be defined as the average $d_j^* := \frac{1}{N_{\text{data}}} \sum_{i=1}^{N_{\text{data}}} d_j(X)$.

4.2. Numerical results

We calibrate the model design parameters by solving the stochastic optimization problem. In order to avoid over-sampling, a progressive batching strategy is applied, when the appropriate number of samples (batch size $|S_k|$) is estimated at each iteration $k$ and is adaptively updated satisfying specific conditions; see \cite{18,19,20,21}. In our implementation, we followed the progressive batching LBFGS algorithm proposed in \cite{56}. Technical details of the algorithm can be found in Appendix \ref{Appendix A}.

The surrogate model generator is implemented using PyTorch \cite{57}, allowing to benefit from algorithmic differentiation for learning the model parameters. In particular, we use PyTorch-LBFGS package \cite{58} for implementation of the progressive batching minimization.

The target material is the octet-truss lattice structure manufactured using an SLM printer \cite{59} from 316L stainless steel. The relative density of the structure is 0.3. The images of the octet lattice have been obtained on the as-printed specimens at the In Situ Innovative Set-ups for X-ray micro-tomography on the ISIS4D platform \cite{60}. Reconstruction of the tomographic data is performed with a filtered back-projection algorithm \cite{61} using X-Act software. Similar X-ray tomography reconstructions have been used for exploring plasticity and fatigue phenomena on various material, see, e.g., \cite{62,63,64}.

We use 6 different lattice cells obtained from the CT image and fit the surrogate model individually on each of these targets, comparing at the end the results of these different fittings. We fix $\nu = 2$ assuming moderate smoothness of the imperfect interface. Therefore, our three parameters to calibrate are the strut thickness $2\tau$, the imperfection level $\alpha$ and the correlation length $\ell$. The initial guess for the model parameters: $2\tau_0 = 0.3$, $\alpha_0 = 0.1$, $\ell_0 = 0.1$. The stopping criterion is reached when the loss increment is less than the fixed tolerance, precisely, $\nabla_{\theta} F_k : \Delta \theta < 10^{-4}$. Figure 7 shows the convergence of the loss function, its increment and the max-norm of its gradient. And Figure 8 shows the evolution of the model parameters. Comparison of a calibrated model sample with an initial guess sample as well as with the target (the first cell) can be found in Figure 9. The progress of the batch size $|S_k|$ is depicted in Figure 10 for each individual cell fitting. For all our samples the stopping criterion is reached within 35 iterations, but in some cases 15 iterations were sufficient. Although only one data sample was considered for each case,
Figure 7: Convergence of the loss function (a), the loss increment (b) and the gradient norm (c) for each individual cell fitting.

Figure 8: Convergence of the model parameters for each individual cell fitting: (a) strut thickness; (b) imperfection level; (c) correlation length.

Figure 9: Calibration of the surrogate model for the first cell: sample examples for the initial guess model (a), the resulting model (b) and the target cell (c).
we can observe that the deviation of the resulting parameters is small; see (9) below. This is due to the fact that the distribution of the imperfections over the material surface is statistically homogeneously, and even one sample provides enough information on the statistical properties of the uncertainties. Note that in the general case, the required number of data samples can be larger depending on the deviation of the resulting design parameters. In case more data samples are available, Bayesian inference techniques can also be employed.

4.3. Uncertainty quantification

Owing to the structure imperfection, the material properties, such as effective bulk and shear moduli, computed on one material sample are random variables. Once the surrogate material model is calibrated with respect to the real material data, we can proceed with uncertainty quantification of the material properties and, in particular, estimation of their probability distribution function (PDF). To this end, using synthetic samples, we employ a crude Monte Carlo method to approximate the mean and the standard deviation of the quantities of interest (QoIs).

Moreover, we assume the design parameters \( \theta \), defined by (7), to be random i.i.d. normally distributed with the mean and the standard deviation estimated using the calibration results for different cells from the previous section, precisely,

\[
\theta \sim \mathcal{N}\left(\begin{bmatrix} -1.8 \\ -1.94 \\ -3.21 \end{bmatrix}, \begin{bmatrix} 0.018^2 & 0.046^2 & 0.043^2 \\ 0.046^2 & 0.04^2 & 0.031^2 \\ 0.043^2 & 0.031^2 & 0.023^2 \end{bmatrix}\right). \tag{9}
\]

Thus, for each surrogate sample \( \omega \), we first sample the design parameters \( \theta(\omega) \) and then the corresponding phase field realization \( \varphi(\theta(\omega), \omega) \).

