A TOPOLOGY OPTIMIZATION APPROACH APPLIED TO METAMATERIAL MECHANISM DESIGN

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Abstract. *Metamaterials are artificial structures that perform unconventional mechanical properties. These structures are obtained by a repetitive cell patterns, rather than the material they are made of. Each cell of the metamaterial can be designed to have a controlled directional movement. This allows to create devices with a desired mechanical function, such as the mechanisms. In this work, compliant mechanism is designed by using the Topology Optimization (TO) method to generate microstructure unit cells that simulate the effect of metamaterials that have negative Poisson's ration (auxetic materials). The unit cell (microstructure) of metamaterial is driven to have the same characteristics of a compliant mechanism, that is, a monolithic body that delivers a desired motion when is loaded in a certain way. Thus, the topology optimization problem of compliant mechanisms is proposed to design more efficient these microstructures for a certain specific structural mechanical property, such as the auxetic behavior. Polygonal finite element meshes are introduced in the TO formulation to avoid the hinges (one-node connections) in the compliant mechanism design. Moreover, a pattern repetition constraint is applied to generate an auxetic macrostructure, allowing to create a metamaterial mechanism efficiently. Computational simulations are also carried out to verify the results of the metamaterial design.*

Keywords: *topology optimization, compliant mechanism, polygonal elements, auxetic structure, metamaterial*

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1 INTRODUCTION

Unlike conventional mechanisms, which are structures composed of rigid bodies connected by joints, a compliant mechanism is a monolithic structure that explores the deformation property as source of motion (Howell, 2001). Compliant mechanisms have wide application in devices that involve precision mechanics, such as the well-known MEMS (micro-electro-mechanical systems) (Gad-el-Hak, 2002). Moreover, compliant mechanism can also be used in the design of grippers, jaws or scissors that require precise motion, such as medical surgical instruments.

This work focuses on using the topology optimization to compliant mechanism design applied to create a microstructure that simulates the behavior of auxetic materials, which have negative Poisson ratio. Unlike conventional materials, an auxetic material has very unusual property of becoming laterally thinner when compressed and thicker when stretched. The auxetic behavior can provide to structural materials notable mechanical properties, such as increased resistance to shear and better energy absorption capacity (Mir el al., 2014).

However, the obtaining of an auxetic material is an activity that is not completely explored, since its design technique is new and can be improved. Auxetic materials can be obtained through structural transformation of conventional materials, such as foams or polymers (Alderson et al., 2002). Another way to obtain an auxetic material (macrostructure) is to design a reentrant unit cell (microstructure) with auxetic behavior and apply a periodic repetition of this cell over a design domain (Fig. 1). Thus, one obtains the auxetic behavior from the mechanism deformation that arises from the geometric configuration of the periodic reentrant unit cell (Liu & Hu, 2010), in which each member rotates about the junctions when is loaded to produce expansion of the structure in both directions (horizontal and vertical).

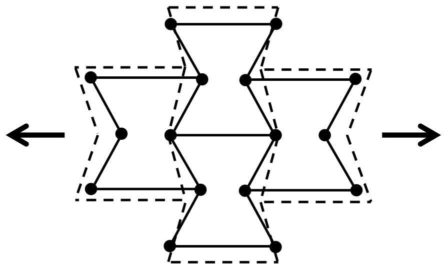


Figure 1. Reentrant structure with auxetic behavior

The design of the unconventional reentrant structures is traditionally based on the designer experience. However, in order to make the design of these structures more systematic, it has recently been improved through the application of the optimization methods. Thus, a very powerful method for this purpose is the topology optimization method (TOM) (Bendsøe & Sigmund, 2003), which systematically seeks the optimized distribution of material within a fixed design domain by removing and adding material in each point of that domain. Sigmund (1994) used the TOM to design materials with any prescribed properties, such as negative Poisson's ratio, in which the unit cell is modeled as a truss structure. Schwerdtfeger et al. (2011) applied the TOM to design a material having a negative Poisson's ratio, using a previously known auxetic cell structure as starting point for the optimization process.

