A Survey of Modeling and Optimization Methods for Multi-Scale Heterogeneous Lattice Structures

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Abstract：

This paper aims to provide a comprehensive review of the state-of–the-art modeling and optimization methods for multi-scale heterogeneous lattice structures (MSHLS) to further facilitate the more design freedom. In this survey, a design process including optimization and modeling for MSHLS is proposed. Material composition and multi-scale geometric modeling methods for representation of material and geometry information are separately discussed. Moreover, the optimization methods including multi-scale and multi-material optimization design methods, as well as the simulation methods suitable for MSHLS are respectively reviewed. Finally, the relationship, advantages and disadvantages of MSHLS modeling and optimization methods are summarized with discussion and comparison, which provides a guidance to further take advantage of MSHLS to improve the performance and multifunctional purpose of production for software developers and researchers concerning the design approaches and strategies currently available.

Keywords: modeling, optimization, multi-scale, heterogeneous lattice structures

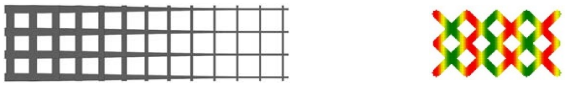
1 Introduction

Recently, Additive Manufacturing (AM) technologies, which fabricate parts by joining materials usually layer by layer, have attracted great interests from both industry and academia. Compared to other manufacturing methods, such as machining or casting, AM processes have the following unique capabilities. Firstly, parts with extremely complex shape can be built by AM process without increasing fabrication cost. Secondly, AM technologies are suitable for processing multiple materials either simultaneously or sequentially; therefore, parts with complex material compositions can be fabricated by this manufacturing method. Thirdly, manufacturing preparation time can be substantially reduced, since the part is directly fabricated from its 3D model. These unique capabilities of AM technologies have brought great application potentials in several major industries such as aerospace [1] and medical implants manufacturers [2]. For example, in the aerospace industry, lightweight, strong and sometimes electrically conductive parts are more desired. AM process can produce lightweight components by replacing solid material with lattice structures. Gradient electrical conductivity can also be achieved by changing the composition of materials at each

fabrication point or each fabrication layer. Major airplane manufacturers such as Boeing, Airbus, and Northrop Grumman have all identified AM technologies to be the emerging and revolutionary manufacturing method [3].

To take advantages of the design freedom enabled by AM processes, several Design for Additive Manufacturing (DfAM) methods have been developed [4]. These methods aim to optimize the performance and/or other key product life-cycle considerations such as manufacturability, reliability, and cost with respect to the capabilities of AM. A recent published literature review [5] shows most existing DfAM methods such as topology optimization method or inverse homogenization. However, it only focusses on a single component design with a single type of material. This review also indicates that in order to further improve the performance of AM fabricated parts, structures with multiscale heterogeneous material distributions are the good choice.

As shown in Fig. 1, the heterogeneity referred in this paper has two aspects: heterogeneous structure (lattice cell and strut size and dimension vary) but with single material composition, and heterogeneous materials (multi material constituent in the lattice structure).



(a) (b)

Fig. 1 Heterogeneous lattice structure: a) Heterogeneous lattice with gradient strut dimensions, b) Heterogeneous lattice with variational material compositions.

A heterogeneous material is composed of different constituent materials and exhibits continuously varying composition and/ or microstructure. In this paper, we refer to lattice structures which are made of heterogeneous structures or heterogeneous materials as heterogeneous lattice structure. The heterogeneous information of such lattice structure can be described and categorized into composition and microstructure [6]. The composition of the graded composite material can be described by the volume fractions of individual constituents that compose the material [7]. Heterogeneity are employed in design, often when both aspects of the resulting lattice structure would be across scale.

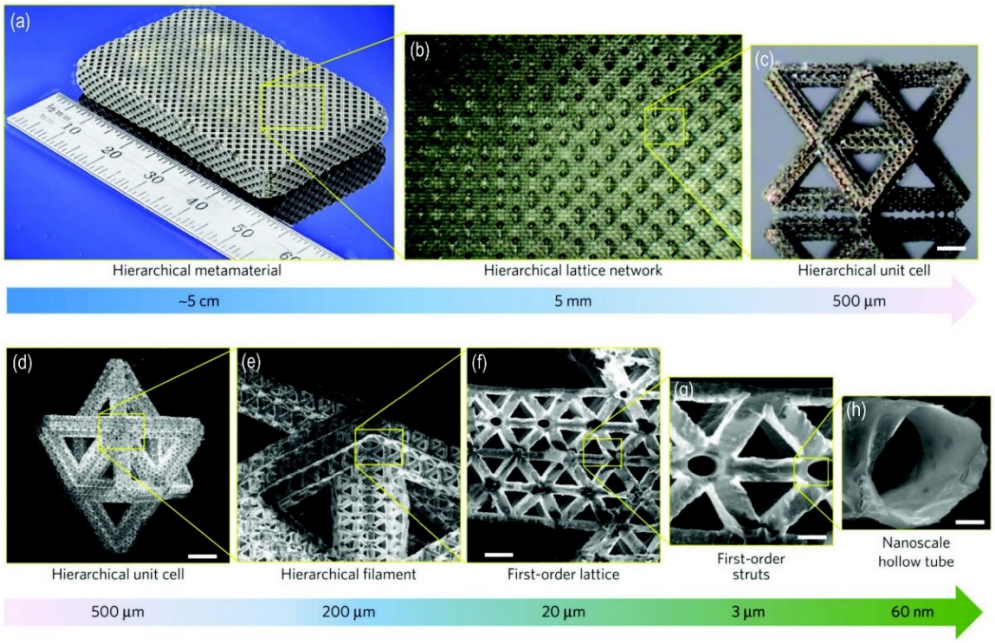


Fig. 2 Multiscale structures with hierarchical lattice architectures. Permission to reprint from Springer Nature copyright 2016 [8].

The length-scale breakdown of multiscale structures with hierarchical architectures is shown in Fig. 2. On the macroscale (~5 cm) (Fig. 2c), the bulk metallic structures is comprised of a network of hierarchical stretch-dominated octet unit cells which are designed to carry load via axial stress (Fig. 2d). Each stretch-dominated unit cell (Fig. 2e, f) from the hierarchical lattice network contains ~200 µm hierarchical strut members (Fig. 2g) that are comprised of a network of stretch-dominated unit cells (Fig. 2h). These first-order unit cells (Fig. 2i) are comprised of microscale thin-walled hollow tube nickel-phosphorus struts with the thickness ranging from 50 to 700 nm at the lowest hierarchy (Fig. 2j).

Therefore, the multiscale lattice structure usually has the following features: the overall structure can be further divided into multiple design scales. The structures defined in the upper scale is made of the material whose microstructure is defined at the lower scale.

Comparing to those structures made of homogeneous materials or even Functional Graded Materials (FGM) [9], multi-scale heterogeneous lattice structures (MSHLS) provides more design freedom for designers to further control the distribution of effective properties of materials on macroscale by controlling both material compositions and their microstructures. Thus, the performance of this type of structures can be further improved comparing to those structures made of conventional materials.

The results of some recent primary research [10, 11] have already proven that the multiscale heterogeneous structures can exhibit better performance. This type of structures is extremely useful especially for multifunctional purposes [12].

Even though, the merits of MSHLS have already been unveiled, it is still difficult for designers to take full advantages of these type of structures in their product design. There are two major barriers-modelling and optimization. Among these two major barriers, modelling is the most important, as it is the key to link the fabrication, simulation and optimization. However, most existing commercial CAD software cannot be used to model the lattice structure with heterogeneous material or structural variance. It is mainly due to the underlying geometric modeling methods used by the software which cannot efficiently handle and manipulate the heterogeneous material or property information. To deal with this issue, several heterogeneous object modelling methods [13] have been developed. However, most of these methods only focus on a single scale, where only the distribution of material compositions is considered. These methods cannot be used to describe the microstructure distribution of materials on multiple design scales. Moreover, the size of geometric model represented by these methods are usually large.

On one hand, MSHLS provides a great design freedom for designers. On the other hand, it also brings challenges for optimizations. There are two main challenges to optimize MSHLS. Firstly, there are a large number of design parameters that needs to be considered. These parameters are from different design scales. If designers want to solve the defined optimization directly, it usually requests high computational resource. Secondly, the design parameters from different design scales may be coupled together, which make the optimization problem even harder to be solved.

The two major issues summarized above must be solved in order to allow designers to take further advantage of MSHLS. The aim of this review is to reflect on the MSHLS design process detailing the various phases. Actually, the current literature on the design of MSHLS are mainly focused on discussing a specific phase of the process lacking a comprehensive view. To create such a view, this work has been conceived to build a link among the main research findings available in the literature and related to the optimization design and modeling of MSHLS.

In general, this review can be beneficial for various experts working in the AM field and provides a comprehensive review of the state-of-the-art approaches to further

take advantage of MSHLS to improve the performance of designed product. For example, designers could retrieve indications for better organizing their decisional process when looking for the most suitable MSHLS considering functional and manufacturing constraints. Software developers could get insights for the development or adjustment of design tools to represent the information of designed and optimized structures for industry and engineering applications. Researchers could get a comprehensive view on the topic together with indications for developing more integrated and evolutionary design methods.

After the introduction above, this paper is organized as follows: firstly, material composition modeling methods and multi-scale geometric for representation of material and geometry information are separately discussed in Sec.2. Moreover, optimization methods including multi-scale optimization and multi-material optimization design methods suitable for MSHLS are respectively reviewed in Sec.3. In addition, a design process of MSHLS is discussed in Sec.4. Finally, this paper is wrapped up with a conclusion and some prospects for the future research in Sec.5.

2 Modeling methods of multi-scale heterogeneous lattice structure

Generally speaking, if a heterogeneous object is composed of n_2 different materials and attached with n_3 different physical properties, the modelling space of heterogeneous object can be denoted as the tensor product of n_1 dimensional geometry space E^{n_1}, n_2 dimensional material space M^{n_2} and n_3 dimensional property space IE^{n_3} [14]. Within such a modeling space, every point in the base space is attached with a vector for the description of its material compositions and property, which can be symbolically described as:

$$\begin{aligned} &P=\left(P_g,\ P_m,\ P_p\right),\\ &P_g \in \Omega_g \subset E^{n_1},\\ &P_m \in \Omega_m \subset M^{n_2},\\ &P_p \in \Omega_p \subset IE^{n_3} \end{aligned} \tag{1}$$

where P_g is the location of a point P in the geometric domain Ω_g, P_m is the material composition defined at P_g, Ω_m is the material domain (subspace of M^{n_2}),

and P_p is the material property defined at P_g, and Ω_p is the property domain (subspace of IE^{n_3}).

Without considering the differences in the definition scales of heterogeneous objects, heterogeneous objects regarded as components are analyzed, recognized and defined uniformly from three levels: integration, element and information (Fig. 3 Multi-material-property configuration [15].). Among which, the element level is subdivided into two levels, namely, the component element and material unit and the information level consists of geometric, material and property information [15]. In general, heterogeneous object modeling embraces two fundamental processes: material composition modeling and geometric modeling [16]. Geometric modeling is concerned with the geometric representations of the objects and material modeling is targeted at modeling material composition distributions defined over the geometric domain. Therefore, material composition and multi-scale geometric modeling methods for representation of material and geometry information are separately discussed in Subsections 2.1 and 2.2.