For each such sample, we compute the linear elastic material response, the macroscopic strains \( \hat{\varepsilon} \), to the applied macroscopic stress

\[
\sigma = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}
\]

Given a linear problem, we simply assume the Young’s modulus of the base material equal to one (zero in the void phase). The material Poisson ratio is set to 0.3. We use the FFT-based numerical scheme proposed in [65, 66], which is designed to handle an infinite contrast. Then we compute the corresponding effective bulk \( K \) and shear \( G \) moduli:

\[
K = \frac{1}{3} \frac{\text{tr} \sigma}{\text{tr} \hat{\varepsilon}}, \quad G = \frac{1}{2} \frac{\sigma_{12}}{\hat{\varepsilon}_{12}}.
\]

Using 100 synthetic material samples, we approximate the mean as 0.045 and the standard deviation as 0.0056 for the bulk modulus \( K \), and the mean as 0.0315 and the standard deviation as 0.0023 for the shear modulus \( G \). This corresponds to an expectation of the Young modulus of \( E = KG/(3K + G) = 0.076 \). Given the volume fraction of the material in the cell near 0.3, these values are in a good agreement with the numerical and experimental results, e.g., in [67, 68, 69].

Remark 3. More sophisticated estimators of the probability distributions of QoIs can also be considered. For example, computing a number of statistical moments of QoIs, one can construct an approximation of the associated PDF using a moment-matching method (such as the maximum entropy principle). In the current numerical example, since the computed variance of elastic moduli of the imperfect lattice cell is relatively small, we used only two statistical moments.

5. Discussions and perspectives

We proposed a hybrid surrogate material model which combines the topological shape and random imperfections. Given in a unified form, the model is able to reproduce a variety of imperfect structures: porous media, fibers, cracks, lattice structures. We used an imperfect octet-truss lattice cell for an illustration of the surrogate model application. From a small amount of the real samples, we calibrated the model design parameters minimizing the misfit between the corresponding geometrical descriptors. The implementation can benefit from algorithmic differentiation and progressive batching techniques.

Note that we used only geometrical descriptors obtained from the target material samples to calibrate the model and to use it consequently to sample the effective material properties in the linear elasticity framework. In the general case, the effective moduli themselves can be also used as descriptors. That is, in addition to the geometrical descriptors, one can use mechanical descriptors, such as effective material moduli, maximum stress, etc.. In this case, while the mechanical descriptors of the surrogate samples have to be computed numerically, the corresponding target descriptor \( d^* \) can be provided by experimental measurements.

Risk-aversion. Note that the optimization algorithm can be used not only for calibration of a surrogate model, but also for material design, i.e., for construction of a surrogate material with desired mechanical properties. In this case, the expectations of the relevant quantities of interest can be used as the statistical descriptors. Moreover, in the context of material design there naturally arises the risk aversion problem, when it is more important to minimize the probability of extreme values (tail of the
Real grain texture plastification or failure, lower values of \( \xi \) (maximum of von Mises stress). When high values correspond to \( \beta \) (taken from [69]), and a zoom showing the interfaces between layers, cluster of small grains at interfaces and the morphological grain angles for both direction of printing.

Figure 11: (a) Example of a synthetic multi-phase sample imitating polycrystalline grain texture in a manufactured material (not calibrated design parameters).

CVaR [70]: conditional value-at-risk (CVaR) is a quantile VaR (value-at-risk) distribution) than the expectation. In many industrial applications, a common choice for such risk measures is the so-called \( \beta \)-quantile of \( \xi \), 0 < \( \beta \) < 1. For example, let the random variable \( \xi \) denote a stress measure of a structure (e.g., the maximum of von Mises stress). When high values correspond to plastification or failure, lower values of \( \xi \) are preferable. The \( \beta \)-quantile of \( \xi \) represents the most optimistic state which can be achieved in the worst (1 - \( \beta \)) \cdot 100% of possible events, while \( \text{CVaR}\_\beta(\xi) \) represents the expected value of \( \xi \) in these events. It is known (see [71]) that \( \text{CVaR} \) can be written via a scalar minimization problem:

\[
\text{CVaR}_\beta(\xi) = \inf_{q \in \mathbb{R}} \mathbb{E}[q + \frac{1}{1-\beta}(\xi - q)_+],
\]

where \( (\cdot)_+ := \max(0, \cdot) \). Therefore, minimization of \( \text{CVaR} \) can be written in the form [69] with an additional parameter \( q \), which converges to the \( \beta \)-quantile.

Multi-phase fields. Further extension of the discussed surrogate model, one can consider a multi-phase field:

\[
\varphi(x) = \arg\max u_W(x),
\]

where \( u = \{u_1, \ldots, u_k\} \) is a vector random fields, and \( W \) is a matrix of weights, such that \( u_W \) is a vector of intensities corresponding to \( n \) different phases. The \( \arg\max \) activation returns the index of the most intense phase at the point. Its smooth approximation is based on the softmax function. We remark that for \( n = 2 \), \( u = \{u_1, u_2\} \) and \( W \) being diagonal with the entries \( \alpha = 1 \) and \( \alpha \), we recover the hybrid model [11][12]. This extended model is a possible direction for following up work. Here, we only provide a 2D example in Figure 11 in order to outline the potential of this model in application to simulation of the morphologic and crystallographic textures of the polycrystalline grains in the additively manufactured materials [69][72].

