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Efficient biscale design of semiregular porous structures with desired deformation behavior

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ABSTRACT

Porous materials/structures are observed in many natural objects, exhibit exceptional properties, and have wide industrial applications. The rapid advance in additive manufacturing has also facilitated the process to fabricate such complex porous structures with fine accuracy control. However, the design of optimal porous structures with the desired deformation behavior is still very challenging because of its high computational complexity. In this study, a novel and efficient approach was developed to solve this problem by designing a *semiregular* porous structure with a hole within each mesh element of a given quad/hex-mesh layout of the design domain. The proposed approach ultimately analytically expresses the displacement of the design model as a function of the design variables, and consequently solves the optimization problem of porous structure design efficiently. The novelty was mainly achieved by representing a compact design space, building approximate analytical structure-property relation, and estimating the displacement variations of material property. The good property was achieved using the advanced numerical techniques: model reduction, homogenization theory, metamodeling, and the combined approximations. Various numerical examples were also tested to demonstrate the performance of the approach.

1. Introduction

With the development of additive manufacturing technology, many research studies have been conducted to explore its potential utilities to product design and manufacturing. One of the most exciting problems is to design internal structures that achieve the desired physical properties. The main challenges are to (i) find an effective representation of the structure, (ii) accurately predict the relationship between the physical properties and structure, and (iii) design highly efficient numerical methods for structure optimization under specific constraints.

In this study, we show that the novel *semiregular porous structure* has great advantages of low-dimensional presentation, accurate property and performance prediction, and efficient optimization. Porous structures are observed in many natural materials or objects, such as human bones, woods, plant stems, and bird beaks. Porous structures are produced by million years natural evolution, exhibit exceptional properties [1,2] in the case of wave absorption [3,4], shock resistance [5,6], damping enhancement [7,8], defect tolerance [9–11], and multifunctional usage [12–16], at a relatively low density. These superior properties are very important for industrial usage, and have attracted much research interest.

According to the cell arrangements, two main categories of engineered porous structures have been studied previously: periodic and stochastic. Both of them have wide industrial applications. See the first two structures in Fig. 1. The periodically arranged regular structures were first studied, where *completely identical* cell elements (called *Representative Volume Element (RVE)*) are assumed to be periodically distributed under periodic physical boundary conditions. Based on this assumption, various analytical or numerical homogenization theories have been proposed to predict the associated material properties [17]. The design of a topological structure for such an RVE of extreme material properties, such as negative Poisson's ratio, has also been recently studied [18].

Among the excellent works in studying periodic structures, Bertoldi and co-workers showed the great potential of these structures both in 2D [19–21] and 3D [22] spaces. When exploring a nonlinear adaptive response [19,20] of structures, they identified procedures to guide the design of 3D soft and active metamaterials, where buckling provides dramatic changes in the structures [21,23,24]. Bertoldi's work opened the way for performance-oriented cellular structure design and inspired more work on this

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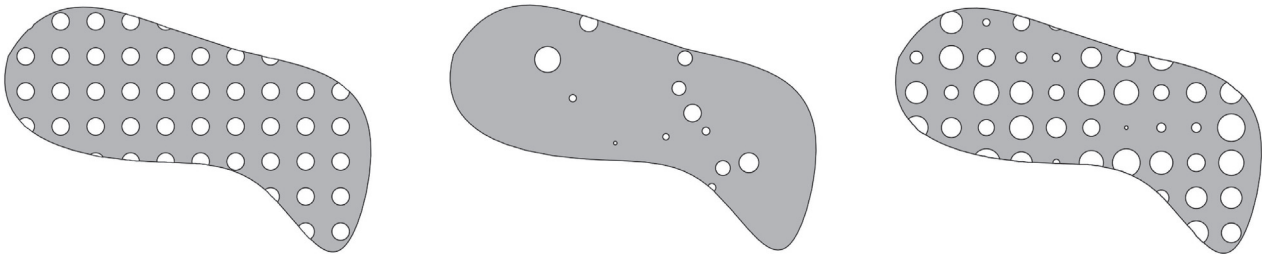

Fig. 1. Porous structures: regular, stochastic or semiregular structures.

issue afterwards. However, these studies mainly focused on the experimental studies of such cellular structures, and did not explore approaches to automatically design and optimize such structures.

