Topological optimization of microstructures with isogeometric analysis

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Abstract

This paper will develop a topology optimization method for computational design of architected microstructures based on isogeometric analysis (IGA). The NURBS (non-uniform rational B-splines) is applied to represent the geometry in both the design and analysis processes, as well as interpolate a material density distribution function (DDF) with the desired smoothness and continuity to represent the material layout in the design domain. An isogeometric topology optimization formulation is then formulated based on the DDF, with the energy-based homogenization method (EBHM) to evaluate the effective properties of the microstructure. Several numerical examples are used to demonstrate the effectiveness of the proposed method for computational design of micro-structured periodic composite structures.

Keywords: Topology optimization; Isogeometric analysis; Microstructures

Introduction

Architected materials with a series of periodically distributed microstructures, a kind of rationally artificial materials, are featured with the superior performance, such as the higher specific stiffness and strength, the better fatigue strength and improved corrosion-resistance and etc. [1, 2]. It is known that the performance of architected materials is mostly dependent on the microstructural information, namely the configuration, rather than the constituent properties. Hence, how to develop a rational design framework for architected materials has accepted enormous attentions in recent years.

Topology optimization has made remarkable progress in creating architected materials with new properties [3], which can be viewed as a numerically iterative procedure to optimize material layout in a given design domain, under the specified objective function and constraint(s) [4], Several topology optimization methods have been developed, like the homogenization method [4], the Solid Isotropic Material with Penalization (SIMP) method [5,6], the Evolutionary Structural Optimization (ESO) method [7] and the level set method (LSM) [8-10]. Since an inverse homogenization method was proposed for the architected materials [11], topology optimization combined with the homogenization method has become more and more popular for the design of architected materials with the specific properties [12, 13] and even more advanced topological designs [14,15].

Although the research on how to obtain architected materials has been extensively studied in recent years, only a limited number of works are devoted to obtaining architected materials with the low density. In this paper, we aim to develop an effective and efficient isogeometric topology optimization (ITO) method for the rational design of the low-density architected materials. Firstly, most of the previous works are studied based on the conventional finite element method (FEM). However, the FEM is also one factor to influence the effectiveness of the topology optimization for the design of architected materials. This is because: (1) The finite element mesh is just an approximation of the original shape of the design domain; (2) The lower-order (C0) continuity of the responses between the neighboring finite elements; (3) The lower efficiency to achieve a finite element mesh with the high quality. Isogeometric analysis (IGA) [16] has attracted much interests, due to its favorable features in numerical analysis, such as the consistency between the computer-aided design (CAD) model and the computer-aided engineering (CAE) model, and the high-order continuity between different elements. Secondly, in the developed ITO method, a sufficiently smooth and continuous DDF is constructed to represent the topological changes during the optimization. Thirdly, the IGA is applied to numerical implement the energy-based homogenization method. Finally, the corresponding isogeometric topology optimization is developed for the design of architected materials with the low-density. Several numerical examples are tested to show the effectiveness and efficiency.

NURBS-based IGA

(1) NURBS

An example of a square modelled by NURBS is shown in **Figure 1**. The NURBS basis functions are linearly combined with a series of control points plotted with the red color to construct the geometrical model shown in **Figure 1** (*b*), and the mathematical form of the NURBS surface $\mathbf{S}(\xi,\eta)$ is given as:

$$\mathbf{S}(\xi,\eta)=\sum_{i=1}^{n}\sum_{j=1}^{m}R_{i,j}^{p,q}(\xi,\eta)\mathbf{P}_{i,j} \tag{1}$$

where n and m are the numbers of control points in two parametric directions, and ξ and η denote the corresponding parametric directions. p and q are the polynomial orders. The detailed information for the square is listed below **Figure 1**. $\mathbf{P}_{i,j}$ correspond to the $(i,j)_{th}$ control point. It should be noted that control points are not necessarily on the structural design domain. R are the bivariate NURBS basis functions, and which are constructed by the B-spline basis functions, as:

$$R_{i,j}^{p,q}(\xi,\eta)=\frac{N_{i,p}(\xi)M_{j,q}(\eta)\omega_{ij}}{\sum_{\hat{i}=1}^{n}\sum_{\hat{j}=1}^{m}N_{\hat{i},p}(\xi)M_{\hat{j},q}(\eta)\omega_{\hat{i}\hat{j}}} \tag{2}$$

