

IH-GAN: A Conditional Generative Model for Implicit Surface-Based Inverse Design of Cellular Structures

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Abstract

Variable-density cellular structures can overcome connectivity and manufacturability issues of topologically-optimized, functionally graded structures, particularly when those structures are represented as discrete density maps. One naïve approach to creating variable-density cellular structures is simply replacing the discrete density map with an unselective type of unit cells having corresponding densities. However, doing so breaks the desired mechanical behavior, as equivalent density alone does not guarantee equivalent mechanical properties. Another approach uses homogenization methods to estimate each pre-defined unit cell's effective properties and remaps the unit cells following a scaling law. However, a scaling law merely mitigates the problem by performing an indirect and inaccurate mapping from the material property space to single-type unit cells. In contrast, we propose a deep generative model that resolves this problem by automatically learning an accurate mapping and generating diverse cellular unit cells conditioned on desired properties (*i.e.*, Young's modulus and Poisson's ratio). We demonstrate our method via the use of implicit function-based unit cells and conditional generative adversarial networks. Results show that our method can 1) generate various unit cells that satisfy given material properties with high accuracy (relative error < 5%), 2) create functionally graded cellular structures with high-quality interface connectivity (98.7% average overlap area at interfaces), and 3) improve the structural performance over the conventional topology-optimized variable-density structure (84.4% reduction in concentrated stress and extra 7% reduction in displacement).

Keywords: Inverse design, cellular structure design, homogenization, generative adversarial network, topology optimization

1. Introduction

Complexity-free manufacturing techniques such as additive manufacturing (AM) have enabled the fabrication of intricate geometric features. This permits the design of complex structures that fulfill specific functional criteria while possessing lower weight. Access to this new design space makes complex structural designs (*e.g.*, cellular structures) coveted in various engineering applications [1, 2, 3, 4, 5, 6]. In this context, topology optimization (TO) plays a major role in designing light-weight structures that satisfy functional goals [7]. However, the most widely used TO algorithms (*e.g.*, solid isotropic material with penalization or SIMP) [8] deliver discrete density maps as the outcome, leading to poor manufacturability due to 1) connectivity issues within variable-density bulk materials and 2) the limited resolution of the density map. To manufacture quality products, one needs to post-process the density map into a smoothed geometric model, which is then physically realized by turning to expensive multi-material (*e.g.*, functionally graded material) design and manufacturing techniques [9, 10].

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To solve this geometric connectivity issue and simplify the manufacturing process, researchers typically replace the density map with variable-density cellular unit cells (Figure 1), enabling functionally graded structure design and manufacturing with a single material [11]. However, a naïve one-to-one replacement with unit cells having corresponding densities/volume fractions (without considering the unit cell shape) can break the optimized behavior because, unlike continuum solids, equivalent density alone does not guarantee equivalent mechanical properties for unit cells. The unit cell shape also affects its mechanical properties. To address this issue, researchers commonly *homogenize* each unit cell by pre-computing their effective properties [12, 13] such that they can approximate the continuum solid domain with the homogenized cellular structure, hopefully retaining equivalent properties. By establishing a mapping between densities and homogenized properties (*e.g.*, elastic tensors) following a scaling law¹ [14], TO can generate an optimized density map for a specific type/shape of cellular unit cells.

However, there are several issues in building such a mapping. First, the scaling law creates a mapping between the material property space and the unit cell density space. This means the unit cell's material property is controlled only by its density (volume fraction), while variable unit cell types are not allowed. Second, being subject to that setting, the scaling law only allows bijective mapping, whereas the mapping from a material property space to a unit cell shape space can be one-to-many. Finally, the mapping itself is hard-coded (polynomial) and has limited flexibility/accuracy under different scenarios.

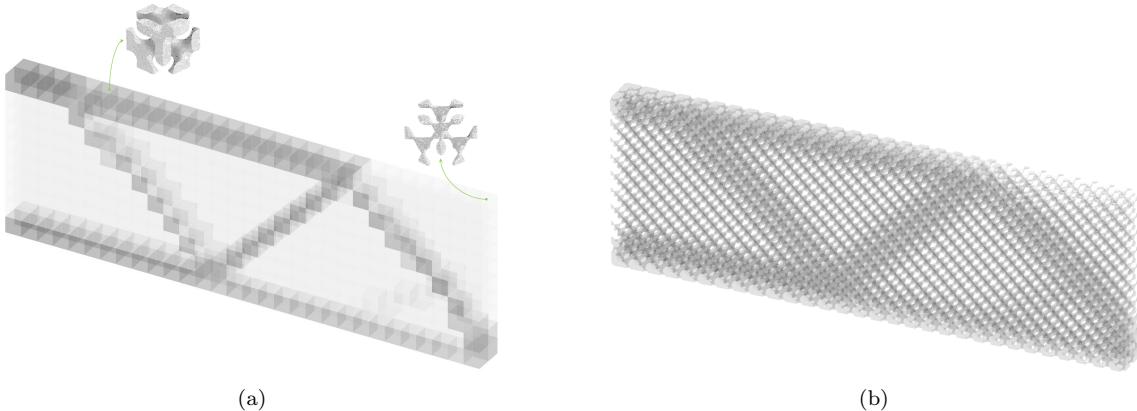


Figure 1: Variable-density cellular structure. (a) Density map obtained from TO. (b) Replacement with variable-density unit cells.

We solve these issues by constructing an *inverse homogenization (IH) mapping*—a generalized, direct, and accurate mapping from material properties to multi-type unit cell shapes. The IH mapping allows designers to efficiently retrieve correct unit cell shapes given the optimized material properties. Rather than the previous approaches that were limited to polynomial scaling and enforced bijectivity (*i.e.*, using the scaling law and level set field [15, 16]), we propose an end-to-end generative model that automatically learns a data-driven one-to-many IH mapping and suggests unit cell shapes conditioned on the input material properties. Figure 2 illustrates the role of our work in assisting the topology optimization of functionally graded cellular structures.

Our generative model is developed by training a conditional generative adversarial network (GAN) upon a family of implicit function-based cellular structures—*i.e.*, triply periodic minimal surfaces (TPMS) [17]. The implicit function representation (FRep) modeling method represents cellular structures as iso-surfaces that enable control of unit cell shapes by manipulating the functions' coefficients and level set constants. Compared to expensive volumetric representations [18], the FRep minimizes the number of design variables representing unit cell geometries. We propose a deep generative model, named *Inverse Homogenization*

¹The scaling law hypothesizes the mechanical properties of cellular structures have polynomial law relationships with their relative densities.

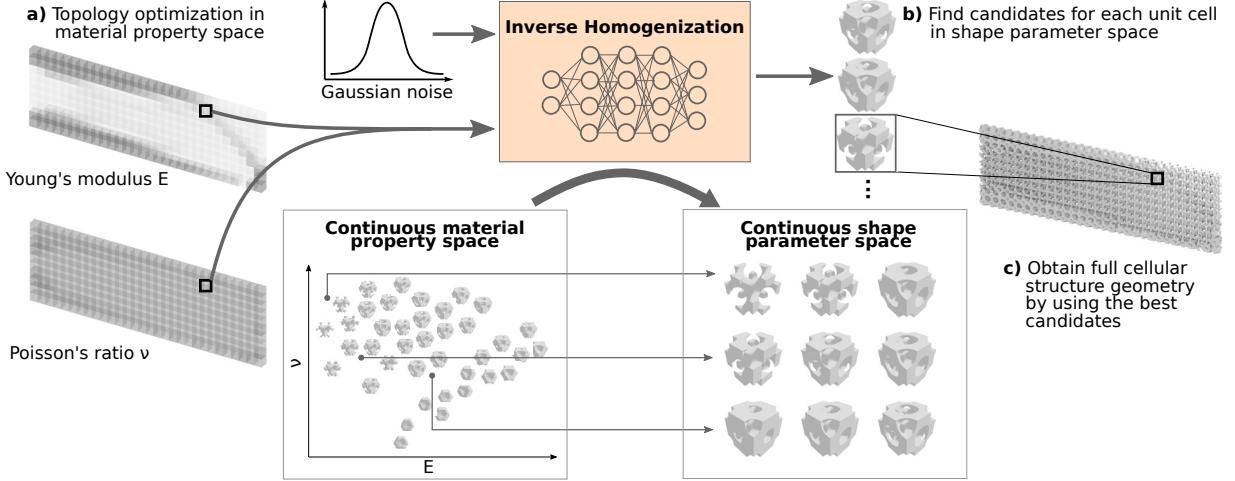


Figure 2: Inverse homogenization mapping for topology optimization of functionally graded cellular structures.

