

MULTISCALE ISOGEOMETRIC OPTIMIZATION FOR CELLULAR STRUCTURE WITH MULTIPLE PROTOTYPES

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Abstract. This paper presents a multiscale concurrent isogeometric design method for the cellular structure composed of the multiple prototype microstructures. Based on the unified-skeleton modeling scheme, the graded microstructures obtained from a same prototype have similar topology and good connectivity between each other. For the different prototypes, the configurations are rearranged and added the thin-wall material in common interfaces. Thus, the geometric features as well as the structural skeletons can have a smooth transition. Through combining the numerical homogenization method with the interpolation technique, the effective properties of graded microstructures can be estimated efficiently. For the multiscale scheme, the allocation of microstructures is optimized by a material distribution-based method while the configurations of prototypes are designed by the isogeometric parameterized level set method. The proposed method inherits the high accuracy and high efficiency of isogeometric analysis and the smooth boundaries and distinct interfaces of level set method. The cellular structure can be freely customized with favorable connectivity.

1 INTRODUCTION

The artificial functionally graded materials consisting of the spatially-varying cellular microstructures have been extensively studied and utilized in engineering applications [1]. Instead of choosing different base material, the key issue for gaining the desired performance is to design configurations and layouts of cellular materials. Currently, the so-called concurrent design or hierarchical design [2] are the effective methods for multiscale cellular structure. By optimizing the prototype microstructure and deriving the corresponding graded microstructure, the assembled macrostructure shows flexible and modular design freedom. Moreover, the multiple prototypes [3] are employed to extend the diversity of microstructure, thereby realizing the complex and spatially varying cellular structure. However, it is difficult to maintain the connectivity between adjacent microstructures without extra geometric constraints in design process. Hence, this paper proposes a multiscale concurrent design method for cellular structure with multiple well-connected prototypes.

The multiscale design for cellular structure can be divided into the single-scale structure design in both macro scale and micro scale. The topology optimization is an effective structure optimization tool for achieving the optimal material distribution under predefined constraints. Compared to the density-based

representation [4] such as the homogenization method, solid isotropic material with penalization method (SIMP) and evolutionary structural optimization method (ESO), the boundary-based representation [5] avoid the numerical artifacts like checkerboard and mesh dependency without the extra filtering process and stabilization. The level set method (LSM) can flexibly handle the complex topology evolution with distinct interfaces. By adopting the non-uniform rational basis splines (NURBS) as basis functions for both parameterized level set model and isogeometric calculation model [6], the configuration design for prototypes inherits the high accuracy and high efficiency [7].

For bridging the design between different scales, the asymptotic expansion theory based numerical homogenization method [8] is employed to estimate the effective elasticity tensors for microstructures. Thus, the configuration design of microstructure can be regarded as the inverse design problem for achieving desired properties. Da et al. [9] optimized the material microstructures for maximum effective elastic modulus. Ye et al. [10] utilized the inverse method to design the gradually stiffer mechanical meta-material for cushioning and vibration damping in engineering. For spatially varying graded microstructures, the effective property is no longer fixed and can be used to analyze the displacement field of macro structure providing that the neighboring cellular microstructures have sufficiently small change in gradient of shape and property. Combining the shape metamorphosis method [11] with unified-skeleton modeling scheme [12], the interpolation process of effective property estimation can be simplified by fitting function.

However, the scale separate assumption in homogenization method gives rise to the uncertainty for connectivity of microstructural geometry. The filtering technique [13] and predefined connected region [14] as the candidates of geometric constraints can address the issue, but increase complexity of algorithm. In addition, the transitional connection method [15] interpolated the level set function of prototypes to generate the transition microstructure. In our previous work [12], the graded microstructures generated from the same prototype have unified structural skeleton and similar topology feature, thereby ensuring the connected components at common interfaces. This paper extends the multiscale design method for the cellular structure composed of the multiple prototypes. By adjusting periodicity interval of prototype microstructure, the different structural skeletons as well as components connect together as a whole. In regional boundary, the thin-wall material is added to avoid the hang caused by the difference of component numbers.

In this paper, we achieve a multiscale concurrent isogeometric topology optimization for the cellular structure derived from the multiple prototypes. In Section 2, by integrating level set method and isogeometric analysis [16], the proposed method inherits the high accuracy and high efficiency. Then the unified-skeleton modeling scheme and the periodicity interval adjusting technology are introduced to construct the cellular structure with well connectivity. Section 3 presents the formulation and the sensitivity analysis. The numerical examples in Section 4 demonstrate the validity.