In general, the unit cell structure (microstructure) has the same characteristics of a compliant mechanism, that is, it consists of a monolithic body that delivers a desired motion when is loaded in a certain way. Therefore, the topology optimization problem of compliant mechanisms can be applied to design more efficient periodic microstructures for a certain specific structural property, such as the auxetic behavior (Kaminakis et al., 2015).

Next sections are organized as follows. Section 2 describes the topology optimization problem and the sensitivity analysis. Section 3 shows the numerical implementation using polygonal finite elements. Section 4 presents some results. Finally, Section 5 gives the conclusions.

2 TOPOLOGY OPTIMIZATION PROBLEM

Let's consider the input and output to be a tensile load (F_{in}) and a displacement (u_{out}), respectively. Thus, in order to obtain the auxetic behavior, the mechanism structure domain should be necessarily designed to expand (u_{out}) in the perpendicular to direction of the applied tensile load (F_{in}). Now, considering a very small square region of the structure domain, in the plane, the Poisson's ratio can be written as (Kaminakis and Stavroulakis, 2012):

$$\nu = -\frac{\Delta_y}{\Delta_x} = -\frac{u_{\text{out}}}{u_{\text{in}}} \tag{1}$$

where u_{in} is the input displacement produced by the input force (F_{in}). Δ_x and Δ_y are the axial and transversal elongations, respectively. Thus, to obtain an optimized compliant mechanism that mimics a microstructure of an auxetic material, the topology optimization problem can be formulated to maximize the Poisson's ratio given by Eq. (1).

Here, the classical formulation of topology optimization applied to compliant mechanism design has been adopted, in which a spring with stiffness k_{in} is included at the input displacement (u_{in}) region, in order to control the stress level in the mechanism structure (Sigmund, 1997). Therefore, the objective function of the optimization problem can be given to maximize the output displacement (u_{out}). In other words, maximize u_{out} is equivalent to maximizing the output work performed on a gripped or pinched object modelled by a spring with stiffness k_{out} (Bendsøe & Sigmund, 2003).

Thus, the topology optimization problem is stated as follows:

$$\begin{aligned} &\underset{\mathbf{0}<\mathbf{d}\leq\mathbf{1}}{\text{maximize}} && u_{\text{out}} \\ &\text{subject to} && \boldsymbol{\rho} = f(\mathbf{d}) \\ & && \sum_{i=1}^{N} \rho_i v_i \leq f_r V \\ &\text{with } \mathbf{K}(\boldsymbol{\rho})\mathbf{u} = \mathbf{f} && \text{(equilibrium equations)} \end{aligned} \tag{2}$$

where v_i is the volume of i-th element, V is the volume of the design domain, f_r is the prescribed volume fraction, and N is the number of elements of the discretized domain. Moreover, in the nested formulation $\mathbf{u}$ is the global displacement vector, which depends on design variables $\mathbf{d}$, $\mathbf{K}$ is the global stiffness matrix, and $\mathbf{f}$ is the global load vector. It is noticed that k_{in} and k_{out} are implicitly considered in the equilibrium equations of the problem.

The first constraint, $\boldsymbol{\rho} = f\ (\mathbf{d})$, is defined on the unified projection-based approach proposed in Vatanabe et al. (2016), which is applied for implementing a minimum member size constraint. Thus, this constraint is given by:

$$\rho_i = \left(\sum_{j \in \Omega_k} d_j^q \right)^{\frac{1}{q}} \quad with \quad q > 0 \tag{3}$$

where a set of variables d_j are calculated and projected onto the domain of pseudo-densities (ρ_i). In this approach, projection and mapping techniques (Guest et al., 2004; Le, 2006) are combined for generating manufacturing constraints that is able to control the optimization solution without adding a large computational cost.