Besides these regular porous structures, randomly arranged porous structures and their associated physical properties have also been studied, mainly in the computational material communities [25]. From the material composition knowledge, the relation between the physical property and the microstructure distribution was mainly studied statistically, i.e., predicting the macroproperty in terms of the statistical parameters of the microstructures [26]. Approaches have also been proposed to find such optimal statistical parameters for performance optimization [27].

Unlike the two main types of porous structures, the study focuses on a novel *semiregular* porous structure, as shown in Fig. 1(c). This has a similar but not identical cellular shapes arranged at a certain layout control. The semiregular structure does not only consider the geometry of cellular elements, but also their global arrangements. This is very different from the regular porous structures whose layouts have been fully determined, and also very different from the stochastic porous structures, which only consider the statistical information of the cells' arrangement. As further explored in this study, the semiregular structure also allows a possible efficient physical simulation owing to its special geometric structures. The differences among the three types of porous structures shown in Table 1 were compared.

Based on the above observations, the problem of designing semiregular porous structures for the desired deformation behaviors of linear elasticity was studied, specifically, certain vertices of the porous structure deforming to specified locations under given external forces. The design problem has wide applications in medical or engineering industrials [28]. Owing to the special structure representations of semiregularity, the problem was reformulated as a biscale design problem, by building sequentially the structure-property relationship, and the property-performance relationship. Ultimately, the displacement of the design model is expressed as an analytical function in terms of the design variables using advanced numerical techniques such as reduced structure representations, homogenization theory and metamodeling [29–31], and combined approximation (CA) [32]. Based on this design, the problem of semiregular porous structure can be efficiently solved as an optimization problem. Various numerical examples were also tested to demonstrate the performance and efficiency of the approach.

The remainder of the paper is arranged as follows: The related work is first given in Section 2. The design problem and overall approach are described in Section 3. Then, the technical details are described in detail in Sections 4 and 5. Various numerical examples are also shown in Section 6 to test the accuracy and efficiency of the approach. The conclusion is given in Section 7.

2. Related studies

Porous structure design has attracted much interest in different research communities such as computational physics, mechanical engineering, computational materials and computer graphics. The research work closely related to the problem includes topology optimization, descriptor-based material design optimization, and fabrication-oriented design optimization.

2.1. Descriptor-based material design optimization

The use of computational tools or informatics knowledge to accelerate the process of novel material discovery is a long-term goal in material research. The stochastic porous structures are mainly studied using statistical tools, probably because of the limitations of material fabrication technology at the beginning. Kalidindi and co-workers [25,33,34] conducted a systematic study on microstructure-sensitive design for performance optimization. The main idea behind their work was to represent the distribution of cells or their relative locations in the spectral space, called *first-order*, or *second-order descriptors*, using a small number of descriptor parameters. Based on this, the structure-property relationship can be expressed using an explicit function based on homogenization theory. Chen and co-workers also systematically studied problem of stochastic multiscale material design [35–37].

These studies have provided promising results and shown practical engineering applications, but are still limited in several aspects. First, the statistical geometry representations lose the geometric detail information, and consequently the predicted physical property may vary in a large range and even has no practical application. Second, even if the statistical descriptors are successfully derived, reconstructing the microstructure from them is still challenging - usually not unique and expensive to compute, particularly for higher-order descriptors.

Table 1
Difference between regular, stochastic and semiregular structures.

Types	Geometry (1)	Arrangement (2)	Design DOFs	Representation	Physical property
Regular (a)	Identical	Along *X*, *Y*, *Z* axis	Only (1)	Compact	Homo., exact
Random (b)	Random	Random	(1), (2) without exact control	Statistical	Homo., large range
Semiregular (c)	Similar	Given	(1), (2) with exact control	Reduced	Homo., approximate