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Topology Optimization of Architected Lattices with Geometric Primitives

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This thesis advances novel computational techniques to design multi-material, multi-scale and programmable truss lattices. The architecture of lattice materials can be engineered to exhibit desired behavior. I focus on truss lattices made of cylindrical struts, which lead to open-cell designs that are more amenable to additive manufacturing. In this work, I use topology optimization to determine the optimal design of the periodic unit cell to attain extremized mechanical properties. Finite element analysis of the unit cell and numerical homogenization are employed to determine the effective properties of the lattice. To efficiently perform the analysis of the unit cell for any lattice layout without having to re-mesh, this work uses the geometry projection method, in which a high-level parametric representation of the struts is mapped onto a density field discretized on a fixed mesh. The techniques advanced in this work aim to push the performance limits of lattices by formulating novel design methodologies that exploit design possibilities beyond merely optimizing the spatial layout of the struts. Three mechanisms are considered towards this end. First, I formulate a topology optimization technique to design multi-material lattices, whereby each strut is made of a single material out of a prescribed set, and in which the optimization simultaneously determines the struts layout and selects the best material for each strut. Second, I advance techniques to design two-scale lattices with transversely isotropic struts that are either hollow or reinforced by long fibers. I extend this formulation to consider the simultaneous design of a structural component made of a uniform-thickness skin and a two-scale lattice infill. The third mechanism considers programmable lattices whose struts can be activated/deactivated by some physical means, thus rendering different effective properties. I advance topology optimization techniques to simultaneously design the layout and program the open/close state of the struts to obtain multiple desired properties.
Topology Optimization of Architected Lattices with Geometric Primitives

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Topology Optimization of Architected Lattices
with Geometric Primitives

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To my amazing and beautiful mom, who hearing her miraculous voice everyday helped me get through my hardest days.

To my wonderful dad, who sees only beauty in me, and has loved me like no one ever will.

To my brother, who has always had my back, and is forever in the deepest place of my heart.

And to you, who have stood by me, been with me through it all, and given my life the beautiful shine of being loved.
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Chapter 1

Introduction

1.1 Motivation

Topology optimization is a design method that determines the layout of material in a prescribed design space for optimal structural performance. One of the applications of topology optimization is to design architected materials. These are materials made of one or more natural materials, and their properties are attained both by the choice of the bulk constituent materials and, importantly, by the spatial arrangement of these constituents. In some cases, the properties of architected materials may lie outside of the envelope of properties attainable by natural materials, in which case they are also called metamaterials.

Architected materials have been employed in various fields, such as in electromagnetic [1, 2, 3, 4, 5], optical [6, 7, 8], thermal [9, 10, 11, 12], and elastic and phononic applications [13, 14, 15, 16, 17, 18, 19, 20]. A particular type of architected materials corresponds to truss lattices consisting of a network of struts. These materials can outperform bulk materials for low relative densities, cf., [21, 22, 23, 24, 25, 26, 27]. Another advantage of truss lattices is that they are open-cell structures, and therefore easier to manufacture using additive manufacturing techniques, due to the possibility of using sacrificial soluble materials for supports. Architected truss lattices have been used in different applications, including heat transfer [28, 29, 30], energy absorption [31, 32, 33] and vibration control [34, 35, 36]. This type of materials constitutes the focus of this dissertation.
1.2 Background and Literature Review

This section presents an overview of the literature on general design approaches for archi-
tected materials. There are two approaches to design periodic lattices for optimal prop-
erties: ground-structure approaches and density-based topology optimization. In ground-
structure approaches (cf. [37, 38]), the unit cell is modeled as a truss or thin frame structure,
and the location of the endpoints of the members as well as their thickness are optimized. 
These methods are computationally efficient and produce designs that consist of struts, and 
they are open-cell. However, the 1-dimensional representation of the struts cannot accu-
rately capture the mechanical properties in the overlaps. In addition, the connectivity of 
the struts is fixed and therefore the optimal design is always a subset of the ground struc-
ture, which restricts the design freedom and consequently the possibility of achieving better 
designs.

Another method that has been used to design periodic lattices is density-based topology 
optimization [39, 40, 41, 42, 43, 44, 45, 46, 47, 48]. In this method, the design space is 
discretized and a pseudo-density is assigned to each element to indicate the presence of ma-
terial, such that a zero value for an element signifies void and a value of unity corresponds 
to the presence of solid material. Although only discrete values of 0 and 1 are physically 
meaningful for elemental pseudo-densities if a purely solid structure is desired, these den-
sities are relaxed for the sake of differentiability. This allows for the use of gradient-based 
optimization methods, which are considerably more computationally efficient than, e.g, 
nature-inspired methods. Lattices optimized using density-based topology optimization 
are significantly better in terms of performance, and that is due to more design freedom. 
However, they are mostly closed-cell designs, which makes their manufacturing more dif-
ficult.

To overcome the aforementioned issues, several methods have been used to obtain 
open-cell lattices while using a 3-dimensional representation of the struts. One of them 
is the geometry projection method [49, 50, 51], wherein the design is solely made of spe-
cific geometric primitives (e.g. bars), which can ‘move’ freely inside the design domain 
to obtain the optimal layout. In this method, the analytical description of the geometry is
smoothly mapped onto a density field subsequently discretized with a fixed finite element mesh. A size variable is ascribed to each bar, that is relaxed and penalized in the spirit of density-based topology optimization and determines the presence of the bar, thus enabling the entire removal of the bar from the design.\(^1\) A similar method to design structures made of distinct geometric components is the method of moving morphable components (MMC) [52], which employs level-set functions to represent primitives and their union. The techniques advanced in this thesis employ the geometry projection method, because the aforementioned ability to entirely remove struts from the lattice allows the optimizer to more easily find good local minima and thus better designs, and because geometry projection techniques in general exhibit good convergence in the optimization.

1.3 Statement of Work

One problem I aim to solve in this dissertation is the design architected lattices made of geometric components such as struts, in which each strut can be made of one of a set of available materials. Using multiple materials with different properties and physical densities opens up the possibility of obtaining better performance than that of a single-material optimal lattice of the same weight. Fig. 1-1 shows a schematic of the proposed multi-material lattice design. The figure on the left-hand side depicts the initial design for the optimization, where struts have near-zero length (and thus appear as spheres) and are made of a mixture of three available materials with different moduli and physical densities. The right-hand side figure shows the result of the optimization, where the optimizer has determined the optimal spatial layout of the struts (including removing struts from the design where necessary) and the best material choice for each strut.

In addition to using multiple materials, it is possible to further improve the properties of the lattice by employing struts with tunable anisotropic properties. Anisotropic materials are known to render designs with better stiffness-to-weight ratios than isotropic materials. Fig. 1-2a shows an example of a strut with anisotropic properties, in which the strut itself is made of a periodic microstructure with a cylindrical inclusion in the unit cell. The inclusion

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\(^1\)In this document, the terms ‘strut’ and ‘bar’ are used interchangeably).
Figure 1-1: Example of multi-material lattice design strategy. Left: initial design; right: optimal design. The color indicates the choice of material for each strut out of the available materials.

can be a hole, in which case the strut is porous, or it can be made of a stiff material, in which case it constitutes a fiber reinforcement. The volume fraction of the inclusion, given by the ratio $D/L$ of the inclusion diameter to the separation between axes, can be modified continuously in the manufacturing process, and thus constitutes an additional design variable. The simultaneous design of the topology of the lattice unit cell and of the inclusion volume fraction effectively constitutes a two-scale design.

I also advanced a formulation to simultaneously design the shape and topology of a structural component made of a uniform-thickness skin and filled with a two-scale lattice like the one previously described. This simultaneous component/lattice/strut design effectively constitutes a three-scale design. The proposed formulation combines the geometry projection techniques advanced in my dissertation with recent developments in density-based topology optimization for the design of skin-and-infill structures.

Finally, in this dissertation I formulate a method for the design of programmable lattices. These are lattices in which each strut can be activated/deactivated through some actuation (for instance, electromagnetic (EM) joints as shown in Fig. 1-3), so that the strut can effectively be opened and closed. The open/close state of the struts, which we refer to as the lattice program, can render different effective properties. In the design methodology advanced in this work, I employ topology optimization to simultaneously determine
the optimal spatial layout of the struts in the unit cell, and the programs to obtain multiple desired properties.

Common across all the techniques I advanced in this dissertation is the geometry projection methodology to map the high-level geometric representation of the struts onto a fixed finite element mesh for efficient analysis. In what follows, I briefly describe the geometry projection technique for structures made of a single material, of a single scale (i.e., no porous struts), and monolithic (i.e., not programmable).

1.4 Geometry Projection

In this work, each strut is modeled as the offset surface of a line segment (the strut’s medial axis), which renders a cylinder with semi-spherical ends. The strut is parameterized by the positions of the endpoints of the medial axis, $x_{b_0}$ and $x_{b_f}$ (cf. Fig. 1-4). We assume that the radius of all the struts is fixed. The projected density at point $p$ is computed as the volume fraction of the intersection of a sample window $B_p^r := \{x : \|p - x\| \leq r\}$ and the
Figure 1-3: Schematic representation of the design of programmable lattices. The design variables that determine the layout are denoted by $X$ and the state of the EM joint for strut $j$ and program $i$ is given by $\alpha_{ij}$.

solid structure $\omega$:

$$\rho(p, r) := \frac{|B_p \cap \omega|}{B_p^r}. \quad (1.1)$$

This projected density for a single strut can be approximated as the volume ratio of the spherical cap of height $r - \varphi_b$ (cf. Fig. 1-4), i.e.,

$$\rho_b(\varphi_b, r) = \begin{cases} 
0 & \text{if } \varphi_b > r \\
\frac{1}{2} + \frac{\varphi_b^3}{4r^3} - \frac{3\varphi_b}{4r} & \text{if } -r \leq \varphi_b \leq r \\
1 & \text{if } \varphi_b < -r. 
\end{cases} \quad (1.2)$$

The signed distance $\varphi_b(p)$ from $p$ to bar $b$ is computed as

$$\varphi_b(d_b, w) := d_b(x_{b_o}, x_{b_f}, p) - \frac{w}{2}. \quad (1.3)$$

In this expression, $d_b$ is the distance from $p$ to the medial axis of bar $b$, given by

$$d_b(x_{b_o}, x_{b_f}, p) = \begin{cases} 
\|b\| & \text{if } a \cdot b \leq 0 \\
\|g\| & \text{if } 0 < a \cdot b < a \cdot a \\
\|e\| & \text{if } a \cdot b > a \cdot a, 
\end{cases} \quad (1.4)$$
where
\[ \mathbf{a} := \mathbf{x}_{bf} - \mathbf{x}_{ho}, \quad \mathbf{b} := \mathbf{p} - \mathbf{x}_{ho}, \quad \mathbf{e} := \mathbf{p} - \mathbf{x}_{bf}, \quad \mathbf{g} := \mathbf{P}_a^\perp \mathbf{b}, \]

and \( \mathbf{P}_a^\perp = \mathbf{I} - (\mathbf{a} \otimes \mathbf{a})/\|\mathbf{a}\|^2 \) is the perpendicular projection matrix on \( \mathbf{a} \).

For a single component made of a single isotropic material, the effective density (cf. [50] and [51]) is defined as
\[ \hat{\rho}_e := (\alpha)^p (\rho_e)^q, \quad (1.5) \]

where \( \rho_e \) is the projected density evaluated at the centroid of element \( e \), and \( \alpha \) denotes a size variable ascribed to the strut. The penalization powers \( p \) and \( q \) encourage the size variables to be either 0 or 1 in the optimal design by penalizing intermediate values. To compute the elasticity tensor, we employ an ersatz material wherein the material properties are weighted with the effective density as
\[ \mathbb{C}^e = \mathbb{C}_\text{void} + \hat{\rho}_e (\mathbb{C}_0 - \mathbb{C}_\text{void}). \quad (1.6) \]

In this expression, \( \mathbb{C}^e \) is the elasticity tensor evaluated at the centroid of element \( e \), \( \mathbb{C}_0 \) denotes the elasticity tensor of the isotropic material, and \( \mathbb{C}_\text{void} \) is the elasticity tensor of a weak material that is used to avoid an ill-posed analysis. If \( \alpha = 0 \), \( \hat{\rho}_e \) is zero resulting in
an elasticity tensor equal to $\mathbb{C}_{\text{void}}$, meaning the bar has no effect on material properties and is therefore completely removed from the design.

To consider multiple components made of a single isotropic material, a combined density is computed as the maximum of the effective densities for all components

$$\bar{\rho}^e = \max_b \hat{\rho}_b^e, \ b = 1, \ldots, n_b.$$  \hfill (1.7)

The smooth approximation $\tilde{\max}$ of the maximum function is employed to ensure differentiability, so that efficient gradient-based optimizers can be used. In the ersatz material of (6.3), $\hat{\rho}^e$ is replaced with $\bar{\rho}^e$.

## 1.5 Research Contributions

Prior to my work, geometry projection techniques were primarily used to design structures and lattices made of a single material. In this thesis, I formulate topology optimization techniques that substantially advance the geometry projection method to design: 1) multi-material 3D structural frames with bars made of any number of available materials; 2) multi-material lattice structures; 3) lattice structures with struts made of anisotropic materials (the first method of its kind); 4) skin-and-infill components where the infill is a truss lattice with anisotropic struts; and 5) programmable lattices made of struts that can be activated/deactivated (the first method of its kind).

List of Publications:


1.6 Thesis Outline

Chapter 2 formulates a topology optimization method for structures made of multiple available materials. Chapter 3 presents a topology optimization method for the design of multi-material periodic lattices. Chapter 4 introduces a topology optimization method for design of periodic lattices with struts made of anisotropic materials. Chapter 5 presents a topology optimization method to simultaneously design a shell component with a lattice infill made of anisotropic struts. Chapter 6 formulates a topology optimization technique to design programmable lattices with struts that can be activated/deactivated. Chapters 2 and 3 have each already been published in peer-reviewed journals [53, 54, 55], whereas Chapters 4, 5 and 6 correspond to manuscripts that have been submitted and are in review at the time of writing this thesis.
Chapter 2

Design of Multi-material Structures

2.1 Summary

This chapter presents a new method for the simultaneous topology optimization and material selection of structures made by the union of discrete geometric components, where each component is made of one of multiple available materials. Our approach is based on the geometry projection method presented in Section 1.4. As opposed to the case where all components are made of a single material, as described in Section 1.4, a size variable $\alpha_{m}^{b}$ per available material $m$ is ascribed to each strut $b$. A value $\alpha_{m}^{b} = 1$ indicates the strut $b$ is made exclusively of material $m$. All size variables for a strut can be zero, signifying the strut is entirely removed from the design. We penalize intermediate values of the size variables via an aggregate constraint in the optimization. A mutual material exclusion constraint is also introduced that ensures that at most one material has a unity size variable in each strut. In addition to these constraints, we propose a novel aggregation scheme to perform the union of geometric components with dissimilar materials. These ingredients facilitate the treatment of the multi-material case. Our formulation can be readily extended to any number of materials. We demonstrate our method with several numerical examples.
2.2 Introduction

Topology optimization has been used extensively in order to generate novel designs that improve structural performance while decreasing the cost. One important option to improve the structure is to employ multiple materials. By having an appropriate distribution of materials, multi-material designs can outperform designs made of each of the materials separately. Moreover, besides decreasing cost, multi-material designs can take advantage of substantial differences in properties to perform multiple functions.

Methods for multi-material topology optimization were first introduced in density-based approaches. In [39], a method is developed to determine the optimal distribution of multiple phases to obtain composite materials with extreme thermal expansion behavior. This work employs an extension of the power-law interpolation used in solid isotropic material penalization (SIMP) [56, 57] to three-phase material designs (two solid materials and void). The interpolation uses two design variables, one that indicates where to put material or void and another that determines which material to choose. This and similar formulations are applied to various problems, such as design of multi-phase composites with extremal bulk modulus [40], design of multi-phase piezoelectric actuators [58, 59], combined optimization of material and voltage distribution [60] and optimal reinforcement of concrete structures [61]. As indicated in [62], this formulation violates the Hashin-Shtrikman bounds and renders different designs if the phases are interchanged. In [62], a formulation that combines the power-law penalization with an interpolation of every material property within its Hashin-Shtrikman bounds is proposed to circumvent the foregoing limitations to design multi-material actuators. In all of these applications, the maximum number of phases involved is three (including two solid phases and a void phase) as the generalization of their interpolation schemes to more than three phases becomes quite involved.

A method for topology optimization of multi-material compliant mechanisms using an alternative material interpolation scheme that employs only one density variable is proposed in [63]. As opposed to the single-material topology optimization, where the optimal density indicates either void (zero) or solid (unity), in this method, the density variable in the optimal design can take any real value. The proximity of this value to one of the means
of a sum of Gaussian distributions with given mean locations and with modes corresponding to the property values for different materials indicates the choice of material. To avoid premature convergence to undesired local minima, this method starts with a large standard deviation for each material’s property distribution and decreases it gradually in order to sharpen the peaks.