Appendix A. Sub-sampled quasi-Newton minimization

In this appendix, we present the details of the sub-sampled quasi-Newton minimization algorithm used for calibration of the surrogate model. The method is proposed in [56]. We also refer the interested reader to [73][19][20][21].

Let us consider a minimization problem in the form

\[
\min_{\theta} J(\theta) = \mathbb{E}_\omega [J(\theta; \omega)].
\]

We define each particular sample with a random seed \( \omega \in S = N \cap [0, 10^3] \) of the pseudo random generator used to sample the uncertainties. The sub-sampled quasi-Newton method iteratively computes a sequence \( \theta_k \) of approximations of the optimal vector of design parameters, using the update formula

\[
\theta_{k+1} = \theta_k - \alpha_k H_k \hat{g}_k^{\varepsilon_k},
\]

where \( \hat{g}_k^{\varepsilon_k} \) is the batch (sub-sampled) gradient of \( J \):

\[
\hat{g}_k^{\varepsilon_k} := \frac{1}{|S_k|} \sum_{\omega \in S_k} g_k(\omega), \quad g_k(\omega) := \nabla J(\theta_k; \omega),
\]

with a set (batch) of material samples (random seeds) \( S_k \) of the size \( |S_k| \). Above, \( H_k \) is a positive definite quasi-Newton operator – an approximation of the inverse Hessian matrix. Using the

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Algorithm 1: Sub-sampled L-BFGS

**Result:** Approximated optimal design parameters $\theta_{opt}$

**Input:** initial guess $\theta_0$, initial sample size $|S_0|

1. repeat
2. Sample batch $S_k \subset S$ of the size $|S_k|$
3. Compute the bound $b_k$ by \((A.1)\)
4. if $|S_k| < b_k$ then
5. Sample $\Delta S_k \subset S \setminus S_k$ with $|\Delta S_k| = |b_k| - |S_k|$;
6. Set $S_k = S_k \cup \Delta S_k$
7. end
8. Compute $\bar{S}_k$
9. Compute $p_k = -H_k \bar{S}_k$ using two-loop recursion;
10. Compute initial steplength $\alpha_k$
11. while the Armijo condition \((A.2)\) is not satisfied do
12. $\alpha_k = \alpha_k / 2$
13. end
14. Update $\theta_{k+1} = \theta_k + \alpha_k p_k$
15. Update the curvature pairs $(\Delta g_k, \Delta \theta_k)$
16. Set $|S_{k+1}| = |S_k|$
17. Increment $k$
18. until convergence;

limited memory BFGS method \([23]\), it is defined by the recursive formula

\[
H_{k+1} = \left( I - \frac{\Delta \theta_k \Delta g_k^T}{\Delta \theta_k^T \Delta g_k} \right) H_k \left( I - \frac{\Delta \theta_k \Delta g_k^T}{\Delta \theta_k^T \Delta g_k} \right)^T + \frac{\Delta \theta_k \Delta \theta_k^T}{\Delta \theta_k^T \Delta g_k},
\]

with the curvature pair $\Delta g_k := \bar{S}_{k+1}^S - \bar{S}_k^S$ and $\Delta \theta_k := \theta_{k+1} - \theta_k$.

A common approach to compute the operator $H_k$ is given by the L-BFGS two-loop recursion algorithm \([75]\).

The key idea of a progressive batching approach is that at each iteration, the sample size is selected such that it satisfies the inner-product quasi-Newton test \([23]\):

\[
|S_k| \geq b_k := \frac{\text{Var}_{\omega \in S_k}[f(\omega)^T H_k^{-1} \bar{S}_k^S]}{\kappa^2 \|H_k^{-1} \bar{S}_k^S\|^4}, \tag{A.1}
\]

with some scalar parameter $\kappa$ (we use $\kappa = 1$). Here, we denoted by Var the sampled variance of some random variable $f_k$ given by

\[
\text{Var}_{\omega \in S_k}[f_k(\omega)] := \frac{1}{|S_k| - 1} \sum_{\omega \in S_k} [f_k(\omega) - f_k^S]^2.
\]

Whenever condition \((A.1)\) is not satisfied, the sample size $|S_k|$ is increased.

To find the steplength $\alpha_k$, we perform a backtracking line search, satisfying the Armijo condition (see also \([56]\)):

\[
\bar{f}_k^S(\theta_k - \alpha_k \bar{S}_k^S) \leq \bar{f}_k^S(\theta_k) - c_1 \alpha_k \bar{S}_k^S^T H_k^{-1} \bar{S}_k^S, \tag{A.2}
\]

where $\bar{f}_k^S := \frac{1}{|S_k|} \sum_{\omega \in S_k} J(\theta_k; \omega)$ and the constant $c_1 = 10^{-4}$.

The initial steplength is $\alpha_k = \left( 1 + \frac{\text{Var}_{\omega \in S_k}[f_k]}{|S_k| \|H_k^{-1} \bar{S}_k^S\|^2} \right)^{-1}$. The full procedure is schematically outlined in Algorithm \([1]\).
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