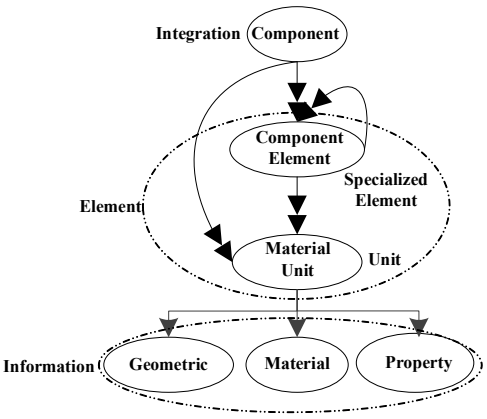


Fig. 3 Multi-material-property configuration [15].

2.1 Material composition modeling

Many scholars have carried out an in-depth research on the techniques of material composition modeling. It mainly includes decomposition-based models, set-based models, explicit function-based models, control feature-based models, control point-based models. A brief review of the methods is provided here to clarify the difference and limitations of present works:

2.1.1 Decomposition-based models

Based on the idea of space segmentation, the space body is divided into grid elements in the decomposition-based models, such as voxel element [17-19] and

volume mesh element [20, 21], and the material composition is defined within each element. The material information of the voxel element is stored in the voxel center point, which is suitable for the irregular distribution of the material. As shown in Fig. 4, 2D [22] and 3D [23] heterogeneous lattice structures with multi-material composition are represented by voxel-based model. It not only supports the efficient query of the material composition, but also facilitates the realization of visualization. However, the pitfall of the voxel model is that the accuracy of the method is directly related to the voxel's resolution. Moreover, voxel methods are inexact in terms of the geometric and material accuracies.

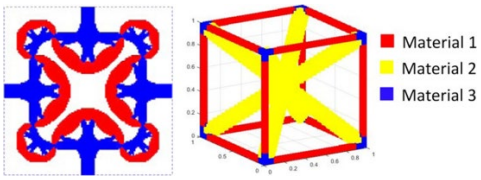


Fig. 4 2D and 3D heterogeneous lattice structures. Permission to reprint from Elsevier copyright 2014 and ASME copyright 2019 [22, 23].

On the contrary, the material information of the volume mesh-based model is stored in the grid node, and the material information of the non-grid node is saved by interpolation function. Therefore, the representation is a more compact data structure, which solves the huge storage problem in voxel unit to a certain extent. Representation of material composition using these decomposition-based depends on the resolution of the mesh or voxels that may not conform to the material distribution, leading to discretization error. In addition, any change in material function would lead to re-discretization of the whole geometry to re approximate the new material distribution.

2.1.2 Set-based models

According to the geometric representation, set-based models are divided into two types. The first one is r_m-set, which is an extension of solid modeling to handle heterogeneous objects by using r-sets (a form of B-rep modeling) with information about material variation. This geometry model is further decomposed into atlases over which material variations are mapped. In order to define FGM models, a set of Boolean operators [24] for modifying the geometry and composition stored in the data structure, therefore, the heterogeneous objects with more complex geometry and material distribution are obtained. Another set-based model is based on implicit function such as level-set [25], R function [26] and convolution surfaces [27] to generate exact

geometric data representations. These models use the functional representation (F-Rep) as the basic model for both the point set geometry and the material distribution. Essentially, the implicit function is used to model spatial partitions and the function determines whether a given point is “inside” or “outside” a subset. When a point is within the subset, the corresponding material distribution is then assigned to that point/point set. Tsukanov and Shapiro [28] proposed the construction of field modeling using sampling distance field and interpolated physics field by way of extended R-functions, however, the limitations of R-functions results in the difficulties in complex shaped heterogeneous object modeling. A level set based scheme was proposed by Wang et al. [29], which adapted a variational model as the objective function to locate any point in the material region of a well-defined gradient or on the boundary edges and surfaces of discontinuities. The set of discontinuities was represented implicitly, using a multi-phase level set model. The compact and exact in data representation capacity makes level set model suitable for multi-material structural representation. In addition, parameterized level set method can be used for CSG (Constructive Solid Geometry) type feature-based CAD modeling. The rectangular frame and the interior hole are the two zero-value level set contours, i.e. the material source profiles. All results demonstrated in Fig. 5 have realized the smooth material transitions between the source profiles [30].

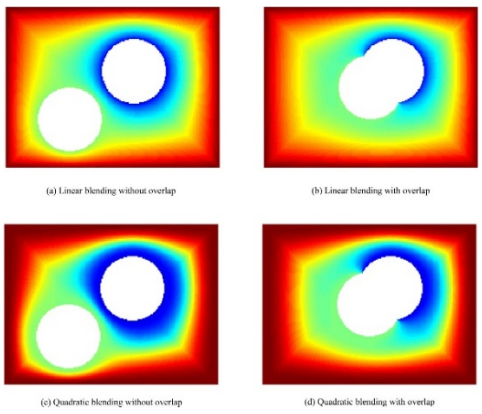


Fig. 5 Material blending with three material source profiles. Permission to reprint from Elsevier copyright 2019 [30].

2.1.3 Control feature-based models

Control feature-based model developed by Siu and Tan [31] employs source profile features as references to determine the functionally graded material (FGM)

distribution with the source profile-based material composition functions [32]. The common material composition variation features (Fig. 6) in MSHLS are: (a) and (b) represent material composition variation in axial and radial direction of struts, (c) represents a circle or spherical strut joint, and (d) represents hollow feature.

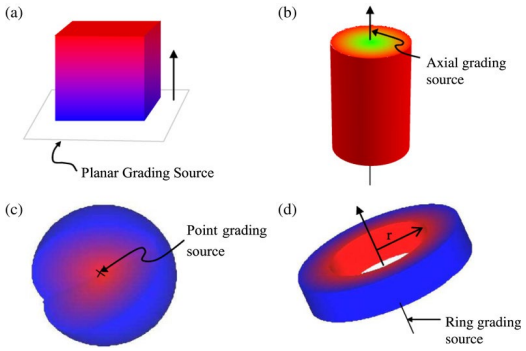


Fig. 6 Common material composition variation features in MSHLS. Permission to reprint from Elsevier copyright 2019 [31].

As shown in Fig. 7, distance-based material distribution function, e.g., Piecewise, Polynomial, Power, Gaussian, Cauchy, etc, can realize different material gradients. The material distribution is invariant under some transformations, such as rotation or translation. Due to the effective evaluation of point-to-feature distances, the representation supports efficient query of material composition. Moreover, the user can select the reference features and material distribution function through the predefined function library and can intuitively and flexibly complete the interaction modeling of multi-material objects.

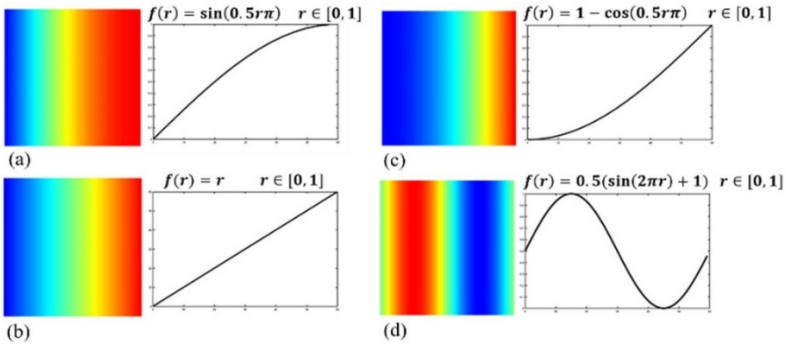


Fig. 7 Effect of different material functions on material-distribution. Permission to reprint from IEEE copyright 2018 [33].

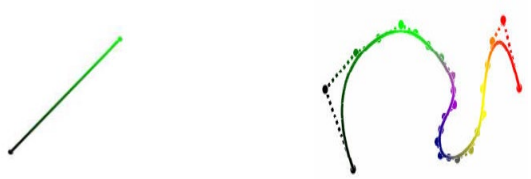
2.1.4 Control point-based models

The material information is stored in the control points of Bezier, B spline, NURBS, parameter curve, surface and volume, and the representation method of parameter control points is obtained [14, 34-36]. Control point-based models have some

appealing properties. They are compact in both geometry and material representations. Given the parametric coordinate (u,v,w), the material composition of a point can be also efficiently interrogated. In addition, this representation method can effectively represent complex (2D or 3D dependent) material distributions. Local modifications on both geometries and material definitions are also straightforward. The drawback of this method is that it relies heavily on spatial parameterizations and for arbitrary 3D objects such parameterizations remain a rather non-trivial task. Kou et al. [37] proposed a more general definition for 1D heterogeneous features (Fig. 8) described in Eq. (2).

$$P = \sum_{i=0}^{n-1} W_i P_i \qquad (2)$$

where P is an arbitrary point on the 1D feature, P_i is constructive point (e.g., starting point, ending point of the line and the control points of the B-Spline curve), W_i is the blending weight of the *i*th constructive point in material gradation. For different types of 1D features, the weight generation methods might be different. Similarly, these approaches could be extended to 2D and 3D features.



(a) (b)

Fig. 8 1D heterogeneous features: a) a heterogeneous line, b) a heterogeneous B-spline. Permission to reprint from Elsevier copyright 2005 [37].

To more clearly compare the methods that investigate the representation abilities of material heterogeneity, both the advantages and disadvantages of existing models for heterogeneous materials are summarized in Table 1. It serves as a reference tool for selecting appropriate models in the downstream applications.

However, the above research approaches only focus on continuous distribution of material composition modeled parametrically by volume fraction, which is applied to solid part model on macro scale instead of material microstructure on lower scale. It is inaccurate because microstructures with the same material volume fraction may have different topological geometry and properties. The appropriate representation is that material microstructure forms the basis for material volume fraction. For instance, nanotechnology enables engineers to create or modify details of atoms at nanoscales so as to realize more desirable material properties. As this technology becomes more

pervasive, it is foreseen that some materials modeling modules will be embedded in future CAD systems so that the geometry and materials of a product can be designed concurrently [38]. Rosen et al. [39-41] firstly proposed a new multi-scale geometric and materials modeling methods that uses a surfacelet-based implicit representation to efficiently capture internal and boundary information of materials. It serves as the foundation for modeling structure-property relationships for materials design. Therefore, multi-scale geometric modeling methods are reviewed in the following section.

Table 1 Comparison of existing models for heterogeneous materials

Methods	Including	Advantages	Disadvantages
Decomposition-based models	Voxel-based model volume mesh-based model	Voxel model is suitable for visualization Volume mesh model is easy for FEA	Inexact and computationally expensive Non-trivialness to manually manipulate the material distribution
Set-based models	R_m-set F-Rep model	R_m-set model is easy to integrate constructive operation F-Rep model facilitates topology optimization	Incompatible with other modeling formats and cannot store topology information
Control feature-based models	Single and multiple feature-based model	More favorable in capturing the designers' intents Suitable for FGM representation	Heavily based on the features with predefined material distributions
Control point-based models	B-spline and radial basis function	Compact in both geometry and material representations	Heavily based on spatial parameterizations

2.2 Multi-scale geometric modeling

2.2.1 Multi-scale problem

Before approaching the topic of multi-scale geometric modeling, it is important to cover issues emerging from multi-scale mathematical models describing reality. These issues come from the fact that on different scales different laws of physics act and different mathematical models are used to describe what happens on these scales and how different entities react to each other on these scales. The main challenge of multi-

scale modeling is the lack of a unified theory that could correctly describe geometry both down from its structure ($\sim 10^{-9}$ m) up to boundary conditions and processes present in it ($\sim 10^{0}$ m) [42]. A common example of a multi-scale problem comes from theoretical physics and lies in finding a theory of everything – a hypothetical ultimate framework that would allow describe physical relations on every possible scale. Nowadays, in physics there are two major models describing our world: quantum field theory (comes from merging quantum mechanics with special relativity) and general relativity (comes from merging Newtonian mechanics with special relativity); there is nothing similar between these models as the first one works well for nano- and lower scales while the second one works for macro- and higher scales [43].