The discrete material optimization method (DMO) [64] simultaneously optimizes the stacking sequence, reinforcement orientation and choice of material of composite shell structures. In this method, there is a set of materials from which each finite element can be made in order to minimize the objective function. A material interpolation scheme is formulated, whereby an increase in the weighting factor for one material decreases the weighting factors for all other materials. The weighting factor for a given material indicates the relative influence of that material on the properties of the corresponding finite element. If the weighting factor for a given material is unity, it indicates that finite element is made solely of that material (e.g., pure phases). One challenge with this formulation is that the weighting factors do not add up to unity except for pure phases. The proposed solution is to normalize each weighting factor by the summation of all weighting factors. However, this alters the penalization effect and the monotonic convergence. The DMO method is used in [65] to optimize the buckling behavior of multi-material composite shell structures, and in [66] to compare topology optimization of multi-material structures with a mass constraint using both this method and the one presented in [39]. The work in [67] formulates simpler multi-material interpolations by imposing one linear constraint per finite element that ensures that it is made of only one material (or no material).

Other density-based methods employ a heuristic rule for the multi-material interpolation. The work in [68] uses a homogenization approach with a unit cell made of two materials and a square hole. The optimization allows for continuous mixtures of the three phases. Then, a post-processing heuristic rule is applied to every finite element in the optimal design to determine if it is made of one of the two materials or void. In [69], material is iteratively removed from a fully solid initial design by applying a rule to each finite element that changes its material, or that makes it solid or void based on the elemental change in compliance incurred by these changes.
There also exist several level set methods for topology optimization of multi-material structures. In the color level-set method [70], the boundaries of multiple regions made of different materials are given by the zero level-sets of multiple functions. Instead of using a level set function per material, this method employs \( m \) level-set functions whose combinations can represent up to \( 2^m \) materials. This strategy circumvents the need for an equality constraint that would be required to avoid overlapping materials if one level set per material was used. Since the combination of level sets renders one and only one material at any point, this method eliminates the need for material interpolation. This method is applied to topology optimization of multi-material compliant mechanisms in [71] and stress-based topology optimization of continuum structures involving multiple materials in [72]. In [73], the color level-set method is combined with a variational approach for optimization of structures made of functionally graded materials.

In the level set method of [74], only one level-set, piece-wise constant function is used as an ‘index’ that indicates the choice of material. A constraint is applied to ensure that the level set function converges to the index values. This method is applied to design of piezoelectric actuators [75]. In [76], \( n \) level-set functions are used to represent \( n \) solid materials and void (i.e. \( n + 1 \) phases). This method employs a material interpolation similar to the one proposed in [39], except it uses the Heaviside of the level-set functions instead of density variables.

The design of multi-material structures has also been studied with phase-field topology optimization methods. The generalized SIMP interpolation scheme proposed in [64] in combination with the mutual material exclusion constraint of [67] are employed in the phase field methods of [77, 78, 79]. In [80], the volume fraction of each phase in phase field model directly represents the contribution of the corresponding material to the material properties. A constraint on these volume fractions ensures that they add up to unity, while a penalization term added to the objective function ensures the volume fractions are zero or unity upon convergence. Phase field methods for topology optimization of multi-material structures require a very large number of iterations, typically in the order of thousands.

All the aforementioned methods produce organic designs that cannot be readily manufactured with stock material. The geometry projection method presented in [49, 50, 51],
generates designs that can be made of stock material such as bars and plates, by smoothly mapping an analytical description of the geometric elements onto a density field over a fixed finite element grid. A size variable is ascribed to each geometric component that is penalized in the spirit of SIMP, allowing the optimizer to entirely remove that component from the design. In the moving morphable components method of [52] and [81], a parametric description of bars is mapped onto a level set representation (termed the ‘topological description function’) for the analysis. The foregoing methods for design with discrete geometric elements use a single material. Recently, the work in [82] proposed a geometry projection method for the topology optimization of multi-material, 3-dimensional lattice structures. This method adapts the material interpolation scheme of [39] to the geometry projection framework, by assigning additional variables to each geometric component that determine the choice of material. Although possible, the extension of this interpolation scheme to more than two materials is not straightforward and it is more prone to getting locked into undesired local minima, as reported in [64]. Also recently, the work in [83] extends the moving morphable components method to accommodate multiple materials by seeding the initial design of geometric components made of different materials (i.e., the material of a component does not change during the optimization). The material interpolation scheme in regions where two or more geometric components intersect chooses the stiffer material of any intersecting component.

In this chapter, we extend the geometry projection method so that it can be readily applied to structures whose geometric components can be made of one of any number of available materials. We achieve this by means of several key ingredients. The first ingredient corresponds to a new aggregation function used to perform the union of geometric components, since the function used in previous geometry projection schemes cannot accommodate components made of dissimilar materials. A second important ingredient pertains to the interpolation of properties from the multiple material candidates. Here, we adapt the DMO formulation to accommodate discrete geometric components made of different materials. Unlike DMO, however, we impose two separate aggregate constraints in the optimization to a) penalize the size variables of geometric components (discreteness constraint), and b) to ensure each component is made of at most one of the available materi-
als (mutual material exclusion constraint). We demonstrate the effectiveness of our method via numerical examples.

The rest of the chapter is organized as follows. Section 2.3 describes the projection of geometric components onto the analysis mesh for analysis, including the aggregation function for the union of geometric components and the interpolation of material properties. Sections 2.4 and 2.5 detail the constraints to penalize intermediate values of size variables, and to ensure geometric components are made of at most one material respectively. The modification of the geometry projection to enforce a symmetric design is presented in Section 2.6. Section 2.7 describes the optimization problem. We present numerical examples to demonstrate our method in Section 2.8, and draw conclusions of our work in Section 2.9.

### 2.3 Geometry Projection

To perform the analysis for any given design made of the union of geometric components, we use the geometry projection method described in Section 1.4, wherein a parametric description of the components is smoothly mapped onto a density field over a fixed grid.

Since several components can intersect, in Section 1.4 we aggregated the corresponding densities in the intersection by using a $p$-norm, which smoothly approximates the maximum projected density of any of the intersecting components. While this approach is effective for single-material structures, it does not accommodate components made of multiple materials. In this chapter, we consider a different aggregation strategy, which we explain in the following.

Let us first consider components made of the same material. We want the contribution of a bar $b$ to the projected density at point $p$ to be 1.0 if $p$ is in the interior of the bar, and 0.0 if it is outside the bar. We can achieve this by using the Heaviside function of the signed distance to express the effective density as:

$$\rho_{eff}(z, p) = \frac{\sum_{b=1}^{N_b} H(-\phi_b(z, p)) \rho_b(z, p)}{\sum_{b=1}^{N_b} H(-\phi_b(z, p))}$$  \hspace{1cm} (2.1)
In the expression above, \( z = [z_1^T \ z_2^T \ldots z_{N_b}^T]^T \) is the vector of design variables, with \( z_b = [x_{b_0}^T \ x_{b_f}^T]^T \) the vector of design variables for bar \( b \). \( N_b \) is the number of bars in the design. With the Heaviside weighting factor, a component contributes to the effective density when \( \phi_b \leq 0 \), i.e, if \( p \) is inside the component. The sum of all weighting factors in the denominator ensures \( \rho_{\text{eff}} \in [0, 1] \). Since the exact Heaviside function is not differentiable, we replace it with a smooth approximation \( \tilde{H}_\varepsilon \) so that design sensitivities are well defined and we can use gradient-based optimizers:

\[
\tilde{H}_\varepsilon(x) = \begin{cases} 
0 & \text{if } x < -\varepsilon \\
\left[\frac{1}{2} + \frac{x}{2\varepsilon} + \frac{1}{2\pi} \sin \left(\frac{\pi x}{\varepsilon}\right)\right]^p & \text{if } -\varepsilon \leq x \leq \varepsilon \\
1 & \text{if } x > \varepsilon
\end{cases}
\] (2.2)

We introduce the exponent \( p > 1 \) as a parameter to sharpen the Heaviside (i.e. to reduce the range over which it attains an intermediate value). In the case of single-material structures, the material properties are modified by some function of the foregoing effective density, as in our previous work. With the smooth Heaviside, it is clear that material properties vary continuously within a narrow band around the boundary of the bars.

To extend this interpolation to components made of one of \( N_m \) materials, we express the effective elasticity tensor at point \( p \) as

\[
C(z, p) = C_{\text{void}} + \sum_{m=1}^{N_m} (C_m - C_{\text{void}}) \rho_{\text{eff}}^m(z, p)
\] (2.3)

where \( C_m \) is the elasticity tensor for material \( m \), \( C_{\text{void}} \) is the elasticity tensor of a weak isotropic material that prevents the analysis from being ill-posed, and \( \rho_{\text{eff}}^m \) is an effective density per material given by

\[
\rho_{\text{eff}}^m(z, p) = \frac{\sum_{b=1}^{N_b} \tilde{H}_\varepsilon(-\phi_b(z, p)) \rho_b(z, p) w_m^b(z)}{\sum_{b=1}^{N_b} \tilde{H}_\varepsilon(-\phi_b(z, p))}
\] (2.4)

In this expression, \( w_m^b \) is a weighting factor for bar \( b \) and material \( m \). Here, we adapt the
DMO interpolation scheme to our method, and define these weights as:

\[ w_m^b(z) = (\alpha_m^b) \prod_{n=1}^{N_m} (1 - (\alpha_{n \neq m}^b)) \]  

(2.5)

The main difference between this expression and the original DMO approach for density-based topology optimization is in the variables \( \alpha \). In the density-based approach, these variables correspond to element-wise densities per material. In our approach, we ascribe a size variable \( \alpha_m^b \in \{0, 1\} \) to geometric component \( b \) that indicates if it is made of material \( m \) when \( \alpha_m^b = 1 \). Correspondingly, the vector of design variables for bar \( b \) is now given by

\[ z_b = [x_{b_0}^T \ x_{b_f}^T \ \alpha_b^T] \]  

(note that \( w_m^b \) only depends on \( \alpha_b \) and not on \( x_{b_0}^T \) or \( x_{b_f}^T \), but we use the foregoing notation for simplicity).

These size variables are discrete, which precludes the use of nonlinear programming methods; therefore, we relax them so that they can take any value between 0.0 and 1.0. To ensure that the optimizer converges to a design with pure phases, we penalize intermediate values in the same spirit as the SIMP method. The second difference between our approach and the original DMO method lies in that the penalization is not imposed through the weights of Eq. 2.5, but through an optimization constraint, as described in Section 2.4. Furthermore, as we desire each component to be made of one and only one material, a mechanism to ensure that \( \alpha_m^b \) is 1.0 for at most one material is required. We detail a constraint to enforce this requirement in Section 2.5.

One problem with the expression for \( \rho_{eff}^m \) in Eq. 2.4 is that in the intersection between a solid bar made of material \( m \) (i.e. with \( \alpha_m^b = 1 \) and \( \alpha_n^b = 0 \) for \( n \neq m \)) and a void bar (i.e. with \( \alpha_m^b = 0 \ \forall m \)), the effective density for material \( m \) is 0.5. Consequently, the effective elasticity tensor of Eq. 2.3 equals 0.5(\( C_m + C_{\text{void}} \)), which is clearly incorrect. This occurs because the denominator is counting all the bars in the intersection, and not only the solid bars. To remedy this, we modify the denominator so that it only counts the non-void bars (i.e., those for which \( \sum_m \alpha_m^b > 0 \)) as follows:

\[ \rho_{eff}^m(z, p) = \frac{\sum_{b=1}^{N_b} \tilde{H}_e(-\phi_b(z, p)) \rho_b w_m^b(z)}{\sum_{b=1}^{N_b} (\tilde{H}_e(-\phi_b(z, p)) \sum_{m=1}^{N_m} \alpha_m^b)} \]  

(2.6)
However, another problematic situation arises: if all bars in an intersection have a zero size variable for all materials, the denominator would be zero. In this case, we want the denominator to be replaced by 1, hence we redefine the effective density per material as:

$$\rho_{eff}^m(z, p) = \frac{\sum_{b=1}^{N_b} \tilde{H}_e(-\phi_b(z, p))\rho_b w^b_m(z)}{A + B}$$  \hspace{1cm} (2.7)

wherein

$$A = \sum_{b=1}^{N_b} \left( \tilde{H}_e(-\phi_b(z, p)) \sum_{m=1}^{N_m} \alpha^b_m \right)$$  \hspace{1cm} (2.8)

$$B = 1 - \max \left( \tilde{H}_e(-\phi_b(z, p)) \sum_{m=1}^{N_m} \alpha^b_m \right)$$  \hspace{1cm} (2.9)

The term $B$ equals 1 if all intersecting bars have zero size variables, and 0 if at least one size variable equals 1. We note that both situations occur only when all intersecting bars have pure phases. Finally, the maximum function is not differentiable, hence we replace it with a Kreisselmeier-Steinhauser (KS) approximation [85]:

$$\rho_{eff}^m(z, p) = \frac{\sum_{b=1}^{N_b} \tilde{H}_e(-\phi_b(z, p))\rho_b w^b_m(z)}{A + C}$$  \hspace{1cm} (2.10)

where

$$C = 1 - KS(\tilde{H}_e(-\phi_b(z, p))) \sum_{m=1}^{N_m} \alpha^b_m$$  \hspace{1cm} (2.11)

and

$$KS(x) := \frac{1}{k} \ln \left( \sum_{i} e^{kx_i} \right)$$  \hspace{1cm} (2.12)

The KS function approximates better the maximum as the paremeter $k$ increases.

## 2.4 Discreteness Constraint

Since the relaxed size variables $\alpha^b_m$ can take any value between 0.0 and 1.0, a penalization scheme is needed to push them toward these values throughout the optimization in order to have a physical meaning. Unlike the DMO method, which performs the penal-
ization through the weighting factors directly, we enforce this penalization via an equality constraint in the optimization:

\[ g_d(z) := 4 KS_m(\alpha^T (1 - \alpha)) = 0 \quad (2.13) \]

in which we use the lower-bound KS function:

\[ KS(x) := \frac{1}{k} \ln \left( \frac{1}{N} \sum e^{kx_i} \right) \quad (2.14) \]

where \( \alpha = [\alpha_1^T \alpha_2^T \ldots \alpha_N^T]^T \) is the vector of size variables \( \alpha^{mb} \) for all components and all materials, and \( \mathbf{1} \) is a vector of size \( N = N_m N_b \) with all components equal to 1.0. The lower-bound KS function approaches the maximum from below, therefore we circumvent the need to adaptively adjust the constraint limit (cf. [86]) and guarantee that \( g_d \in [0, 1] \). As before, we denote \( g_d \) as being dependent on \( z \) for notational simplicity, however it only depends on the size variables. If all size variables are 0.5, the above constraint will attain its largest value, 1.0. If all size variables are either zero or unity, the constraint value will be zero.

Since enforcing equality constraints is more difficult than enforcing inequality constraints in nonlinear programming methods, we replace the constraint of Eq. 2.13 with the inequality constraint

\[ g_d(z) \leq \varepsilon_d \ll 1 \quad (2.15) \]

For the penalization to be effective, the positive bound \( \varepsilon_d \) should be small enough. However, if we start the optimization with a very small value, the size variables will quickly converge to 0.0 or 1.0 as the optimizer tries to reach the feasible region, which means that a geometric component can prematurely get ‘locked’ into one of the available materials. Consequently, the optimization can get locked into undesirable local minima. To prevent this, we use a continuation strategy, whereby we start the optimization with a relatively large value of \( \varepsilon_d^{(0)} \). Then, we slowly start decreasing it at every iteration by an amount \( \Delta \varepsilon_d \) once the relative change in the objective function in consecutive iterations falls below a
specified value $\Delta f^*$, i.e.:

If $\Delta f^{(I+1)} \leq \Delta f^*$ then $\epsilon_{d}^{(I+1)} \leftarrow \max(\epsilon_{d}^{(I)} - \Delta \epsilon_{d}, \epsilon_{d}^*)$ \hfill (2.16)

where $\epsilon_{d}^*$ is the final constraint limit we want to attain, and the relative change in the objective function at iteration $I + 1$ is defined as

$$\Delta f^{(I+1)} := \frac{|f^{(I+1)} - f^{(I)}|}{f^{(I)}}$$ \hfill (2.17)

2.5 Mutual Material Exclusion Constraint

By applying the discreteness constraint, we can ensure pure phases in the optimal design. However, this constraint does not prevent more than one material from having a size variable of 1.0 for a bar. To avoid this situation, we introduce a mutual material exclusion constraint in the optimization, defined as:

$$g_{m}(z) := KS_q \left( \sum_{m=1}^{N_m} \alpha_{m}^b \right) - 1 \leq 0 \hfill (2.18)$$

in which we again use the lower-bound $KS$ function of Eq. 2.14 with $N = N_b$.

When all the size variables $\alpha_{m}^b$ for bar $b$ satisfy the discreteness constraint, the term in parenthesis equals 1.0 if the bar is solid (in which case it is made of one and only material) or 0.0 if the bar is void. We employ a similar continuation strategy as in Section 2.4 to avoid premature convergence to an undesired local minimum. To this end, we write:

$$g_{m}(z) \leq \epsilon_{m} \ll 1 \hfill (2.19)$$

As before, we start with a relatively large value of $\epsilon_{m}^{(0)}$, and start decreasing it once the relative change in the objective function in consecutive iterations is smaller than a specified value, i.e.

If $\Delta f^{(I+1)} \leq \Delta f^*$ then $\epsilon_{m}^{(I+1)} \leftarrow \max(\epsilon_{m}^{(I)} - \Delta \epsilon_{m}, \epsilon_{m}^*)$ \hfill (2.20)
Note that $\varepsilon_m^{(0)}$ must be smaller than 1.0, as otherwise it is possible for a bar to be made of more than one pure phase. In this situation, a decrease in one of the material size variables can increase the violation of the discreteness constraint, making it difficult for the optimizer to find feasible designs with bars made of at most one material.