GAN (IH-GAN), to learn a mapping from material properties to the implicit function describing the cellular unit cell geometry. We demonstrate our method’s efficacy by rapidly generating various TPMS unit cells with accurate (relative error $< 5\%$) elastic properties (*i.e.*, Young’s modulus and Poisson’s ratio). To further demonstrate IH-GAN’s practical usage in designing functionally graded cellular structures, we show a cantilever beam design example where the structure is assembled by variable types of unit cells generated from IH-GAN. This paper’s primary contributions are as follows:

1. We describe a conditional generative model, IH-GAN, to enable an accurate (relative error $< 5\%$) and efficient IH mapping. After 38 seconds of training, IH-GAN can generate corresponding unit cell shapes in less than one second given any feasible Young’s modulus and Poisson’s ratio.
2. We improve the IH mapping learned by the conditional GAN by adding an auxiliary material property regressor. We show through ablation experiments that this additional regressor reduces about half of the average mapping error.
3. We reduce the IH mapping complexity by representing unit cell shapes as implicit function parameters, a more compact but precise representation compared to volumetric or boundary representation.
4. We ensure high-quality connections between different types of adjacent unit cells in designing functionally graded cellular structures by taking advantage of the material property filter kernel used in TO and the continuous shape variation of IH-GAN’s generated unit cells in the 2D material property space.
5. We demonstrate that our method can improve the structural performance over the conventional topology-optimized variable-density structure (84.4% reduction in concentrated stress and extra 7% reduction in displacement).
6. We create a unit cell shape database for future studies on data-driven cellular structure design (available at https://github.com/available_if_accepted).

2. Related work

Our proposed method constructs the IH mapping from material properties to cellular unit cells using a GAN-based model. In this section, we first review prior work in cellular structure modeling. We then review

generative models pertinent to the inverse design of cellular structures. Finally, we introduce conditional GANs (cGANs) [19], which our proposed IH-GAN builds upon.

2.1. Cellular structure modeling

Main approaches to representing cellular structures include boundary (*e.g.*, NURBS surfaces) representations (BRep) [20, 21, 22], volume (*e.g.*, voxels) representations (VRep) [18, 23, 24], and FRep (*e.g.*, trigonometric periodic functions) [25, 26, 27]. Given the high complexity of cellular structures, BRep and VRep incur large data size and processing costs (*e.g.*, in the number of voxels or polygons), limited geometry precision (*e.g.*, cracks in surfaces and self-intersections of polygons), limited or no support for parameterization (*e.g.*, VRep models need to be regenerated using a separate, high-level procedure or method), and poor manufacturability (*e.g.*, voxels have aliasing problems unless they are given at high resolutions requiring large amounts of memory) [28]. FRep is a shape parameterization that maps a set of parameters to points along the iso-surface of an implicit function. It offers a compact but precise representation of cellular structures that solves most of the above issues. To enable an accurate and efficient IH mapping using a deep neural network, we benefit from the compactness of FRep that allows representing cellular unit cells by a small set of parameters.

2.1.1. FRep of TPMS-based cellular structures

Surfaces whose mean curvature is everywhere zero are minimal surfaces. A *triply periodic* minimal surface is infinite and periodic in three independent directions. A TPMS is of special interest because it has no self-intersections and partitions space into two labyrinthine regions. These regions commonly appear in various natural and human-made structures, providing a concise description of a wide variety of cellular structures [29, 30, 31]. Compared to the other families of periodic surfaces [25, 32, 33, 34], TPMS are particularly fascinating because a TPMS derives one of the crystallographic space groups as its symmetry group [35]. Those with cubic symmetry simplify the homogenization process by having the same properties along three orthogonal axes [16]. Additionally, TPMS-based cellular structures afford high specific surface area, high porosity, and low relative density while maintaining outstanding mechanical properties [36, 37].

TPMS can be approximated by the periodic implicit surfaces of a sum defined in terms of Fourier series [38, 39, 17]:

$$f(x, y, z) = \sum_{hkl} |F(hkl)| \cos[2\pi(hx + ky + lz) - \alpha(hkl)] = 0 \quad (1)$$

where (h, k, l) are the reciprocal lattice vectors for a given lattice, $\alpha(hkl)$ is a phase shift, and the structure factor $F(hkl)$ is an amplitude associated with a given vector $(h, k, \text{ and } l)$.

Other than the concise representation and cubic symmetry, TPMS-based cellular unit cells can also be diversified by combining several functions and adjusting corresponding coefficients [25, 40].

2.1.2. Variable-density cellular structures and inverse homogenization mapping

Topology optimization is a computational process that optimizes the material distribution in a design space by literally removing material within it, intending to reveal the most efficient design given a set of constraints. Conventional TO methods (*e.g.*, SIMP, ESO/BESO², and level set) [8, 41, 42] often output the optimal structural design as a discrete field (*e.g.*, SIMP produces discrete densities and BESO generates discrete mesh elements). Thus, the TO outputs failed to consider aesthetics, manufacturability, or any other design constraints that one would normally need in a design process. To overcome these limitations, one needs to convert a discrete field into concrete geometries that can be physically realized while maintaining the same performance.

Variable-density cellular structures are a promising candidate to replace the density map (generated by SIMP). They resolve the geometric connectivity and manufacturability issues and possess unique combinations of physical properties (*e.g.*, high strength-to-weight ratio, high energy absorption, and high thermal

²Evolutionary structural optimization (ESO) and its later version bi-directional ESO (BESO).

conductivity) [43, 44, 45]. In addition, variable-density cellular structures make the density map manufacturable with a single material to avoid using costly multi-material techniques [46, 47, 48, 49]. First-generation variable-density cellular structures were designed using simple repeating elements such as cubic trusses with variable strut thickness [50] or hexagonal cells with variable hole diameter [51, 52]. Since then, the three main approaches, namely BRep (e.g., B-splines) [53], VRep (e.g., voxels) [54], and FRep [16], have been investigated for topology optimization of more complex cellular structures. FRep have become a more versatile representation that can produce miscellaneous cellular structures as implicit surfaces whose volume fraction can be conveniently controlled by the level set constant to resemble the given density map. By forming specific implicit functions like TPMS, one can even mimic complicated real-world structures, such as silicates (e.g., Schwartz Diamond structures in diamonds) [55] and biomorphic formations (e.g., Gyroid structures in butterfly wing scales) [56]. These implicit surfaces also take care of geometric continuity and coherence at the connections or interfaces between variable-density unit cells.

Besides the geometric modeling challenge, we need to ensure that generated variable-density cellular structures still preserve desired property performance to complete the density map conversion. To do that, one needs to homogenize the variable-density cellular unit cells to acquire their effective material properties and construct an IH mapping from the homogenized properties to their geometries. Most existing work builds the IH mapping by following the scaling law—*i.e.*, the mechanical properties of cellular structures have polynomial law relationships with their relative densities (Gibson-Ashby model [57, 14]). These relationships have been successfully fitted for low dimensional properties like elastic constants and thermal conductivity constants using polynomial and exponential functions [16]. For material properties with higher dimensionality, a level set field has been proposed to construct a continuous gamut representation of the material properties [15].

As mentioned previously, the scaling law performs a preliminary and simplified version of IH mapping with limited data to be fitted. However, it can only be applicable to approximating the low dimensional (e.g., one-dimensional) property space with simple relationships (e.g., one-to-one mapping). Every time the unit cell type changes, one needs to repeat that fitting process; this forces the mapping to be bijective and difficult to generalize across cell types. The level set method supports the IH mapping for a higher dimensional property space but suffers from a costly manual process requiring extensive computation. For example, Zhu *et al.* [15] needed to perform a series of procedures, including a discrete sampling of the microstructures, a continuous optimization of the microstructures, and a continuous representation of the material gamut by computing a signed distance field (up to 93 hours computational cost in total) to construct an accurate mapping in their application. Unlike these methods, our work eliminates these limitations by training an end-to-end deep generative model (*i.e.*, conditional GAN) to automatically learn the IH mapping from three-dimensional elastic properties (*i.e.*, Young’s modulus and Poisson’s ratio) to multiple types of unit cells.

2.1.3. Structures assembled by multiple types of cellular unit cells

Rather than using single-type variable-density unit cells that can limit the spectrum of physical properties, researchers have explored assembling structures with different types of unit cells to expand the range of physical behaviors. The major bottleneck in the assembly is the lack of sufficient interface connection area due to significantly different geometries at the intersection between two adjacent unit cells. Some existing works have focused on solving this bottleneck by optimizing geometric compatibility between adjacent unit cells. Zhou and Li [58] have summarized three methods (*i.e.*, connective constraint, pseudo load, and unified formulation with nonlinear diffusion) to ensure the connectivity between adjacent 2D unit cells. Li *et al.* [59] used a similar kinematic approach to solve the compatibility issue. Radman *et al.* [60] performed topology optimization of three adjacent base cells by considering the connectivity constraints simultaneously: the base unit cells were designed for the target stiffness while maintaining smooth connectivity. Garner *et al.* [61] focused on finding the optimal connectivity between more diverse topology optimized unit cells while maximizing bulk moduli of the graded structures. Schumacher *et al.* [18] precomputed a database of tiled unit cells indexed by the elastic properties and applied a global optimization to select the optimal tiling that can best connect adjacent tile. Another approach was to use geometric interpolation to obtain intermediate structures that have no geometric frustration [62]. A similar interpolation strategy was commonly used to

design variable-density cellular structures to generate a smooth connection between unit cells with different volumes [16]. Wang *et al.* [63] tackled the geometric compatibility by proposing non-periodic implicit functions that can generate two compatible unit cells with good overlap at the intersection face. In this paper, our approach takes advantage of the integrated TO and IH-GAN framework to generate functionally graded cellular structures with multiple types of unit cells and address the connectivity bottleneck simultaneously without a need for compatibility optimization. The generated structures are also precise and manufacturable for AM techniques.