The sensitivity of the objective function with respect to the design variables (d_j) is given by (Vatanabe et al., 2016):

$$\frac{\partial f\left(\rho\left(d_j\right)\right)}{\partial d_j} = \sum_{i \in \Omega} \frac{\partial f}{\partial \rho_i} \frac{\partial \rho_i}{\partial d_j} \tag{4}$$

where Ω is the design domain. $\partial \rho_i / \partial d_j$ is calculated by direct differentiation of Eq. (3).

The objective function of the optimization problem, Eq. (2), can be written as:

$$u_{\mathrm{out}} = -\mathbf{l}^T \mathbf{u} = f \tag{5}$$

where $\mathbf{l}$ is a vector composed of zeros except for the position at the output displacement (u_{out}) point which is one. Thus, by applying the adjoint method, the sensitivity $\partial f / \partial \rho_i$ is given by:

$$\frac{\partial f}{\partial \rho_i} = \boldsymbol{\lambda}^T \frac{\partial \mathbf{K}}{\partial \rho_i} \mathbf{u} \tag{6}$$

where the adjoint vector $\boldsymbol{\lambda}$ is the solution of the system $\mathbf{K}\boldsymbol{\lambda} = -\mathbf{l}$.

The derivative $\partial \mathbf{K} / \partial \rho_i$ is calculated from direct differentiation of the global stiffness matrix, considering a penalization imposed by the material model. In this work, a version of the Solid Isotropic Material with Penalization (SIMP) (Bendsøe, 1989; Zhou & Rozvany, 1991) is adopted as material model, in which a very weak material (E_{min}) is used to represent the void region ($\rho = 0$) and, thus, allowing to avoid singularity of the finite element stiffness matrix.

3 NUMERICAL IMPLEMENTATION

The optimization problem, Eq. (2), is solved by the iterative algorithm shown in Fig. 2, which depicts the topology optimization (TO) implementation containing the unified based-projection technique adopted in this work. Initially, guess design variables (d_j) are provided as input to TO algorithm, which are used to obtain the initial pseudo-densities (ρ_i) by using the projection function, Eq. (1). After that, the implemented TO algorithm follows the usual procedure outlined in the references on topology optimization (Bendsøe & Sigmund, 2003), that is, the algorithm calculates the objective function value and performs the sensitivity analyses, which are used for the optimization solver as guidance for recalculating material distribution along the design domain. A new set of design variables is generated after each iteration and the optimization cycle continues until convergence is achieved for the objective function.