### 2.6 Symmetry

If the boundary conditions and design envelope are such that a symmetric design is expected, density-based and level set topology optimization methods have significant design freedom that allows them to readily produce symmetric designs. However, as discussed in [50], the more restrictive design representation enforced by discrete geometric components can lead to asymmetric designs as the optimizer satisfies exactly the resource constraint. Specifically, if the design can only be made of a finite number of discrete geometric components, it is entirely possible to find an asymmetric design that exactly satisfies the weight fraction constraint and it has lower compliance than the best symmetric design that can be obtained with the available set of components.

In cases where a symmetric design is expected or desired, we employ a simple approach to enforce symmetry that consists of reflecting the geometry projection for elements on the opposite side of the symmetry plane. This approach was introduced in [82]. We define geometric components only on one side of the symmetry plane and bound their location to ensure they remain on that side. To compute the projected density for a point on the reflected side, we reflect the point with respect to the symmetry plane, and then compute the projected density for the reflected point as usual. The sensitivities are modified accordingly to account for this reflection.

In the case of a symmetry line for two-dimensional problems, the reflected point is given by

$$\hat{p} := Rp + 2s$$

$$R := \begin{bmatrix} \cos(2\phi) & \sin(2\phi) \\ \sin(2\phi) & -\cos(2\phi) \end{bmatrix}$$
where \( \mathbf{s} \) is a vector from the origin to the closest point on the line of symmetry, \( \phi \) is the angle between the symmetry line and the \( e_1 \) axis, and \( \mathbf{R} \) is the reflection matrix. We use this approach to enforce symmetry in the example of Section 2.8.3.

### 2.7 Optimization Problem

In this work we aim to minimize the structural compliance. Since we have multiple materials, a total volume constraint results in the exclusive use of the stiffest material. To avoid this, most of the works cited in Section 2.2 impose individual volume constraints for each one of the available materials. While this is an effective strategy, the determination of constraint limits for each material is somewhat arbitrary in practice. Instead, here we impose a weight fraction constraint. The space occupied by the structure and the design envelope are denoted by \( \omega \) and \( \Omega \), respectively with \( \omega \subset \Omega \). We consider linearly elastic problems without a body load. The weight fraction constraint is computed as

\[
g_w := \frac{1}{\gamma_{ref}} \sum_{m=1}^{N_m} \gamma_m \int_{\Omega} \rho_{eff}^m(z, \mathbf{p}) d\mathbf{v} \leq w_f^*.
\]  

The compliance minimization problem is then stated as

\[
\min_{\mathbf{z}} f(\mathbf{u}(\mathbf{z})) := \int_{\Gamma_i} \mathbf{u}(z) \cdot \mathbf{t} ds
\]

subject to

\[
a(\mathbf{u}(z), \mathbf{v}) = l(\mathbf{v}), \forall \mathbf{v} \in \mathcal{V}_\Omega, \mathbf{u} \in \mathcal{U}_\Omega
\]

\[
g_w(z) \leq w_f^* 
\]

\[
g_d(z) \leq \varepsilon_d^{(f)} 
\]

\[
g_m(z) \leq \varepsilon_m^{(f)} 
\]

\[
\mathbf{x}_{b_0}, \mathbf{x}_{bf} \in \Omega
\]

\[
0.0 \leq \alpha_m^p \leq 1.0
\]
where $\gamma_i$ is the physical density for material $m$, $\gamma_{ref}$ is a reference density that we choose to be 1 here, $|\Omega|$ denotes the volume of the design region, $v$ denotes the virtual displacement, $t$ denotes the design-independent traction, and $w_f$ is the weight fraction. $\mathcal{Z}_\Omega := \{u| u \in H^1(\Omega), u|_{\Gamma_a} = 0\}$ is the set of admissible displacements, and $u$ is the displacement obtained from the solution to Eq. 4.30, with $a$ and $l$ the energy bilinear and load linear forms respectively given by:

$$a(u, v) := \int_{\Omega} \nabla v \cdot C(z, p) \nabla u dv$$ \quad (2.31)

$$l(u, v) := \int_{\Gamma} v \cdot t ds$$ \quad (2.32)

We impose move limits on the design variables at every iteration to improve convergence by normalizing the design variables by some reference value so that $0 \leq \hat{z} \leq 1$, where $\hat{z}$ denotes the scaled design variable. The coordinates of the end points $x_{b_0}$ and $x_{b_f}$ are normalized by the corresponding dimensions of the design region. The $\alpha_{bm}$ do not need normalization, as they already lie within the desired magnitude range. A single move limit $0 \leq m \leq 1$ is imposed on all normalized variables as

$$\max(0, \hat{z}^{(l-1)} - m) \leq \hat{z}^{(l)} \leq \min(1, \hat{z}^{(l-1)} + m)$$ \quad (2.33)

We stop the optimization when the discreteness and mutual material exclusion constraints are feasible, and when the relative change of the objective function between consecutive iterations falls below the specified value $\Delta f^*$. 

### 2.8 Examples

To illustrate the effectiveness of our method we present several examples. In all examples, we employ bilinear quadrilateral elements for the analysis. The entire code, including the finite element analysis, the sensitivities calculation and the optimization is implemented in MATLAB. To solve the optimization problem, we use the method of moving asymptotes (MMA) \cite{87, 88} with the default parameters described in \cite{88}, i.e., $a_0 = 1$ for the objective
function, and \( a_l = 0, c_l = 1000 \) and \( d_l = 1 \) for every constraint \( l \) in the optimization (we refer the reader to [88] for a description of these parameters). Unless noted, the stopping criterion on the relative change in compliance between consecutive iterations is \( \Delta f^* = 10^{-4} \). Also, unless specified, we employ a move limit of \( m = 0.3 \). We use \( \varepsilon_d^0 = 1.0 \) and \( \varepsilon_d^* = 0.01 \) for the discreteness constraint of Eq. 2.16, and \( \varepsilon_m^0 = 0.3 \) and \( \varepsilon_m^0 = 0.01 \) for the mutual material exclusion constraint of Eq. 2.20. We use a power of \( p = 2 \) in the smooth Heaviside approximation of Eq. 2.2. The constant \( k = 25 \) is used for the KS functions of Eqs. 2.12 and 2.14. All the materials considered are homogeneous, isotropic, and linearly elastic with Poisson’s ratio \( \nu = 0.3 \), but with different Young’s moduli and material densities.

### 2.8.1 Two-bar Cantilever Beam

The first example is a short cantilever beam made of two bars. The design envelope, boundary conditions and initial design are shown in Fig. 2-1. The design envelope is meshed with a regular grid of 80 \( \times \) 80 elements. There are two available materials with Young’s moduli \( E_1 = 10 \) and \( E_2 = 5 \), and physical densities \( \gamma_1 = 0.9 \) and \( \gamma_2 = 0.45 \) respectively. The initial design, shown in the same figure, consists of two horizontal bars of width \( w = 0.25 \) and with \( \alpha_1^b = \alpha_2^b = 0.5 \), \( b = 1, 2 \). For this problem, we use a looser stopping criterion on the relative change in compliance between consecutive iterations of \( \Delta f^* = 10^{-3} \).

We perform the optimization for several weight-fraction limits \( w_f^* \), and the results are
presented in Table 2.1. The choice of \( w_f^* \) for each run corresponds to expected configurations. For example, \( w_f^* = 0.0520 \) corresponds to a design made of a single horizontal bar made of material 2 and completely inside the design envelope. Some of the weight-fraction limits account for the fact that half of the horizontal bar may be outside of the design envelope.

Two interesting cases are worth noting. For the second run, the weight-fraction limit \( w_f^* = 0.1020 \) corresponds to the weight fraction of a single horizontal bar made of material 1 and completely inside the design envelope. However, the optimization produces a better design by using a short diagonal bar made of material 2. For the third run, the weight-fraction limit \( w_f^* = 0.115 \) corresponds to a V-shape design made of the lighter material. However, the optimizer finds a better design whereby the horizontal bar is partially outside the design envelope.

In Fig. 2-2 we plot the compliance versus the weight fraction for the optimal designs of all six runs to illustrate that the compliance decreases as the weight fraction increases. As expected, for the lowest weight-fraction limit, the optimal design corresponds to a single bar made of the lighter (and weaker) material. As the weight-fraction constraint increases, the optimizer first introduces a second bar made of the heavier (and stiffer) material, and eventually obtains a two-bar design made of the stiffest material. Finally, Fig. 2-3 shows the effective density for each of the two materials for the initial and optimal designs of run 4 in Table 2.1.

2.8.2 MBB Beam

The second example corresponds to the Messerschmitt-Bölkow-Blohm (MBB) beam widely studied in topology optimization. The design envelope, boundary conditions and initial design are shown in Fig. 2-4. We note that, as we have discussed in previous work (cf., [50]), geometry projection methods are more prone to converging to different local minima than free-form topology optimization methods due to the more restrictive design representation. The design envelope is meshed with a regular grid of \( 160 \times 40 \) elements. We use the same two materials of the preceding example. The initial design consists of 21 bars of width
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Table 2.1: Optimization results for two-bar cantilever beam problem. Red indicates material 1 and green indicates material 2. The last column indicates the number of iterations to convergence.
Figure 2-2: Compliance versus weight fraction for optimal two-bar cantilever beams. Red indicates material 1 and green indicates material 2. The circled numbers indicate the corresponding runs in Table 2.1.

Figure 2-3: Effective density $\rho_{eff}^m$ for materials $m = 1$ (left) and $m = 2$ (right) for initial (top) and optimal (bottom) designs for run 4 in Table 2.1.
Figure 2-4: Design envelope, boundary conditions and initial design for the MBB beam.

\( w = 0.4 \) and with \( \alpha^b_1 = \alpha^b_2 = 0.5, b = 1, \ldots, 21 \). We consider two configurations of bars. In one configuration, as in the previous example, the endpoints \( x_{b_0} \) and \( x_{b_f} \) for each bar are independent from other bars, so that bars are ‘floating’ inside the design envelope. In the second configuration, bars share common endpoints, so that the design remains connected at all times.

We perform the optimization for several weight-fraction limits, \( w^*_f = 0.1, 0.11, \ldots, 0.19 \). The optimal designs for the floating and connected configurations are shown in Figs. 2-5 and 2-6 respectively. Several of the designs obtained resemble known solutions for the MBB beam. As expected, the runs with floating bars produce better designs than their connected bars counterparts since they have more design freedom. Also, the smallest ‘solid’ size variable \( \alpha^b_m \) is 0.988249 for all floating bars runs and 0.983790 for all connected bars runs; and the largest ‘void’ size variable \( \alpha^b_m \) is 0.036276 for all floating bars runs and 0.038084 for all connected bar runs. This is an indication that the discreteness constraints is very effective in penalizing intermediate values of the size variables.

### 2.8.3 Michell Cantilever

We now present an example that shows that the proposed formulation can be readily extended to any number of materials. It corresponds to a cantilever frame considered in Michell’s work [89], with design envelope and boundary conditions as shown in Fig. 2-7. The design envelope is meshed with 9700 elements. We enforce symmetry of the design with respect to the horizontal center line shown in Fig. 2-7. For this example, we use a tighter move limit of \( m = 0.2 \) to improve convergence. The initial design is made of twelve
Figure 2-5: MBB optimal designs with floating bars. Red indicates material 1 and green indicates material 2.
Figure 2-6: MBB optimal designs with connected bars. Red indicates material 1 and green indicates material 2.
near-zero length bars of width $w = 0.25$ and with $\alpha_{mb}^b = 0.5$, $b = 1, \ldots, 12$.

We perform the optimization using four materials with Young’s moduli $E_1 = 6.5$, $E_2 = 5.0$, $E_3 = 4.5$ and $E_4 = 3.5$ and physical densities $\gamma_1 = 0.55$, $\gamma_2 = 0.4$, $\gamma_1 = 0.35$ and $\gamma_2 = 0.25$. We use a weight-fraction limit of $w_f^* = 0.028$ that allows us to obtain a design with four materials, as otherwise we would get designs made only of the stiffer material(s) if $w_f^*$ is larger, or made only of the weaker material(s) if $w_f^*$ is smaller. Fig. 2-8 shows the optimal designs using one, two, three, and four materials. As expected, the designs improve as we increase the number of materials available. Also, the smallest ‘solid’ size variable $\alpha_{mb}^b$ is 0.999817 for all runs, and the largest ‘void’ size variable $\alpha_{mb}^b$ is 0.003536 for all runs, once again indicating the effectiveness of the penalization scheme.

### 2.8.4 3D Cantilever Beam

In the last example we perform the optimization for a 3D cantilever beam. For this example, we migrated our MATLAB code to C++ using the deal.II library [90, 91]. The design envelope, boundary conditions and initial design are shown in Fig. 2-9. The design envelope is meshed with a regular grid of $64 \times 32 \times 32$ elements. We use the same two materials of the first example. The initial design consists of 42 bars of width $w = 0.2$ and with $\alpha_{mb}^b = \alpha_{mb}^b = 0.5$, $b = 1, \ldots, 42$. We consider an initial design with connected bars as in the previous MBB beam example of Section refsubsec:mbb-beam. The optimal designs corresponding to weight-fraction limits of $w_f^* = 0.01$, 0.02, 0.03 and 0.04 are shown in
Figure 2-8: Michell cantilever optimal designs. Red indicates material 1 (stiffest/heaviest), green indicates material 2, blue indicates material 3 and magenta indicates material 4 (weakest/lightest).
2.9 Conclusions

This chapter introduced a method for the design via topology optimization of structures constructed as the union of geometric components, where each component is made of one of several available materials or removed from the design. Several examples that minimize the structural compliance subject to a weight fraction constraint demonstrate the proposed method. The available materials have different moduli but also different physical densities, hence a combination of materials is most advantageous for some weight fraction limits.

The examples demonstrate our method’s effectiveness in producing structurally efficient multi-material designs. By penalizing intermediate size variables and enforcing the mutual material exclusion requirements as constraints in the optimization and not through the interpolation scheme, our technique makes it easier to incorporate any number of materials. Unlike density- and level set-based topology optimization methods for design with multiple materials, which produce material phases with geometries that are difficult to manufacture and assemble, the use of geometric components that are readily fabricated makes it easier to physically realize the multi-material structures. Also, instead of imposing arbitrary volume fraction constraints on each of the available materials, we directly constrain the weight, which is a more natural design requirement.
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Table 2.2: Optimization results for 3D cantilever beam problem. Red indicates material 1 and blue indicates material 2.
We have demonstrated our method for 2- and 3-dimensional bars modeled with offset surfaces. Since the computation of the effective density $\rho_{eff}$ of Eq. 2.10 is uncoupled from the calculation of the projected density $\rho_b$ of Eq. 1.2, the scheme to interpolate the material properties from various discrete geometric components should work for any geometry representation, and thus we believe our method can be applied to other component geometries.
Chapter 3

Design of Multi-material Lattices

3.1 Summary

This chapter presents a computational method for the design of architected truss lattice materials where each strut can be made of one of a set of available materials. It constitutes an extension of the method presented in the previous chapter to multi-material lattice design. We design the lattices to extremize effective properties. As customary in topology optimization, we design a periodic unit cell of the lattice and obtain the effective properties via numerical homogenization. As in the previous chapter, lattice struts are represented as cylindrical offset surfaces. The geometry projection and material interpolation, as well as the constraints that ensure that each strut in the optimal lattice design is made of at most a single material are the same as those described in the previous chapter. As before, the proposed scheme readily accommodates any number of materials. To obtain lattices with desired material symmetries, we design only a reference region of the unit cell and reflect its geometry projection with respect to the appropriate planes of symmetry. Also, to ensure struts remain whole upon reflection inside the unit cell or with respect to the periodic boundaries, we impose a no-cut constraint on the struts. This constraint renders designs that are more amenable to manufacturing. We demonstrate the efficacy of our method via numerical examples of bulk and shear moduli maximization and Poisson’s ratio minimization for two- and three-material lattices with cubic symmetry.
3.2 Introduction

Topology optimization techniques generate novel structural designs by optimizing the material layout within a prescribed design region. One important application is the design of architected materials with desired effective properties. This chapter focuses on the design of multi-material, periodic lattice structures via topology optimization. Open-cell designs, and in particular open lattices, readily allow for removal of supports—for instance, if supports are made of a sacrificial, soluble material that is dissolved after fabrication—and therefore they are easier to manufacture than closed-cell designs. As all methods to design periodic structures, the goal of the proposed method is to design the unit cell, which we refer to in this chapter as the microstructure.

Methods to design microstructures were first introduced in ground-structure approaches. Inverse homogenization methods to design the microstructure by modeling the unit cell as a truss or thin frame structure are presented in [37, 38]. These methods benefit from efficient computation and naturally enforce a uniform cross-sectional area for the struts that simplifies the fabrication of the microstructure. However, the 1-dimensional representation of the struts does not capture strut overlaps or the 3-dimensional stress states at strut intersections, and the optimal design may be suboptimal as it is a subset of the ground structure.

Topology optimization of continua to design microstructures was first introduced in density-based methods to design materials with extreme thermal expansion in [39], and later employed in [40] to optimize the effective bulk modulus. This and similar approaches were also employed in [41, 42, 43, 44, 45, 46, 47]; cf. the recent review [48]. Compared to ground-structure approaches, these methods produce more efficient structures and are less dependent on the initial design. However, these structures can be more difficult to manufacture, specially closed-cell designs. Other topology optimization approaches to design microstructures include evolutionary approaches [92, 93, 94, 95] and level-set methods [96, 97, 98, 99].