The ability of modeling in meso- and macro-scale is crucial in many research fields involving computer graphics and geometric modeling. For example, Prada et al. [44] apply multi-scale modeling concepts for 3D mesh generation process for multiscale bone analysis. Engquist et al. [45] identified the need for an appropriate multi-scale geometric modeling tool for porous materials. Predictive nonlinear theories are being applied for multiscale modeling of heterogeneous materials [46].

Multi-scale geometric modeling methods are also critical in medical research. For example, Youssef [47] introduced a bio-inspired framework for the simulation of 3D multicellular tissue growth. However, there is no geometric modeling tool to implement this framework due to high geometric complexity. The need for such a geometric modeling approach for modeling a human heart both as a whole and in details (as even small defects are crucial) is identified [48]. Another common application for multi-scale geometric modeling is visualization of online geographic maps: when a user zooms in to a map, e.g. *Google Maps*, more and more details appear to the extent that even 3D shapes of buildings render [49].

2.2.2 Geometric modeling of heterogeneous lattice structures

Geometric modeling in engineering is mainly used for visualizing engineering systems such as parts, assemblies, etc., and represented by computer-aided design (CAD) software. While conventional CAD software is normally sufficient for engineering design in industry, there is no geometric modeling tool that would be able to appropriately represent complex heterogeneous lattice structures due to inability of existing geometric modeling tools to represent a model in multi-scale, which forms a research gap that is yet to be filled. Another issue is the computational cost of such

geometric modeling tools because heterogeneous lattice structures have high geometrical complexity resulting in high computational needs using conventional methods [50].

Multi-scale modeling becomes a crucial add-on to conventional geometric modeling tools when dealing with lattice structures. It is required to consider not only the whole structure in its macro-scale, but also each joint and strut of the lattice as they form at meso-scale [51].

2.2.3 Level of detail

In computer graphics, a far-away object in a virtual environment appears obscured (similar to the effect people with myopia experience), which means that there is no need for representing all details of the object on a screen [52]. However, the details appear to be more concrete when approaching the object or zooming into it. Such effect of manipulating the *level of detail* (LOD) can be achieved, for example, by reducing the polygon count for distant objects by vertex and edge removal [53]. However, decreasing LOD of a lattice structure down to a certain level can result in complete homogenization of lattice, i.e. removing from view all geometrical features corresponding to lattice structures [54].

Normally, LOD is manually or automatically associated with CAD-features of solid bodies as illustrated in Fig. 9, e.g. extrusions, revolutions, etc. [55]. However, lattice structures are designed not with CAD-features but with nodes connected by struts which are not so well-defined from the CAD-perspective [56]. Moreover, in heterogeneous lattice even periodicity of the lattice is not obvious.

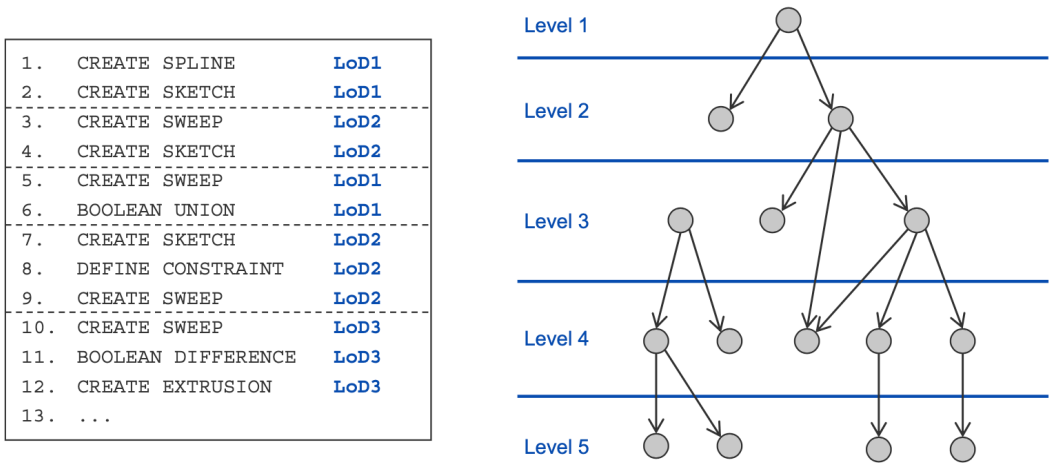


Fig. 9 An example of LODs associated with CAD features. Permission to reprint from John Wiley

and Sons copyright 2014 [55].

As mentioned, simplifying a lattice structure by reducing the LOD of its model eventually results in complete homogenization of the structure. Such model does not provide the user with sufficient information about structure and topology.

Another way to simplify a lattice structure is to represent it as a beam-element model. This approach, however, avoids representing detailed geometrical information that can be important for an appropriate analysis of a lattice structure, especially in node regions as beam models simply do not take high material concertation at nodes into the account [5].

Setting up a limit for the maximum distance for an object to be shown on screen is a common practice in computer graphics. This limit is called a *draw distance* [57]. It is mainly used for optimizing the overall performance of a 3D model [58].

The described model complexity reduction methods have proven their effectiveness in the video game industry when developing game engines, such as *AnvilNext* developed by *Ubisoft Montreal*, in particular for rendering 2D or 3D graphics and providing a physics engine [59]. Some other geometric modelling approaches also can be adapted from *game engines* that are being used for videogames design.

Considering applying the LOD concept and multi-scale modeling to lattice structures, Liu and Shapiro [60] propose a framework for multi-scale modeling of parts with lattice structures. The framework's first scale describes the shape-material model; the second scale describes identity mapping for the solid regions of the part, as well as it includes downscaling and neighborhood functions for lattice structures; the third scale includes downscaling and neighborhood functions for lattice structures in case beams of the lattice structures are made of the fine scale structures. Such division into scales and phases essentially corresponds to the LOD concept, as the complexity of the solid model iteratively rises with downscaling.

2.2.4 Voxel modeling

One more topic worth considering when discussing multi-scale geometric modelling is application of multi-scale voxel modeling. The word 'voxel' derives from combining words 'volumetric' and 'pixel' and it is defined as 'a unit of volume containing the value of the corresponding raster element in a 3D space' [61]. Voxelized objects allow the same set of operations with polygonal objects [62]. Voxel-based object simplification has been used for eliminating high-frequency details of the object

ever since the introduction of voxels [63]. Similar voxel-based approaches are used for simplification and repair of polygonal models [64]. Voxels have an advantage in terms of downsampling and acquisition of real-world data, i.e. any geometrical complexity is feasible which, however, comes at a cost due to rise of computational resources required for rendering [65]. Note that as lattice structures cannot be produced without AM techniques, there is no need in voxel size higher than 3D-printer resolution [66]. Voxel models do not handle zooming efficiently [65].

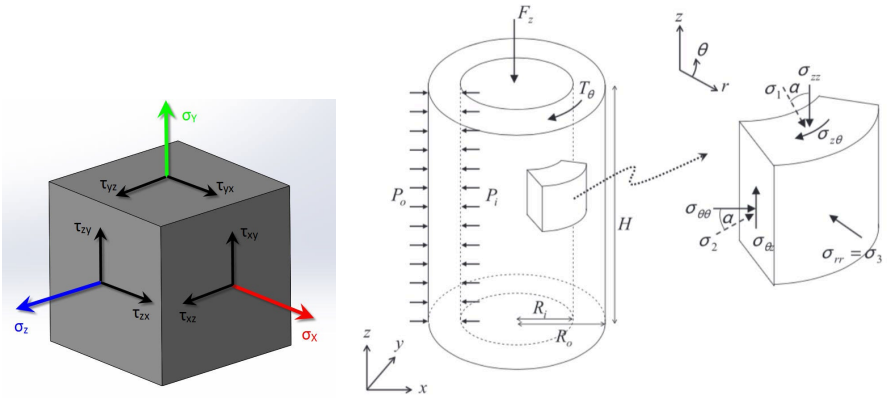
One of the most popular voxel-based simplification methods involves using sparse voxel octrees which are based on generating multi-scale voxels which could be visible or invisible depending on the resolution and size of the screen. Moreover, recent researches show that octree-based neural networks can be applied for 3D shape analysis and learning and thus can be adapted for feature recognition. For example, Wang et al. introduced an octree-based convolutional neural networks (CNN) for 3D shape analysis [67]. Liu et al. [68] proposed an octree-based variational shape learning model for the same purpose. Wu et al. [69] developed a Bayesian volumetric shape recognition based on voxel octrees.

Recent research on voxel-based surface approximation investigates the possibility of applying the previously discussed LOD concept to voxel models. The results have proven themselves encouraging, as a 12 GB voxel model can be approximated to a 2 GB while still accurately visualizing the details [70]. However, in this method, the depth of rendering (which is required for fully adaptive multi-scale voxel modeling [71]) is assumed to be given and the voxelization algorithm is not adaptive, which does not allow performing multi-scale modeling. Moreover, current approaches are unable to represent crucial features of a part on a larger scale with voxels [72] and become significantly slow on a smaller scale [73].

Lattice structure is essentially a structure of some size that is defined by a topology of a significantly smaller size. Thus, voxelization of lattices introduces visible discreteness of its model as illustrated in Fig. 10, which affects user experience.

Fig. 10 Lattice structure voxelization, adapted from [74].

Voxels normally have cubic shape which is explained by render simplicity: one cubic voxel can be defined only by its position in 3D space (assuming that every voxel has the same size). Cubic shape also fits well for simulations, e.g. a cube is a common unit element for stress analysis within structures as noted in Fig. 11a since it easily allows modeling of normal stresses σ_x, σ_y and σ_z, as well as shear stresses τ_{xy}, τ_{xz}, τ_{yz}, τ_{yx}, τ_{yz} and τ_{zy}. However, representing cylindrical shapes illustrated in Fig. 11b as a combination of cubes introduces an obvious distortion which gets lower as the number of cubes approaches infinity, which is not feasible from the computational point of view. Similarly, not cubic but cylindrical sector unit elements are used for simulations of cylindrical shapes, which allows modeling of normal stresses σ_{rr}, $\sigma_{\theta\theta}$ and σ_{zz}, as well as shear stresses $\sigma_{\theta z}$ and $\sigma_{z\theta}$ [75].



(a) (b)

Fig. 11 A standard cubic unit element: a) and a cylindrical shape with its cylindrical sector unit element, b) used for stress analysis. Permission to reprint from Elsevier copyright 2013 [75].