2.2. Generative models for inverse design of microstructures

Generative modeling, a branch of unsupervised learning techniques in machine learning, has been used to build the statistical model of data distributions. In recent years, deep generative models like variational autoencoders (VAEs) or GANs have drawn much attention and are used to generate realistic data. These models are primarily applied in the computer science domain for image synthesis and nature language processing [64]. Unlike these typical applications, generative models have been used in the microstructural design, including crystalline porous structures, nanophotonic structures, and metamaterial structures. Kim *et al.* [65] developed a ZeoGAN model to generate realistic zeolite materials and their corresponding energy shapes via training the combined data of three grids (*i.e.*, the energy, silicon atom, and oxygen atom grids). Liu *et al.* [66] enabled the inverse design of nanophotonic metasurfaces (2D image data) by adopting a conditional GAN model where a pre-trained simulator was added to approximates the transmittance spectrum for a given geometric pattern at its input. Ma *et al.* [67] revealed the non-intuitive and non-unique relationship between metamaterial structures and their optical responses by incorporating a VAE in their generative model, which encodes the designed pattern together with the corresponding optical response into a latent space. A VAE model (combined with a regressor of the mechanical properties of interest) was also used by Wang *et al.* [68] to generate the pixel-based 2D metamaterial microstructures. Kumar *et al.* [69] designed the spinodoid non-periodic cellular structures inversely via the use of two multi-layer perceptron—an inverse network and a forward network—the former takes a queried stiffness as input and outputs design parameters defining a cellular unit cell, and the latter takes the predicted design parameters as input and reconstructs the stiffness and verifies the prediction from the inverse network. In this paper, we use a conditional GAN model to realize the inverse design of cellular structures by learning the mapping from the material properties (*i.e.*.. Young's modulus and Poisson's ratio) to the shape parameters that define the implicit surfaces of the cellular unit cells. To the best of our knowledge, the conditional GAN model has never been used in the inverse design of cellular structures.

2.3. Conditional generative adversarial networks

Generative adversarial networks [70] model a game between a generative model (*generator*) and a discriminative model (*discriminator*). The generative model maps an arbitrary noise distribution to the data distribution (*i.e.*, the distribution of designs in our scenario), thus can generate new data; while the discriminative model tries to perform classification, *i.e.*, to distinguish between real and generated data. The generator G and the discriminator D are usually built with deep neural networks. As D improves its classification ability, G also improves its ability to generate data that fools D . Thus, a vanilla GAN (standard GAN with no bells and whistles) has the following objective function, which includes a discriminator loss term and a generator loss term:

$$\min_G \max_D V(D, G) = \mathbb{E}_{\mathbf{x} \sim P_{data}} [\log D(\mathbf{x})] + \mathbb{E}_{\mathbf{z} \sim P_{\mathbf{z}}} [\log(1 - D(G(\mathbf{z})))] \quad (2)$$

where \mathbf{x} is sampled from the data distribution P_{data} , \mathbf{z} is sampled from the noise distribution $P_{\mathbf{z}}$, and $G(\mathbf{z})$ is the generator distribution. A trained generator thus can map from a predefined noise distribution to the distribution of designs. The noise input \mathbf{z} is considered as the latent representation of the data, which can be used for design synthesis and exploration.

The *conditional GAN* or *cGAN* [19] further extends GANs to allow the generator to learn a conditional distribution. This is done by simply feeding the condition, \mathbf{y} , to both D and G . The loss function then

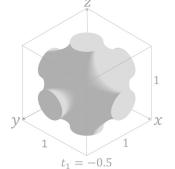
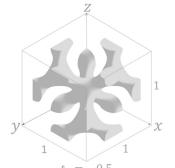
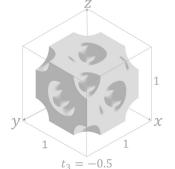
becomes:

$$\min_G \max_D V_{\text{cGAN}}(D, G) = \mathbb{E}_{\mathbf{x} \sim P_{\text{data}}} [\log D(\mathbf{x}|\mathbf{y})] + \mathbb{E}_{\mathbf{z} \sim P_{\mathbf{z}}} [\log(1 - D(G(\mathbf{z}|\mathbf{y})))]. \quad (3)$$

3. TPMS-based cellular structures

Our cellular structures are created as a composition of three different TPMS surfaces that have a cubic symmetry, namely Schwarz P (P), Diamond (D), and Schoen's F-RD [71]. Table 1 lists their implicit functions and corresponding geometric models.

Table 1: TPMS surfaces with cubic symmetry

Morphology	TPMS function	Model
Schwarz P (P)	$f_P(x, y, z) = \cos(X) + \cos(Y) + \cos(Z) + t_1 = 0$	(4a) 
Diamond (D)	$f_D(x, y, z) = \cos(X) \cos(Y) \cos(Z) - \sin(X) \sin(Y) \sin(Z) + t_2 = 0$	(4b) 
F-RD	$f_{FRD}(x, y, z) = 8 \cos(X) \cos(Y) \cos(Z) + \cos(2X) \cos(2Y) \cos(2Z) - (\cos(2X) \cos(2Y) + \cos(2Y) \cos(2Z) + \cos(2Z) \cos(2X)) + t_3 = 0$	(4c) 

where $X = 2\pi x$, $Y = 2\pi y$, $Z = 2\pi z$.

The three TPMS surfaces are merged as a weighted sum of their implicit functions using Equation (5):

$$\begin{aligned} f_{\text{merge}}(x, y, z) &= \alpha_1(4f_P(x, y, z)) + \alpha_2(4f_D(x, y, z)) + \alpha_3 f_{FRD}(x, y, z), \\ \alpha_1 + \alpha_2 + \alpha_3 &= 1, \\ 0 \leq \alpha_1, \alpha_2, \alpha_3 &\leq 1 \end{aligned} \quad (5)$$

where α_1 , α_2 , and α_3 are randomized with a fixed sum of 1 to generate diverse cellular unit cells. The weights of P and D surfaces are augmented by a multiplier ($= 4$) to balance the proportion of P and D surfaces when merging the three basic TMPS surfaces (shown in Table 1). The level set value (t_1 , t_2 , and t_3) in Equation (4a)-(4c) determines the volume fraction (*i.e.*, relative density) of a unit cell by thickening or thinning the surfaces. By picking different level set values, we can further increase the variations of these merged unit cells. Figure 3 displays some merged unit cells generated by Equation (5).

4. Effective properties of homogenized cellular structures

In this paper, a voxel-based numerical homogenization method [72] is employed to compute the effective elasticity tensor of the TPMS unit cells. From the homogenized constitutive matrix, one can obtain the

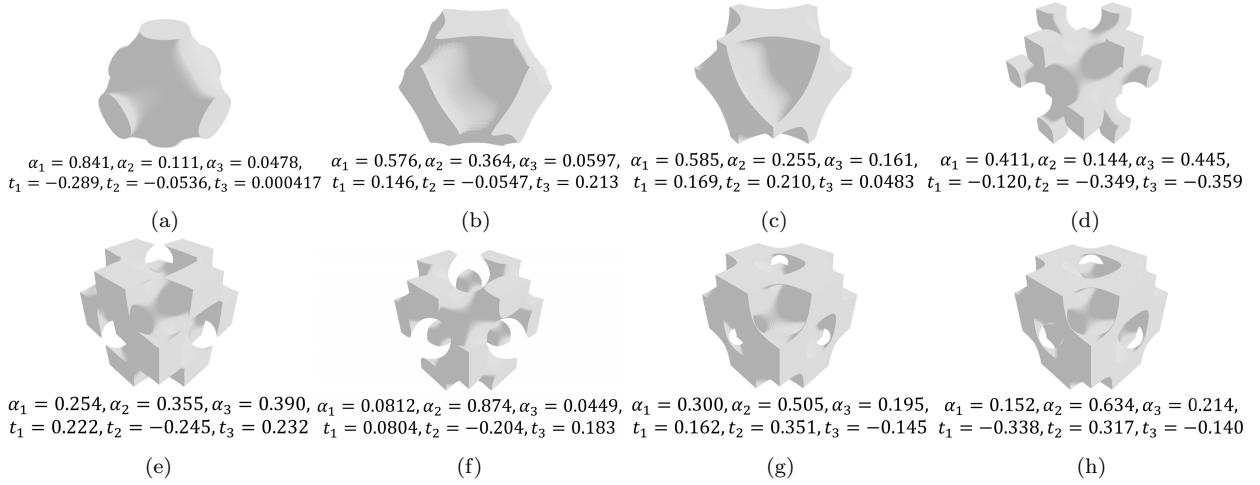


Figure 3: Merged unit cells using different shape parameters.

identical Young's modulus and Poisson's ratio along the axial directions ($x-$, $y-$, and $z-$) due to the cubic symmetry of those TPMS-based cellular structures (orthotropic materials).