The use of multiple materials with different mechanical properties (i.e., moduli) and different physical densities can render designs that outperform single-material designs. The multi-material topology optimization of continuous microstructures was first demonstrated
in the aforementioned works [39] and [40]. Other interpolation schemes (i.e., [100, 101]) have also been used to design multi-phase materials with extreme thermal conductivity [102, 103]. The reader is referred to Section 2.2 for a more detailed description of these approaches.

Several techniques have been advanced to obtain open-cell lattice designs while using a 3-dimensional analysis model. A technique that has been used to perform the topology optimization of a structure exclusively made of, e.g., cylindrical bars while using a fixed mesh for the analysis is the geometry projection method [49, 50, 51]. In this method a high-level parameterization of the geometry is smoothly mapped onto a density field over a fixed finite element grid. By assigning a size variable to each geometric component that is penalized in the spirit of density-based methods, the geometry projection enables the entire removal of a component from the design. A similar family of methods to design structures made of distinct geometric primitives is the method of moving morphable components [52], in which primitives and their union are represented using level set functions. Unlike the geometry projection method, this method does not employ penalized size variables for the components and therefore can only remove components by engulfing them inside other components or by making their size small enough that they do not affect the analysis.

An advantage of lattice designs is that it is arguably easier to manufacture a lattice in which each strut is made of a single material than a microstructure with a continuously varying mixture of materials. The geometry projection method was employed in [82] in conjunction with an adaptation of the multi-material interpolation scheme of [39] to design two-material, 3-dimensional lattice structures. The effectiveness of this method is demonstrated via the design of two-material lattices for maximal bulk modulus and for minimal Poisson’s ratio. While this interpolation scheme is very effective, extending its application to more than two materials is not straightforward and requires changes to the material interpolation formulation, as noted in [64]. In the context of topology optimization with discrete geometric components using geometry projection, a new interpolation scheme was presented in [53] to accommodate the design of multi-material structures. A size variable per material is ascribed to each geometric component. This interpolation is an adaptation of the discrete material optimization (DMO) method [64]. However, unlike DMO, this
method employs optimization constraints to ensure these size variables are 0 or 1, and to
guarantee that each component has at most one material with a size variable of 1. The
moving morphable components method has been applied to the design of multi-material
structures [83] with geometric components made of different materials; however, unlike all
of the aforementioned multi-material methods, the choice of material for each component
is fixed and therefore not part of the optimization.

This chapter focuses on the topology optimization of multi-material lattice structures
using the geometry projection method. By employing the multi-material interpolation and
optimization constraints introduced in [53], the proposed method can readily accommodate any number of materials. It employs inverse homogenization to design the unit cell
for extremizing the effective properties of the macrostructure. To enforce desired sym-
metries in the lattice, the geometry projection of a reference region is reflected onto other
regions with respect to the symmetry planes corresponding to the desired symmetry. To
ensure bars remain whole upon reflection inside the unit cell or with respect to the periodic
boundaries and thus facilitate fabrication, we impose a volume difference constraint on the
bars. This work builds on the preliminary results presented in [54] for maximal bulk mod-
ulus design by adding a no-cut constraint to ensure that bars remain whole upon reflection,
which results in significantly different designs. We demonstrate the efficacy of our method
by designing two- and three-material lattices with maximal bulk modulus, maximal shear modulus and minimal Poisson’s ratio subject to a weight constraint.

The rest of the chapter is organized as follows. In Section 3.3 we describe the ho-
mogenization method that we use to calculate effective properties of the macrostructure by
considering a unit cell. In Section 3.4 we employ reflection matrices to enforce symmetries
on the lattice. Section 3.5 presents a new constraint to enforce the bars to stay in the sym-
metry reference region. The optimization problem in described in Section 3.6. We present
numerical examples to demonstrate our method in Section 3.7, and we draw conclusions
in Section 3.8.
3.3 Homogenization

We approximate the effective properties of the lattice by using homogenization (cf., [104]). The components of the effective elastic tensor $C^H$ are given by

$$C_{ijkl}^H = \frac{1}{|Y|} \int_Y C_{pqrs} (\varepsilon_0^{0(ij)} - \varepsilon_*^{*ij}) (\varepsilon_0^{0(kl)} - \varepsilon_*^{*kl}) \, dy$$

(3.1)

with $\varepsilon_0^{0(kl)} = e_k \otimes e_l$ corresponding to six unit strains applied on the unit cell, $Y$ denoting the domain of the unit cell, $C_{pqrs}$ indicating the components of the elasticity tensor of Eq. 2.3, and

$$\varepsilon_*^{*kl} = \frac{1}{2} \left( \frac{\partial \chi_{p}^{(kl)}}{\partial y_q} + \frac{\partial \chi_q^{(kl)}}{\partial y_p} \right)$$

(3.2)

The fields $\chi^{(kl)} \in \mathcal{U}_{adm}$ are the solutions to the six problems

$$\int_Y C_{ijpq} \frac{\partial \chi_p^{(kl)}}{\partial y_q} \frac{\partial v_i}{\partial y_j} \, dy = \int_Y C_{ijkl} \frac{\partial v_i}{\partial y_j} \, dy, \forall v \in \mathcal{U}_{adm}$$

(3.3)

with $v$ denoting the test function and $\mathcal{U}_{adm} := \{ u | u \in H^1(Y), u \text{ is } Y-\text{periodic} \}$ being the set of admissible solutions.

3.4 Symmetry

We impose symmetry with respect to an arbitrary number of planes on the unit cell to obtain desired material symmetries on the lattice. The intersection of these planes defines a number of similar regions, among which we choose one as the reference region, wherein we define the bars. To compute the projected density at a point in any of the other regions, we reflect the point with respect to the appropriate symmetry planes so that the reflected point lies on the reference region, and then we perform the geometry projection as usual. This strategy is employed in [53] and is similar to the one introduced in [82]. To perform the reflection with respect to the appropriate symmetry planes, we multiply all the corresponding reflection matrices (we assume all symmetry planes pass through the origin of the
unit cell coordinate system). The reflected point is obtained as

\[ \hat{p} := \prod_{s=1}^{N_s} R_s p \]  

(3.4)

with \( N_s \) denoting the number of symmetry planes and \( R_s \) being the reflection matrix corresponding to symmetry plane \( s \).

### 3.5 No-Cut Constraint

A significant difference of the proposed method with the preliminary results of [54] is that here we introduce a constraint in the optimization to ensure components remain whole in the design space, that is, that lattice bars are not cut upon reflection or across boundaries, which would make fabrication more difficult. A mechanism to achieve this is introduced in [82] by imposing constraints on the positions of the endpoints of the medial axes so that bars entirely lie within the reference region; in the case of cubic symmetry, for instance, this amounts to lower and upper bounds on the endpoint positions (which render orthotropic symmetry) plus four additional constraints per bar to restrict the positions to the reference tetrahedral region.

Here, we follow a simpler but equally effective approach, whereby we introduce a constraint on the difference between the volume of the bars in the reference region computed using the geometric parameters, and the volume that would be computed using the geometry projection. If these two volumes are different, it means a portion of the bar is lying outside of the reference region and the bar is cut. Therefore, if we impose a constraint that this difference cannot be larger than a small value, we consequently force bars to be wholly placed within the reference region. To account for multiple bars, we place the constraint on the maximum volume difference violation of all bars, which we smoothly approximate using a lower-bound Kreisselmeier-Steinhauser (LKS) function

\[ g_n(z) := \frac{LKS}{\nu} (V_{\text{geom}} - V_{\text{num}}^b) \leq \epsilon_n, \]  

(3.5)
with
\[
LKS(x) := \frac{1}{k} \ln \left( \frac{1}{n} \sum_i e^{kx_i} \right), \quad x \in \mathbb{R}^n,
\]
where \(V_{\text{geom}}^b\) is the volume of bar \(b\) calculated using its geometric parameters (i.e., end-point locations and width), and \(V_{\text{num}}\) is the sum of projected densities for bar \(b\) inside the symmetry reference region. The advantages of this approach are that it does not require formulating different placement constraints on the points for different types of material symmetries, and it renders a single optimization constraint regardless of the number of bars and of symmetry planes. We use the LKS function instead of the KS function of Eq. 2.12 because it approximates the maximum from below and therefore the approximation does not exceed the desired maximum value of zero. Also, we do not need to use adaptive constraint scaling strategies to compensate for the approximation error similar to those used in, e.g., stress-based topology optimization (cf., [86]) because the constraint limit is zero and we are approximating from below. A similar idea was used in the context of level set methods for topology optimization in [105] to prevent the overlap of embedded, primitive-shaped components in a free-form structure. This is achieved by comparing the analytical volume of all the embedded components to the volume obtained from integrating a smooth Heaviside projection of the components. Our method is different in that the comparison is made for each component individually, which only prevents the struts from leaving the reference region, but it does not prevent overlaps among struts. Since the comparison is made component by component, we thus require the aggregation function of Eq. 3.6.

### 3.6 Optimization and Computer Implementation

We consider three problems in this work: maximization of the effective bulk modulus, maximization of the effective shear modulus and minimization of the effective Poisson’s ratio of the lattice structure, all subject to a weight fraction constraint, a discreteness constraint (Section 2.4), and a mutual material exclusion constraint (Section 2.5).
3.6.1 Optimization Problem

In this work, we only consider effective lattices with cubic symmetry. The effective bulk ($K$) and shear ($G$) moduli for an isotropic material are calculated as

$$K(z) := \frac{1}{3} C_{1111} + \frac{2}{3} C_{1122}$$  \hspace{1cm} (3.7)

and

$$G(z) = C_{1212},$$  \hspace{1cm} (3.8)

respectively. The Poisson’s ratio is given by

$$\nu(z) = \frac{C_{1122}}{2(C_{1122} + C_{1212})}.$$  \hspace{1cm} (3.9)

The weight fraction constraint is computed as

$$w_f := \frac{1}{|\Omega| \gamma_{max}} \sum_{m=1}^{N_g} \gamma_m \int_{\Omega} \rho_{eff}(z,p) \, dv \leq w_f^*. \hspace{1cm} (3.10)$$

The optimization problem is given by

$$\min_{z} f(z) \hspace{1cm} (3.11)$$

subject to

$$a(u^{(kl)}(z), v) = l(v, \varepsilon^{0(kl)}), \forall v \in \mathcal{V}_0, u^{(kl)} \in \mathcal{U} \hspace{1cm} (3.12)$$

$$g_w(z) \leq w_f^* \hspace{1cm} (3.13)$$

$$g_d(z) \leq \varepsilon_d^{(l)} \hspace{1cm} (3.14)$$

$$g_m(z) \leq \varepsilon_m^{(l)} \hspace{1cm} (3.15)$$

$$g_n(z) \leq \varepsilon_n \hspace{1cm} (3.16)$$

$$x_{b_0}, x_{b_f} \in \Omega \hspace{1cm} (3.17)$$

$$0.0 \leq \alpha^b_m \leq 1.0, \hspace{1cm} (3.18)$$
with \( f(z) \equiv -K(z) \) for the bulk modulus maximization, \( f(z) \equiv -G(z) \) for the shear modulus maximization, and \( f(z) \equiv \nu(z) \) for the Poisson’s ratio minimization. In addition to the foregoing constraints, and as is customary for this problem (cf. [37]), for the Poisson’s ratio minimization we also impose a lower limit on the effective bulk modulus, \( K(z) \leq K_{\text{min}} \) to avoid removal of all the material. In the expressions above, \( w_f \) is the weight fraction, \( \gamma_m \) the physical density for material \( m \), and \( \gamma_{\text{max}} \) is the largest physical density of all available materials, so that if the heaviest material occupies the entire unit cell, \( w_f = 1 \). The domains \( \Omega \) and \( \omega \subseteq \Omega \) correspond to the region occupied by the design envelope and the design, respectively. The test functions are denoted by \( v \), and \( u^{(kl)} \) are the displacements corresponding to the six applied unit strains \( \epsilon^{(kl)} \), \( k, l = 1, \cdots, 3 \). The admissible sets for trial and test functions are \( \mathbb{V} := \{ u | u \in H^1(\Omega), u \text{ is } Y\text{-periodic}, u(c) = 0 \} \) and \( \mathbb{V}_0 := \{ v | v \in H^1(\Omega), v|_\Gamma = 0, v(c) = 0 \} \), respectively. We prevent rigid-body motions by imposing zero displacements at the center of the unit cell \( c \). The energy bilinear form \( a \) and the load linear form \( l \) in Eq. 4.30 are computed as

\[
a(u, v) := \int_\Omega \nabla v \cdot C(z, p) \nabla u \, dv \tag{3.19}
\]

and

\[
l(v, \epsilon) := \int_\Omega \nabla v \cdot C(z, p) \epsilon \, dv. \tag{3.20}
\]

For the design variables \( z \) to fall within the range \([0, 1]\), we scale them as in our previous works [50, 51, 53], and at each optimization iteration \( I \) we impose a move limit \( m \) on each design variable as

\[
\max(0, z^{(I-1)} - m) \leq z^{(I)} \leq \min(1, z^{(I-1)} + m). \tag{3.21}
\]

### 3.6.2 Computer Implementation

A flowchart describing the proposed method is shown in Algorithm 2. Our code is implemented in C++ using the deal.II library [90, 106] as a backbone for the finite element solutions. We parallelize the assembly of the stiffness matrix, the computation of the ge-
ometry projection, and the solution of the linear system of equations by employing the data structures provided by parallel linear algebra libraries. We employ an element-wise uniform effective density, which we compute at the element centroid $x_e$. The geometry projection is computed using a window radius $r$ equal to $c$ times the radius of the sphere that circumscribes the element, i.e., $r = c\sqrt{3}h/2$, where $h$ is the element size. As the optimizer, we employ the parallel implementation of the method of moving asymptotes (MMA) of [87, 88], presented in [107]. We use the default MMA parameters presented in [88]. We stop the optimization when the relative change $\Delta f$ in compliance between consecutive iterations falls below a specified value $\Delta f^*$. The optimization parameter values we employed for all examples are listed in Table 3.1.
Algorithm 1 Multi-material Topology Optimization of Lattice Structures

1: $k \leftarrow 0$ ▷ Iteration counter
2: $z^{(0)} \leftarrow z_0$ ▷ Initial design
3: $f_{old} = -objtol$
4: repeat
5: for $q = 1, \ldots, N_b$ do
6: for $e = 1, \ldots, N_{el}$ do
7: Compute signed distance $\phi_b$ to bar $b$ ▷ §1.4
8: if element $e$ outside of the reference region then
9: Computed reflected element centroid $\hat{x}_e$ ▷ Eq. (3.4)
10: end if
11: Compute projected density $\rho_b$ ▷ Eq. (1.3)
12: end for
13: end for
14: for $e = 1, \ldots, N_{el}$ do
15: Compute element stiffness matrix $K_e$ using $C(z, p)$ ▷ Eq. (2.3)
16: Assemble $K_e$ into global stiffness matrix $K$
17: end for
18: for $k = 1, \ldots, 6$ do
19: for $e = 1, \ldots, N_{el}$ do
20: Compute element force $f^k_e$ contributions from applied unit strains ▷ Eq. (4.30)
21: Assemble $f^k_e$ into global force vectors $f_k$
22: end for
23: Solve $K_k(z)u_k(z) = f_k$ for $u(z)$
24: end for
25: Compute $f(z), \nabla f(z)$ ▷ Eq. (3.7) or Eq. (3.8) or Eq. (3.9)
26: Compute $g(z), \nabla g(z)$ ▷ $g$ denotes vector of constraints
27: Impose move limits and update $z_{low}$ and $z_{upp}$ ▷ Eq. (3.21)
28: $z^{(k+1)} \leftarrow \text{opt}(z^{(k)}, f, \nabla f, g, \nabla g, z_{low}, z_{upp})$ ▷ Update design
29: $k \leftarrow k + 1$
30: Compute relative change in objective $\Delta f = |(f - f_{old})/f_{old}|$
31: $f_{old} \leftarrow f$
32: until $\Delta f \leq objtol$

46
### Parameter Table

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**Table 3.1: Optimization parameters**

## 3.7 Examples

We now present examples to illustrate the effectiveness of the proposed method. We employ hexahedral, trilinear elements to mesh the unit cell. We employ a system with six compute nodes with 24 Intel Haswell cores each, CPU speed of 2.59 GHz and 128 GB of memory per node to perform all the examples.

### 3.7.1 Maximal Bulk Modulus of Two- and Three-material Lattices with Cubic Symmetry

In this example, we maximize the bulk modulus for lattices with cubic symmetry and made of two and three materials. To enforce the cubic symmetry, we define nine symmetry planes, including the three orthogonal planes perpendicular to the faces that pass through the center of the unit cell, and the six planes that pass through the origin and two opposite edges that divide the cube into two equal partitions. The initial design consists of 10 bars with near-zero length (which resemble spheres) and width $w = 0.1$, as shown in Fig. 3-1.

All materials are homogeneous, isotropic, and linearly elastic, with Poisson’s ratio $\nu = 0.3$. The unit cell is meshed with a regular grid of $64 \times 64 \times 64$ elements.

For the two-material designs, the available materials have Young’s moduli $E_1 = 10$ and $E_2 = 5$, and physical densities $\gamma_1 = 0.9$ and $\gamma_2 = 0.45$. We set the initial size variables corresponding to these two materials to $\alpha_1^b = \alpha_2^b = 0.5$. 
The results of the optimization for different weight fraction limits are presented in Table 3.2. It is worth noting that small changes in the weight fraction limit produce completely different designs. This is expected, since this problem is known to have many local minima [108]. The overall trend is that the maximal bulk modulus increases as we increase the weight fraction limit as expected. We posit the exceptions to a strict monotonic behavior correspond to convergence to local minima. One possibility to obtain better minima would be to employ the tunneling method proposed in [109]; however, this is outside the scope of this work.