2 MODELING FOR CELLULAR STRUCTURE

2.1 Isogeometric level set method

In IGA, the NURBS [17] is utilized for the numerical discretization. For the B-spline with p order and n spline basis function, the non-decreasing knot vector $H = \{\vartheta_1, \vartheta_1, \dots, \vartheta_{n+p+1}\}$ describes the parametric coordinates of a curve. Then the B-spline functions are recursively defined according to the Cox-de Boor

formula [18] as:

$$\begin{cases} B_{i,0}(\vartheta) = \begin{cases} 1 & \text{if } \vartheta_i \leq \vartheta < \vartheta_{i+1} \\ 0 & \text{otherwise} \end{cases} \\ B_{i,p}(\vartheta) = \frac{\vartheta - \vartheta_i}{\vartheta_{i+p} - \vartheta_i} B_{i,p-1}(\vartheta) + \frac{\vartheta_{i+p+1} - \vartheta}{\vartheta_{i+p+1} - \vartheta_{i+1}} B_{i+1,p-1}(\vartheta) \end{cases} \quad (1)$$

They constitute a partition of unity. When k is the multiplicity of the knots, the continuity among knot spans is C^{p-k} . Thus, the curve shows favorable smoothness. The two-dimensional B-spline basis function is constructed as $B_{i,p}^{j,q}(\vartheta, \zeta) = B_{i,p}(\vartheta) B_{j,q}(\zeta)$, which can be further used to generate the bivariate B-spline surface. NURBS basis functions as extension of B-spline are constructed by introducing the positive weight ω_i , then the two-dimensional NURBS basis functions are expressed as:

$$N_{i,p}^{j,q}(\vartheta, \zeta) = \frac{B_{i,p}(\vartheta) B_{j,q}(\zeta) \omega_{i,j}}{\sum_{k=1}^n \sum_{l=1}^m B_{k,p}(\vartheta) B_{l,q}(\zeta) \omega_{k,l}} \quad (2)$$

Based on the basis functions, a NURBS surface can be defined as a bivariate piece-wise rational function as:

$$R(\vartheta, \zeta) = \sum_{i=1}^n \sum_{j=1}^m N_{i,p}^{j,q}(\vartheta, \zeta) P_{i,j} \quad (3)$$

where $P_{i,j}$ denote the control points.

The parameterized level set function is defined in a similar way [19]. The structural boundary is implicitly traced as the zero set of high-dimensional function:

$$\Phi(x, t) = \mathbf{N}^T(x) \Lambda(t) = \sum_i^n N_i(x) \kappa_i(t) \quad (4)$$

Difference both side of Eq. (4) with respect to pseudo time t , the Hamilton-Jacobi equation is obtained as:

$$\mathbf{N}^T(x) \frac{\partial \Lambda(t)}{\partial t} - \mathbf{v}_n \left| (\nabla \mathbf{N}(x))^T \Lambda(t) \right| = 0 \quad (5)$$

Then the normal velocity can be represented as $\mathbf{v}_n = \left(\mathbf{N}^T(x) / \left| (\nabla \mathbf{N}(x))^T \Lambda(t) \right| \right) (\partial \Lambda(t) / \partial t)$.

In order to calculate the initial level set values as well as the expansion coefficients, the Greville abscissae is employed as the selection strategy of collocation points. When order and control point number of NURBS are p, m respectively. The Greville abscissae are defined by:

$$\zeta_i = \frac{1}{p} (\xi_{i+1} + \xi_{i+2} + \dots + \xi_{i+p}), \quad i = 1, 2, \dots, m \quad (6)$$

2.2 Geometry model of cellular structure with multiple prototypes

Referring to [12], the level set based prototype microstructure is used to generate the unified-skeleton graded microstructures to ensure the connectivity between adjacent cells. In [20], the structural skeletons are defined as the center set of the maximal inscribable sphere. As shown in Figure 1, the blue dotted line represents the skeleton, at point x_s of which the normal and tangential direction are defined as $n(x_s)$, $\tau(x_s)$. Due to the signed-distance modeling scheme, the level set function meets the equation:

$$\frac{\partial \Phi(x_s)}{\partial n(x_s)} = 0, \quad \frac{\partial \Phi(x_s + n \cdot d)}{\partial n(x_s + n \cdot d)} < 0 \quad (7)$$

Setting the level set values at structural skeleton as maximum of Φ , reconstructing the level set function as

$$\tilde{\Phi}(x, t) = \begin{cases} \frac{R_b}{R_s + R_b} \max(\Phi(x, t)) & x \in \Omega \\ \frac{R_s - R_b}{R_s - R_b} \max(\Phi(x, t)) & x \notin \Omega \end{cases} \quad (8)$$

where R_b and R_s denote the minimum distances of point x to structural boundary and skeleton respectively.