Strand [76] conveyed research in the area of using non-cubic voxels and tested various voxel shapes such as body-centered cubic (BCC) and face-centered cubic (FCC)

Note that BCC is similar to a truncated octahedron and FCC is similar to a rhombic dodecahedron. Non-cubic grids appear more sparse than cubic grids which provide the most information about the structure. However, there is no evidence of research that had been conveyed on combining different shapes of voxels within one model. Such research would contribute to not only AM of heterogeneous lattice structures but also to 4D printing technique, i.e. AM with smart materials [77].

There is evidence that volumetric meshes can support multi-scale modeling. Volumetric meshes are similar to polygon meshes that are used in the majority of CAD-software with the difference in discretizing the whole solid body and not only its surface, i.e. the whole body is considered to be subdivided with polyhedrons instead of polygons [78]. For instance, volumetric mesh models of macromolecules are able to provide sufficient visual information in chemistry [79]. However, the computation of curvature values of polygon and polyhedron meshes is non-trivial due to their discrete nature. Moreover, a volumetric finite element is always convex since it is bounded by a finite number of planes. Therefore, FEV introduces even more distortion when applied to non-convex geometric shapes such as lattice structures and surfaces with genus 1 and higher [80]. This implies the need in a proper meshing algorithm that takes convexity and curvature into the account and affects quality of meshed models, especially ones requiring multi-scale modeling. Note that non-convex volume selection is a topic of interest in geometric modeling [81, 82].

Table 2 compares polygon mesh methods with voxel-based method when applied to MSHLS. Note that the table does not include F-Rep method as it is incompatible with other modeling formats and cannot store topology information [83]. The hybrid modeling approach introduced by Tang et al. [84] has certain features (e.g. using boundary representation for lattice struts) that can assuage the disadvantages of both geometric modeling methods described in Table 2.

Note that as the size of a lattice structure approaches nano-scale, new properties arise, some of which are of quantum nature [85]. As there is no tool that can efficiently produce a lattice structure with tolerance down to its nanoscale, this work does not support geometric modeling of lattice structures at nanoscale.

Table 2 Comparison between polygon mesh modeling and voxel-based modeling approaches for MSHLS

Methods	Advantages	Disadvantages
Polygon mesh modeling	Computational efficiency	Not suitable for complex geometrical shapes
	LOD concept is applicable	
Voxel-based modeling	Handles high complexity	Not computationally efficient
	No need for resolution higher than required for printing	Introduce distortion when modeling on low resolution
	Efficient Boolean operations	Applying the LOD concept is not straightforward and does not achieve as good results as for polygon mesh modeling
	Feature recognition is well applicable	

3 Optimization methods of heterogeneous lattice structures

Lattice structures are often produced to solve engineering optimization problems and AM itself prompts research in computational optimization [84]. In heterogeneous lattice structures, optimization of structural topology and thickness of lattice struts results in satisfaction of given functional requirements [86]. Heterogeneity of a structure provides unique properties which are required to be optimal and which cannot be provided by homogeneous structures, e.g. gradual elasticity of the structure or structural stiffness [87]. Research on optimizing the internal structure to provide an optimal strength-to-weight ratio is identified as crucial, for example, in the aerospace sector [88]. Topology optimization methods are often being applied for lattice structures [89]. For example, Zhu et al. [11] proposed a two-scale topology optimization framework of microstructures. One of the ways to optimize a lattice structure is by adding porosity to the internal structure. Moreover, the approaches that are being used for the porosity generation (such as the ones that are based on Voronoi tessellation [90]) produce a tessellation that is visually similar to the tessellation of cells in a living organism. Based on this, it is crucial to analyze multi-scale and multi-material optimization methods of heterogeneous lattice structures covered in Subsection 3.2 and

3.3, respectively, as well as the ability to perform computational simulation on them as covered in Subsection 3.1.

3.1 Simulation methods of multi-scale heterogeneous lattice structures

This section of the design workflow is the evaluation of the MSHLS performance through simulation methods to support optimization design.

The simplest way is to directly apply the rules of mixtures, where the property of heterogeneous composite can be considered as a linear or non-linear combination of its base materials [91, 92]. Comparing to other ways to evaluate the effective properties of the heterogeneous objects, the rule of mixtures is the simplest and most straightforward method. The effective properties $\overline{X}$ of a point with material composition values $m(\rho_1, \rho_2, ..., \rho_n)$ corresponding to the properties $(X_1, X_2, ..., X_n)$ could be calculated by Eq. (3).

$$\overline{X} = X_0\rho = X_1\rho_1 + X_2\rho_2 + ... + X_n\rho_n \quad (3)$$

However, rules of mixtures are not accurate and flexible enough for MSHLS. Some numerical analysis methods suitable for MSHLS including physics-based method, homogenization method, finite element analysis (FEA) method, and isogeometric analysis (IGA) are reviewed as follows.

3.1.1 Physics-based method

There are many established methods and implementations for simulating deformable soft bodies. Considering the large deformations and relatively low stiffness of the materials involved, the physics-based dynamics are often significant. When our proposed MSHLS consist of multiple materials, it's important to consider deformation simulation for further application such as feature films, video games, and virtual surgery, among others. Much of the development in simulating soft bodies has been driven by the computer graphics community. In this method each voxel is modeled as a lattice point with mass and rotational inertia. Voxels are connected (from their centers) by three-dimensional beam elements with appropriate translational and rotational stiffness leading to realistic deformation under applied forces and moments. These beams form a 3D lattice frame, which acts as a backbone (or a control structure) of the whole shape. The frame is what holds the multi-material objects together and that governs the

deformation of the whole geometry. Based on this method Sossou G et al. [77, 93] developed a computational design tool, which has been implemented in the Rhinoceros® add-on Grasshopper®(GH).

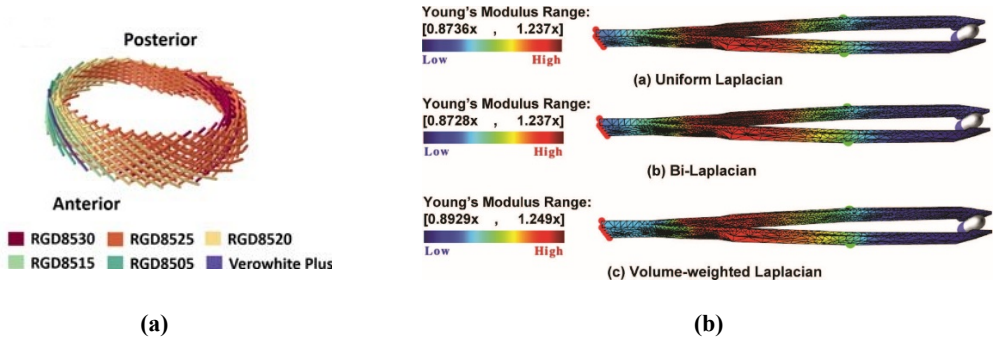
3.1.2 Homogenization method

The homogenization usually refers to a way to replace the composite with a kind of equivalent material model, which can overcome the difficulty in the analysis of the boundary value problem with high heterogeneities. It is used to obtain the effective properties of homogenized material for periodic heterogeneous continuous media in many physical and engineering applications [50]. Homogenization methods can also be applied to calculate the effective properties of the heterogeneous objects at any points [94, 95]. It can be applied to the cells with any arbitrary material compositions and can also be applied for the calculation of several different types of material effective properties including stiffness, heat transfer coefficients and Poisson's ratio. This method is applied for material effective properties simulation of lattice cell with geometric heterogeneity [96] but also material composition heterogeneity [22, 23]. Based on the calculated effective properties of the lattice unit, the overall performance of designed objects can be easily evaluated. A typical procedure of simulation of solid-lattice hybrid structure with homogenization method has been introduced by Dong [97]. However, this method has its own limitations. It cannot be applied to the structure based on heterogeneous density gradients, and it is not easy to manage in case of complex geometries.

3.1.3 FEA-based method

FEA-based simulation method is usually used in interactive inverse design method to create continuous heterogeneous material distributions on 1D beam [98], truss element with truss-like lattice structure [99] or 3D volumetric meshes with arbitrary geometry [100-102]. The material distributions are designed to conform to prescribed displacements and internal elastic forces at the selected vertices of the 1D element or 3D mesh [103]. Such a capability has numerous applications as many mechanical components, structures, and mechanisms have to produce predictable displacements under known forces or pressure distributions. With smooth varying heterogeneous material distributions, multiple properties (functions) can be obtained in the same object,

and high-stress regions at the material boundaries can be avoided. The method is applicable not only to small deformations, linear mesh elements but also to nonlinear materials under large deformations. Each mesh element is assumed to be homogeneous and made of an isotropic material parameterized by Young's modulus and Poisson's ratio. Two applications of FEA-based simulation aided design with 1D truss element and 3D tetrahedral mesh, respectively are shown in Fig. 12. FEA method with 1D element has a moderate computational cost and can be used for MSHLS with heterogeneous density gradients. Its limitations are the following: when the strut is not thin enough, it is difficult to provide accurate results and the ability to predict the stress distribution at struts joints is poor. While, FEA method with 3D mesh is of high computation cost and time consuming.



(a) (b)

Fig. 12 FEA-based simulation aided design: a) multi-material fiber network of artificial disc. Permission to reprint from ASME copyright 2019 [98], b) medical tweezers with spatial material distribution. Permission to reprint from ACM copyright 2015 [100].

3.1.4 IGA-based method

A common approach to the analysis and optimization of metamaterials and lattices is multiscale simulation through homogenization of unit cell behavior. However, due to the functional grading and curved topology, which lead to non-periodicity of the microstructure, as well as the nonlinearity of a soft lattice, common homogenization approaches cannot be applied, and the lattice needs to be simulated at full scale. In addition, nonlinear simulation based on continuum mechanics and 3D finite elements is not feasible due to the huge computational effort involved and linear modelling with 3D truss elements will not capture the nonlinear behavior of a soft lattice [104]. While, IGA uses B-spline function and NURBS basis function, which are commonly used in CAD environment, to accurately describe any complex geometry and approximate

unknown solution fields in the analysis [105]. It provides an accurate and efficient numerical discretization of the model and enables a seamless integration of the simulation method with the design approach through the concept of IGA. The rod formulation and IGA method also allow to accurately represent graded design parameters of the cross-sections, such as a spatially variable material distribution, e.g. in terms of Young's modulus. These properties are highly desirable for many types of applications, such as reusable energy absorbing devices based on nonlinear elastic rather than plastic deformations, vibration mitigation through curved ligaments, tailored energy absorption response through functional grading of material properties or hierarchical microstructures, tissue-like medical implants, soft robotic actuators and devices, 4D printing, or structures with complex constitutive behavior such as negative Poisson's ratio effects. Weeger O et al. [106] proposed a digital design and manufacturing framework for soft lattice structures (Fig. 13). The design approach was implemented in the 3D modeling software Rhinoceros® (also Rhino® or Rhino3D®) using the algorithmic design environment Grasshopper™ and the open-source plugin IntraLattice.