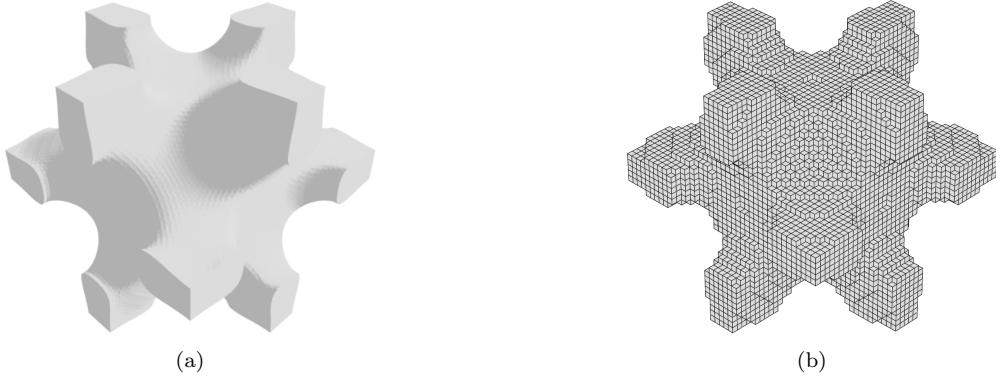


Figure 4: Voxelization of a TPMS-based unit cell. (a) Implicit surface. (b) Voxels.

The finite element used in this homogenization is an eight-node hexahedron. Therefore, each unit cell is voxelized into $40 \times 40 \times 40$ cubes (Figure 4). The homogenized constitutive matrix \mathbf{C}^H of a unit cell can be calculated as an assembly of the finite elements using the following equation:

$$\mathbf{C}^H = \frac{1}{|V|} \sum_e \int_{V_e} (\mathbf{I} - \mathbf{B}_e \boldsymbol{\chi}_e)^T \mathbf{C}_e (\mathbf{I} - \mathbf{B}_e \boldsymbol{\chi}_e) dV_e \quad (6)$$

where V is the total volume of the unit cell, V_e is the element volume, \mathbf{B}_e and $\boldsymbol{\chi}_e$ are strain-displacement matrix and displacement matrix of each hexahedral element, and \mathbf{I} is a 6×6 identity matrix (\mathbf{I}_6). \mathbf{C}_e is the element constitutive matrix of the elementary material that is isotropic over each finite element, and thus

can be expressed by Lamé's parameters [73] as:

$$\mathbf{C}_e = \begin{bmatrix} \lambda + 2\mu & \lambda & \lambda & 0 & 0 & 0 \\ \lambda & \lambda + 2\mu & \lambda & 0 & 0 & 0 \\ \lambda & \lambda & \lambda + 2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & \mu & 0 & 0 \\ 0 & 0 & 0 & 0 & \mu & 0 \\ 0 & 0 & 0 & 0 & 0 & \mu \end{bmatrix} \quad (7)$$

where the Lamé's first and second parameters λ and μ are:

$$\begin{aligned} \lambda &= \frac{\nu E}{(1+\nu)(1-2\nu)}, \\ \mu &= \frac{E}{2(1+\nu)} \end{aligned} \quad (8)$$

where E and ν are Young's modulus and Poisson's ratio of the elementary material³. The global stiffness matrix \mathbf{K} of the unit cell is assembled as:

$$\mathbf{K} = \sum_e \int_{V_e} \mathbf{B}_e^T \mathbf{C}_e \mathbf{B}_e dV_e \quad (9)$$

The load \mathbf{f}^i is calculated by the macroscopic volumetric straining:

$$\mathbf{f}^i = \sum_e \int_{V_e} \mathbf{B}_e^T \mathbf{C}_e \boldsymbol{\varepsilon}^i dV_e \quad (10)$$

where the macroscopic strains $\boldsymbol{\varepsilon}^i$ are:

$$\begin{aligned} \boldsymbol{\varepsilon}^1 &= (1, 0, 0, 0, 0, 0)^T, \boldsymbol{\varepsilon}^2 = (0, 1, 0, 0, 0, 0)^T, \boldsymbol{\varepsilon}^3 = (0, 0, 1, 0, 0, 0)^T, \\ \boldsymbol{\varepsilon}^4 &= (0, 0, 0, 1, 0, 0)^T, \boldsymbol{\varepsilon}^5 = (0, 0, 0, 0, 1, 0)^T, \boldsymbol{\varepsilon}^6 = (0, 0, 0, 0, 0, 1)^T \end{aligned} \quad (11)$$

The global displacement fields $\boldsymbol{\chi}^i$ of the unit cell are achieved by solving the following equation:

$$\mathbf{K} \boldsymbol{\chi}^i = \mathbf{f}^i \quad (12)$$

Finally, each entry in \mathbf{C}^H can be obtained by using the following equation:

$$\mathbf{C}_{ij}^H = \frac{1}{|V|} \sum_e \int_{V_e} (\boldsymbol{\chi}_e^{0(i)} - \boldsymbol{\chi}_e^{(i)})^T \mathbf{C}_e (\boldsymbol{\chi}_e^{0(j)} - \boldsymbol{\chi}_e^{(j)}) dV_e \quad (13)$$

where $\boldsymbol{\chi}_e^{0(i)}$ is the element displacement field that corresponds to the i -th unit strain in Equation (11), and $\boldsymbol{\chi}_e^{(i)}$ is the corresponding displacement field obtained from globally enforcing the unit strains in Equation (12). After iterating the six unit strains, the 6×6 homogenized constitutive matrix \mathbf{C}^H is attained. To achieve the unit cell's effective Young's modulus and Poisson's ratio, one still needs to find the inverse of \mathbf{C}^H —i.e., the homogenized compliance matrix \mathbf{S}^H . From the compliance matrix, the cubic symmetric unit cells have:

$$\begin{aligned} E^H &= E_x = E_y = E_z = \frac{1}{S_{11}^H} = \frac{1}{S_{22}^H} = \frac{1}{S_{33}^H}, \\ \nu^H &= -S_{12}^H E = -S_{13}^H E = -S_{21}^H E = -S_{23}^H E = -S_{31}^H E = -S_{32}^H E \end{aligned} \quad (14)$$

³In this paper, we assume the material has Young's modulus of 200 GPa and Poisson's ratio of 0.3. Using Equation (8), the Lamé's first and second parameters λ and μ are calculated as 115.4 and 76.9, respectively.

Figure 5 shows the coverage of effective material properties of our training data. Note that no training data is present in some regions (*e.g.*, the lower right region) of the material property space. This means that IH-GAN cannot faithfully generate the unit cells with the material properties from those regions since it has not seen any data there during training. Therefore, in downstream tasks like topology optimization, we need to constrain the solution space of the material properties based on the distribution of our training data. We will describe later how we consider the training data distribution while performing topology optimization.

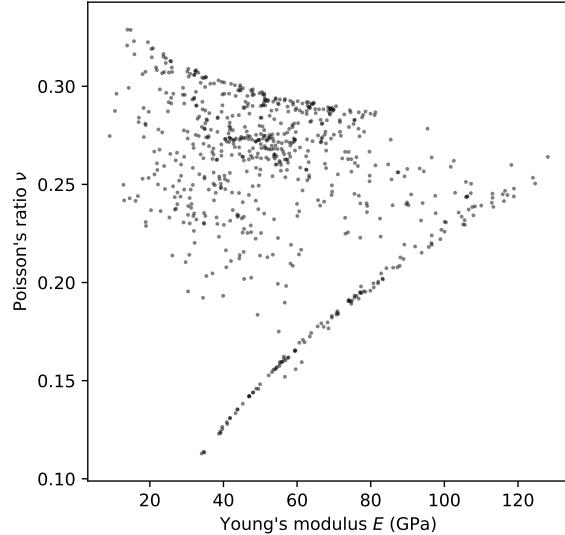


Figure 5: Effective material properties of training data.

5. Inverse homogenization GAN

We propose a conditional GAN, Inverse Homogenization GAN (IH-GAN), to learn the IH mapping — a one-to-many mapping from the material property space \mathcal{M} in \mathbb{R}^2 to the shape parameter space \mathcal{S} in \mathbb{R}^6 (Figure 6). Specifically, \mathcal{M} is defined by the Young's modulus E and the Poisson's ratio ν of a unit cell; while \mathcal{S} is defined by the six shape parameters $\alpha_1, \alpha_2, \alpha_3, t_1, t_2$, and t_3 from Equation (4a)-(4c) and (5). The generator G has both the material properties and the noise vector \mathbf{z} as inputs. The noise is drawn from a predefined prior distribution $P_{\mathbf{z}}$ (*e.g.*, multivariate normal distribution). Given E and ν , we can draw multiple unit cell shapes as the output of G by sampling noise vectors from $P_{\mathbf{z}}$ as the input to G .

We further improve the IH mapping by ensuring the generated shape parameters can be accurately mapped back to their corresponding material properties. Specifically, we add an *Auxiliary Material Property Regressor* (R) to predict each design's material properties (Figure 6). This leads to an additional loss term:

$$L(G, R) = \mathbb{E}_{\mathbf{x} \sim P_{data}} [|\mathbf{y} - R(\mathbf{x})|] + \mathbb{E}_{\mathbf{z} \sim P_{\mathbf{z}}} [|\mathbf{y} - R(G(\mathbf{z}|\mathbf{y}))|], \quad (15)$$

where $\mathbf{x} = (\alpha_1, \alpha_2, \alpha_3, t_1, t_2, t_3)$, and $\mathbf{y} = (E, \nu)$.