where ω_{ij} is the positive weight for the $(i,j)_{th}$ control point $\mathbf{P}_{i,j}$. $N_{i,p}$ and $M_{j,q}$ are the univariate B-spline basis functions in two parametric directions, respectively. The B-spline

basis function is defined by the Cox-de-Boor formula [16], and the recursive formula in ξ direction with a non-decreasing knot vector $\Xi = \{\xi_1, \xi_2, \cdots, \xi_{n+p+1}\}$ is defined as:

$$\begin{cases} N_{i,0}(\xi) = \begin{cases} 1 & if\ \xi_i \le \xi_{i+1} \\ 0 & otherwise \end{cases}, & p = 0 \\ N_{i,p}(\xi) = \frac{\xi - \xi_i}{\xi_{i+p} - \xi_i} N_{i,p-1}(\xi) + \frac{\xi_{i+p+1} - \xi}{\xi_{i+p+1} - \xi_{i+1}} N_{i+1,p-1}(\xi), & p \ge 1 \end{cases} \tag{3}$$

It is noted that the fractions with the form 0/0 in Eq. (3) are defined as zero. Similarly, the basis functions $M_{j,q}$ in the η direction are also defined by Eq. (3) with the knot vector. The NURBS basis functions of the square in two parametric directions are respectively displayed in **Figure 1** (*d*) and (*e*). The bivariate basis functions are also plotted in **Figure 1** (*f*).

We can easily see that the NURBS basis functions are featured with several important properties: (1) **Nonnegativity**: $N_{i,p}(\xi) \ge 0$; (2) **Local support**: the support of each basis function $N_{i,p}$ is contained in the interval $[\xi_i, \xi_{i+p+1}]$; (3) **Partition of unity**: for an arbitrary knot span $[\xi_i, \xi_{i+1}]$, $\forall \xi \in [\xi_i, \xi_{i+1}]$, $\sum_{j=i-p}^{i} N_{j,p}(\xi) = 1$; (4) **Continuity**: The continuity between knot spans is equal to C^{p-k} where k is the multiplicity of the knots.

(2) Numerical discretization in the IGA

The NURBS basis functions are firstly applied to parametrize the structural domain, and then construct the space for structural responses. As far as the latter, the key principle is that the continuous solution space is approximately defined by a linear combination of all NURBS basis functions with the nodal responses on control points. The mathematical formula of the space keeps the same as the geometrical model in Eq. (1), while control coefficients correspond to the structural responses on control points, expressed as:

$$\mathbf{x}(\xi, \eta) = \sum_{i=1}^{n} \sum_{j=1}^{m} R_{i,j}^{p,q}(\xi, \eta) \mathbf{x}_{i,j} \tag{4}$$

where $\mathbf{x}$ is the field of structural responses in design domain, and $\mathbf{x}_{i,j}$ is the structural response on the control point $(i,j)_{th}$. Considering the linearly elastic in IGA, the system stiffness matrix is obtained by assembling the element stiffness matrix which is calculated by the Gauss quadrature method, as:

$$\mathbf{K}_e = \sum_{i=1}^{3} \sum_{j=1}^{3} \{ \mathbf{B}^T(\xi_i, \eta_j) \mathbf{D} \mathbf{B}(\xi_i, \eta_j) |\boldsymbol{J}_1(\xi_i, \eta_j)| |\boldsymbol{J}_2(\xi_i, \eta_j)| \omega_i \omega_j \} \tag{5}$$

where $\mathbf{B}$ is the strain-displacement matrix calculated by the partial derivatives of NURBS basis functions with respect to parametric coordinates.