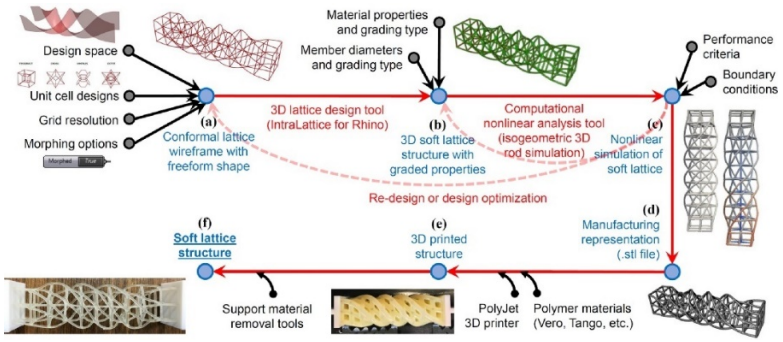


Fig. 13 Overview of the digital design and manufacturing framework for soft lattice structures. Permission to reprint from Elsevier copyright 2019 [106].

Based on the simulation methods introduced above, a comparison between different simulation approaches is made and summarized in Table 3, and it helps designers select a suitable simulation method for MSHLS.

Table 3 Comparison of existing simulation methods for MSHLS

Methods		Advantages	Disadvantages
Physics-based method		Realistic visual effects in real time Able to simulate multiple interspersed materials of varying properties Computationally efficient	Low accuracy
Homogenization method		Computationally efficient Easy to conduct multiscale simulation through repeated unit cell behavior	Satisfying local periodicity hypothesis owing to scale effect
FEA-based method	3D element	Suitable for arbitrary geometry High accuracy and heterogeneity	High computation cost and time consuming
	1D element	Suitable for truss-like structure Low heterogeneity Relatively low computation cost	Unable to simulate multiple interspersed materials at joints Low heterogeneity
IGA-based method		Suitable for curves frame The parameters control points of the model can be directly optimized, and the boundary of the optimization results is smooth and continuous	The stiffness matrix of higher order basis function is dense and does not satisfy the orthogonal condition

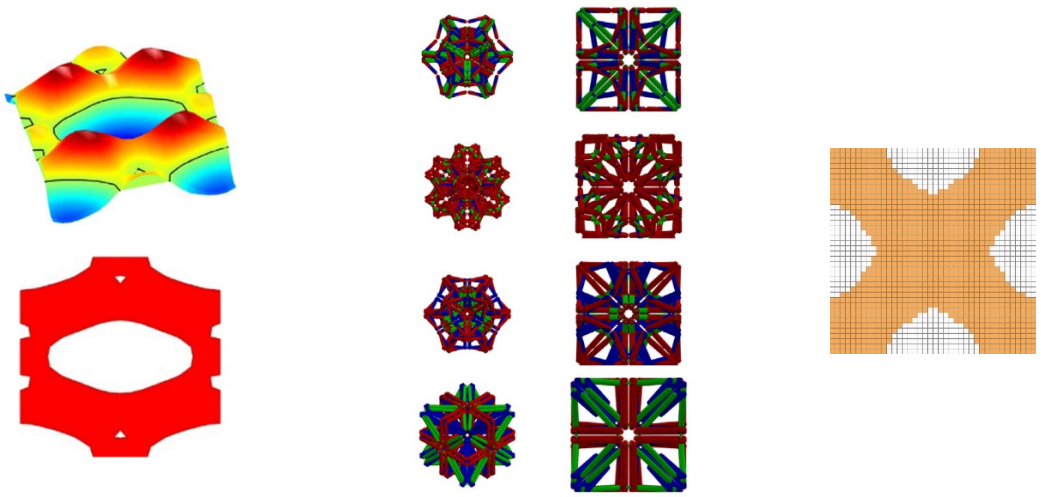
3.2 Multi-scale optimization methods of heterogeneous lattice structures

As to the optimization of the heterogeneous lattice structures, the existing methods can be roughly divided into three groups according to their design scales. It mainly includes the optimization design of microstructure, optimal distribution of material compositions or microstructures in macroscale and the two-scale concurrent optimization.

3.2.1 Optimization design of microstructures

The inverse homogenization technique can be applied to determine the optimal distribution of material in micro-cell at a certain point of the microstructures to achieve their desired properties[107]. In this process, a microstructure periodically arranged in

macro design domain actually behaves like a material, whose length scale is much smaller than that of the macroscopic structure. This method has originally been developed for the structural related properties, such as extreme elastic modulus, Poisson's ratio, and extreme thermal expansion coefficients. Also, it can be easily extended to many other fields for multifunctional purposes. Li et al. [108] produced periodic cellular composite for each layer, by integrating the numerical homogenization into a level set approach (Fig. 14a). Kazemi et al. [109] proposed 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 (Fig. 14b). Schumacher et al. [110] solved the inverse problem to the numerical coarsening method, obtaining a microstructure that coarsens to a given stiffness tensor (Fig. 14c). The difference among the three methodology is that the representations of microstructures are continuous method (Fig. 14a) and discrete method, in which the discrete method uses 1D truss element (Fig. 14b) and voxel element (Fig. 14c), respectively.



(a) (b) (c)

Fig. 14 Material microstructures design: a) level-set-based design. Permission to reprint from Elsevier copyright 2016 [108], b) design of architected truss lattice materials with three base materials. Permission to reprint from Elsevier copyright 2020 [109], and c) voxel-wise material distribution. Permission to reprint from ACM copyright 2015 [110].

3.2.2 Optimal distribution of material compositions or microstructures in macroscale

Optimal distribution of material compositions. Instead of only focusing on microscale, the second group of optimization methods is developed to determine the

optimal distribution of material compositions or microstructures. Due to the limitations of traditional manufacturing technologies, most of the existing optimization methods mainly focus on the optimization of material compositions distributions. During the optimization of material compositions, the material distribution functions are usually preselected. Then, the optimization formulation is generated to find the optimal coefficients which are defined in the preselected functions. For example, in the optimization of Functional Graded Materials (FGM) which is a typical heterogeneous object, power law and exponential functions are widely used [92, 111, 112]. Instead of using functions, SIMP-based topology optimization results with relative density distribution have also been used for the design of the heterogeneous lattice structure. For example, Brackett et al. [113] suggested mapping volume fractions of the lattice unit cells onto the intermediate densities of an un-penalized SIMP solution, making the greyscale density solution of topology optimization possible to manufacture with AM. This work utilized the tessellation of the unit cell for the lattice generation, i.e. where a selected unit cell template was tessellated across the design domain in a regular fashion. To generate lattice with varying cell sizes, Brackett et al. [114] offered an error diffusion-based method which enabled the mapping of irregular unit cell lattice onto a grey scale input. This was achieved by generating dithered points from the greyscale image followed by connecting them, using either Delaunay triangulation or Voronoi tessellation. Tang et al. [115] developed a function-performance-property-design parameter model (F-P-P-D) (Fig. 15) for heterogeneous lattice structures where the result of density-based topology optimization has been mapped to the relative density of lattice structures. Its result shows the optimized heterogeneous lattice structures can significantly achieve both low thermal conductivity and high stiffness without increasing its weight.

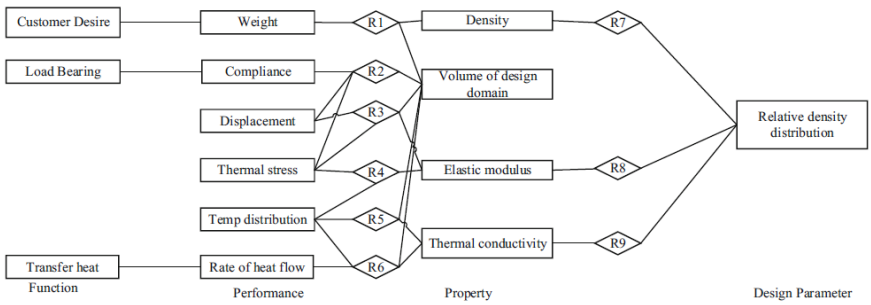


Fig. 15 An example of F-P-P-D model. Permission to reprint from Springer Nature copyright 2018

[115].

Alzahrani et al. [116] proposed method utilizes the relative density information (Fig. 16) obtained from a solid topology optimization to automatically determine the diameter of each individual strut in the structure, which collectively represents the set of design variables. This allows the method to produce lattice structures that can perform reliably under multiple loading conditions and also reduce the computational cost associated with the design of these structures.

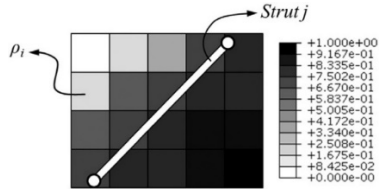


Fig. 16 Relative density mapping to strut diameter. Permission to reprint from Elsevier copyright 2015 [116].

Li et al. [117] presented a novel optimization strategy for designing functionally graded cellular structures with desired mechanical properties. In the strategy a complex functionally graded gyroid lattice structure is generated by implicit surface reconstruction algorithm in 3D space, which maps the corresponding material properties (Fig. 17a) to geometric parameter (Fig. 17b) perfectly.

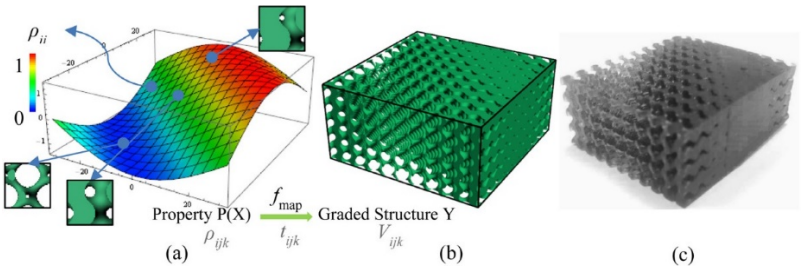


Fig. 17 Example of mechanical properties mapping process and its manufacturability verification by 3D printing: a) material properties diagram, b) 3D mapping result, c) 3D printing result. Permission to reprint from Elsevier copyright 2018 [117].

Panesar et al. [118] presented a number of strategies that enable lattice structures to be derived from topology optimization results suitable for AM. As shown in Fig. 18, the structures with different strategies such as solid (Fig. 18a), intersected lattice of D-P (Fig. 18b), intersected lattice of BCC (Fig. 18c), graded lattice of D-P (Fig. 18d), scaled lattice of D-P (Fig. 18e), and uniform lattice of D-P (Fig. 18f) are used for FEA and made a comparison for several objectives.

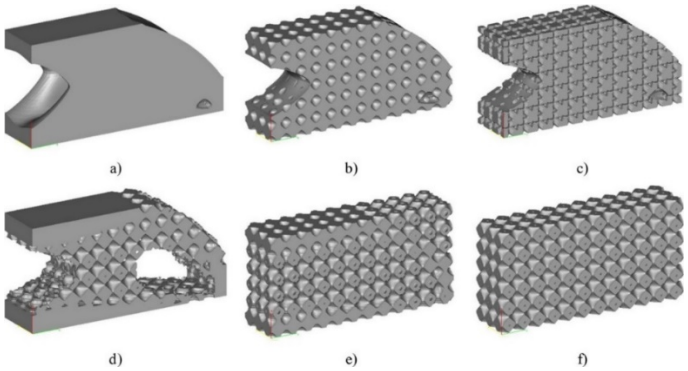


Fig. 18 Structures used for FEA: a) Solid (SIMP solution), b) Intersected Lattice of D-P, c) Intersected Lattice of BCC, d) Graded Lattice of D-P, e) Scaled Lattice of D-P, and f) Uniform Lattice of D-P [118].