Similar architecture is also used in two existing GAN variants: (1) To maximize the mutual information between the generated sample \mathbf{x} and its latent code \mathbf{c} , InfoGAN [74] uses an auxiliary network to approximate the conditional latent code distribution $P(\mathbf{c}|\mathbf{x})$; and (2) To improve sample quality, the auxiliary classifier GAN (AC-GAN) [75] uses an auxiliary classifier to predict the probability distribution $P(\mathbf{l}|\mathbf{x})$ over the class labels \mathbf{l} .

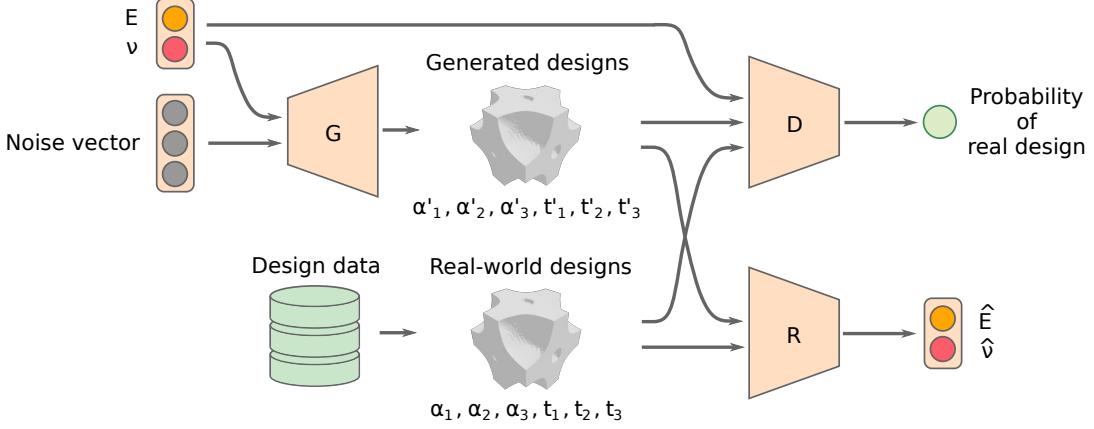


Figure 6: Architecture of the IH-GAN. Notations G , D , and R represent the generator, the discriminator, and the auxiliary material property regressor, respectively.

The overall loss function of IH-GAN thus combines the conditional GAN’s loss and Equation (15) with a hyperparameter γ :

$$\min_{G,R} \max_D V_{\text{IH-GAN}}(D, G, R) = V_{\text{cGAN}}(D, G) + \gamma L(G, R). \quad (16)$$

During training, we fix G when updating D and R , and fix D and R when updating G .

6. Topology optimization for IH-GAN

As the proposed IH-GAN model can accurately generate cellular structures possessing the desired material properties, it can be useful in designing functionally graded cellular structures composed of multiple types of cellular unit cells. Rather than typical TO algorithms (*e.g.*, SIMP) that optimize a density map by assuming an approximate relation between Young’s modulus (E) and the density (ρ), our IH-GAN model uses a modified version of a TO algorithm that can output maps of both E and ν . Based on the E and ν maps, our IH-GAN generates corresponding cellular unit cells to replace the two maps and end up with a functionally graded cellular structure.

We use the compliance (C_c) as the elasticity objective as used in other TO benchmarks. With E and ν as the design variables, our new TO problem is defined as:

$$\begin{aligned} & \underset{E, \nu}{\text{minimize}} \quad C_c = \mathbf{u}^T \mathbf{K}(E, \nu) \mathbf{u} \\ & \text{subject to} \quad \mathbf{K}(E, \nu) \mathbf{u} - \mathbf{f}_{ext} = 0, \\ & \quad \Phi(E_i, \nu_i) \leq 0, \quad i = 1, \dots, N_e, \\ & \quad \sum_{i=1}^{N_e} E_i \leq E_c, \\ & \quad E_{min} \leq E_i \leq E_{max}, \\ & \quad \nu_{min} \leq \nu_i \leq \nu_{max} \end{aligned} \quad (17)$$

where \mathbf{E} and $\boldsymbol{\nu}$ are the vectors of the element Young’s modulus and Poisson’s ratio, \mathbf{K} is the global stiffness matrix, \mathbf{u} is the displacement vector, and \mathbf{f}_{ext} represents the external loads applied to the object. The equality constraint is the static elasticity (Hooke’s law) equilibrium equation.

The first inequality constraint $\Phi \leq 0$ guarantees each cellular unit cell's material properties have high probability density in the training data distribution (Figure 5) so that IH-GAN can faithfully generate shape parameters given E and ν . It can have the following form:

$$\Phi(E_i, \nu_i) = \tau - \Pr(E_i, \nu_i; \theta), \quad (18)$$

where the probability density function $\Pr(E_i, \nu_i; \theta)$ can be estimated by methods like kernel density estimation (KDE), θ denotes the parameters of the estimated distribution, and τ is a threshold on the probability density. To simplify this problem, in this paper, we use the convex hull of the training data's material property instead to form a linear constraint:

$$\Phi(E_i, \nu_i) = A (E_i, \nu_i, 1)^T, \quad (19)$$

where $A \in \mathbb{R}^{n \times 3}$ contains the coefficients of n hyperplane equations.

The second inequality constraint controls the overall Young's modulus, which indirectly impacts the total mass of the object (a high E often corresponds to a large ρ). The last two constraints limit the lower and upper bounds of the element E and ν , respectively.

The solution of this modified TO problem contains two maps (*i.e.*, \mathbf{E} and $\boldsymbol{\nu}$), which are combined and fed into the IH-GAN model to generate the 6 shape parameters $(\alpha_1, \alpha_2, \alpha_3, t_1, t_2, t_3)$. The corresponding unit cell shapes are then created using Equation (5).

7. Experiments

In this section, we introduce a new unit cell shape dataset and our experimental settings. We release both our dataset and code at https://github.com/available_if_accepted.

7.1. Datasets

To train the IH-GAN, we use a unit cell shape database containing the shape parameters and the effective material properties of 924 unit cells.

Shape parameters. Using the design method in Section 3, each cellular unit cell can be represented by six parameters $(\alpha_1, \alpha_2, \alpha_3, t_1, t_2, t_3)$. To produce a diverse dataset, we first randomly generate N groups of α_1 , α_2 , and α_3 with a fixed sum of 1. Next, we generated N groups of t_1 , t_2 , and t_3 through a Latin hypercube sampling [76] strategy to evenly cover the level set space. In this paper, we have $t_1, t_2, t_3 \in [-0.4, 0.4]$ to avoid modeling failures—*i.e.*, breaks due to a low density and fully solid due to a high density. We excluded shapes having small cross section areas or having zero contact areas with neighboring cells. The final dataset contains 924 different unit cells.

Effective material properties. The dataset of effective material properties is collected by homogenizing each of the 924 unit cells using the approach described in Section 4. In our material dataset, each unit cell's material properties are represented as a set of two parameters (*i.e.*, E^H and ν^H).

The database is then split with a ratio of 8:2 for training (739) and evaluation (185), respectively.

7.2. IH-GAN model configuration and training

The generator, the discriminator, and the auxiliary regressor are fully-connected neural networks with the architectures shown in Figure 7. The unit cell shapes are represented as 6-dimensional vectors. The condition vectors (*i.e.*, material properties E and ν) are 2-dimensional vectors. We set the noise input \mathbf{z} as a 3-dimensional vector drawn from a standard multivariate normal distribution. We set $\lambda = 20$ in Equation (16). We used 5000 training iterations during training, with each iteration randomly sampling 32 examples as a mini-batch. The same learning rate of 0.0002 is used for optimizing the generator, the discriminator, and the auxiliary regressor. This simple neural network configuration allows a wall-clock training time of 38 seconds on a GeForce GTX TITAN X. The inference time is less than one second.