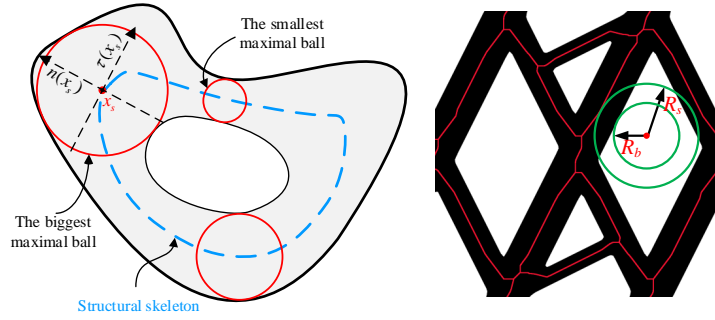


Figure 1: Based on structural skeleton, reconstructing the level set function.

According to [11], for reproducing the property of the base material, the solid microstructure must be contained in the graded microstructures. Therefore, the geometric description of microstructures should retain the feature of prototype. The level set function of solid microstructure and void microstructure are defined as:

$$\begin{cases} \tilde{\Phi}_{solid}(x) = \tilde{\Phi}(x) - \min(\tilde{\Phi}) \\ \tilde{\Phi}_{void}(x) = \tilde{\Phi}(x) - \max(\tilde{\Phi}) \end{cases} \quad (9)$$

Then the graded cellular microstructures are expressed by:

$$\tilde{\Phi}_{gm}(x) = (1 - f(\rho)) \tilde{\Phi}_{void}(x) + f(\rho) \tilde{\Phi}_{solid}(x) \quad (10)$$

where ρ denotes the relative density. $f(\rho)$ is the increasing function which can be solved by the method of bisection.

For the cellular structure with multiple prototypes, we rearranged and added the thin-wall material in common interfaces. As shown in Figure 2, several prototypes from the reference [6] are arranged from left to right. Because they have different topology as well as the structural skeletons, there are some mismatch and hang in the common interfaces. In consideration of the periodicity of prototypes, the microstructure can be freely captured providing fixed length of interval. Setting the points where level set function reaches the maximum value as new nodes x_{new} , the skeleton will go through them. Then all the skeletons of different prototypes connect to each other at the nodes.

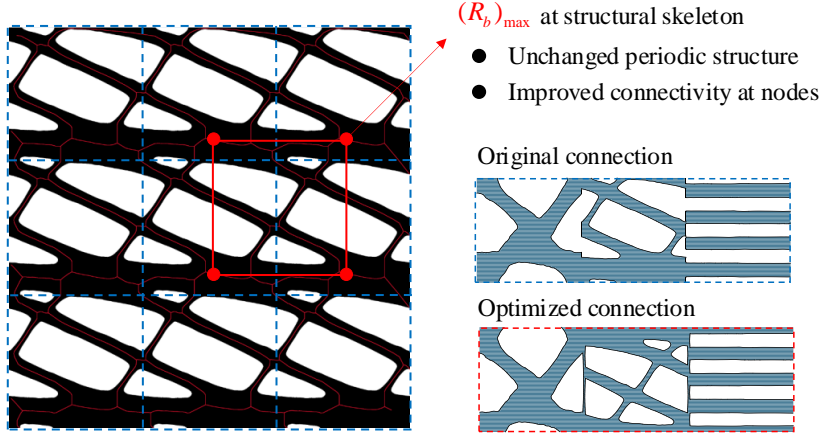


Figure 2: Rearranging prototypes and adding thin-wall at interfaces.

In Figure 2, the red box surrounds the new prototype when the red nodes locate at x_{new} , they can be represented as:

$$\Phi_{new}(x, t) = \Phi_{ori}(x + (x_{new} - x_{old}), t) \quad (11)$$

Although the rearranged prototype microstructure is different from the original one, the periodically assembled macrostructures have roughly the same topology. The nodes having the maximal level set value means that the microstructural components for connection possess the biggest size. Hence, this method can improve the connectivity at nodes effectively.