An important difference between these results and those previously published in [54] is that the no-cut constraint is effective in rendering struts that do not have cuts that would be difficult to manufacture. The no-cut constraint also performs an important function, namely to ensure open-cell designs by preventing struts that are cut by a face of the unit cell from agglomerating on that face in a manner that effectively produces a thin closed wall (this situation was observed in [54]). Some of the designs either resemble the well-known octet truss configuration (for instance the one for $w_f^* = 0.0722$), or have an ‘embedded’ octet truss made of one material (cf. the designs with $w_f^* = 0.05$ and $w_f^* = 0.0889$). The design for $w_f^* = 0.0444$ resembles the two-material octahedral rectified cubic (ORC) design shown in [82]. Other designs, however, are less intuitive.

In Fig. 3-2a, we compare the effective bulk moduli for the designs of Table 3.2 to the Hashin-Shtrikman-Walpole (HSW) bounds for three-phase materials (with one phase being void) [40]. As expected, all the bulk moduli for the optimal designs are below the bounds. We also note that the moduli are not close to the bounds. This is contrary to what has been

Figure 3-1: Initial design after reflection for cubic symmetry. Blue region indicates reference region.
<table>
<thead>
<tr>
<th>$K$</th>
<th>$w_f^*$</th>
<th>iso</th>
<th>side</th>
<th>$K$</th>
<th>$w_f^*$</th>
<th>iso</th>
<th>side</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.07</td>
<td>0.0444</td>
<td></td>
<td></td>
<td>0.1385</td>
<td>0.0778</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0803</td>
<td>0.05</td>
<td></td>
<td></td>
<td>0.1203</td>
<td>0.0833</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.0923</td>
<td>0.0556</td>
<td></td>
<td></td>
<td>0.1391</td>
<td>0.0889</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1171</td>
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<td></td>
<td></td>
<td>0.1574</td>
<td>0.0944</td>
<td></td>
<td></td>
</tr>
<tr>
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<td>0.0667</td>
<td></td>
<td></td>
<td>0.1865</td>
<td>0.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.1237</td>
<td>0.0722</td>
<td></td>
<td></td>
<td>0.1753</td>
<td>0.1056</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3.2: Maximal bulk modulus designs for cubic two-material lattices and different weight fraction limits $w_f^*$. Red bars are made of material 1, blue bars are made of material 2, and bars that have been removed from the design (i.e., with $\alpha_1^b, \alpha_2^b \approx 0$) are not shown.
shown for designs obtained using density-based topology optimization [40]. The reason for this is that the design representation is significantly more restrictive (i.e., a truss made of cylindrical struts of constant diameter) and we impose an additional geometric requirement (the no-cut constraint). Moreover, the lattice representation ensures an open-cell design (which we desire, as justified in Section 3.2); however, closed-cell designs are known to render higher bulk moduli [108].

![Effective bulk modulus and shear modulus](image)

Figure 3-2: Comparison of effective moduli to HSW-bounds for the designs corresponding to Tables 3.2 and 3.4. Arrows point from the optimal design to the HSW-bound surface.

We now perform the optimization for this same problem by adding a third material with elastic modulus $E_3 = 7.5$ and physical density $\gamma_3 = 0.675$. The results for different weight fraction limits are shown in Table 3.3. An important note about these results is that the range of weight fraction limits that produces three-material designs is narrower than for two-material designs. This is expected, since above and below that range two-material designs (and eventually, single-material designs) are more weight-efficient. The designs produced in this example are intricate and not intuitive; to the best of our knowledge there are no published designs for three-material lattices.

### 3.7.2 Two- and Three-material Lattices with Maximal Shear Modulus and Cubic Symmetry

In this section we present results for maximization of the effective shear modulus, both for two-material and three-material lattices. The material properties are the same as in...
Table 3.3: Maximal bulk modulus designs for cubic three-material lattices and different weight fraction limits $w_f^*$. Red, blue and green bars are made of materials 1, 2, and 3, respectively; and bars that have been removed from the design (i.e., with $\alpha_1^b, \alpha_2^b, \alpha_3^b \approx 0$) are not shown.
Table 3.4: Maximal shear modulus designs for cubic two-material lattices and different weight fraction limits \( w_f^* \). Red bars are made of material 1, blue bars are made of material 2, and bars that have been removed from the design (i.e., with \( \alpha_1^b, \alpha_2^b \approx 0 \)) are not shown.

<table>
<thead>
<tr>
<th>( G )</th>
<th>( w_f^* )</th>
<th>iso</th>
<th>side</th>
<th>( G )</th>
<th>( w_f^* )</th>
<th>iso</th>
<th>side</th>
</tr>
</thead>
<tbody>
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<td>0.0778</td>
<td></td>
<td></td>
</tr>
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<td></td>
</tr>
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<td></td>
<td></td>
<td>0.0861</td>
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<td></td>
<td></td>
</tr>
<tr>
<td>0.0502</td>
<td>0.0667</td>
<td></td>
<td></td>
<td>0.1518</td>
<td>0.1</td>
<td></td>
<td></td>
</tr>
<tr>
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<td></td>
<td></td>
<td>0.1243</td>
<td>0.1056</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The results of the optimization for this same problem with three materials (with the same properties as before) are shown in Table 3.5. Once again, the range of weight fraction limits that produces three-material designs is narrower than for two-material designs.
<table>
<thead>
<tr>
<th>$G$</th>
<th>$w_f^*$</th>
<th>iso</th>
<th>side</th>
</tr>
</thead>
<tbody>
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<td><img src="image2.png" alt="Image" /></td>
</tr>
<tr>
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<td>0.0722</td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
</tr>
<tr>
<td>0.0859</td>
<td>0.0944</td>
<td><img src="image5.png" alt="Image" /></td>
<td><img src="image6.png" alt="Image" /></td>
</tr>
<tr>
<td>0.1288</td>
<td>0.1056</td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
</tr>
</tbody>
</table>

Table 3.5: Maximal shear modulus designs for cubic three-material lattices for different weight fraction limits $w_f^*$. Red, blue and green bars are made of materials 1, 2, and 3, respectively; and bars that have been removed from the design (i.e., with $\alpha_1^b, \alpha_2^b, \alpha_3^b \approx 0$) are not shown.
Finally, we present results for the minimization of the effective Poisson’s ratio for two- and three-material cubic lattices. The material properties are the same as before. As detailed in Section 3.6, for this problem we add a constraint that ensures a minimum bulk modulus of $K_{\text{min}}$, cf. Table 3.1. The results for two-material lattices are shown in Table 3.6. For the weight fraction limits we employed, the resulting effective Poisson’s ratios are all negative, therefore the lattice is auxetic. In this case, the effective Poisson’s ratio monotonically decreases as we increase the weight fraction limit. We also present a three-material lattice design in Table 3.7. In this case, we could only find a narrow weight fraction limit range that would render a three-material design with negative Poisson’s ratio. We note, however, that the three-material design performs better than the two-material design for the same weight fraction limit shown in Table 3.6. Interestingly, the side views of most of these designs resemble the well-known re-entrant honeycomb design for auxetic materials. However, the 3-dimensional arrangement seen in the isometric views is not necessarily intuitive.
Table 3.7: Minimal Poisson’s ratio design for cubic three-material lattice. Red, blue and green bars are made of materials 1, 2, and 3, respectively; and bars that have been removed from the design (i.e., with $\alpha_1^b, \alpha_2^b, \alpha_3^b \approx 0$) are not shown.

3.8 Conclusions

This chapter presented a topology optimization method for the design of multi-material lattice structures using the geometry projection technique. The numerical examples demonstrate that the proposed method is effective in producing multi-material lattices for the maximization of effective bulk and shear moduli, and for the minimization of effective Poisson’s ratio. The proposed formulation effectively imposes any number of symmetry planes to obtain desired material symmetries; in the case of the numerical examples, cubic symmetry is imposed on all lattices. Moreover, the no-cut constraint is also effective in preventing struts from being cut by the unit cell boundaries or the symmetry planes that would make the manufacturing more difficult, and that may produce closed-cell structures. As expected, the designed lattices satisfy theoretical bounds on effective bulk and shear moduli, and are in fact away from these bounds since they are open-cell structures. The designs produced by the proposed method still pose some fabrication challenges, as some of the struts may have overlaps that are difficult to realize. The minimum angle constraint discussed in Section 4.4.2 alleviates this problem.
Chapter 4

Design of Multi-scale Lattices

4.1 Summary

This chapter presents a topology optimization method for design of architected truss lattices made of anisotropic struts. Previous works on lattice design, including the one presented in the previous chapter, have used a single or multiple isotropic materials for the struts. Employing anisotropic materials, however, can result in better effective properties. In this chapter we focus on lattice struts that are either hollow or fiber-reinforced, which effectively result in transverse isotropy.

As before, we design a unit cell of the lattice to extremize its effective properties. The proposed method simultaneously optimizes the spatial configuration of the struts and the volume fraction of the reinforcing fibers or the hole in each strut. Each strut is represented via a 3-dimensional offset surface. We employ the geometry projection method to map the parametric description of the lattice geometry onto a density field for analysis, however we employ the material interpolation of [110] to accommodate the overlap of struts with different anisotropic properties. As in the method of the previous chapter, the technique proposed here accommodates any number of specified material symmetries by performing appropriate reflections of the projected density with respect to the symmetry planes. As before, we impose a discreteness constraint to ensure 0 or 1 size variables in the optimal design. We again impose a no-cut constraint to ensure that struts are not partially cut upon reflection by the symmetry planes or by the faces of the unit cell. We also constrain the
smallest angle at which two struts can intersect to avoid overlaps that are difficult to man-
ufacture. We demonstrate the effectiveness of our method with examples of maximization of the effective bulk modulus of the lattice.

4.2 Introduction

Topology optimization has been extensively employed to determine the optimal layout of material in a prescribed design region. One of the applications of topology optimization techniques is the design of periodic architected materials, also referred to as design of microstructure. Lattices made up of struts are one of the most popular types of architected materials. One way in which lattices are advantageous is that they are open-cell structures, and thus easier to manufacture in comparison with closed-cell structures due to the possibility of using sacrificial, soluble support materials. Furthermore, they have been shown to outperform bulk materials for low relative densities. This chapter focuses on designing the unit cell of a periodic lattice with anisotropic struts using topology optimization.

One of the limitations in the design of multi-material, polymeric lattices is that the physical densities of the materials employed in multi-material 3d-printing processes are very similar; this is likely a result of the need to tightly control the rheology in the printing process. Therefore, optimal lattices for maximal moduli with a weight fraction constraint end up employing only the stiffest material. To overcome this practical limitation, it is possible to employ porous struts with designable porosity that render a range of material properties by using a single printable material. If the porous microstructure of the struts is such that the effective properties of the porous material are isotropic, the optimizer converges to either fully solid or void struts. This is due to the fact that isotropic materials obey bounds on the effective properties (the Hashin-Shtrikman bounds) and exhibit low stiffness-to-density ratios for intermediate porosity values, and therefore using isotropic porosity is not advantageous in stiffness-based optimization. All the aforementioned methods have employed isotropic materials to design the microstructure. Anisotropic materials, on the other hand, are not subject to these bounds and thus a porous microstructure that renders anisotropic effective properties can be beneficial in such problems.
In this chapter we propose a geometry projection method for the topology optimization of lattices with struts made of a porous, anisotropic material. Specifically, we consider struts that are transversely isotropic, either by reinforcing a weak matrix with stiff fibers along the strut, or by having a hollow strut with one or more holes running along the axis of the strut. The proposed method aims to determine the optimal layout of struts to extremize the effective properties of the lattice. Unlike previous works, however, we must account for the fact that the struts are made of a porous, anisotropic material. This has two important consequences. The first is that in addition to the layout of the struts, the porosity of the struts can be controlled in the manufacturing and is also a design parameter. The second is that we must model the porosity in the struts. To do this in a simple way, we employ a homogenized material for the struts whose effective properties are a function of the porosity. Since this homogenized material is anisotropic, we must align the material properties with the orientation of the strut upon design changes. To achieve the latter, we build on the recent work of [110] to design frame structures made of anisotropic bars. To obtain desired material symmetries, the geometry projection of the symmetry reference region is reflected with respect to appropriate symmetry planes onto other regions. A no-cut constraint is imposed to ensure that struts remain whole upon reflection to facilitate manufacturing. We demonstrate the effectiveness of our method by designing lattices with maximal bulk modulus subject to a weight constraint.

The remainder of the chapter is organized as follows. In Section 4.3 we describe the geometry projection method in more details. In Section 4.4 we describe the optimization problem. Section 4.5 presents numerical examples to demonstrate our method, and the conclusions are drawn in Section 4.6.

4.3 Geometry Projection

To represent the lattice using specified geometric primitives (such as bars), we use the geometry projection method presented in the introduction. To account for anisotropic materials, we employ the formulation presented in [110] for the design of structures made of geometric components, where each component is made of an anisotropic material. In this
method the material for each component is specified in the initial design and fixed during
the optimization, and thus there is no material selection by the optimizer. We adopt that
formulation in this work to account for the anisotropy of the struts, and we now briefly
describe it for completeness.

The penalized element density is computed as

\[ \tilde{\rho}_e := \sum_b w_{be} \hat{\rho}_b, \]  

(4.1)

where the weights \( w_{be} \in [0, 1], \sum_b w_{be} = 1 \) denote the fractional contribution of each strut to
the penalized element density. These weights are very much in the spirit of the discrete ma-
terial optimization (DMO) method for multi-material, density-based topology optimization
[64, 67]. The ersatz material elasticity tensor is computed as

\[ C^e = C_{\text{void}} + \sum_b w_{be} \hat{\rho}_b (C_b - C_{\text{void}}). \]  

(4.2)

The above equation is essentially equivalent to the softmax function [111] with the weights
given by

\[ w_{be} = \frac{e^{\hat{\rho}_b}}{\sum_b e^{\hat{\rho}_b}}. \]  

(4.3)

This interpolation has the advantage that when multiple struts intersect, it chooses the best
material at the intersection region, thus there is no mixture of materials at strut intersections.

An important difference between this formulation and the methods mentioned in the
previous section is that since the material properties of each geometric component are no
longer isotropic, they need to be aligned with the strut. This can be done using a coordinate
transformation from the strut coordinates to the global coordinates. The principal material
direction is along the medial axis, and by selection of two orthogonal vectors, a Cartesian
coordinate system for the material can be defined. Since there is no obvious choice for
these vectors in 3-dimensions, the orthogonal vector is chosen to be the unit coordinate
vector \( \hat{e}_\alpha \) that is closer to being orthogonal to the medial axis, i.e., that has a minimal \( \mathbf{a} \cdot \hat{e}_\alpha \):

\[
\hat{e}_{1b} := \frac{\mathbf{a}}{\| \mathbf{a} \|} \tag{4.4}
\]
\[
\hat{e}_{2b} := -\left( \mathbf{a} \times \hat{e}_\alpha \right) / \| (\mathbf{a} \times \hat{e}_\alpha) \| \tag{4.5}
\]
\[
\hat{e}_{3b} := \hat{e}_{1b} \times \hat{e}_{2b}. \tag{4.6}
\]

The coordinate transformation matrix for strut \( b \) is thus computed as

\[
R_{ij}^b = \hat{e}_i \cdot \hat{e}_{jq}, \tag{4.7}
\]

and the elasticity tensor for strut \( b \) is then transformed to the global coordinate system as

\[
\mathbb{C}_b = (R_b \boxtimes R_b)^T \mathbb{C}_b (R_b \boxtimes R_b^T) \tag{4.8}
\]

where \( \boxtimes \) is the conjugate product—also called the square tensor product or tensor product of transformation [112, 113]. The components of the transformation matrix \( R_{ij}^b \) depend on the choice of \( \hat{e}_\alpha \). However, that will not affect the components of the transformed elasticity tensor due to transverse isotropy. Unlike the work of [110], in this work the material properties of each strut are a continuous function of the porosity or material fraction of the strut. The material properties of the fiber-reinforced strut \( b \) correspond to those of a unidirectional fiber composite with cylindrical continuous fibers, and are given by (cf.
$E_L = E_m(1 - V_f) + E_f V_f + \frac{4(V_f - V_m)^2(1 - V_f) V_f K_f K_m G_m}{(1 - V_f) K_m G_m + V_f K_f G_m + K_f K_m}$ \hspace{1cm} (4.9)

$\nu_L = \nu_m(1 - V_f) + \nu_f V_f + \frac{G_m(V_f - V_m)(K_f - K_m)(1 - V_f)V_f}{(1 - V_f) K_m G_m + V_f K_f G_m + K_f K_m}$ \hspace{1cm} (4.10)

$G_L = G_m G_m (1 - V_f) + G_f (1 + V_f)$ \hspace{1cm} (4.11)

$G_T = G_m + \frac{2V_f G_m(K_m + G_m)}{(1 - V_f)(K_m + 2G_m) - 2(K_m + G_m)}$ \hspace{1cm} (4.12)

$K = \frac{K_m(K_f + G_m)(1 - V_f) + K_f(K_m + G_m)V_f}{(K_f + G_m)(1 - V_f) + (K_m + G_m)V_f}$ \hspace{1cm} (4.13)

$E_T = 4 \left( \frac{1}{G_T} + \frac{1}{K} + \frac{4\nu_L^2}{E_L} \right)^{-1}$ \hspace{1cm} (4.14)

$\nu_T = \frac{E_T}{2G_T} - 1$ \hspace{1cm} (4.15)

In these expressions, $V_f$ is the volume fraction of the fiber in strut $b$ (the subscript $b$ is omitted in these expressions for conciseness), however we note that $V_{fb}$ is an additional design parameter for each strut. $E_m$, $G_m$, $K_m$ and $\nu_m$ are the Young’s modulus, shear modulus, bulk modulus and Poisson’s ratio of the isotropic matrix material, respectively; $E_f$, $G_f$, $K_f$ and $\nu_f$ are their isotropic fiber material counterparts. $E_L$, $\nu_L$ and $G_L$ are the effective longitudinal modulus, Poisson’s ratio and shear modulus, respectively; $K$ is the effective bulk modulus; and $G_T$ and $\nu_T$ are the transversal shear modulus and Poisson’s ratio respectively. These expressions are obtained from micromechanics formulations, and they are all exact, except for the transverse shear modulus $G_T$ which is an upper bound for the case where the fiber is stiffer than the matrix (i.e., $K_f > K_m$) and a lower bound if the matrix is stiffer than the fiber (i.e., $K_m > K_f$) [114].