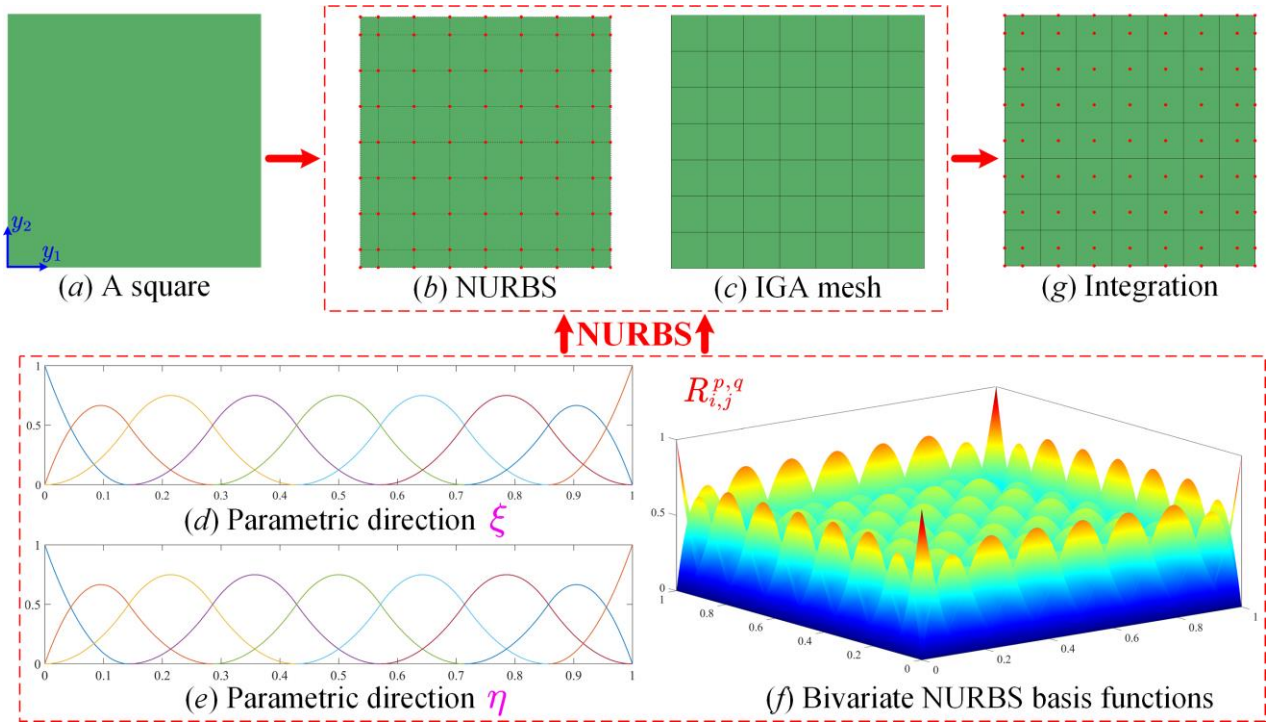

Figure 1. NURBS-based IGA for a square: $\Xi = \{0,0,0,0.1429,\cdots,0.8517,1,1,1\}$, $\mathcal{H} = \{0,0,0,0.1429,\cdots,0.8517,1,1,1\}$; $n = m = 9$; $p = q = 2$.

IGA-based EBHM

The principle of the homogenization is that the macroscopic effective properties of the bulk material are determined by using the information from the microstructure, where the microstructure is described in the coordinate system **y**. Considering the linear elasticity, only the first-order variation term with respect to the parameter expansion ϵ is considered. The effective elastic tensor of the bulk material D^H_{ijkl} can be computed as:

$$D^H_{ijkl} = \frac{1}{|\Omega|}\int_\Omega \left(\varepsilon^{0(ij)}_{pq} - \varepsilon_{pq}\left(u^{ij}\right)\right) D_{pqrs} \left(\varepsilon^{0(kl)}_{rs} - \varepsilon_{rs}(u^{kl})\right) d\Omega \tag{6}$$

where $|\Omega|$ is the area (2D) or volume (3D) of the microstructure, and D_{pqrs} is the locally varying elastic property. $\varepsilon^{0(ij)}_{pq}$ is the linearly independent unit test strain field, containing three components in 2D and six in 3D. $\varepsilon_{pq}\left(u^{ij}\right)$ denotes the unknown strain field in the microstructure, which is solved by the following linear elasticity equilibrium equation with **y**-periodic boundary conditions (PBCs):

$$\int_\Omega \varepsilon_{pq}\left(u^{ij}\right) D_{pqrs} \varepsilon_{rs}\left(\delta u^{ij}\right) d\Omega = \int_\Omega \varepsilon^{0(ij)}_{pq} D_{pqrs} \varepsilon_{rs}\left(\delta u^{ij}\right) d\Omega, \quad \forall \delta u \in H_{per}(\Omega, \mathbb{R}^d) \tag{7}$$

where δu is the virtual displacement in the microstructure belonging to the admissible displacement space H_{per} with **y**-periodicity, and d denotes the dimension of material

microstructure.