Instead of using relative density distribution results, stress distribution results of the structures could also be used for optimization. Teufelhart and Reinhart [119] optimized the strut diameters of an irregular lattice structure by capitalizing on the flux of force within a solid structure. They showed that enhancement in performance can be achieved when compared to a regular (uniformly tessellated) counterpart, mainly due to a much smoother distribution of stresses owing to the stress conformal nature of the lattice. Also Tang et al. [86] proposed a BESO-based design method for truss-like lattice structure optimization. In this method, Functional Volumes (FVs) and Functional Surfaces (FSs) are first determined based on an analysis of the functional requirements. FVs can be further decomposed into several sub-FVs. These sub-FVs can be divided into two types: FV with solid and FV with lattice.

Optimal distribution of microstructures. Besides material compositions, the microstructure distribution is another type of design parameter which are considered during the optimization process. For instance, to achieve the given elasticity gradients, an inverse-homogenization technique-based design optimization is proposed for functional graded cellular structures [120]. In this method, a precomputed data-based of tiled cell structures is built to cover a wide range of elastic properties. Then, a global optimization algorithm is proposed to synthesize the cells from the pre-computed database to achieve desired elasticity distribution with the consideration of connections between neighborhood cells. To simultaneously update the topology of unit cell as well as the morphology of cells in the different region of design domain, Liu et al. proposed a new approach to generate functional graded cellular structures based on moving

morphable components/voids (MMV/MMC) topology optimization [121, 122]. In this method, the topology of the unit cell is represented by a set of explicit functions, while the basis perturbation functions have been applied to control the morphology of cell distribution. This innovative design parameterization method enables designers to control both cell topology and its morphology distribution simultaneously without a large number of design parameters. Similarly, Schumacher et al. [110] proposed a method for fabricating deformable objects with spatially varying elasticity using 3D printing. A database of microarchitectures is assembled prior to large-scale optimization, consisting of different families derived through topology optimization targeting defined material properties. A tiling algorithm then maps the discrete microarchitectures to the large-scale domain in order to fulfil functional objectives. Liu et al. [123] considered the connectivity between lattice cells, and divided the lattice cells of constructed unit-cell library into seven series to ensure that lattice cells of each series could be connected. Panetta et al. [124] explored a wide space of truss-like, symmetric 3D patterns to obtain a small family. This pattern family can be printed without internal support structure on a single-material 3D printer and can be used to fabricate objects with prescribed mechanical behavior. As shown in Fig. 19, the microstructures from same family are mapped to each voxel according to the property distribution of the designed objects.

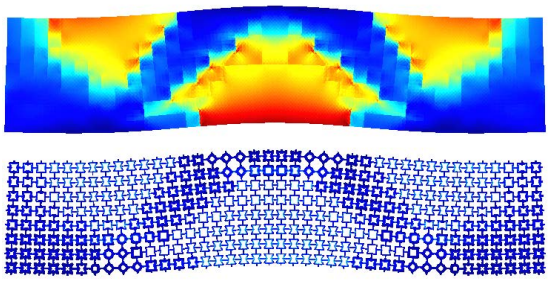


Fig. 19 Deformation of an object with varying material properties per voxel, and the same object with the material in each voxel replaced with the corresponding pattern. Permission to reprint from ACM copyright 2015 [124].

3.2.3 Two-scale concurrent optimization

However, above works are restricted to a single scale (either macro or microscale), while the concurrent optimization at both scales is limited. The concurrent topology optimization refers to simultaneously devise the best structural topology with the most

compatible material microstructure, with the aim of increasing the design freedom to find the optimal performance in the macrostructure [125]. The development of the AM can provide a feasible solution to fabricate the concurrent multiscale designs with either single material [126] or multiphase materials [127, 128]. In the existing concurrent topology optimization framework, macro and micro densities are introduced as independent design variables for macro structure and material microstructure, respectively. Optimizations at two scales are integrated into one system with the homogenization theory. Penalization approaches are adopted in both scales to ensure clear topologies, i.e., SIMP in the micro scale and PAMP (Porous Anisotropic Material Penalization) in the macro scale. Two classes of design variables (density fields) are independently defined [129].

As illustrated in Fig. 20, the two-scale concurrent topology optimization framework, where the material microstructure is assumed to be the same throughout the macroscopic structure, is the focus of this work. The macrostructure is assumed to be composed of uniform materials, whose material microstructures could be regarded as composed of repetitive unit cells in which a voxel-based representation specifies whether a finite element contains base material (voxel=1) or not (voxel=0).

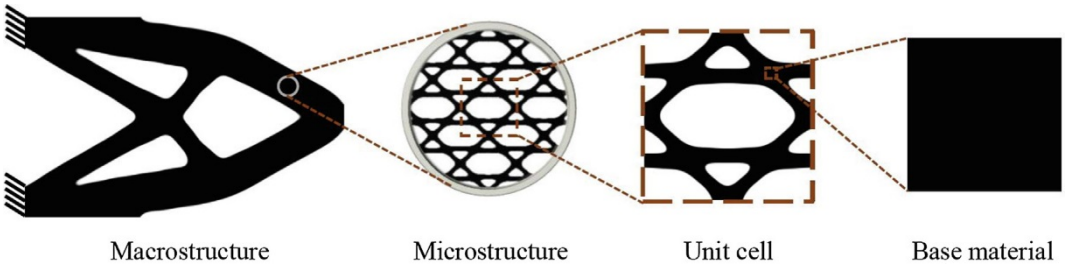


Fig. 20 Two-scale hierarchical structure with uniform microstructure. Permission to reprint from Elsevier copyright 2019 [130].

The most commonly applied strategy is designing a uniform material microstructure at the microscopic scale either for a fixed or concurrently changed structure at the macroscopic scale. Obviously, such designs have not yet released the full potentiality of concurrent two-scale designs. A further step has been made by Xia and Breitkopf [131], where several different cellular materials are designed for a layered structure following a two-step design procedure. Another concurrent topology optimization model with multiple porous materials is proposed by Deng and Chen [129]. By combining the concurrent topology optimization framework and the discrete material optimization interpolation model, the distribution of subdomains on the

macroscale and the topology of the material microstructure in each subdomain can be automatically determined. L-Beam optimized design by a generic approach [10] allowing any number of unique microstructures indicates that increasing the number of allowable microstructures leads to a solution with an improved objective. Li et al. [132] introduced a larger number of material microstructures in architected thermoelastic materials optimization, the overall performance was improved due to the expanded design space. However, when multiple architected materials with spatial variations in a structure are considered, a challenge arises in topological solutions, which may not be connected between adjacent material architecture. Du et al. [133] introduced connectivity index (CI) to quantify the topological connectivity, and added it as constraint in multiscale topology optimization to achieve connected architected materials.

However, the unit cell of microstructure is composed of single base material with single base material property. In order to further explore design freedom provided by multi-material AM (e.g., Polyjet), Zhu et al. [11] proposed a two-scale topology optimization with microstructures consisting of two base materials (soft material and rigid material). As shown in Fig. 21, a continuous gamut of material properties is derived from a precomputed database of discrete microarchitectures prior to large-scale optimization. Topology optimization is then used to optimize the material properties of the large-scale domain within the gamut to satisfy functional objectives. The continuous solution from the topology optimization is then mapped to discrete microarchitectures from within the database. This effective approach requires a large computational resource to assemble the databases prior to large scale optimization.

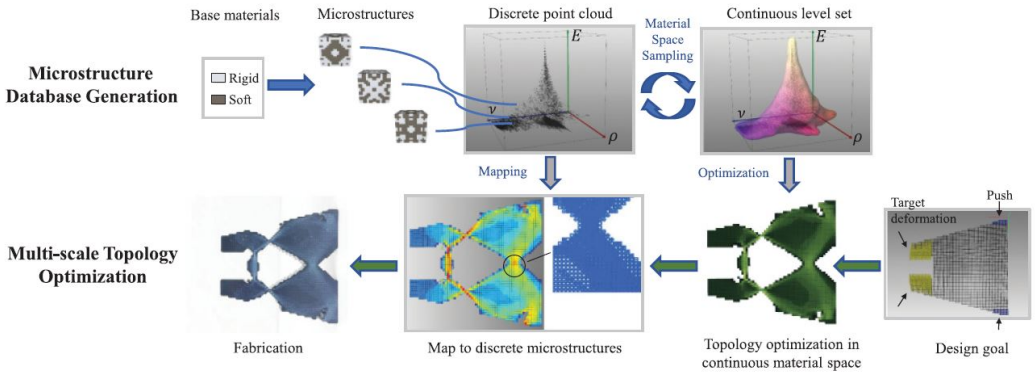


Fig. 21 Multi-scale topology optimization framework with microstructure database. Permission to reprint from ACM copyright 2018 [11].

3.3 Multi-material optimization methods of heterogeneous lattice structures

From the multi- material point of view, the material space of the multi- material objects is no longer confined to a single material, it has been extended to multi-material space. Therefore, compared with the topology optimization of a single material object, multi-material topology optimization (MMTO) refers to finding the optimal layout form of a variety of materials in the design space under a given design domain, a given constraint and a load. Then, the best way to pass force is obtained to achieve a predetermined function or movement, and to achieve a certain design goal. For MMTO, the problem could be generalized to

$$\begin{aligned} &\underset{\Omega_{k=1,2,\cdots,M\subset D}}{\text{Min}}\ \varphi \\ &\Omega_i \cap \Omega_{j\neq i} = \varnothing \\ &g_i\left(u,\Omega_k\right) \le 0 \\ &\text{Subject to} \\ &Ku = f \end{aligned} \tag{4}$$

where φ is the objective, such as compliance, stress, or volume; Ω_k is the topology to be computed for material "k" to be computed; M is the number of materials; D is the domain within which the topology must lie; u is the finite-element displacement vector K is the finite-element stiffness matrix; f is the external force vector, and g_i is the constraints on volume, stress, buckling, etc.

The MMTO problem assumes that every point within the design space has a distinct material associated with it (or is void). This differs from functionally graded material optimization, where a mixture of base materials is allowed [134]. It mainly includes Solid Isotropic Microstructure with Penalty (SIMP), Level Set Method (LSM) and Discrete Element Method (DEM).

3.3.1 SIMP for MMTO

SIMP method needs different material interpolation schemes to meet the requirements of different base materials and material properties. Thomsen et al. [135] firstly extended multiple materials to SIMP in 1992. Sigmund proposed [136] a two-material interpolation scheme for designing electrically and thermally driven micro-actuators. Kruijf et al. [137] find the optimal structures with the maximum stiffness and minimum resistance to heat dissipation and tailor composite materials with effective thermal conductivity and bulk modulus. Two-phase ill-ordered base materials (i.e. one

has a higher Young's modulus, but lower thermal conductivity while another has a lower Young's modulus but higher conductivity) are assumed in order to observe competition in the phase distribution defined by stiffness and conduction. Hvejsel et al. [138] proposed two multi-material interpolation schemes as direct generalizations of the well-known SIMP and RAMP material interpolation schemes originally developed for isotropic mixtures of two isotropic material phases. Jeong et al. [139] presented a new regional constraint method based on the sorting algorithm and the applicability and limitations of the newly developed framework were discussed in the context of its application to several stress-based topology optimizations with multiple materials. Gaynor et al. [140] manufactured compliant mechanism designs based on three-phase (2 solid phases plus void) topology optimization using PolyJet AM technology, which can print bulk materials covering a wide range of elastic moduli (Fig. 22).