We note that the third term in Eq. 4.9 is typically negligible, which renders the well known rule of mixtures; and when the Poisson ratios of the fiber and the matrix are identical (as it is the case for the fiber-reinforced examples considered in this work), this term is zero. In the case of hollow struts, we simply set $E_f = G_f = 0$. It can be shown that in this case $\nu_L = \nu_m$.

The elasticity tensor for the isotropic material of bar $b$ is given by $C^0_b = (S^0_b)^{-1}$, where
$S_0^b$ is the bar compliance tensor given by

$$
S_0^b = \begin{bmatrix}
\frac{1}{E_L} & -\frac{\nu_L}{E_L} & -\frac{\nu_L}{E_L} & 0 & 0 & 0 \\
-\frac{\nu_L}{E_L} & \frac{1}{E_T} & -\frac{\nu_T}{E_T} & 0 & 0 & 0 \\
-\frac{\nu_L}{E_L} & -\frac{\nu_T}{E_T} & \frac{1}{E_T} & 0 & 0 & 0 \\
0 & 0 & 0 & 2(1+\nu_T) & 0 & 0 \\
0 & 0 & 0 & 0 & \frac{1}{\rho_L} & 0 \\
0 & 0 & 0 & 0 & 0 & \frac{1}{\rho_L}
\end{bmatrix}
$$

(4.16)

4.4 Optimization and Computer Implementation

We consider maximization of the effective bulk modulus, subject to a weight fraction constraint, a discreteness constraint, a no-cut constraint and an angle constraint. We impose a weight fraction constraint instead of separate volume fraction constraints on different materials, which allows the optimizer to determine the right proportion of materials in the optimal design. The no-cut constraint ensures struts are not cut upon reflection or by the unit cell boundaries. The purpose of this constraint is to prevent the optimizer from creating closed-cell designs by agglomerating cut struts on the unit cell faces. These closed-cell designs are more difficult to manufacture. Additionally, we impose a constraint on the minimum angle between struts to avoid overlaps that are difficult to manufacture. We discussed the discreteness constraint in Section 2.4 and the no-cut constraint in Section 3.5. In the following, we briefly describe the weight fraction constraint and the angle constraint.

4.4.1 Weight Fraction Constraint

Imposing a constraint on the total volume of the unit cell in a multi-material design typically results in the exclusive use of one of the materials, e.g., the stiffest material available in the case of bulk modulus maximization. To avoid this, most works in multi-material topology optimization impose separate volume constraints for each material. The limits for these constraints, however, are arbitrary. Here, we instead impose a weight fraction constraint that takes into account the physical density of the strut. The strut physical density $\gamma_b$ is
computed as a linear interpolation of the physical densities of the fiber and matrix materials, \( \gamma_f \) and \( \gamma_m \), respectively, and it is a function of the fiber volume fraction:

\[
\gamma_b = \gamma_m(1 - V_{fb}) + \gamma_f V_{fb}.
\]  

(4.17)

Similar to the penalized element density of 4.1, we define a physical element density as

\[
\bar{\gamma} := \sum_b w_{be} \hat{\rho}_b \gamma_b.
\]  

(4.18)

Note that thanks to the weights \( w_{be} \), this expression ensures the correct \( \gamma_b \) is used in this computation. The weight constraint is thus given by

\[
g_w := \frac{1}{|\Omega| \max(\gamma_f, \gamma_m)} \sum_e \bar{\gamma}^e v_e \leq g_w^*,
\]  

(4.19)

where \( v^e \) is the element volume and \( \Omega \) denotes the design space. We note that \( \gamma_m > \gamma_f \) (\( = 0 \)) in the case of hollow struts, while typically \( \gamma_f > \gamma_m \) for fiber-reinforced struts. It should also be noted that if the lattice were made of a single homogeneous material, then the weight fraction would be equivalent to a volume fraction.

### 4.4.2 Angle Constraint

We impose an angle constraint to prevent struts from overlapping at very acute angles and facilitate manufacturing. To this end, we use the technique presented in [115], wherein the angle between struts \( b \) and \( b' \) is computed as

\[
\theta_{ss'bb'} = \begin{cases} 
\arccos \hat{n}_b \cdot \hat{n}_{b'} & \text{if } s = s' \\
\pi - \arccos \hat{n}_b \cdot \hat{n}_{b'} & \text{otherwise},
\end{cases}
\]  

(4.20)

where \( \hat{n}_b = a / \|a\| \) denotes the unit normal along the medial axis of strut \( b \), and the indices \( s \in \{1, 2\} \) correspond to the endpoints \( x_{bo} \) and \( x_{bf} \) of bar \( b \).

We restrict the consideration to pairs of bars whose angles are below the minimum angle specified, and also to bars that are close to each other. To achieve the former, we use
the regularized Heaviside function to compute a weight $\rho_\theta$ which is an indicator of whether a strut should be considered. This indicator is computed as

$$\left(\rho_\theta\right)_{s'b'b'} = \begin{cases} 0 & \text{if } b = b' \\ \tilde{H} \left( \theta^* - \frac{\theta_{s'b'b'}}{e} - 1 \right) & \text{otherwise}, \end{cases} \quad (4.21)$$

where $\tilde{H}(x) = \frac{1}{2} \left( 1 + \text{erf} \left( \frac{3x}{\sqrt{2}} \right) \right)$ and $e = \pi / 32$.

To restrict the consideration to nearby struts, $\rho_{s'}$ is computed as

$$\left(\rho_{s'}=1\right)_{sbb'} = \begin{cases} 0 & \text{if } b = b' \\ \tilde{H} \left( -1 + \frac{2}{r_b} \hat{n}_b \cdot b_{sbb'} \right) & \text{otherwise} \end{cases} \quad (4.22)$$

$$\left(\rho_{s'}=2\right)_{sbb'} = \begin{cases} 0 & \text{if } b = b' \\ \tilde{H} \left( -1 - \frac{2}{r_b} \hat{n}_b \cdot b_{sbb'} \right) & \text{otherwise}, \end{cases} \quad (4.23)$$

where $\tilde{H}$ is a smooth Heaviside.

The indicators $\rho_\theta$ and $\rho_{s'}$ are then combined to define the angle indicator as

$$\left(\rho_{\text{angle}}\right)_{sbb'} = \sum_{s'} \left(\rho_{s'}\right)_{sbb'} \left(\rho_\theta\right)_{s'b'b'}. \quad (4.24)$$

The angle constraint is then computed as

$$g_a = \frac{1}{N_b^2} \sum_{s,b,b'} \tilde{\alpha}_b \tilde{\alpha}_{b'} \left(\rho_{\text{angle}}\right)_{sbb'} \left(\rho_{\text{dist}}\right)_{sbb'}. \quad (4.25)$$

In this equation, $\rho_{\text{dist}}$ is computed as

$$\left(\rho_{\text{dist}}\right)_{sbb'} = \tilde{H} \left( 1 - \frac{2d_{sbb'}}{r_b + r_{b'} + \delta} \right), \quad (4.26)$$
where $\delta$ is the minimum separation between the struts and

$$
\delta_{sbb'} = \begin{cases} 
\|b_{sbb'}\| & \text{if } \hat{n}_b \cdot b_{sbb'} < 0 \\
\|e_{sbb'}\| & \text{if } \hat{n}_b \cdot e_{sbb'} > 0 \\
\|g_{sbb'}\| & \text{otherwise,}
\end{cases}
$$

and

$$
b_{sbb'} = x_{sb} - x_{1b'}$$

$$
e_{sbb'} = x_{sb} - x_{2b'}$$

$$
g_{sbb'} = x_{sbb'} - (\hat{n}_{b'} \cdot b_{sbb'}) \hat{n}_{b'}.
$$

The reader is referred to [115] for more details on this angle constraint.

### 4.4.3 Optimization Problem

The design of lattices we consider in this work corresponds to the extremization of some effective property of the periodic lattice, such as the maximization of the effective bulk modulus. To compute these properties, we employ the homogenization method discussed in previous chapters. Once we have the effective elasticity tensor, the effective bulk modulus ($K$) is computed as

$$
K(z) := \frac{1}{3} C_{1111} + \frac{2}{3} C_{1122}.
$$
The optimization problem is

\[
\min_z f(z) \equiv -K(z) \tag{4.29}
\]

subject to

\[
a(u^{(kl)}(z), v) = l(v, e^{0(kl)}), \forall v \in \mathcal{V}_0, u^{(kl)} \in \mathcal{U} \tag{4.30}
\]

\[
g_w(z) \leq w_f, \tag{4.31}
\]

\[
g_d(z) \leq \varepsilon_d, \tag{4.32}
\]

\[
g_a(z) \leq \varepsilon_a, \tag{4.33}
\]

\[
g_n(z) \leq \varepsilon_n, \tag{4.34}
\]

\[
x_{b_o}, x_{b_f} \in \Omega, \tag{4.35}
\]

\[
0 \leq \alpha_b \leq 1, \tag{4.36}
\]

In the above expressions, \( \Omega \) denotes the region occupied by the design envelope and \( \omega \subseteq \Omega \) corresponds to the design region. The energy bilinear form \( a \) and the load linear form \( l \) in Eq. 4.30 are computed as

\[
a(u, v) := \int_\Omega \nabla v \cdot C(z, p) \nabla u \, dv \tag{4.37}
\]

and

\[
l(v, \varepsilon) := \int_\Omega \nabla v \cdot C(z, p) \varepsilon \, dv. \tag{4.38}
\]

As in our previous works [50, 53], we scale the design variables \( \tilde{z} \) so that they fall within \([0, 1]\) and we impose a move limit \( m \) on each design variable at each optimization iteration \( I \) as

\[
\max(0, z^{(I-1)} - m) \leq z^{(I)} \leq \min(1, z^{(I-1)} + m). \tag{4.39}
\]

As customary in gradient-based optimization, the move limits prevent drastic design changes that could produce a poor design, particularly in early iterations of the optimization. The variable scaling allows us to use the same move limit on all variables.
### Table 4.1: Optimization parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Equation/Section</th>
</tr>
</thead>
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<td>2.15</td>
</tr>
<tr>
<td>$\varepsilon^0_d$</td>
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<td>$\varepsilon^2_\alpha$</td>
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</tr>
<tr>
<td>$\varepsilon_a$</td>
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</tr>
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</tr>
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<tr>
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<tr>
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<td>§4.4.4</td>
</tr>
</tbody>
</table>

#### 4.4.4 Computer Implementation

Algorithm 2 contains a flowchart describing the proposed method. Our code is implemented in MATLAB. We compute the uniform elemental density at the element centroid $x_e$. The radius $r$ of the sample window equals to $c$ times the radius of the sphere that circumscribes the element, i.e., $r = c\sqrt{3h}/2$, where $h$ is the element size. We employ the method of moving asymptotes (MMA) of [87, 88] as the optimizer, with the default parameters listed in Table 4.1. We stop the optimization when the relative change $\Delta f$ in the objective function between consecutive iterations falls below a specified value $\Delta f^*$. The optimization parameter values we employed for all examples are also listed in Table 4.1.

#### 4.5 Examples

In this section we provide numerical examples to demonstrate the effectiveness of the method. In all the examples, we enforce cubic symmetry by defining nine symmetry planes. These symmetry planes include three orthogonal planes that pass through the origin and are perpendicular to the faces of the unit cell, and six planes that pass through the origin and two diagonally opposed edges of the unit cell, dividing the cube into two equal partitions.
Algorithm 2 Multi-material Topology Optimization of Lattice Structures

1: \( k \leftarrow 0 \)  \hspace{1cm} \triangleright \text{Iteration counter}
2: \( z^{(0)} \leftarrow z_0 \)  \hspace{1cm} \triangleright \text{Initial design}
3: \( f_{\text{old}} = -\text{objtol} \)
4: repeat
5: \hspace{1cm} for \( q = 1, \ldots, N_b \) do
6: \hspace{2cm} for \( e = 1, \ldots, N_{\text{el}} \) do
7: \hspace{4cm} Compute signed distance \( \phi_b \) to bar \( b \)  \triangleright \S \ref{sec:1.4}
8: \hspace{4cm} if element \( e \) outside of the reference region then
9: \hspace{6cm} Computed reflected element centroid \( \hat{x}_e \)  \triangleright \Eq \ref{eq:3.4}
10: \hspace{4cm} end if
11: \hspace{4cm} Compute projected density \( \rho_b \)  \triangleright \Eq \ref{eq:1.3}
12: \hspace{2cm} end for
13: \hspace{1cm} end for
14: \hspace{1cm} for \( e = 1, \ldots, N_{\text{el}} \) do
15: \hspace{2cm} Compute element stiffness matrix \( K_e \) using \( C(z, p) \)  \triangleright \Eq \ref{eq:4.2}
16: \hspace{2cm} Assemble \( K_e \) into global stiffness matrix \( K \)
17: \hspace{1cm} end for
18: \hspace{1cm} for \( k = 1, \ldots, 6 \) do
19: \hspace{2cm} for \( e = 1, \ldots, N_{\text{el}} \) do
20: \hspace{4cm} Compute element force \( f^k_e \) contributions from applied unit strains  \triangleright \Eq \ref{eq:4.30}
21: \hspace{4cm} Assemble \( f^k_e \) into global force vectors \( f_k \)
22: \hspace{2cm} end for
23: \hspace{2cm} Solve \( K_k(z)u_k(z) = f_k \) for \( u(z) \)
24: \hspace{2cm} end for
25: \hspace{1cm} Compute \( f(z), \nabla f(z) \)  \triangleright \Eq \ref{eq:4.28)}
26: \hspace{1cm} Compute \( g(z), \nabla g(z) \)  \triangleright \text{g denotes vector of constraints}
27: \hspace{1cm} Impose move limits and update \( z_{\text{low}} \) and \( z_{\text{app}} \)  \triangleright \Eq \ref{eq:4.39}
28: \hspace{1cm} \( z^{(k+1)} \leftarrow \text{opt}(z^{(k)}, f, \nabla f, g, \nabla g, z_{\text{low}}, z_{\text{app}}) \)  \triangleright \text{Update design}
29: \hspace{1cm} \( k \leftarrow k + 1 \)
30: \hspace{1cm} Compute relative change in objective \( \Delta f = |(f - f_{\text{old}})/f_{\text{old}}| \)
31: \hspace{1cm} \( f_{\text{old}} \leftarrow f \)
32: until \( \Delta f \leq \text{objtol} \)
Fig. 4-1 shows the initial design, which consists of 10 near-zero length struts of width $w = 0.1$. In all the examples, the strut width is assumed fixed. An initial matrix volume fraction of $V_m = 0.5$ is used for both fiber-reinforced and hollow struts. The initial size variables for all struts are set to $\alpha_b = 0.5$. For the matrix material, we use PLA12 with $E_m = 1650 \text{ MPa}$ and $\gamma_m = 0.93 \text{ g/cm}^3$ and for the fiber material we use PPSF with $E_m = 2100 \text{ MPa}$ and $\gamma_m = 1.28 \text{ g/cm}^3$. Both materials are used by some multi-material 3d-printers. The unit cell is meshed with a uniform grid of $64 \times 64 \times 64$ hexahedral, trilinear elements.

4.5.1 Bulk Modulus Maximization of Lattices Made of Hollow Struts

In this example we maximize the bulk modulus using hollow struts. Table 4.2 shows the results of the optimization for different weight fraction limits. We observe that, in general, the maximal bulk modulus increases with the weight fraction limit as expected. We attribute exceptions to this trend to the fact that this design problem is known to have many local minima [116], and therefore in some cases the optimization may converge to a suboptimal design.

Using an anisotropic material for the strut (for example, as shown in Fig. 4-2a) is more advantageous in obtaining higher bulk moduli than using an isotropic material. Fig. 4-3 shows an example of a maximal bulk modulus design obtained using the porous material.
Figure 4-2: Schematic representation of two-scale lattice design. Color scale indicates the fiber volume fraction.

of Fig. 4-2b (which is not isotropic but it has cubic symmetry), starting from the initial design shown in Fig. 3-1. As it turns out, the optimization in this case renders bars that are either completely solid (i.e., with zero hole radius), shown in red; or entirely removed from the design (not shown in the figure) as a result of the hole radius being equal to the separation distance between parallel holes. This is due to the fact that isotropic porous materials have poor stiffness-to-weight ratios as compared to fully-solid material. Indeed, multi-phase isotropic materials have physical bounds on the effective stiffness as a function of the porosity, which are called the Hashin-Shtrikman (HS) bounds ([40]). As a result of these limitations, using a porous isotropic material is not advantageous in stiffness-based optimization. In other words, if the porous material that the struts are made of is isotropic, then the optimization will always find a solid/void design to be better.
Figure 4-3: Maximal bulk modulus design using an isotropic porous material with a volume fraction constraint of 0.07. The bulk modulus of the optimal design is 0.068. All of the bars shown have zero porosity ($D/L = 0$); bars that have $D/L = 1$ are removed from the plot.