The homogenization is numerically performed by discretizing and solving Eq. (8) using the finite element method (FEM), and the utmost importance is the imposing of the PBCs on material microstructure. As an alternative method, the EBHM with a simplified periodic boundary formulation [13] is developed. Here, the numerical analysis of material microstructure is performed by IGA. In IGA, the displacement field in material microstructure is approximately expressed by a combination of the NURBS basis functions with the displacements at control points:

$$\mathbf{u} = \sum_{i=1}^{n}\sum_{j=1}^{m} R_{i,j}^{p,q}(\xi,\eta)\mathbf{u}_{i,j} \tag{8}$$

where $\mathbf{u}_{i,j}$ denote the displacements of the $(i,j)_{th}$ control point. As we can see, NURBS basis functions are linearly combined with nodal displacements to approximate the displacement field in the microstructure. In the application of the EBHM to evaluate material effective properties, the displacement field in material microstructure needs to satisfy the PBCs, and a general form is expressed as:

$$\mathbf{u}_k^+ - \mathbf{u}_k^- = \varepsilon(\mathbf{u}_0)\Delta k \tag{9}$$

where k denote the normal direction of the structural boundary. $\mathbf{u}_k^+$ indicate the displacements of points at the structural boundary with the normal direction k, and the normal direction is in the positive direction of the coordinate axis. $\mathbf{u}_k^-$ correspond to the displacements of points at the opposite structural boundary. Δk is the scale of the material microstructure along the direction of k.

ITO formulation for architected materials

Before developing the DDF, the definition of nodal densities assigned to control points needs to satisfy two basic conditions: (1) non-negativity; and (2) the strict bounds ranging from 0 to 1. Meanwhile, the Shepard function is used to improve the overall smoothness of nodal densities, so as to make sure the smoothness of the DDF. The corresponding mathematical model is given as:

$$\mathcal{G}(\rho_{i,j}) = \sum_{i=1}^{\mathcal{N}}\sum_{j=1}^{\mathcal{M}} \psi(\rho_{i,j})\rho_{i,j} \tag{10}$$

where $\mathcal{G}(\rho_{i,j})$ is the smoothed nodal density assigned to the $(i,j)_{th}$ control point, and $\rho_{i,j}$ is the initial nodal density. $\mathcal{N}$ and $\mathcal{M}$ are the numbers of nodal densities located at the local support area of the current nodal density in two parametric directions. $\psi(\rho_{i,j})$ is the Shepard function of the $(i,j)_{th}$ nodal density.

Assuming that the DDF in the structural domain is denoted by $\mathcal{X}$, the DDF is constructed by the NURBS basis functions with a linear combination of the smoothed nodal densities, expressed as:

$$\mathcal{X}(\xi,\eta)=\sum_{i=1}^{n}\sum_{j=1}^{m}R_{i,j}^{p,q}(\xi,\eta)\mathcal{G}\left(\rho_{i,j}\right) \tag{11}$$

It can be seen that the DDF has the same mathematical formula for NURBS in Eq. (1). The key difference is the physical meaning of control coefficients.