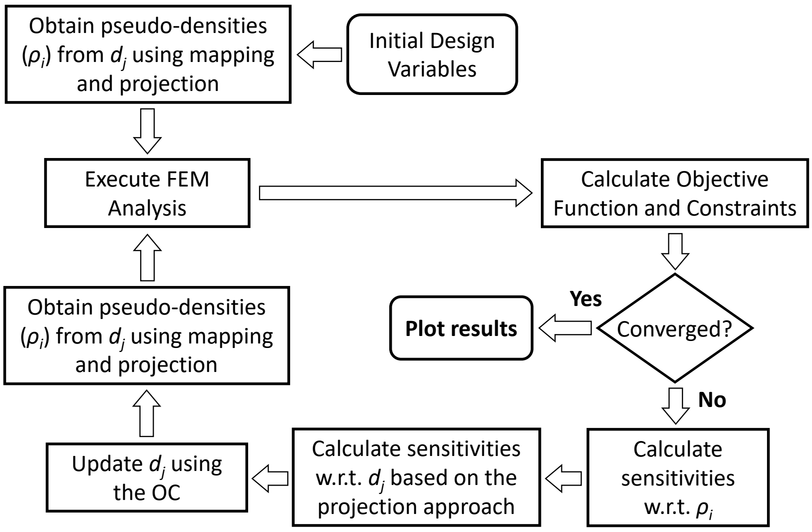


Figure 2. Flowchart of the TO algorithm

In this work, the design domain is discretized using the Polymesher (Talischi et al., 2012a), which is a robust mesh generator solver that uses Centroidal Voronoi diagrams to generate a polygonal mesh. As the traditional finite element discretization, using triangular or quadrilateral elements, are susceptible to exhibit checkboards patterns and one-node connections in topology optimization results the polygonal finite elements (Saxena & Saxena, 2008; Talischi et al., 2010) have employed to overcome this issue. Adjacent polygons always keep an edge in common having two connected vertices, and due to the virtue of its geometry can directly eliminate the occurrence of one-node connection (hinges) in topology optimization applied to compliant mechanism design.

The topology optimization procedure (Fig. 2) is implemented by using an efficient MATLAB code for structural topology optimization called PolyTop (Talischi et al., 2012b, Pereira et al., 2011). In this work, the well-known optimality criteria (OC) method has been employed in the Polytop to update the design variables of the topology optimization problem. Nevertheless, other optimization solvers can be explored for this purpose, such as the method of moving asymptotes (MMA) (Svanberg, 1987). In this case, few changes in the original OC solver, such as using new move limit and damping parameters and replacing positive sensitivities by small positive values (Bendsøe & Sigmund, 2003), are applied to stabilize the convergence of the TO algorithm for compliant mechanism design.

4 RESULTS

The square design domain and boundary conditions (input force F_{in}, output displacement u_{out}, and fixed supports) applied to the compliant mechanism design that simulates an auxetic microstructure are shown in Fig. 3. Due to symmetry and to save computational time, only a quarter of the entire structure domain is used for the topological optimization solution.

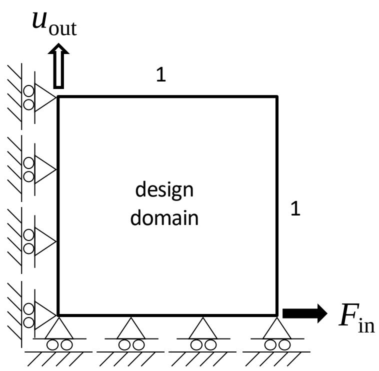
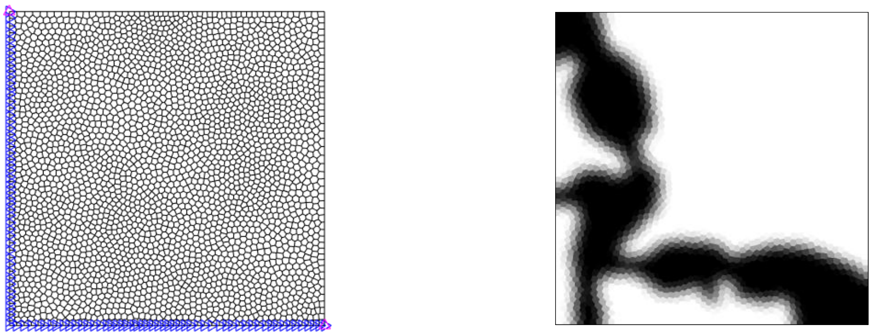


Figure 3. Design domain and boundary conditions

For all examples, the input force F_{in} is equal to 1, penalization factor of the SIMP is equal to 3, and Poisson's ration of the base solid material is equal to 0.3. Moreover, a relation between elastic modules of the solid (E_0) and the weak material is defined as $E_{min} = 10^{-4} E_0$. Consistent units are employed.

4.1 Unit auxetic cell design

In this example, the design domain is discretized in 3,000 polygonal elements, as shown in Fig. 4a. A random polygonal mesh is generated in the PolyMesher algorithm, which allows obtaining a non-structured mesh with different polygonal elements. The bottom and left sides of the polygonal mesh are constrained along the vertical and horizontal directions, respectively. Figure 4b shows the result obtained by the TO algorithm.