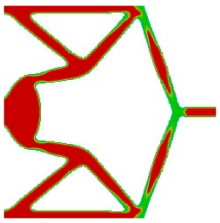


Fig. 22 3-phase inverter result by multiphase SIMP approach. Permission to reprint from ASME copyright 2014 [140].

The advantages of SIMP are as followings: the design variables (cell densities) in the SIMP model are directly linked to the optimization problem, that is, the display of the topology is dependent on the design variables. The model optimization algorithm converges well and can directly calculate the discrete design sensitivity based on finite element method. Moreover, it is suitable for any shape of the design domain and is easier to integrate with existing commercial finite element software. However, SIMP method extended to *m*-phase materials requires (*m*-1) design variables for each finite element, which results in complex interpolation express and large computational cost [141]. In order to enforce the selection of, at most or exactly, one material at each design subdomain, a large number of sparse linear constraints are needed.

3.3.2 LSM for MMTO

The level-set function is originally developed by Osher and Sethian [142] with the fundamental goal of tracking the motion of curves and surfaces. In this work, the structural boundary is implicitly represented by the zero level sets. For the multi-

material structures, multiple level set functions $\phi_k,(k=1,2\cdots M)$ are employed to denote different phases. These level set functions are utilized to define the following subdomains [143]:

$$\begin{cases} \Phi^k(\mathrm{x})>0 & \forall x\in\Omega^k\setminus\Gamma^k \\ \Phi^k(\mathrm{x})=0 & \forall x\in\Gamma^k, \\ \Phi^k(\mathrm{x})<0 & \forall x\in D\setminus\Omega^k \end{cases} \qquad k=1,2\cdots M \tag{5}$$

where D represents the design domain including all admissible shapes. Ω^k denotes the kth material region with positive value of the kth level set function, Γ^k is the boundary of the kth material, negative value of the kth level set function signifies the domain not containing the kth material. x represents a point located in D. M is the number of the level set function. An example for the design domain containing three level set functions is illustrated in Fig. 23.

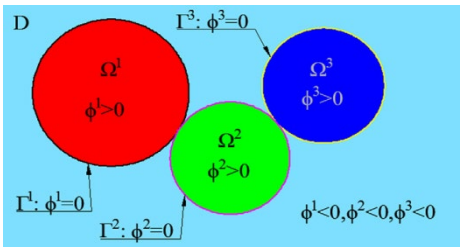


Fig. 23 A schematic diagram of the design domain which includes three level set functions. Permission to reprint from Elsevier copyright 2016 [143].

Wang et al. [144] also introduced a novel level-set approach referred to as a "color" level-set representation which has its unique benefits: it is flexible to handle complex topologies. The multi-level set functions $\phi_k,(k=1,2\cdots M)$ are used to represent $n=2^M$ distinct material phases and substantially reduces the number of model functions. Liu et al. [30] employed multiple level set functions to build the geometry, utilizes zero-value level set contours as material source profiles, and realized FGM blending with a signed distance-based blending function. More importantly, this model supports the concurrent structure and material optimization because of the unified level set framework for both structure and material composition representation. The initial problem setups are demonstrated in Fig. 24a and Fig. 24c. The heterogeneous source profile in Fig. 24a employs the Young's modulus combination of 1.3 and 0.33, while the heterogeneous source profile in Fig. 24c employs the Young's modulus combination of 1.3 and 0.98. The optimization results are demonstrated in Fig. 24b and Fig. 24d, respectively.

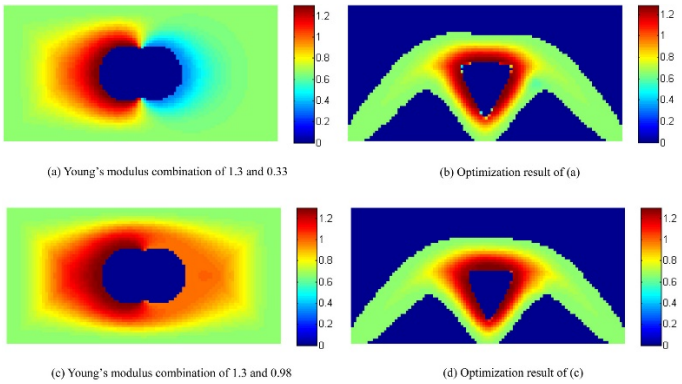


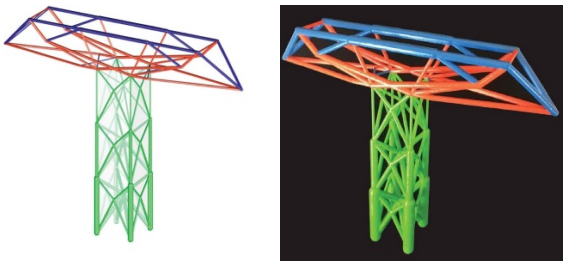
Fig. 24 Optimization results of the Michell structure problem with heterogeneous source profiles. Permission to reprint from Elsevier copyright 2019 [30].

The advantages of level set are as followings: level set-based model is one of a few exceptions that could support both aspects of modeling and optimization. The gray area problem is solved by the unique advantages of smooth and clear boundaries of various materials and convenient extraction of topological configurations, and the optimization results can be directly used for manufacturing. However, since the design variables are indirectly linked to optimization problems, it involves the approximation of finite elements that are cut by the horizontal set, thus affecting the optimization accuracy. Level-set-based topology optimization methods suffer from local minima and dependency of the final result on the initial guess. This property is a consequence of the shape optimization character of LSM. Seeding an initial design with a large number of holes or inclusions may lead to numerical issues and does not necessarily mitigate the dependency of the final result on the initial guess.

3.3.3 DEM for MMTO

Unlike continuous topology optimization method, i.e. SIMP. Discrete elements such as 1D truss element (ground structure method) [145] or 3D bar element (geometry projection method) [146] can be directly applied to MMTO for MSHLS. Recently, several papers about this topic have been published. Zhang et al. [147] proposed an efficient MMTO formulation considering material nonlinearity. The proposed formulation handles an arbitrary number of candidate materials with flexible material properties, features freely specified material layers, and includes a generalized volume constraint setting. An application to MMTO of truss networks considering multiple load cases and nonlinear constitutive behavior is shown in Fig. 25. Kazemi et al. [148] presented a geometry projection 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. Michell cantilever example shows that the proposed formulation can be readily extended to any number of materials (Fig. 26).



(a) (b)

Fig. 25 3D crane design subjected to multiple load cases: a) optimized structure for the 3D crane design with three materials, b) printed model using FDM process. Permission to reprint from Springer Nature copyright 2017 [147].

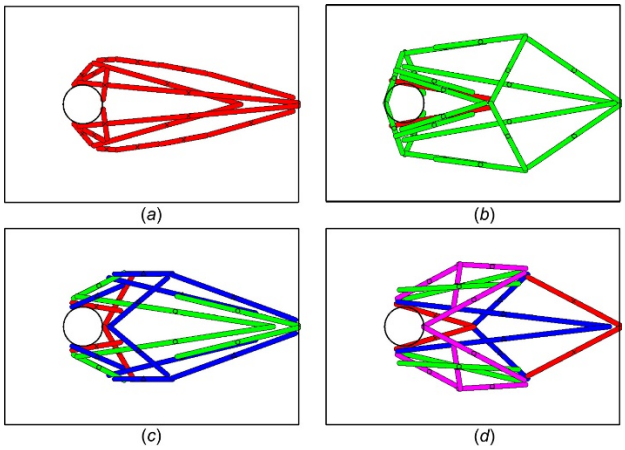


Fig. 26 Michell cantilever optimal designs. Red (3) indicates material (stiffest/heaviest), green indicates material 2, blue indicates material 3, and magenta indicates material 4(weakest/lightest): (a) one material, C=50.233370; (b) two materials, C=50.176354; (c) three materials, C=50.193584; and (d) four materials, C=50.192687. Permission to reprint from ASME copyright 2018 [148].

The advantages of DEM are as followings: Optimal design of truss like structures with discrete design variables share many mathematical properties with multi-material topology optimization. For ground structure method, the final optimal truss structure is realized by selecting an optimal substructure from a pre-defined ground structure. Typically strut cross-section dimensions (such as diameter) are the design variables. Local strain or stress values from the FEA results are used to compute the strut sizes. If a strut size approaches the specified threshold, it can be removed, effectively changing

the topology of the design. This conveniently changes a topology optimization problem into a sizing problem. Unlike ground structure methods, the discrete elements in geometry projection method need not be connected during the optimization, hence giving more freedom to the optimizer to optimally place and size the bars. By having an independent explicit geometry, this method is capable of producing designs with members of predefined cross-sections. Moreover, it can accommodate the case where the thicknesses of the bars are added at their intersections (overlapping bars), and it can compute the volume fraction and its sensitivities directly from the bar's geometry and not from the composite density. However, the discrete nature of the problem makes it difficult to be solved. There exist a large number of both mathematically well-founded as well as heuristic approaches like genetic algorithms, swarms and differential evolution techniques that are not viable alternatives for the vast majority of topology optimization problems. However, none of them is well-suited for the problems with thousands and up to millions of variables that are encountered in topology optimization approaches.

Based on the optimization design methods introduced above, a comparison between different optimization approaches is made and summarized in Table 4. Based on this comparison, it helps designers select a suitable optimization method for different cases.

Table 4 Comparison of existing optimization methods for MSHLS

	Methods	Advantages	Disadvantages
Multi- material optimization methods	SIMP-based method	The algorithm has good convergence, is suitable for any design domain, and is easy to integrate with commercial FEA software	Complex interpolation expresses and large computational cost
	LSM-based method	The boundary of optimization results is clear, which can be directly used in manufacturing	Final results strongly depend on starting guess
	DEM-based method	It is suitable for truss-like MSHLS, and can deal with multiple load cases and nonlinear constitutive behavior	It is difficult to solve the discrete nature of the problem

	Methods		Implementation approach
Multi-scale optimization methods	Optimum design of material microstructure		It uses inverse homogenization method for microstructural topology
	Macro scale	Material composition distribution optimization	It optimizes function coefficients according to material composition distribution function or relative density distribution for cellular cells
		Microstructure distribution optimization	It uses perturbation function or elasticity tensors to control the distribution of microstructures
	Concurrent optimization		It can update material microstructure and macrostructure topology simultaneously

4 Discussion

A general design process of MSHLS including input of design and functional requirements, initial design, optimized design and geometric & material composition models is proposed in Fig. 27. This process is based on the design and fabrication methods for AM proposed by Rosen[4], Tang[5] and Yang[149]. In this paper, we only focus on the design aspect. With the input of design and functional requirements, initial design including either Functional Volumes (FVs) and Functional Surfaces (FSs) with solid & skin or with lattice can be obtained. Then the initial design result is the input to the simulation step. The simulation result then goes back to modeling stage for the optimization of the initial design to get optimized design. During this design process, optimization methods (multi-scale optimization and multi-material optimization), simulation support (mixtures rule and numerical analysis), and modeling methods (material composition modeling and multi-scale geometric modeling) as main design methods support optimized design phase to obtain final geometric & material composition models of MSHLS.