Here, the objective function for the topology optimization of architected materials with the low-density, which is defined by a function of the homogenized elastic tensor, given as:

$$\begin{cases} Find: \boldsymbol{\rho}\ \left\{\left[\rho_{i,j}\right]_{2\mathrm{D}}\ \ \left[\rho_{i,j,k}\right]_{3\mathrm{D}}\right\} \\ Min: J(\mathbf{u},\mathcal{X})=f\left(D_{\hat{i}\hat{j}\hat{k}\hat{l}}^{H}(\mathbf{u},\mathcal{X})\right) \\ S.t: \begin{cases} G(\mathcal{X})=\frac{1}{|\Omega|}\int_{\Omega}\mathcal{X}(\boldsymbol{\rho})v_0\,d\Omega-V_0\le 0 \\ a(\mathbf{u},\delta\mathbf{u})=l(\delta\mathbf{u}),\ \forall\delta\mathbf{u}\in H_{per}(\Omega,\mathbb{R}^d) \\ 0<\rho_{min}\le\boldsymbol{\rho}\le 1,(i=1,2,\cdots,n;j=1,2,\cdots,m;k=1,2,\cdots,l) \end{cases} \end{cases} \tag{12}$$

where $\boldsymbol{\rho}$ denotes the nodal densities assigned to control points, working as the design variables. J is the objective function. d is the spatial dimension of materials. G is the volume constraint, in which V_0 is the maximum value and v_0 is the volume fraction of the solid. $\mathcal{X}$ is the DDF. $\mathbf{u}$ is the unknown displacement field in material microstructure, which have to satisfy the PBCs given in the above. $\delta\mathbf{u}$ is the virtual displacement field belonging to the admissible displacement space H_{per} with **y**-periodicity, which is calculated by the linearly elastic equilibrium equation. a and l are the bilinear energy and linear load functions, as:

$$\begin{cases} a(\mathbf{u},\delta\mathbf{u})=\int_{\Omega}\varepsilon(\mathbf{u})\left(\mathcal{X}(\boldsymbol{\rho})\right)^{\gamma}\mathbf{D_0}\boldsymbol{\varepsilon}(\delta\mathbf{u})\,d\Omega \\ l(\delta\mathbf{u})=\int_{\Omega}\boldsymbol{\varepsilon^0}\left(\mathcal{X}(\boldsymbol{\rho})\right)^{\gamma}\mathbf{D_0}\boldsymbol{\varepsilon}(\delta\mathbf{u})\,d\Omega \end{cases} \tag{13}$$

It should be noted that the elastic tensor is assumed to be an exponential function with respect to the DDF, and γ is the penalization parameter. $\mathbf{D_0}$ is the constitutive elastic tensor of the basic material.

Numerical Examples

In this section, several numerical examples are provided to demonstrate the effectiveness and efficiency of the ITO method. In all examples, the Young's moduli E_0 and the Poisson's ratio v_0 for the basis material are defined as 1 and 0.3, respectively. In the numerical analysis, 3×3

(2D) or 3×3×3 (3D) Gauss quadrature points are chosen in an IGA element. For numerical simplicity, the dimensions of material microstructures in all directions are set to be 1. The penalty parameter is set as 3. Considering 2D materials, the structural design domain is a square with 1×1, shown in **Figure 1**. Here, NURBS surface is applied to parametrize the design domain, where the quadratic NURBS basis functions are chosen and the knot vectors are set as: $\Xi = \mathcal{H} = \{0,0,0,0.01,\cdots,0.99,1,1,1\}$. The corresponding IGA mesh for the design domain has 100×100 elements, and 101×101 (10202) control points are contained in the NURBS surface. In all examples, the maximum material consumption V_0 for different cases is defined as 10%.