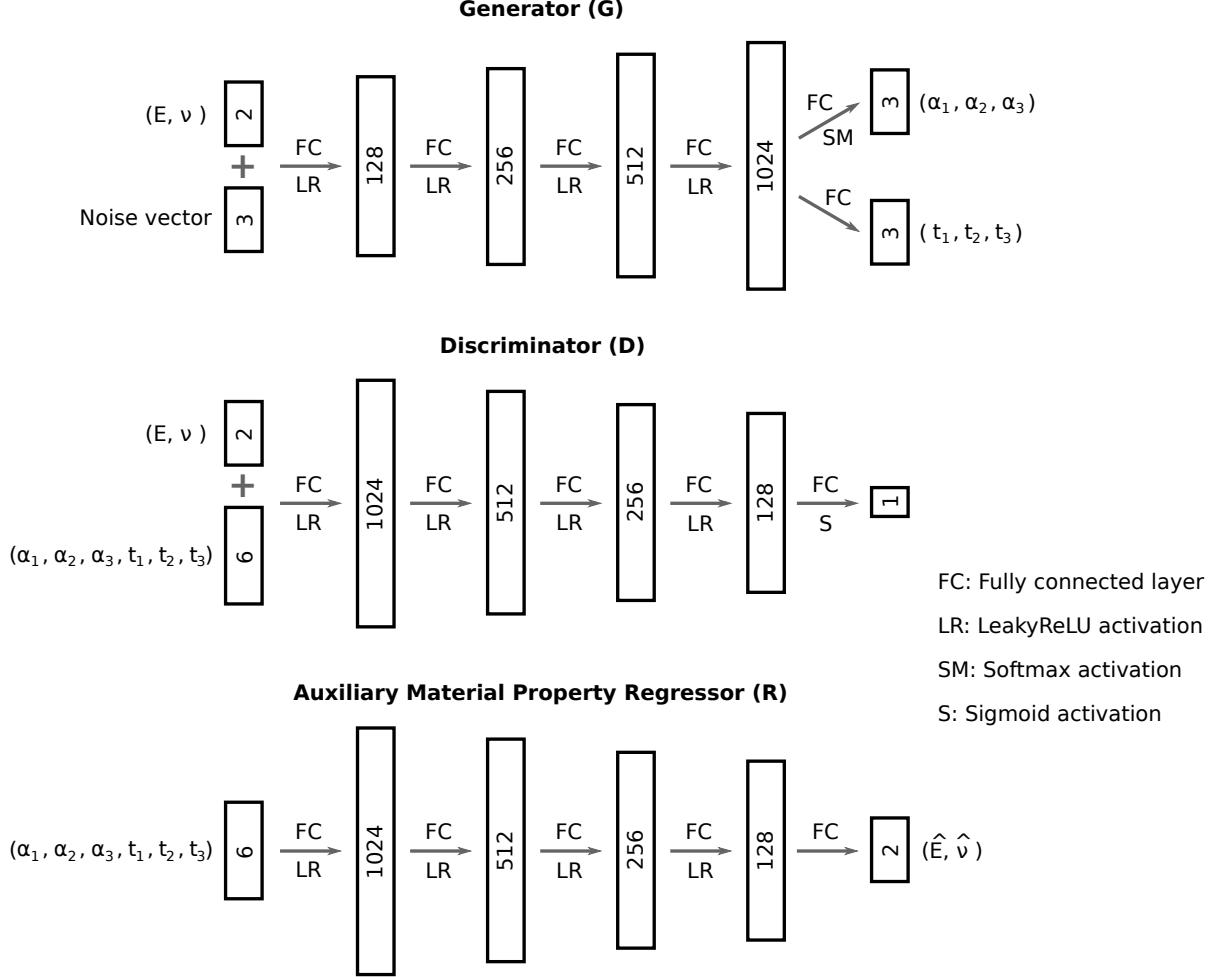


Figure 7: Neural network configuration used for experiments.

7.3. Topology optimization settings

In the training data, E ranges between [9.10, 128.11] (unit: GPa) and ν ranges between [0.11, 0.33]. Thus, in topology optimization, we set the material property upper bounds ν_{max} to 0.33 and E_{max} to 128.11 GPa in Equation (17). However, to avoid generating unfaithful unit cells as discussed earlier, we set the lower bounds ν_{min} to 0.23 and E_{min} to 20 GPa, as training data are sparse below those bounds. In Sec. 8.1, we will show that unit cells generated by conditioning on E and ν from the sparse data regions have connectivity issues and lead to inaccurate effective material properties.

8. Results and discussion

8.1. Performance of IH-GAN

To evaluate whether the generated unit cells have the exact material properties (E, ν) on which the geometries are conditioned, we compute the *material property error* on the test dataset. The material property error measures the percentage error between (E, ν) and the actual material properties (E', ν')

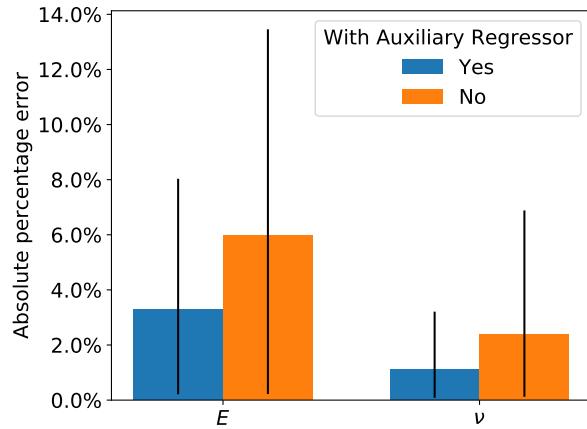


Figure 8: Material property errors of generated unit cells. Bars denote the mean material property errors. Error bars denote the 5%-95% interval.

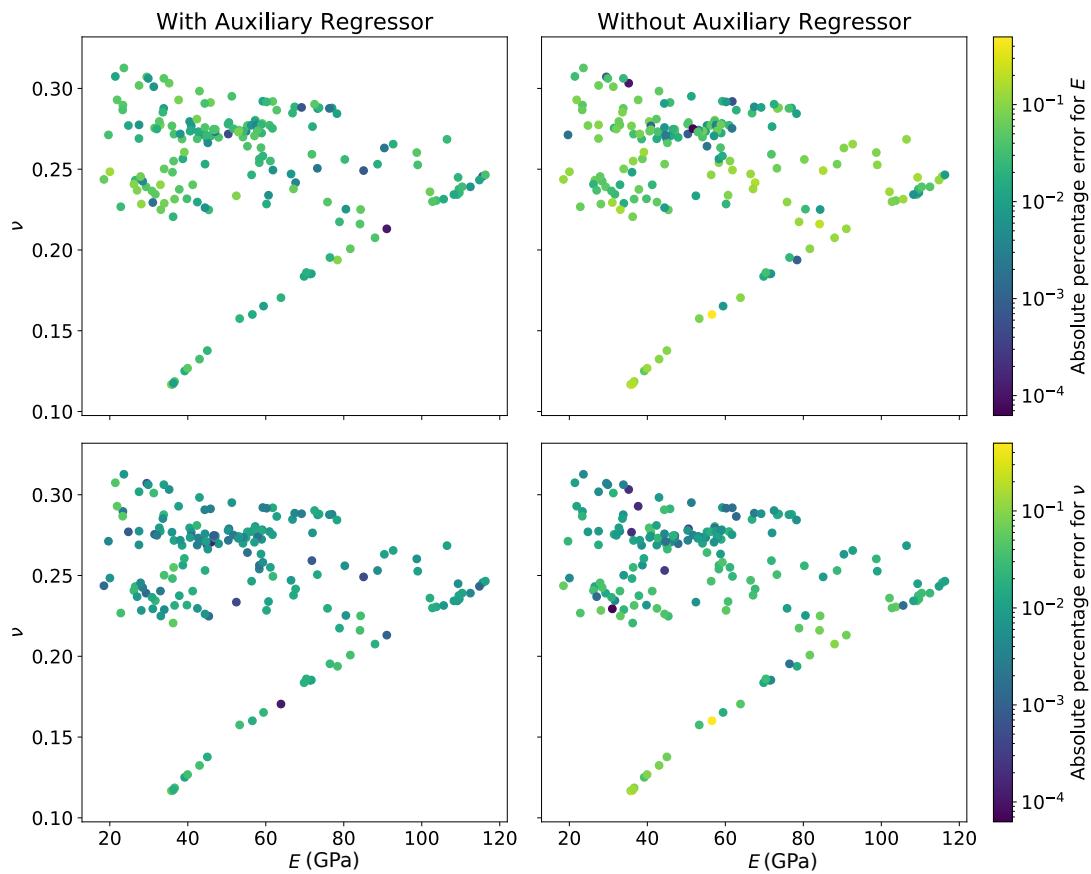


Figure 9: Error maps for generated unit cells in the material property space.

(computed via homogenization) of a generated geometry:

$$\begin{aligned}\epsilon_E &= (E' - E)/E, \\ \epsilon_\nu &= (\nu' - \nu)/\nu.\end{aligned}\quad (20)$$

We compute the errors on the test set. Results are shown in Figures 8 and 9. To demonstrate the effects of the auxiliary regressor, we also compute the errors when it is removed. Figure 8 indicates that using an auxiliary regressor decreases the errors in general. When adding an auxiliary regressor, the mean absolute percentage error decreases 44.9% and 53.1% for Young's modulus and Poisson's ratio, respectively. There is also a substantial decrease in the standard deviation of the absolute percentage errors for both material properties. Figure 9 shows the error maps of Young's modulus and Poisson's ratio. The auxiliary regressor mainly improves the accuracy when the Young's modulus is large, or the Poisson's ratio is small.