It should be noted that there are applications in which it is advantageous to have a porous strut for reasons other than mechanical performance, such as in the design of synthetic bone scaffolds for bone repair, in which the pores in the struts can be impregnated with a bone growth factor to favor bone growth upon implantation ([117]). If an upper bound is imposed on the pore size of each bar, then the optimization renders designs with struts that are either fully solid or that attain the specified bound (i.e., this is effectively a two-material design). An example of such an instance is shown in Fig. 4-4. This is consistent with observations for density-based topology optimization of 2D coated structures with an infill that has square symmetry, whereby the optimal designs only render infill porosity values that equal the imposed bounds [118].

Table 4.3 shows the results of the optimization for different weight fraction limits for a single isotropic material (namely, the matrix material). For most weight fractions, we can see an improvement by employing anisotropic materials. For smaller weight fractions, using hollow bars allows us to find feasible designs that we are unable to obtain using a single isotropic material. This is because for very low weight fractions it may not be possible to find a connected design in which all of the struts are fully solid, which in fact is the case for weight fractions $w_f < 0.03$. A comparison of the optimal lattice designs with hollow struts and those with fully solid struts made of the matrix material is shown in Fig. 4-5, which also includes the HS upper bound for reference. This bound is very close to a

Figure 4-4: Maximal design using an isotropic porous material with a volume fraction constraint of 0.05 and an upper bound on the porosity of $D/L \leq 0.5$. The optimal design has a bulk modulus of 0.029. Red bars are fully solid (i.e., $D/L = 0$) and blue bars are porous with $D/L = 0.5$.

linear interpolation within this low weight fraction range. We observe that the bulk moduli of all the designs are far from the HS upper bound, which we expect due to the fact that these designs are open-cell structures.

### 4.5.2 Maximal Bulk Modulus of Lattices made of Fiber-reinforced Struts

In this example we maximize the bulk modulus of a lattice made with fiber-reinforced struts. Table 4.4 shows the results of the optimization for different weight faction limits. The maximal bulk modulus increases as we increase the weight fraction limit as expected. As shown in Fig. 4-5, using fiber-reinforced struts renders a higher bulk modulus than using hollow struts, which is expected since the fiber material is stiffer than the matrix material. We observe that the optimal designs attain intermediate fiber radii, which is possible because the fiber reinforcement renders an anisotropic material. The fact that a good number of struts is made solely of fully-solid matrix material (shown in blue) is a consequence of the matrix material having a larger stiffness-to-weight ratio than the fiber. It is worth noting that by reinforcing the strut with a fiber that is only 27% stiffer than the matrix, we can get designs that are in some cases 56% stiffer (for $w_f = 0.07$), which is possible because of the anisotropy, justifying the use of fiber-reinforced struts.
Table 4.2: Maximal bulk modulus designs for lattices made of hollow struts and different weight fraction limits $w^*_f$. The color scale indicates the volume fraction of the holes in each strut. Bars that have been removed from the design (i.e., with $\alpha_b \approx 0$) are not shown.
<table>
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</tbody>
</table>

Table 4.3: Maximal bulk modulus designs for lattices made of a single isotropic material and different weight fraction limits $w_f^*$. Bars that have been removed from the design (i.e., with $\alpha_b \approx 0$) are not shown.
Table 4.4: Maximal bulk modulus designs for lattices made of fiber-reinforced struts and different weight fraction limits $w_f^*$. The color scale indicates the volume fraction of the fiber in each strut. Bars that have been removed from the design (i.e., with $\alpha_b \approx 0$) are not shown.

<table>
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</table>
4.6 Conclusions

This chapter introduced a topology optimization method for the design of truss lattices with anisotropic struts via the geometry projection technique. The numerical examples demonstrate the effectiveness of the method in producing truss lattices with hollow or fiber-reinforced struts for the maximization of effective bulk modulus and the minimization of effective Poisson’s ratio. The proposed method can enforce desired material symmetries by imposing any number of symmetry planes. The discreteness constraint ensures 0 or 1 size variables in the optimal design; The no-cut constraint is effective in preventing the struts from being cut by the symmetry planes or the boundaries of the unit-cell; and the angle constraint effectively prevents overlaps at angles below the specified threshold. These constraints render designs that are easier to manufacture. The examples also show that the use of hollow struts enables the design of lattices with weight fractions lower than those that can be obtained with fully-solid struts, and that the use of fiber-reinforced struts can render much stiffer truss designs than a lattice of the same weight fraction that is made of the matrix material alone.

Figure 4-5: Comparison of results using isotropic and anisotropic materials with the HS upper bound.
Chapter 5

Design of Coating-and-Infill Structures

5.1 Summary

This chapter presents a computational method for the design of a component made of a constant-thickness coating filled in with a two-scale lattice. The two-scale lattice is made of fiber-reinforced (or hollow) struts, as presented in the previous chapter. The proposed method simultaneously optimizes the shape and topology of the component, the layout of the struts in the lattice infill, and the volume fraction of the fiber or hole in each strut. The proposed method combines recent techniques to design coating-and-infill components via density-based topology optimization with the geometry projection technique introduced in the previous chapter for the design of the two-scale lattice. The efficacy of the proposed method is demonstrated through a numerical example of compliance minimization.

5.2 Introduction

Advances in additive manufacturing (AM) have facilitated the manufacture of components made of a porous infill coated with a constant-thickness skin. Although AM technologies that support multiple materials are becoming available, in practice the available materials often have very similar properties due to process limitations, such as requiring that these materials possess similar rheological properties for extrusion. Therefore, using multiple materials does not necessarily provide a structural advantage. As shown in the previous
chapter, the use of lattices whose struts are made of an anisotropic material can render effective properties that are better than those obtained with isotropic materials. This opens the possibility of designing highly-performing structural components by simultaneously optimizing the shape and topology of a constant-thickness skin and a two-scale lattice infill. The coating-and-infill configuration is advantageous because lattices have high stiffness-to-weight ratios, good thermal and acoustic insulation properties and good energy absorption characteristics [21]. Porous structures show better performance in response to buckling stability [119], force variations and material deficiency [120], and thermally induced residual stresses arising from the manufacturing process [121, 122].

Different methods have been employed for the design of components made exclusively of an architected porous microstructure. In general, these methods aim to simultaneously design the shape and topology of the macrostructure (i.e., of the component) and of the microstructure. Since the computational cost of modeling the microstructure with a body-fitted mesh for the entire macro component is prohibitive, these methods model the component using the numerically homogenized properties of the microstructure. These properties are computed by numerical homogenization, which requires an analysis of a unit cell of the microstructure. Some methods assign a different microstructure to each finite element in the mesh of the macro component (e.g., [123]). This strategy offers a high degree of design control, but it tends to produce microstructures that are not continuous across element boundaries, and are therefore not manufacturable. Recent works have focused on techniques to render connected microstructures (for instance, [124]). Other strategies employ a single microstructure for the entire component, which sacrifices performance but ensures connectedness and greatly improves manufacturability (e.g., [125]). In other cases, the topology of the microstructure is fixed and only size optimization of the members in the microstructure is performed, with the size being variable throughout the macro component; moreover, with the topology being fixed, these methods can employ efficient surrogate models of the lattice effective properties that are constructed once prior to the optimization, thus they do not require in-line homogenization (for example, [126]). Methods for multi-scale topology optimization have employed density-based, level set and evolutionary strategies. A thorough review of these methods is outside of the scope of this work, and we
refer the reader to [127, 128] and the references therein for a more detailed account. Finally, a strategy that has been recently explored is to perform the topology optimization using a homogenized rank-2 material, and determining the layout of the microstructure as a post-processing “de-homogenization” step by obtaining a layout of members that renders the same properties of the optimized homogenized material (cf., for example, [129, 130, 131]).

Recently, topology optimization techniques have been advanced for the design of coating-and-infill components. In the methods of [132, 133] the infill is made of a porous isotropic base material with fixed microstructure. Since the microstructure design is fixed, this method does not require homogenization. A key aspect of these methods is the use of subsequent filtering operations to render the constant-thickness coating; this is a strategy we employ in this work. Another strategy to design coating-and-infill components is presented in [134], which uses the filter strategy of [132] to obtain the coating, but the infill is obtained by imposing an optimization constraint to render a lower bound on the porosity everywhere. This has the effect of controlling the maximum size of structural members in the infill, which effectively produces a cellular solid. This method does not employ homogenization for the microstructure, but it requires a mesh that is fine enough to capture the slender members in the infill. The level set method of [135] designs a uniform-thickness coating with a specified orthotropic infill. The coating is given by a band of uniform width around the zero level set of a signed distance function. The infill is modeled as a homogeneous orthotropic material and it models an infill pattern specified the user, such as those used in some additive manufacturing methods. The orientation of the material properties is thus given by the orientation of the specified infill pattern. The coating is also endowed with orthotropic properties, aligned with the normal and tangential directions to the coating, to reflect the anisotropy arising from the manufacturing of the coating. [118] extends the work of [133] to simultaneously design a coating-and-infill component with an orthotropic infill. In this method, the design of the microstructure corresponds to a laminated composite, and therefore the effective properties are a function of the dimensions of the laminae, which are design parameters in the optimization. This work takes advantage of the fact that the moduli of orthotropic materials are not bound by the Hashin-Shtrikman bounds, and therefore the optimization favors a porous infill to minimize the structural compliance.
In this work, we present a 3-scale method to design 3-dimensional coating-and-infill structures whose infill is a two-scale truss lattice like the ones discussed in the previous chapter. One of the significant advantages of using a truss-lattice infill is that it is easier to fabricate via additive manufacturing techniques because its unit cell open, and thus it is possible to remove sacrificial support material. We employ the method presented in the previous chapter to design the lattice infill, including the the layout of the struts and the volume fraction of the fiber (or hole) in each strut. We adapt the double smoothing and projection (DSP) approach of [118] to differentiate the regions occupied by the coating, the homogenized infill and void via successive filtering operations. To our knowledge, this is the first topology optimization technique to design these 3-scale structures.

The rest of the chapter is organized as follows. Section 5.3 describes the filtering operations. Section 5.4 discusses the optimization problem. In Section 5.5, we present a numerical example to demonstrate our method, and we draw conclusions in Section 5.6.

5.3 Successive Filtering Operations

We adopt the method presented in [118] to model a 3-dimensional coating-and-infill component by using a single field as design variable to differentiate between coating, infill and void regions and assign the corresponding ersatz material properties to a fixed mesh for analysis. The main difference between our work and that of [118] is that the infill corresponds to a truss lattice with transversely isotropic struts. Fig. 5-1 shows a schematic representation of the sequence of filtering operations to determine distinct boundaries for the aforementioned regions, which we briefly discuss in the following. This presentation follows that of [118].

5.3.1 Smoothing

The first filter corresponds to a Helmholtz-type PDE-based density filter ([136]) employed for smoothing. The filter ensures a minimum size for the structural members in the optimal
topology. The filtered field $\tilde{\phi}$ is obtained from the solution of the Helmholtz equation

$$- \left( \frac{R}{2\sqrt{3}} \right)^2 \nabla^2 \tilde{\phi} + \tilde{\phi} = \phi,$$

(5.1)

where $\phi$ is the unfiltered field and $R$ denotes the length-scale imposed by the filter operation. Homogeneous Neumann boundary conditions are applied at the boundary of the filter domain. The system matrix corresponding to the discretized equation only needs to be factorized once in the optimization, and upon design changes the right-hand side is updated and the filtered density obtained via inexpensive backward and forward substitutions.

### 5.3.2 Projection

The next filtering operation corresponds to a smooth Heaviside projection [137], whose purpose is to sharpen the density field, and it is computed as

$$\hat{\phi} = \frac{\tanh \beta \eta + \tanh \beta (\tilde{\phi} - \eta)}{\tanh \beta \eta + \tanh \beta (1 - \eta)},$$

(5.2)

where $\hat{\phi}$ is the projected field, the parameter $\beta$ determines the steepness of the projection, and $\eta$ is a threshold parameter that determines whether the filter adds or removes material; when $\eta > 0.5$ material is eroded, and when $\eta < 0.5$ material is dilated. Here, we use $\eta = 0.5$, for which material is neither removed nor added.
5.3.3 Combining the filters to obtain a coated structure

We use successive filter operations to obtain the field $\phi$ describing the solid and void portions of the infill, $\Omega_l$ and $\Omega_v$, respectively, and the field $\tau$ describing the coating region $\Omega_c$. These regions are defined via

$$\mathbf{x} \in \begin{cases} 
\Omega_v & \text{if } \phi(\mathbf{x}) = 0 \text{ and } \tau(\mathbf{x}) = 0 \\
\Omega_l & \text{if } \phi(\mathbf{x}) = 1 \text{ and } \tau(\mathbf{x}) = 0 \\
\Omega_c & \text{if } \tau(\mathbf{x}) = 1 
\end{cases} \quad (5.3)$$

The smoothing and projection filters are employed twice using a filter radius $R_1$, and projection parameters $\beta_1$ and $\eta_1$. The purpose of applying these filters twice is to improve convergence to 0-1 designs. The field obtained after these four operations corresponds to $\phi$, as shown in Fig. 5-1. After these steps, the field is smoothed again using $R_2 < R_1$ so that the resulting field $\tilde{\phi}$ has smooth boundaries, which is necessary to compute the gradient of the field. The coating layer is defined by taking the Euclidean norm of the spatial gradient of $\tilde{\phi}$ and normalizing it such that the largest possible norm is unity, by employing a normalization factor $\alpha = \frac{R_2}{\sqrt{3}}$. The normalized gradient norm is subsequently sharpened using a projection filter with $\beta_2$ and $\eta_2$ to define the coating field $\tau$ (see Fig. 5-1). [132] shows an analytical relation between $R_2$ and the maximum coating thickness $t_{ref}$ given by

$$R_2 = \frac{\sqrt{3}}{\ln 2} t_{ref} \approx 2.5 \ t_{ref}. \quad (5.4)$$

Using the filtered fields $\phi$ and $\tau$, we define the ersatz elasticity tensor for analysis as

$$\mathbb{C}^e = \mathbb{C}_{\text{void}} + (\mathbb{C}_l - \mathbb{C}_{\text{void}}) \hat{\phi}^{p_1} + (\mathbb{C}_c - \mathbb{C}_l \hat{\phi}^{p_1}) \tau^{p_2}, \quad (5.5)$$

where $\mathbb{C}_c$ is the elasticity tensor for the coating material (which in our case is an isotropic material), and $\mathbb{C}_l$ is the elasticity tensor of the lattice infill, which in our case is the tensor of Eq. 4.2 obtained from the geometry projection of the two-scale lattice.
5.4 Optimization and Computer Implementation

5.4.1 Optimization Problem

We minimize the compliance of the coating-and-infill component subject to a weight fraction constraint for the whole component. As in the previous chapter, we also impose a no-cut constraint and an angle constraint for the lattice infill to improve manufacturability. The weight fraction of the lattice is computed by Eq. 4.19, and the weight fraction constraint is given by

$$g_w(z, \mu) = \frac{1}{|\Omega| \max(\gamma_f, \gamma_m)} \sum_e \tilde{\gamma}^e v^e \leq g_w^*.$$  \hspace{1cm} (5.6)

In this expression, $v^e$ denotes the element volume, $\Omega$ is the design region of the component, and $\tilde{\gamma}^e = w_f^l \phi + (1 - w_f^l \phi) \tau$.

The optimization problem is stated as

$$\min_{z, \mu} f(u(z, \mu)) := \int_{\Gamma_t} u(z, \mu) \cdot t ds$$ \hspace{1cm} (5.7)

subject to

$$a(u(z, \mu), v) = l(v), \forall v \in \mathcal{V}_\Omega, u \in \mathcal{V}_\Omega$$ \hspace{1cm} (5.8)

$$g_w(z, \mu) \leq w_f^*$$ \hspace{1cm} (5.9)

$$g_n(z) \leq \epsilon_n$$ \hspace{1cm} (5.10)

$$g_a(z) \leq \epsilon_a$$ \hspace{1cm} (5.11)

$$x_{b_0}, x_{b_f} \in \Omega$$ \hspace{1cm} (5.12)

$$0.0 \leq \alpha_i^b \leq 1.0$$ \hspace{1cm} (5.13)

$$0.0 \leq \mu \leq 1.0.$$ \hspace{1cm} (5.14)

As before, we scale the design variables and impose move limits on the scaled variables as described in the previous chapters. The definitions of the no-cut constraint $g_n$, the angle constraint $g_a$ and the equilibrium problem of Eq. 5.8 are the same as those of Section 4.4.
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</table>

Table 5.1: Optimization parameters

### 5.4.2 Computer Implementation

We implement our code in MATLAB. We employ the method of moving asymptotes (MMA) of [87, 88] with the default parameters. We stop the optimization when the relative change $\Delta f$ in compliance between consecutive iterations falls below a specified value $\Delta f^*$. Table 5.1 shows the optimization parameters we employed for the example presented in this chapter.