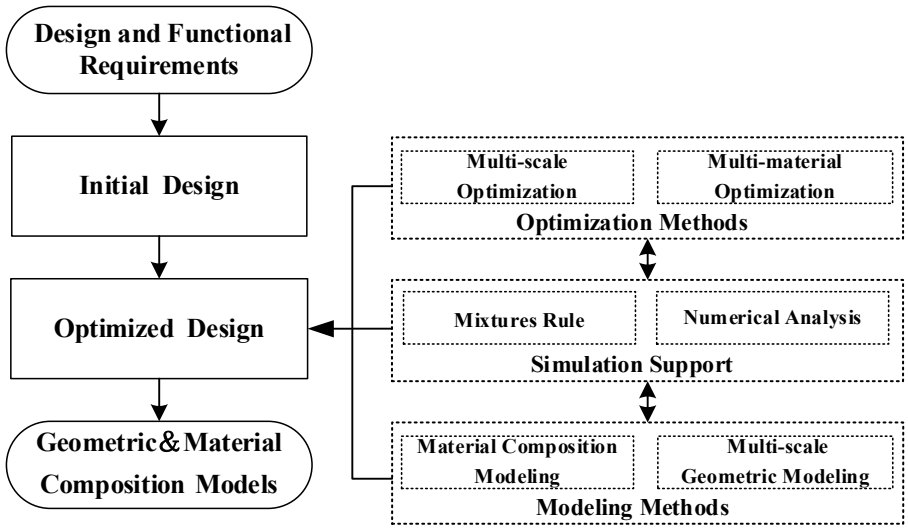


Fig. 27 The design process of multi-scale heterogeneous lattice structure.

To facilitate the use of the above-mentioned modeling, simulation and optimization methods for MSHLS design, it is necessary to describe the scope of application of the method. According to the minimum basic elements describing the material information of MSHLS, voxel-based, volumetric mesh-based, truss or beam-based and curve feature-based design methods are summarized. Among them, voxel-

based modeling, simulation and optimization methods include voxel model (Section2.1.1), physics-based method (Section3.1.1), homogenization method (Section3.1.2), and SIMP method (Section3.3.1); Volumetric mesh-based methods include volume mesh model (Section2.1.1) and FEA-based method (Section3.1.3); Truss or beam-based methods include control feature-based model (Section2.1.3), FEA-based method (Section3.1.3) and DEM (Section3.3.3); Curve feature-based methods include control point-based model (Section2.1.4), IGA-based method (Section3.1.4). Especially, as an implicit function, level set-based method (Section2.1.2) is not only applicable to Boolean operation but also to MMTO (Section3.3.2).

Summarising the overview of modelling methods, there is a gap between geometrical complexity of heterogeneous lattices and inability of current geometric modelling methods to handle such complexity. Moreover, volumetric modelling allows direct transition to structural simulations but is even more complicated. Thus, there is a need in a novel volumetric geometric modelling approach to support MSHLS. Such approach should be extensively tested on numerous use-case of lattice structures and other complex geometries, measuring its performance and speed comparing to existing approaches. Moreover, the concept of level of detail should be adapted for lattice structures, as they do not have CAD-features that are commonly associated with their level of detail in conventional modelling.

Simulation methods such as homogenization can be applied based on the calculated effective properties. However, how to accurately predict the effective properties for MSHLS is a critical issue, since micro cell of this type of structure may dramatically change in a certain local region. RVE (Representative Volume Element) for this type of structure is difficult defined. There is no cell which can strictly satisfy the periodic boundary condition. By directly choosing the smallest unit cell as RVE will cause the significant discrepancy between simulation result and physical testing result. Another method of mixtures rule is the simplest way. However, the accuracy of this method is limited, since it fails to consider the geometric configuration of the microstructures of the material composition. In most cases, it can only provide a rough estimation of upper or lower bound of effective properties. FEA methods could be used based on decomposition-based models (Section2.1.1). However, the computational cost for a fine-meshed model is too heavy to fulfillment.

For the optimization methods, to efficiently solve the proposed optimization

formulation is another critical issue needs to be solved. Comparing to the existing optimization methods for homogenous objects, the proposed optimization formulation contains more design parameters. Moreover, those design parameters may be coupled with each other. For example, during the optimization the stiffness of the heterogeneous structures. The material distribution on macroscale is coupled with the microstructure of materials in different regions. On the one hand, the optimized microstructure can be generated based on predefined material compositions. On the other hand, the effective properties of optimized structures will affect the distribution of material compositions in turn. To solve this complex optimization problem, there are several potential methods which can be adopted in this problem. Given that MSHLS needs to deal with a large number of design parameters, one strategy for MMTO is to introduce multi-resolution method to obtain multiple discretization level. The discretization level for the displacement elements, the density elements, and the design variables can be chosen independently, thus it can realize high-resolution MMTO with relatively low computational cost by employing a coarser discretization for finite elements and a finer discretization for both density elements and design variables. Another strategy is to reduce the number of design parameters by using the heuristic algorithms. Generally, the heuristic algorithm may be applied based on initial analysis of structure to divide the initial design domain on a single design scale into several sub-regions. The material or its microstructure are supposed to be homogeneous in each sub region during the design optimization process. This method can significantly decrease the number of design parameters and computational time for the defined optimization problem. To optimize the structures on different scales sequentially. The method (Section3.2.3) tries to decouple the relation between design parameters on different design scales. The effects of design parameters defined on the lower scale will be pre-estimated during the optimization iteration for the design parameters defined on the upper scale. Additional optimization constraint will be added to limit the discrepancy between the estimated effects and the real effects of the design parameters defined in the lower scales. This strategy has been widely used in the Multidiscinplnary Design Optimization (MDO), and known as IDF (Indiviual Discinplinary Feasible) analysis. It can be used for design and optimization a complex coupled system.

The developed geometric＆material composition model for MSHLS is a universal model. It cannot only be used to represent the information of designed and optimized

structures for industry and engineering applications. This model can be also used to represent the information of bio-tissues which also has hierarchical complexities such as human's bone. Based on the developed model, researchers from bioengineering and biomedical fields can further investigate the mechanical behaviour of these tissues.

5 Conclusion and perspectives

The contribution of this review is to provide a comprehensive view of the MSHLS design process, and of the modeling, simulation and optimization strategies currently available, which are still lacking. In the end, based on the summaries of different modeling, simulation and optimization methods, it comes out that further researches are needed and several future work perspectives concerning the design of MSHLS have been pointed out:

- To develop a multi-scale model which can represent the information of MSHLS. This model should satisfy the following requirements. Firstly, it should be able to store both material and geometry information on multiple design scales. The relations between different design scales are also needed to be clearly defined in this model. Secondly, the developed model should have a compact and efficient data structure, which enable the quick accessing and visualization of data on different design scales. Thirdly, the developed model should be general enough to incorporate different types of MSHLS. Fourthly, this model should also be easily converted manufacturing readable data model, which enable the direct fabrication via selected AM process.
- To develop a multiscale simulation model of MSHLS. In this model the effective properties of material defined in the bottom scale need to be calculated based on the numerical homogenization methods. Different numerical homogenization methods will be developed or modified to evaluate the different type of microstructures. For example, if the microstructures are lattice structure, numerical homogenization methods can be applied. By carefully selecting the suitable numerical homogenization methods, it can significantly shorten the computational time. Moreover, in order to improve the accuracy of the calculation, the modification of calculated effective properties from numerical homogenization methods also needs to be done. The detailed

modification algorithm needs to be further investigated. Based on evaluated effective properties, the numerical simulation model such as FEA model can be applied to evaluate the performance of modeled multiscale MSHLS.

- To investigate general optimization parameterization formulation. On different design scale, the parameters which can efficiently control the distribution of material compositions and its microstructures should be figured out. For example, the coefficient of exponential function can be used to control the material distribution in design domain, while the implicit level set functions can be used to parameterize the microstructures of materials. The selected design parameters can be directly converted to the generalized units defined on each level.

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Figure Captions List

Fig. 1 Heterogeneous lattice structure: a) Heterogeneous lattice with gradient strut dimensions, b) Heterogeneous lattice with variational material compositions.

Fig. 2 Multiscale structures with hierarchical lattice architectures. Permission to reprint from Springer Nature copyright 2016 [8].

Fig. 3 Multi-material-property configuration [15]

Fig. 4 2D and 3D heterogeneous lattice structures. Permission to reprint from Elsevier copyright 2014 and ASME copyright 2019 [22, 23].

Fig. 5 Material blending with three material source profiles. Permission to reprint from Elsevier copyright 2019 [30].

Fig. 6 Common material composition variation features in MSHLS. Permission to reprint from Elsevier copyright 2019 [31].

Fig. 7 Effect of different material functions on material-distribution. Permission to reprint from IEEE copyright 2018 [33].

Fig. 8 1D heterogeneous features: a) a heterogeneous line, b) a heterogeneous B-spline. Permission to reprint from Elsevier copyright 2005 [37].

Fig. 9 An example of LODs associated with CAD features. Permission to reprint from John Wiley and Sons copyright 2014 [55].

Fig. 10 Lattice structure voxelization, adapted from [74].

Fig. 11 A standard cubic unit element: a) and a cylindrical shape with its cylindrical sector unit element, b) used for stress analysis. Permission to reprint from Elsevier copyright 2013 [75].

Fig. 12 FEA-based simulation aided design: a) multi-material fiber network of artificial disc. Permission to reprint from ASME copyright 2019 [98], b) medical tweezers with spatial material distribution. Permission to reprint from ACM copyright 2015 [100].

Fig. 13 Overview of the digital design and manufacturing framework for soft lattice structures. Permission to reprint from Elsevier copyright 2019 [106].

Fig. 14 Material microstructures design: a) level-set-based design. Permission to reprint from Elsevier copyright 2016 [108], b) design of architected truss lattice materials with three base materials. Permission to reprint from Elsevier copyright 2020 [109], and c) voxel-wise material distribution. Permission to reprint from ACM copyright 2015 [110].

Fig. 15 An example of F-P-P-D model. Permission to reprint from Springer Nature copyright 2018 [115].

Fig. 16 Relative density mapping to strut diameter. Permission to reprint from Elsevier copyright 2015 [116].

Fig. 17 Example of mechanical properties mapping process and its manufacturability verification by 3D printing: a) material properties diagram, b) 3D mapping result, c) 3D printing result. Permission to reprint from Elsevier copyright 2018 [117].

Fig. 18 Structures used for FEA: a) Solid (SIMP solution), b) Intersected Lattice of D-P, c) Intersected Lattice of BCC, d) Graded Lattice of D-P, e) Scaled Lattice of D-P, and f) Uniform Lattice of D-P [118].

Fig. 19 Deformation of an object with varying material properties per voxel, and the same object with the material in each voxel replaced with the corresponding pattern. Permission to reprint from ACM copyright 2015 [123].

Fig. 20 Two-scale hierarchical structure with uniform microstructure. Permission to reprint from Elsevier copyright 2019 [129].

Fig. 21 Multi-scale TO framework with microstructure database. Permission to reprint from ACM copyright 2018 [11].

Fig. 22 3-phase inverter result by multiphase SIMP approach. Permission to reprint from ASME copyright 2014 [140].

Table Caption List