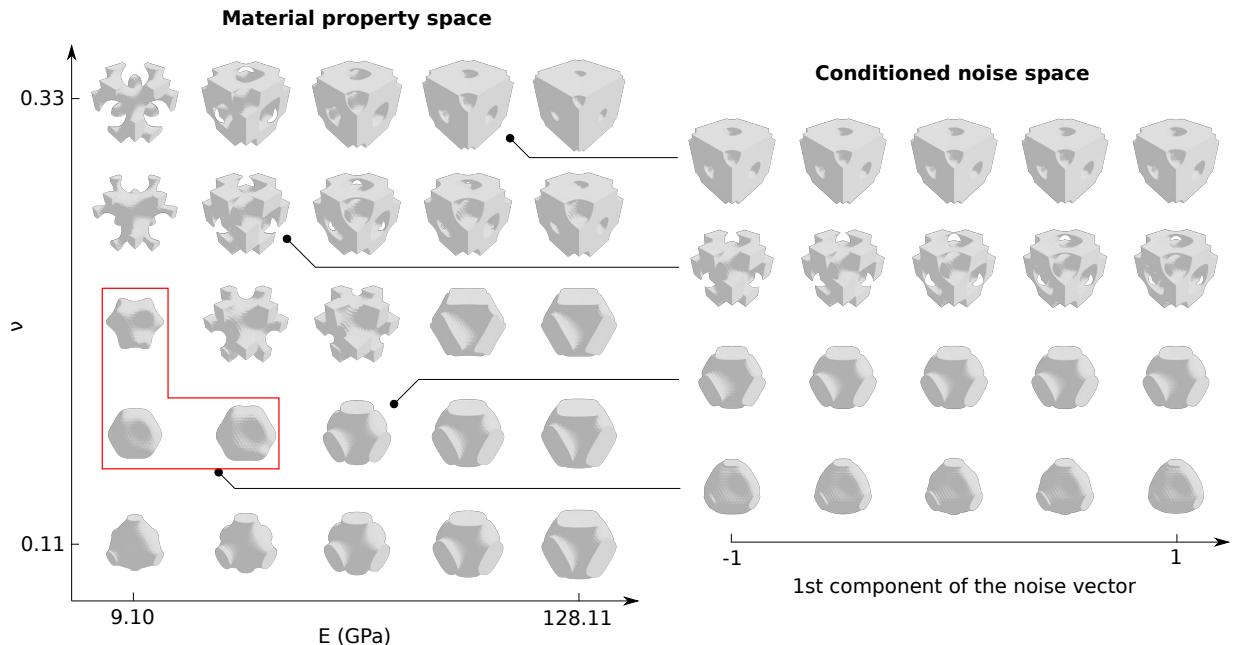


Figure 10: The effects of material properties (E and ν as conditions) and noise on synthesized unit cells. *Left*: synthesized unit cells conditioned on different material properties and fixed noise. Unit cells in the red box are generated in the region of the material property space where there are no real-world material property data. *Right*: each row shows synthesized unit cells by conditioning on certain material properties while varying the first noise variable.

On the left of Figure 10, we visualize the generated shape variation in a continuous 2D material property space, *i.e.*, how the generated unit cell shape changes when varying Young's modulus E and Poisson's ratio ν . It shows that there is a strong correlation between E and the unit cell's volume fraction. Meanwhile, as ν increases, mass transports from the center of the unit cell to the periphery. These observations are consistent with physical intuition. Note that the true material property space may contain infeasible regions where there are no real-world data (*e.g.*, the lower left and lower right regions). In those regions, IH-GAN generates either invalid unit cells (*i.e.*, round-shaped unit cells at the lower left, which have zero contact areas with neighboring cells, as indicated by the red box) or invariant shapes (*i.e.*, shapes at the lower right corner). When IH-GAN is used for downstream tasks, we need to exclude those infeasible regions by bounding E and ν . On the right of Figure 10, we show how shape varies with the noise vector given fixed E and ν as the condition. We obtain different unit cells by perturbing the noise input to the generator.

This results in a one-to-many mapping from the material property space to the shape parameter space. The magnitude of shape variation, however, differs when conditioned on different material properties.

Ideally, for an inverse homogenization mapping, given fixed material properties (E, ν) as conditions, the noise input would only change the geometry of generated unit cells; whereas the material properties they actually possess would be fixed as (E, ν) . In reality, given fixed (E, ν) as conditions of generated geometries, their actual material properties (E', ν') may deviate from (E, ν) as we perturb the noise input. To test how far (E', ν') deviates from (E, ν) , we take 50 sets of (E, ν) as conditions, under each of which we randomly perturb the noise inputs to generate 50 unit cells and compute their material property errors. The results are shown in Figure 11. The errors for Young's modulus have a larger variation caused by noise perturbation than Poisson's ratio. Despite some outliers, most percentage errors for E have mean values within [-3%, 5%] and standard deviations within 6%. Most percentage errors for ν have mean values within [-2%, 1%] and standard deviations within 2%.

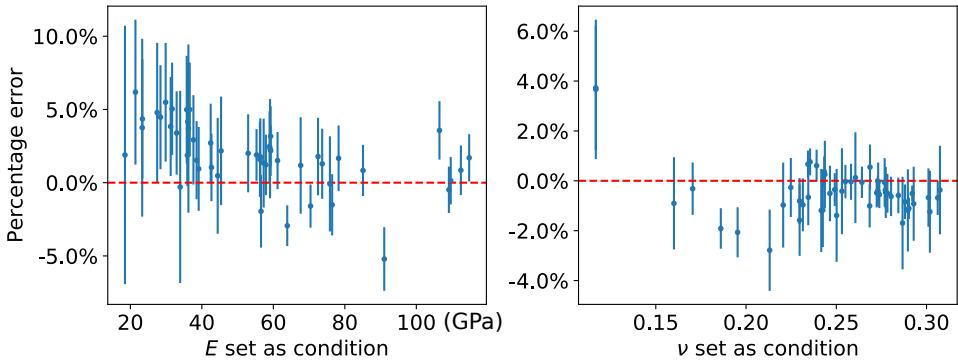


Figure 11: Distribution of material property errors when randomly perturbing the noise input (points and vertical lines denote mean and standard deviation, respectively).

8.2. Functionally graded cellular structural design

This paper optimizes a cantilever beam as an illustrative example to demonstrate the functionally graded cellular structural design using IH-GAN as shown in Figure 12. We obtain the optimized E and ν maps by solving the topology optimization problem described in Section 6. We then combine the two maps and feed them into IH-GAN to generate corresponding cellular unit cells. We finally assemble these cellular unit cells to make a beam.

To find the beam with the lowest weight, we generate n ($n = 10$ in this work) candidate cellular unit cells for each element by varying the noise and picking the one with the lowest density. The synthesized structure on the right of Figure 12 shows the final design with the lowest total mass (47.9% of the original total mass).

8.3. Connectivity

The major risk that arises when merging different types of cellular unit cells is the lack of sufficient interface connection area [63]. If the geometries at the intersection between two adjacent unit cells are significantly different, the common face's potential overlap can be low, leading to poor connectivity. Such poor connectivity can result in a weak link that makes the entire structure vulnerable to failure (under functional needs) and eliminates any advantage obtained using multi-type cellular structures. In this paper, we ensure the quality of interface connectivity by computing the percentage of overlap area:

$$P_o = \frac{|A_A \cap A_B|}{\min\{|A_A|, |A_B|\}} \times 100\%, \quad (21)$$

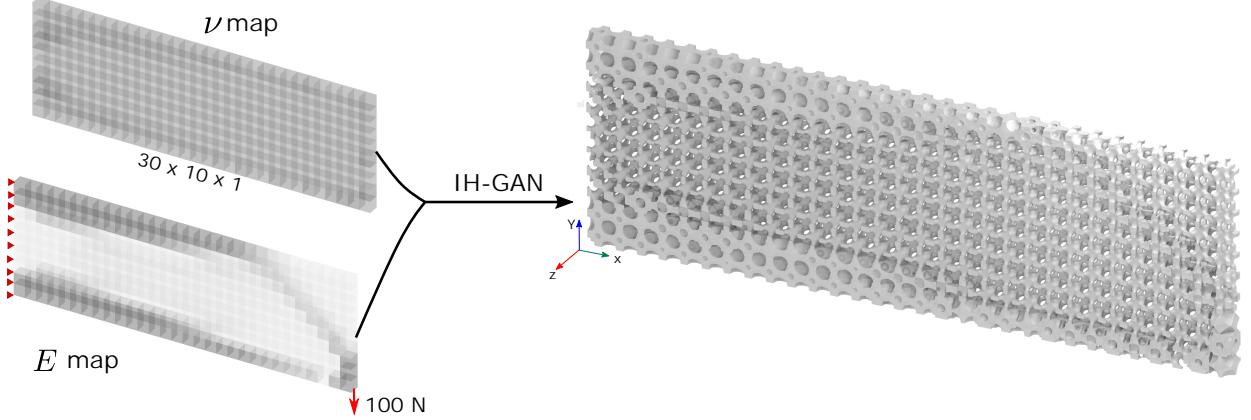


Figure 12: An illustrative example of a cantilever beam built by functionally graded cellular unit cells using IH-GAN. The beam has a dimension of $30 \text{ mm} \times 10 \text{ mm} \times 1 \text{ mm}$ ($x \times y \times z$). *Left:* optimized Young's modulus map and Poisson's ratio map with boundary conditions indicated. The red triangles (\blacktriangle) symbolizes a fixed boundary condition along all three coordinates. The red arrows (\rightarrow) represent a point force loading condition and the direction it is applied. *Right:* the synthesized structure with multiple types of cellular unit cells.

where A_A and A_B are sets of pixels of two connecting unit cell faces after discretization. Figure 13 illustrates the boundary faces of two different unit cells, A and B, with the faces in contact vertically or horizontally when the structure is assembled. The face of unit cell A is represented by red circles, the face of unit cell B is depicted by green crosses, and the overlap areas are shown in red circles with green crosses infilled. In this paper, we utilize TPMS-based unit cells that have cubic symmetry. Therefore, each unit cell has six identical boundary faces. The average percentage of overlap areas within the whole structure is 98.7%.