However, in consideration of difference of component number, there may be the mismatches of geometric features at middle part of interface. The thin-wall material is added to address this issue.

2.3 Estimation of effective property

Homogenization method is used to calculate the effective properties of microstructures. Via the asymptotic homogenization, a physical field such as the displacement field can be expressed as an asymptotic expansion:

$$u^v(x) = u_0(x, y) + \nu u_1(x, y) + \nu^2 u_2(x, y) + \dots \quad (12)$$

where the variables at macroscopic and microscopic are represented as x, y . The aspect ratio $v=x/y$ is very small. Only considering the first order of Eq. (12), the effective stiffness tensor is calculated as:

$$\mathbf{D}_{pqrs} = \frac{1}{|V|} \int_{V_s} M_{pqkl} \mathbf{D}_{klmn} M_{rsmn} dV \quad (13)$$

V is the solid part of the cell, and $|V|$ denotes its volume. \mathbf{D}_{klmn} is the locally elastic matrix, vary from the position of dV . Driving from the test strain $\boldsymbol{\varepsilon}_{kl}^0, \boldsymbol{\varepsilon}_{mn}^0$, the displacement field u^{pq}, u^{rs} as well as the strain field $\boldsymbol{\varepsilon}_{kl}^*(u^{pq}), \boldsymbol{\varepsilon}_{mn}^*(u^{rs})$ can be yielded. Then, the local structural tensor M_{pqkl} and M_{rsmn} can be calculated as:

$$\begin{cases} M_{pqkl} = \boldsymbol{\varepsilon}_{kl}^0 - \boldsymbol{\varepsilon}_{kl}^*(u^{pq}) \\ M_{rsmn} = \boldsymbol{\varepsilon}_{mn}^0 - \boldsymbol{\varepsilon}_{mn}^*(u^{rs}) \end{cases} \quad (14)$$

With regard to the similar shape and property of graded microstructures, the regularized effective elasticity tensor is introduced. Ignoring the parameters of base material, the effective modulus and elasticity matrix are represented as:

$$\begin{cases} E^H = (1 + \mu)(1 - \mu)E_{pqrs}/E_{base} \\ D^H = (1 + \mu)(1 - 2\mu)D_{pqrs}/[(1 - \mu)D_{base}] \end{cases} \quad (15)$$

Through the interpolation between relative density ρ_i and ρ_{i+1} , the effective property of the arbitrary graded cell can be expressed as:

$$D^H(\Phi_{gm}(\rho_e)) = \frac{\rho_{i+1} - \rho_e}{\rho_{i+1} - \rho_i} D^H(\Phi_{gm}(\rho_i)) + \frac{\rho_e - \rho_i}{\rho_{i+1} - \rho_i} D^H(\Phi_{gm}(\rho_{i+1})) \quad (16)$$

Thus, for the isogeometric parameterized level set method, the global stiffness matrix is assembled by the element stiffness matrix which can be estimated from effective properties in Eq. (13). The equation is described as:

$$K = \sum_{e=1}^N k_e \Pi = \sum_{e=1}^N \int_V \frac{\mathbf{B}_e^T [(1 - \mu)D_{base}] \mathbf{D}_e^H \mathbf{B}_e}{(1 + \mu)(1 - 2\mu)} |\mathbf{J}_1| |\mathbf{J}_2| dV \Pi \quad (17)$$

where Π denotes the selection matrix in the common notation. Jacobian \mathbf{J}_1 and \mathbf{J}_2 represent the transformation relationship among the integration parametric space, NURBS parametric space and the physical space.

3 FORMULATION AND SENSITIVITY

The proposed multiscale design is divided into macro scale and micro scale. On one hand, the configurations of multiple prototypes are designed, the corresponding graded microstructures are evolved synchronously. On the other hand, the prototypes are adjusted for their periodicity interval and added the thin-wall materials at interfaces. The distributions of the corresponding microstructures are optimized.