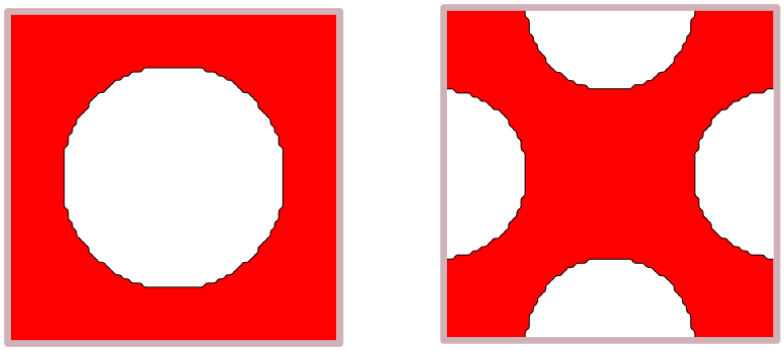

Figure 2. Initial design 1 and Initial design 2

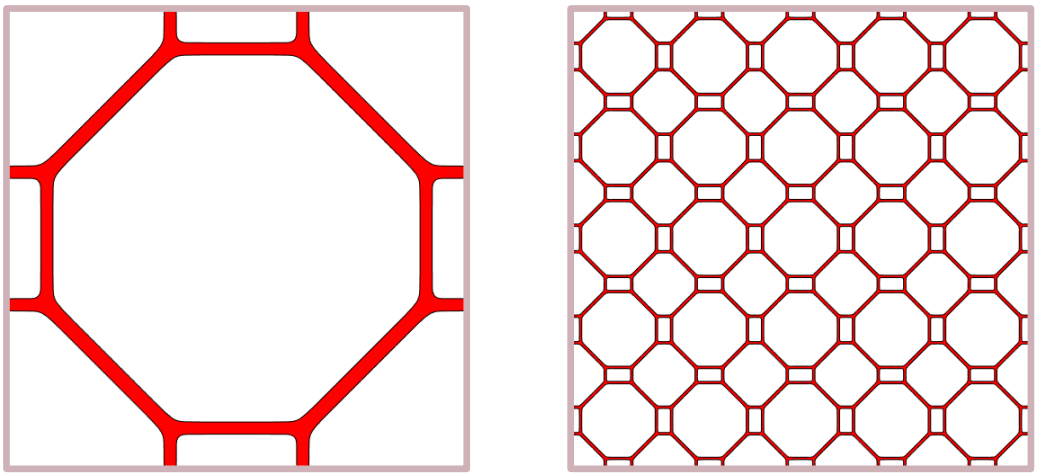

Figure 3. The optimized design 1

In this example, we study the effectiveness of the defined formulation on topology optimization of architected materials with the maximum bulk modulus in an extremely low volume fraction. As shown in Fig. 2, two different initial designs are defined and then discussed into two different cases, respectively. As shown in Figs. 3 and 4, the optimized results of the low-density architected materials with the maximum bulk modulus are provided. It can be easily seen that the optimized results are very similar to the known lattice structures, but the current design is obtained from a rational design using the isogeometric topology optimization framework.

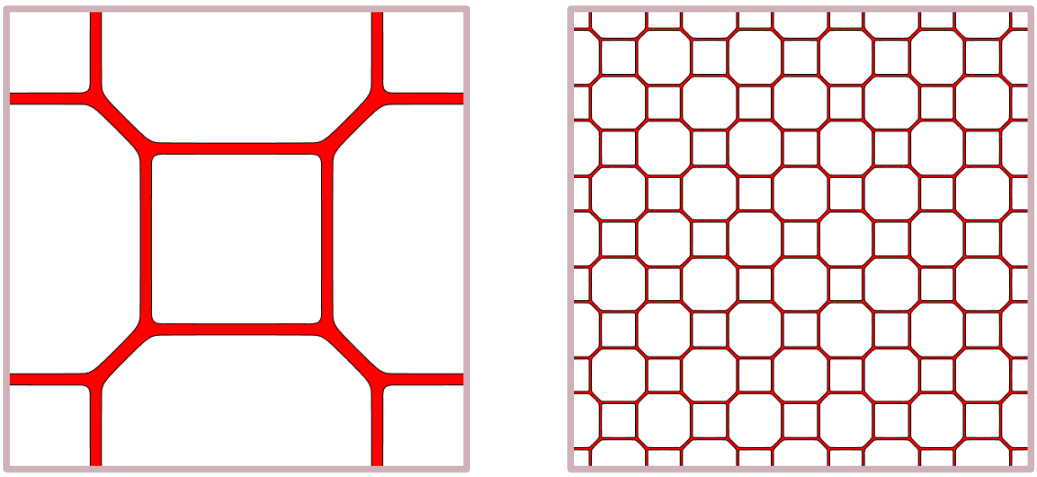

Figure 4. The optimized design 2

Moreover, we also perform the discussions of the ITO method on the optimization of architected materials with the maximum shear modulus. In this example, the parameters are consistent with the above example, and the objective function is defined based on the shear modulus. Two different cases are both discussed with two distinct initial designs, and the optimized topologies of the low-density architected materials with the maximum shear modulus are displayed in Figs. 5 and 6. As we can see, the optimized design with the bars in 45^{o} can provide the sufficient stiffness for affording the load, which shows the effectiveness of the current work. Additionally, the optimized low-density architected materials are also analogous to the known lattice materials, which has gained the extensive applications in the aerospace engineering. Hence, we can easily see that the current ITO method has the capability to seek the low-density architected materials with the sufficiently stiffness.