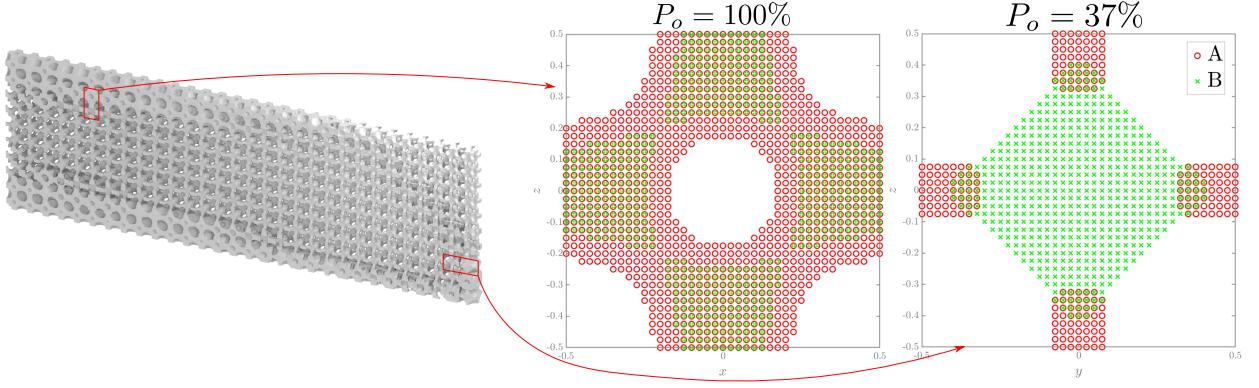


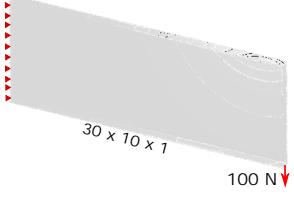
Figure 13: Interface boundaries for adjacent unit cells (A and B) at two locations.

By taking advantage of the material property filter kernel used in TO and the continuous shape variation of IH-GAN's generated unit cells in the 2D material property space, IH-GAN's generated unit cells can naturally guarantee quality connectivity between different unit cells without additional compatibility optimization efforts [18, 61]. Most of the boundary faces have overlap areas close to 100%. There are still some adjacent unit cells that can have relatively low overlap areas. For example, the rightmost subfigure in Figure 13 shows the lowest overlap between two unit cells with a percentage of 37.0%. To avoid possible failure due to insufficient interface connection, we can replace one of the two low-overlap unit cells with another one that has a relatively higher E .

8.4. Validation of structural performance

To demonstrate the efficacy of IH-GAN in designing functional structures, we validate the cantilever beam's structural performance (Figure 12) by performing an FE simulation and comparing it with the single-type cellular structural designs. As seen in Table 2, the solid beam is also redesigned into a variable-density single-type cellular structure and a uniform single-type cellular structure. For the variable-density structure, the density of D surface unit cells is optimized by state-of-the-art proposed in [16]. In comparison, the uniform structure is formed by D surface unit cells with identical densities.

Table 2: Structural performance comparison with different design methods

Design domain	IH-GAN	Variable-density	Uniform
			
Density (ρ)	47.9%	47.9%	47.9%
Displacement (unit: mm)	0.1374	0.1478	0.4373
σ_{max} (unit: MPa)	4,301.4	27,650.8	56,863.2

To enable a fair comparison between different design methods, we apply the same load (a point force of 100 N) and keep the density consistent (47.9%) for the three structures (Table 2). The FE simulation is performed using ABAQUS 2017. The material properties used in the simulation are the same ones used in the homogenization process with $E = 200$ GPa and $\nu = 0.3$. Our proposed IH-GAN-based method slightly reduces the beam's maximum displacement by 7% (from 0.1478 mm to 0.1374 mm) compared to the variable-density structure. In contrast, the uniform structure (without optimization) results in a much larger displacement of 0.4373 mm. While maintaining the displacement performance, the IH-GAN-based method can lower the maximum von-Mises stress (σ_{max}) significantly compared to the other two methods. The IH-GAN structure's maximum stress is 4,301.4 MPa, which is 84.4% lower than the maximum stress of the variable-density structure (27,650.8 MPa) and 92.4% lower than the maximum stress of the uniform structure (56,863.2 MPa). The FE simulated displacement contours of the three structures are compared in Figure 14. The FE simulation results show that our IH-GAN model can successfully generate graded cellular structures with functional performance exceeding current state-of-the-art methods.

9. Conclusion

We proposed a GAN model to learn the IH mapping from material properties to unit cell shapes that can be used to optimize functionally graded cellular structures. The cubic symmetric TPMS surfaces (P, D, and F-RD) were chosen and combined to create the dataset of orthotropic cellular structures and represent each cellular unit cell as a six-dimensional shape vector (*i.e.*, $\alpha_1, \alpha_2, \alpha_3, t_1, t_2, t_3$). The material property space consisting of effective Young's modulus and Poisson's ratio (*i.e.*, E^H and ν^H) were computed using a voxel-based numerical homogenization method. Our proposed IH-GAN's one-to-many IH mapping was learned on the six-dimensional shape parameter space with the two-dimensional material property space as the input conditions.

Our approach offers an end-to-end generative model that automatically learns the IH mapping from data without assuming a bijective polynomial relationship. Except for the unit cell density (volume fraction), we also consider unit cell types when building the mapping. By including an auxiliary regressor in the IH-GAN,

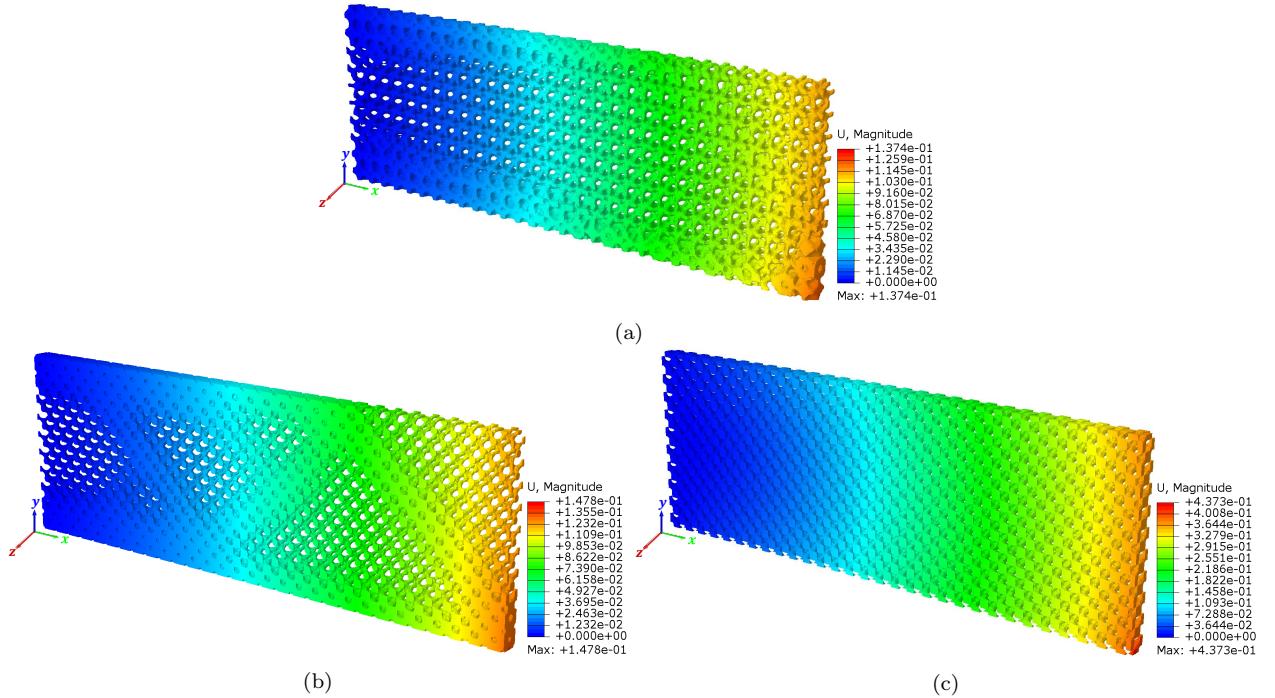


Figure 14: FE simulated displacement contours of the beam redesigned by different methods: (a) IH-GAN-based multi-type cellular structure, (b) variable-density single-type cellular structure, and (c) uniform single-type cellular structure.

we can accurately generate the cellular unit cells that possess the desired material properties (relative error < 5%).

We also demonstrate the IH-GAN model’s efficacy by combining it with a modified TO algorithm to construct functionally graded cellular structures (*e.g.*, a cantilever beam in this paper) using multiple types of cellular unit cells. Our approach addresses the connectivity issue between different types of unit cells simultaneously without a need for further compatibility optimization. The optimized example shown in this paper can save 52.1% of total weight compared to the solid counterpart. By implementing FE simulations, we also validate that the beam constructed by IH-GAN improves the functional performance (*e.g.*, 84.4% reduction in concentrated stress) compared to the conventional topology-optimized variable-density beam structure.

Limitations and future work: As a data-driven model, the IH-GAN cannot faithfully generate unit cell shapes given material properties outside the training data distribution. This brings the need for constraining the solution space when performing topology optimization, which in turn may limit the performance of the optimized cellular structure. Future work could explore how to combine both data-driven and physics models to allow faithful data extrapolation beyond the training dataset.

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