The formulations of topology optimization are written as:

$$\begin{aligned}
 & \text{Design variables : } \mathbf{T} = (\rho_1, \rho_2, \dots, \rho_N), \quad \Lambda^Z = (\kappa_1^Z, \kappa_2^Z, \dots, \kappa_n^Z) \quad Z = 1, 2, \dots, P \\
 & \text{Objective : } J = \mathbf{F}^T \mathbf{U} = \mathbf{U}^T \mathbf{K} \mathbf{U} = \sum_{e=1}^N \mathbf{U}_{N_e}^T \left(\int_{\Omega} \mathbf{B}_e^T \mathbf{D}^H(\chi_e, \Phi^Z(\Lambda^Z, \rho_e)) \mathbf{B}_e d\Omega \right) \mathbf{U}_e \\
 & \text{Constraints : } \mathbf{F} = \left\{ \sum_{e=1}^N \int_V \frac{\mathbf{B}_e^T [(1-\mu)D_{base}] \mathbf{D}_e^H \mathbf{B}_e}{(1+\mu)(1-2\mu)} |\mathbf{J}_1| |\mathbf{J}_2| dV \Pi \right\} \mathbf{U} \\
 & G = \sum_{e=1}^N \rho_e V_0 - V_{\max} \leq 0 \\
 & g_Z = V_Z - V_{Z, \max} = \int_{Y_Z} H(\Phi_Z) dY_Z - V_{Z, \max} \leq 0 \\
 & 0 < \rho_{\min} \leq \rho_e \leq 1 \alpha_{\min} \leq \alpha^Z \leq \alpha_{\max}
 \end{aligned} \tag{18}$$

where Λ^Z are the expansion coefficients set of the multiple prototypes. The relative densities of microstructures are macro-scale design variables to decide the location of the graded ones. The objective function is influenced by a lot of parameters. Thus, it is necessary to find out a simplified representation for implementing the optimization.

The problem will be solved by the gradient based algorithms. Then the method of moving asymptotes method is employed to evolve the design variables in both scales. For the sensitivity analysis, the derivatives of objective function to the densities are expressed as:

$$\frac{\partial J}{\partial \rho_e} = -\mathbf{U}_e^T \left(\int_{\Omega} \mathbf{B}_e^T \frac{\partial \mathbf{D}^H(\chi_e, \Phi^Z(\Lambda^Z, \rho_e))}{\partial \rho_e} \mathbf{B}_e d\Omega \right) \mathbf{U}_e \tag{19}$$

As the regularized effective property can be yielded from the interpolation, the equation is further solved as:

$$\frac{\partial J}{\partial \rho_e} = -\mathbf{U}_e^T \left(\int_{\Omega} \mathbf{B}_e^T \frac{(1-\mu) \mathbf{D}_{base}}{(1+\mu)(1-2\mu)(\rho_{i+1} - \rho_i)} \left[\frac{\nabla \mathbf{D}^H(\Phi_{i+1}^Z(\Lambda_{i+1}^Z, \rho_e))}{\partial \rho_e} \right] \mathbf{B}_e d\Omega \right) \mathbf{U}_e \tag{20}$$

Although the prototype is updated in process of optimization, the modeling scheme for the graded microstructures guarantees that the variation trend of macroscopic response with respect to the relative density is not tremendous. Hence, the evolution of macro-scale design is stable and efficient.

In micro scale, the number of the design variables is $n \times P$, which can be decoupled to perform the sensitivity analysis. It can be seen from Eq. (18) that the regularized effective properties of graded microstructures are too complex to describe in an analytical form. Without special numerical equation treatment, there will be huge amount of computation required in the analysis.

Taking the prototype microstructure as a representation, all the graded ones are related to it. Thus, the sensitivity can be described as:

$$\frac{\partial J}{\partial \kappa_e^Z} = -\sum_{e=1}^{M_Z} \mathbf{u}_e^T \left(\int_{V_e} \mathbf{B}_e^T \frac{\partial \mathbf{D}^H(\chi_e, \Phi^Z(\Lambda^Z, \rho_e))}{\partial \kappa_e^Z} \mathbf{B}_e dV_e \right) \mathbf{u}_e \tag{21}$$

where M_Z is number of graded microstructures from prototype Z, the equations are parallel in a step of optimization. Referring to the shape derivative [21] and the chain rules, the derivatives of objective

function are extended as:

$$\frac{\partial J}{\partial \kappa_e^z} = - \sum_{e=1}^{M_z} \mathbf{u}_e^T \left(\int_{V_e} \mathbf{B}_e^T \frac{1}{|V_{Ne}|} \int_V (\boldsymbol{\varepsilon}_{kl}^0 - \boldsymbol{\varepsilon}_{kl}^*(u^{pq})) \mathbf{D} (\boldsymbol{\varepsilon}_{mn}^0 - \boldsymbol{\varepsilon}_{mn}^*(u^{rs})) H(\Phi) \delta(\Phi) N(x) dV \mathbf{B}_e dV_e \right) \mathbf{u}_e \quad (22)$$

$N(x)$ is the NURBS basis function which is linked to the collocation point and expansion coefficient. The variables of integration are shared for the estimation of effective property and calculation of derivative. Therefore, it prefers to adopt the parallel computation which runs on Graphics Processing Unit using Computing Unified Device Architecture.