### 5.5 Example

We present a numerical example to illustrate the effectiveness of the method. The example corresponds to the minimum compliance design of a cantilever beam, with dimensions, loading and boundary conditions shown in Fig. 5-2a. All the materials considered are homogeneous, isotropic, and linearly elastic with Poisson’s ratio $\nu = 0.3$, but with different Young’s moduli and material densities. We enforce cubic symmetry by defining nine symmetry planes as in the previous chapter. The initial design for the lattice is the same one
Figure 5-2: (a) Design region, mesh and boundary conditions for macro component. (b) Initial design after reflections for cubic symmetry. The blue region indicates the reference region.

employed in the previous chapter, which is shown in Fig. 5-2b. As before, we use an initial fiber volume fraction of $V_f = 0.5$ for each strut. The initial size variables for all struts are set to $a_r = 0.5$. For the matrix and coating material, we use PLA12 with $E_m = 1650$ MPa and $\gamma_m = 0.93$ g/cm$^3$ and for the fiber material we use PPSF with $E_f = 2100$ MPa and $\gamma_f = 1.28$ g/cm$^3$. The unit cell of the lattice and the component are meshed with uniform grids of $64 \times 64 \times 64$ and $60 \times 30 \times 30$ hexahedral trilinear elements, respectively.

Fig. 5-4 shows the optimization results. Fig. 5-4a shows the 0.5 iso-surface of the field $\tau$, corresponding to the boundaries of the coating. We note that the filtering scheme does not preclude the possibility that some regions of the infill are exposed and not covered by the coating, as seen in the figure. Fig. 5-4b shows the 0.5 iso-surface of the field $\phi$, which is the boundary of the lattice infill, and it can be readily seen that it corresponds to the interior of the coating. We can see cross-sections of coating and infill in Figs. 5-4c and 5-4d, respectively. Figs. 5-4e and 5-4f show the optimal design of the lattice for the infill. In this case, the optimizer has pushed the bar volume fractions $V_{fb}$ to either 0 or 1, which indicates that the struts are either made of material 1 or material 2. Fig. 5-3 shows the logarithmic convergence plot of the compliance. We note that even though the cubic-symmetric lattice design is not optimal in terms of stiffness, as discussed in the previous chapter, the optimization still renders an infill region that is not empty, i.e., it does not render a pure 0-1 design for the macro component. This owes to the fact that the
representation of Eq. 5.3 forces the design to be exclusively made of a uniform-thickness coating, a void region, and an infill region. That is, the design representation does not allow for fully solid regions other than the coating. This is consistent with the results of [132, 133].

## 5.6 Conclusions

In this chapter, we introduced a formulation to simultaneously optimize the shape and topology of a coating-and-infill structure whose infill is a lattice made of transversely isotropic struts. The numerical example demonstrates the effectiveness of the method. As in the previous chapter, the geometric constraints on the struts layout render a lattice design that is more amenable to manufacturing. To our knowledge, this is the first topology optimization technique to design a 3-scale structure.
Figure 5-4: Coating-and-infill design of the component for a weight fraction limit of $W_f^* = 0.1$. The compliance is $c = 0.2026$. 
Chapter 6

Design of Programmable Lattices

6.1 Summary

This chapter presents a topology optimization method for the design of programmable lattices. These are lattices in which each strut can be activated/deactivated through some actuation mechanism. For large enough unit cells, this could be achieved using electromagnetic (EM) joints. Another possible actuation mechanism is to have hollow struts full with a magnetorheological fluid that drastically changes its mechanical properties (and consequently, those of the strut it occupies) in the presence of an electromagnetic field. The open/close state of the struts, which we refer to as the lattice program, can render different effective properties. Thus, the designer may obtain a lattice that attains, for example, different effective moduli for different programs.

The method introduced in this chapter designs and programs a unit cell of a periodic truss lattice made of cylindrical struts. This consists of simultaneously designing the spatial layout of the struts in the unit cell and their open/close state for each one of the specified programs. As in the previous chapter, we employ the geometry projection method to smoothly map the high-level geometric description of the struts onto a density field over a fixed mesh for analysis. To model the open/close state of a strut for the different specified programs, we assign a size variable per program to each strut. We impose a constraint in the optimization to ensure these size variables are 0 or 1 in the optimal design. If the size variable of a strut equals 1 for all the programs, the strut need not be actuated and it can be
made of a single material; if the size variable is 0 for one or more programs and 1 for the others, the strut is an actuated strut; and if the size variable is 0 for all programs, the strut is altogether removed from the design. We demonstrate the effectiveness of the proposed method via numerical examples that design a programmable lattice to obtain two and three desired effective bulk moduli.

6.2 Introduction

The majority of applications of architected materials, such as those listed in Chapter 1, use monolithic designs, i.e., those for which the spatial configuration of the unit cell and consequently the effective properties are fixed. There exist, however, applications where it is advantageous to change the material properties in real time. A new class of composite acoustic metamaterials is introduced in [138], where an acoustic cavity is coupled with an array of Helmholtz resonators with flexible cavities that results in a tunable effective bulk modulus. A similar idea is presented in [139] by employing cavities with flexible or piezoelectric diaphragms. In [140], digital metamaterials are introduced that consist of two types of unit cells with two phase responses, or four types of unit cells with four phase responses. Different functionalities are achieved by manipulating electromagnetic waves by coding these elements with controlled sequences. Origami-inspired mechanical metamaterials with tunable compressive moduli that are attained through switching between states are presented in [141]. The work in [142] demonstrates mechanical metamaterials with programmable response to uniaxial compression via lateral confinement. A highly nonlinear coupling of deformations along the primary axes of these materials are obtained through a broken rotational symmetry, which results in monotonic, nonmonotonic and hysteretic behavior. Programmable cellular materials that employ electromagnetic joints to open/close the struts are presented in [143]. All of these works explore different mechanisms to tune the programmed responses, however they do not employ systematic design techniques to determine the spatial layout of the architected material.

To the best of our knowledge, topology optimization techniques have not been previously used to design and program actuated lattices. In this work, we present a topology
optimization method to simultaneously determine the optimal truss layout and open/close programs of the programmable lattice. The techniques to determine the optimal layout of the struts are those employed in the previous chapters. The novelty of the proposed methodology is in determining the open/close state of the struts for the different programs.

The remainder of the chapter is organized as follows. In Section 6.3 we describe the geometry projection of the programmable lattices. We present the optimization problem in Section 6.4. Section 6.5 discusses numerical examples to demonstrate the effectiveness of our method by designing lattices to attain two or three specified bulk moduli, and we draw conclusions in Section 6.6.

6.3 Geometry Projection

We extend the geometry projection presented in Chapter 1 to account for multiple programs. The design of the programmable lattice (i.e., the spatial layout of the struts) is determined by the location of the endpoints of the struts. The program is determined by the state of the switchable struts. Each strut $b$ is ascribed size variables $\alpha^b_p, p = 1, \cdots, n_p,$ where $n_p$ is the number of programs. If $\alpha^b_p = 1$, the strut $b$ is closed (activated) for program $p$, and if $\alpha^b_p = 0$ it is open (deactivated). If $\alpha^b_p = 1$ for all programs, strut $b$ is monolithic, meaning there is no need for a switch in this strut. If $\alpha^b_p = 0$ for all programs, strut $b$ is completely removed from the design. Otherwise, the strut is switchable and can be activated or deactivated for different programs.

The projected density is computed from Eq. 1.2. The effective density for each program $p$ and strut $b$ is accordingly computed as

$$\hat{\rho}^b_p := \alpha^b_p (\rho_b)^q,$$  

where $q = 3$ is the penalization power. We note that in this formulation, we employ an explicit penalization scheme to ensure the size variables converge to 0 or 1, which we detail in the following section. A smooth approximation of the maximum function is used
to combine multiple components

$$\bar{\rho}_p = \max_b \bar{\rho}_p^b, \ b = 1, \ldots, n_b.$$  \hfill (6.2)

The elasticity tensor for the computation of the stiffness matrix of element $e$ and for each program is subsequently computed by employing an ersatz material as

$$C_i^e = C_{\text{void}} + \bar{\rho}_p^e (C_0 - C_{\text{void}}),$$  \hfill (6.3)

where $C_{\text{void}}$ and $C_0$ are the elasticity tensors of the void region and the solid material as before. As in previous chapters, we use homogenization to compute the lattice effective properties for each program.

\section*{6.4 Optimization and Computer Implementation}

We aim to find the optimal struts layout and programs that renders the lightest lattice while achieving two or more target effective properties with different programs. In this work, we specifically consider the design of lattices that attain two or more specified bulk moduli with different programs. The optimization problem corresponds to the minimization of the lattice volume fraction, subject to constraints on the target effective properties for each
program, and it is stated as

$$\min \ V_f(z) := \sum_e \max_{p,b}(\alpha_p^b \rho_b)v_e$$  \hspace{1cm} (6.4)

subject to

$$a(u_p^{(kl)}(z), v) = l(v, \epsilon_0^{(kl)}), \ \forall v \in \mathcal{V}_0, u_p^{(kl)} \in \mathcal{U}, \ p = 1, \cdots, np$$  \hspace{1cm} (6.5)

$$g_p(z) := (K_{p}^{\text{eff}}(z) - K_p^{0})^2 \leq \epsilon, \ p = 1, \cdots, np$$  \hspace{1cm} (6.6)

$$g_n \leq \epsilon_n$$  \hspace{1cm} (6.7)

$$g_d \leq \epsilon_d$$  \hspace{1cm} (6.8)

$$x_{b_0}, x_{b_f} \in \Omega$$  \hspace{1cm} (6.9)

$$0.0 \leq \alpha_p^b \leq 1.0.$$  \hspace{1cm} (6.10)

The evaluation of the volume fraction in Eq. 6.4 takes into account all the struts that are either monolithic or have a closed state in at least one program (i.e., all struts that have a size variable of $\approx 1$ in at least one program). The smooth maximum approximation we use is the LKS function of Eq. 3.6. Each lattice program $p$ requires the solution of a numerical homogenization problem (cf., Eq. 6.5), which, as before, requires the application of six separate unit strains $\epsilon_0^{(kl)}$ (i.e., $k, l = 1, \cdots, 3$). The solution of the homogenization problem is as described in previous chapters.

The goal of each constraint $g_p$ is to minimize the difference between the specified target modulus $K_p^0$ and the lattice effective modulus $K_{p}^{\text{eff}}$ for program $p$. The effective bulk modulus $K_{p}^{\text{eff}}$ for each program $p$ is computed from Eq. 3.7. As in the previous chapters, we impose a no-cut constraint $g_n$ (cf., Eq. 3.5) to ensure struts are not cut by unit cell boundaries or symmetry planes to improve manufacturability. To ensure the size variables converge to 0 or 1, we employ an explicit penalization by imposing a discreteness constraint $g_d$ (cf., Eq. 2.13). As in previous chapters, we impose cubic symmetry of the lattice for all programs by applying appropriate reflections of the position of element centroids outside the reference region (where the projected density is computed) with respect to the appropriate symmetry planes so that the reflected point lies in the reference region. We scale the design variables and impose move limits as described in the previous chapters.
### Table 6.1: Optimization parameters

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#### 6.4.1 Computer Implementation

Our code is implemented in MATLAB. We compute an element-wise uniform effective density at the element centroid $x_e$. The geometry projection is computed using a window radius $r$ equal to $c$ times the radius of the sphere that circumscribes the element, i.e., $r = c\sqrt{3h/2}$, where $h$ is the element size. As the optimizer, we employ the method of moving asymptotes (MMA) of [87, 88] with the default parameters. We stop the optimization when the relative change $\Delta f$ in compliance between consecutive iterations falls below a specified value $\Delta f^*$. The optimization parameter values we employed for all examples are also listed in Table 6.1.

#### 6.5 Examples

We consider the simultaneous design and programming of lattices for two and three specified target bulk moduli. The initial design consists of 10 near-sphere struts of width $w = 0.1$, as shown in Fig. 6-1. We mesh the unit cell with a uniform grid of $64 \times 64 \times 64$ hexahedral, trilinear elements. The material the struts are made of has Young’s modulus $E = 1000$ MPa and Poisson’s ratio $\nu = 0.3$.

The first example has two specified target bulk moduli of $K_1^0 = 3$ and $K_2^0 = 12$. Table 6.2 shows the results of the optimization.
Figure 6-1: Initial design after reflections for cubic symmetry. The blue region indicates the reference region.

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Table 6.2: Minimal volume fraction designs for two target bulk moduli. The optimized volume fraction for this problem is 0.0995. Struts shown in the iso and side columns are shown in gray, blue and red to denote monolithic, open and closed struts, respectively. The columns active/iso and active/side show all of the load-transferring struts for each program.
Table 6.3: Minimal volume fraction designs for two target bulk moduli. The optimized volume fraction for this problem is $V_f = 0.0715$. Struts shown in the iso and side columns are shown in gray, blue and red to denote monolithic, open and closed struts, respectively. The columns active/iso and active/side show all of the load-transferring struts for each program.

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In the second example we specify three target bulk moduli of $K_1^0 = 2$, $K_2^0 = 4$ and $K_3^0 = 8$. Table 6.3 shows the result of the optimization. This result is more interesting than the previous one in that the second program (for $K_2^0 = 4$), some struts are open (blue) and some are closed (red).

### 6.6 Conclusions

This chapter introduced a computational method for the design and programming of programmable lattices using the geometry projection method. The examples show the effectiveness of the proposed method in determining the spatial layout of the struts and the programs for each of the specified bulk modulus targets. To our knowledge, this is the first topology optimization technique to design programmable lattices. Future work should include the experimental validation of these designs.
Chapter 7

Conclusions

Topology optimization is a design method to generate novel structural designs by determining the optimal layout of material in a prescribed design region. It has been employed in the past in the design of architected materials to obtain desired properties, often with the goal of attaining properties outside the envelope of properties in existing natural or man-made bulk materials. A particular type of architected material that has garnered substantial interest is periodic truss lattices, due to their high stiffness-to-weight ratio, and the fact that their manufacturing has become increasingly feasible for smaller and smaller scales thanks to advances in additive manufacturing.

The majority of works in topology optimization of architected truss lattices considers only struts made of a single isotropic material. In this dissertation, I formulated topology optimization techniques to push this envelope by considering struts made of multiple isotropic materials; fiber-reinforced or hollow struts that are transversely isotropic; the simultaneous design of coating-and-infill structural components made of a uniform-thickness coating and a two-scale lattice infill; and the design of programmable lattices whose struts can be activated and deactivated through some actuation mechanisms. All these considerations greatly expand the possibilities of architected lattices. The geometry projection method, whereby a high-level parametric description of the struts in the lattices is smoothly projected onto a fixed finite element mesh for analysis and for the efficient computation of design sensitivities, is the foundation of all these methods.

In this thesis, I formulated topology optimization techniques to design multi-material
3-dimensional structural frames and architectured lattices with bars made of any number of available isotropic materials. The optimization simultaneously determines the spatial layout of bars and selects the best material for each bar out of a set of available materials. While a geometry projection technique had been previously advanced for the design of 2-material architected lattices, the formulation I proposed can be readily extended to any number of materials, as demonstrated by numerical examples. As expected, this method is able to render multi-material designs of frame structures and periodic truss lattices that outperform single-material structures of the same weight; and, as the number of materials available increases, the structural performance of the optimal design improves. Another significant contribution of this method is the imposition of geometric no-cut constraints to ensure struts in the lattices are whole in the optimum design, which greatly facilitates the manufacturing of the lattice.

I also advanced the first topology optimization technique to design 3-dimensional lattices with fiber-reinforced or hollow struts. This method builds on recent developments in our research group to design frame structures with bars made of anisotropic materials. A key contribution of the method I proposed is that the volume fraction of the reinforcing fibers or of the holes in the struts is itself designable, and the optimization determines not only the spatial layout of the struts, but also the optimal fiber/hole volume fraction in each strut, effectively rendering a 2-scale design. Our numerical experiments demonstrate that these 2-scale designs clearly outperform single, isotropic material designs. This is the first topology optimization technique to design two-scale truss lattices.

This dissertation also addressed a problem that has recently captured the attention of the structural design community, namely the design of coating-and-infill structures, which are becoming increasingly popular thanks to the availability of additive manufacturing techniques for their fabrication. I formulated a topology method for designing this type of components, where the infill is made of a 2-scale lattice with fiber-reinforced or hollow struts. The method I advanced not only optimizes the design of the lattice unit cell, but also the shape and topology of the coating and the infill region. Notably, a significant advantage of using a truss-lattice infill is that it is easier to fabricate via additive manufacturing techniques because its unit cell is open, and thus it is possible to remove sacrificial support
material. To our knowledge, this is the first topology optimization technique to optimize 3-scale structures; and it is also the first technique to design a 3-dimensional coating-and-infill structure that is feasible for manufacturing.

Finally, I formulated a topology optimization method for the design of programmable lattices. This is an emerging and exciting area of research that uses actuation mechanisms to open and close struts in architected lattices in order to obtain multiple desired properties depending on the open/close state of the struts. The method I advanced in this dissertation simultaneously determines the optimal spatial layout of the struts, but it also determines what struts are monolithic, which ones must be altogether removed from the design, and which ones must be actuated and what is their open/close state to attain each of the desired properties. The numerical experiments demonstrate the ability to design these programmable lattices to obtain two or three specified bulk moduli. This is the first topology optimization technique to accomplish the design of programmable lattices of any kind.
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