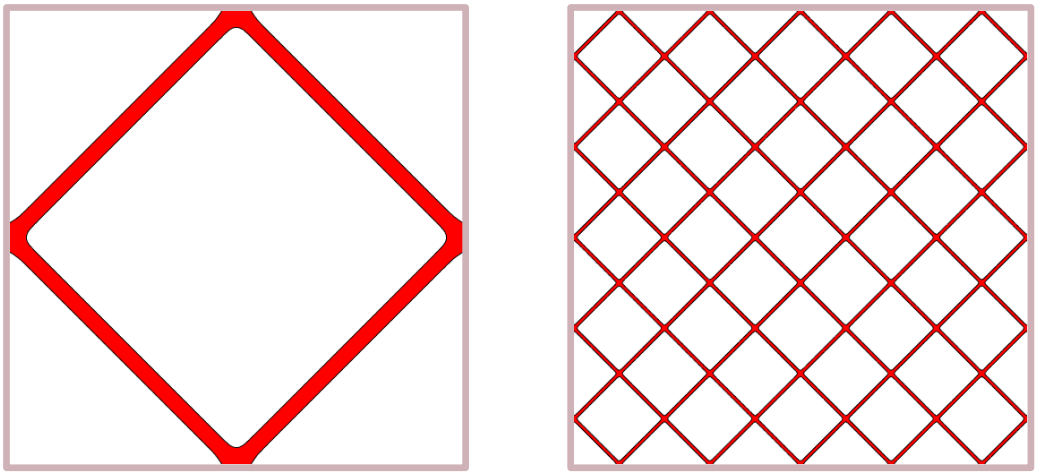

Figure 5. The optimized design 1

Conclusions

In this paper, an effective and efficient ITO method is developed for the rational design of the low-density architected materials with the optimal stiffness, where a DDF with the desired smooth and continuous is constructed to represent the structural topology and IGA is applied to solve the displacement responses in microstructures. The EBHM to predict the macroscopic

effective properties is numerical implemented by the IGA, with the consideration of the periodic boundary conditions. Several numerical examples are given to show the basic features and effectiveness of the proposed ITO method. We can obtain the optimized low-density architected materials, very similar to the lattice materials.

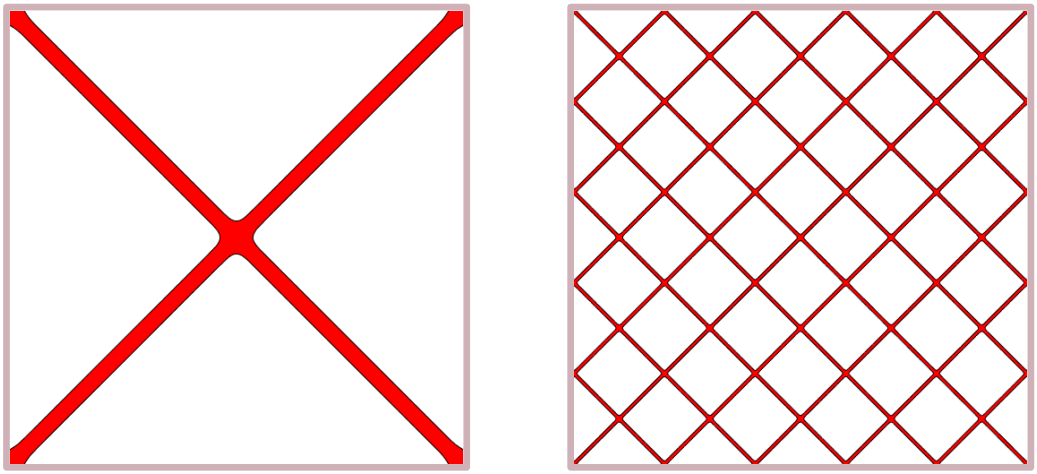

Figure 6. The optimized design 2

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