4 NUMERICAL EXAMPLES

The multiscale minima compliance problems are tested in this Section. We assume that the Young's modulus and Poisson's ratio of base material are 1 and 0.3 respectively. For the alternative one-scale evolution, the optimization will terminate until the relative differences of objective function and design variables are below 0.01.

In Figure 3(a), the cantilever beam is designed for the cellular structure with multiple prototypes. The beam with 60×20 cells is fixed at the left edge, and the vertical force is applied at center of right. There are five prototypes for generating the corresponding microstructures. The distributions of them are optimized at the predefined subdomain which are divided from calculating the orientations of major principal stresses.

With respect to the unconnected microstructural components, an amendment for prototype is implemented. By adjusting the periodicity interval, the effective property as well as the composed cellular structure is almost unchanged. Choosing the points farthest from the boundary as new nodes, the material must be allocated at the corners of cells, then the connectivity can be guaranteed. The optimized solution is illustrated, and the enlarged views of parts are listed below.

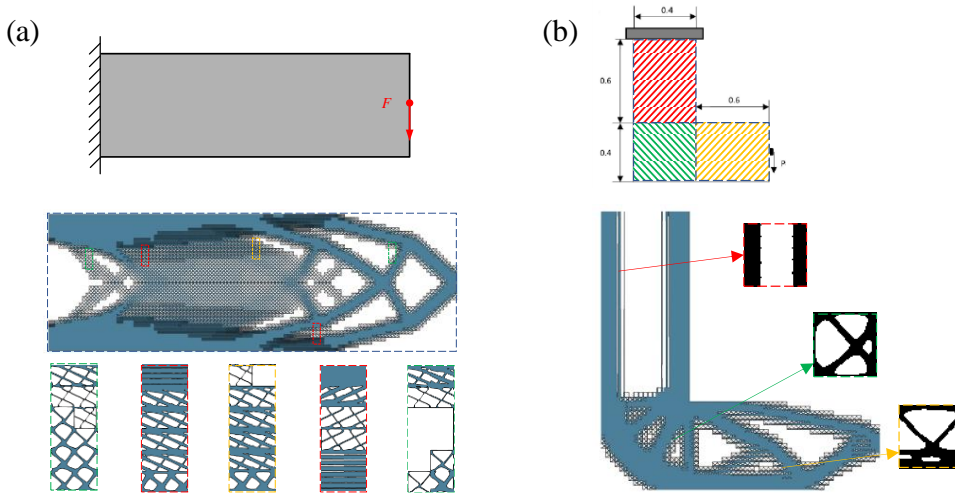


Figure 3: Numerical examples of cantilever beam and L-shape structure.

Another example is the L-shape structure shown in Figure 3(b). The structure is fixed at the upper left side, and a vertical force is applied at the lower right. The macrostructure is divided into three groups which correspond to individual prototype and derived graded microstructures. In comparison to one type of cells, the employment of the multiple prototypes brings more design freedom. The configurations of prototypes can be customized according to the local stress condition. The processing of boundary connections promoted the optimized solution closing to engineering practice.

In addition, the effect of more groups for configurations and distributions of prototypes is studied. The optimized results show the similar distribution to the SIMP method in macro scale. The micro-scale topology shows more detail features as the groups increase.

5 CONCLUSIONS

This paper proposes a multiscale concurrent isogeometric design method for cellular structure constituted by multiple prototype microstructures. There are several highlights as:

- Our work integrates the isogeometric analysis, thus the method has a higher accuracy and fewer design variables.
- The structural skeleton is introduced to generate the graded microstructures. Then the microstructures have unified skeleton and similar topology, thereby promoting the connectivity of the components.
- For the different prototypes, the periodicity intervals are rearranged and the thin-wall material is added at the common interfaces. Thus, the geometric features as well as the structural skeletons can have a smooth transition.

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