(a) (b)

Figure 4. (a) Polygonal FE mesh; (b) topology optimization result

Springs with k_{in} = 0.1 and k_{out} = 0.1 are applied at the input force and output displacement points, respectively. The volume fraction (f_r) is equal to 30% of the fully volume of solid domain, and the radius (R) of minimum member size constraint is equal to 0.05. Figure 5 shows the convergence of the solution, in which random values is adopted to the design variables at the start of the topology optimization process.

As can be seen in Fig. 4b, this result is free for checkerboard pattern, which is attributed essentially to the use of the polygonal elements. It is also verified that the microstructure obtained from the implemented TO algorithm has auxetic behavior with Poison's ratio of ν =

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− 0.131. This value is calculated by applying Eq. (1), considering the heterogeneous domain resulting from the topology optimization process.

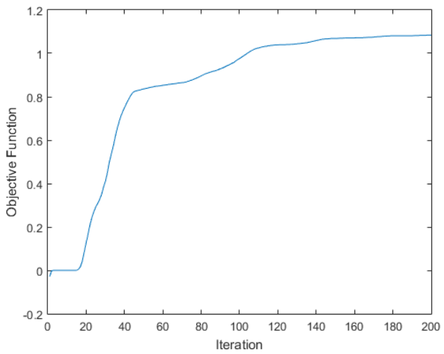
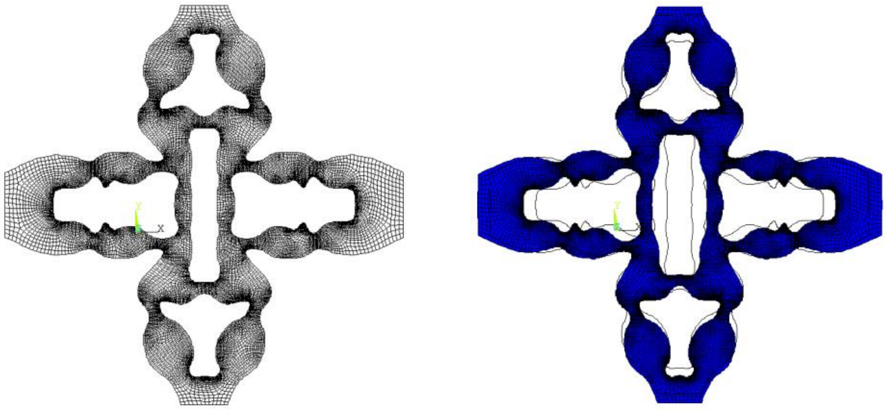


Figure 5. Convergence curve of the optimization process

A post-processing is carried out after the last iteration of the optimization process, by using a CAD software (SolidWorks), to produce a well-defined contour for the topology optimization result (Fig. 4b) and to generate a geometric model to be verified by finite element (FE) analysis. Figure 6 shows the deformed and undeformed shapes of the auxetic microstructure created by topology optimization of compliant mechanism. The deformed shape is simulated through commercial FE software (ANSYS). The unit cell of the microstructure shown in Fig. 4b can be repeated several times into a domain to generate a macrostructure that simulates an auxetic metamaterial mechanism.



(a) (b)

Figure 6. Auxetic microstructure: (a) FE mesh of the post-processed result; (b) deformed shape simulated by FE analysis

4.2 Applying pattern repetition constraint

Nevertheless, a pattern repetition constraint could be included in the topology optimization problem to produce repeated cells in a controlled manner, in such way that different regions in the domain, subjected to different boundary conditions, should assume the same topology for all situations. In this case, a structured polygonal mesh with 120x120 elements are adopted to discretize the design domain.

Analogous to the previous example, a square domain with symmetry conditions (Fig. 3) is taken into account. Springs with stiffness $k_{in} = 0.05$ and $k_{out} = 0.025$ are applied at the input load and output displacement points of the domain. Volume fraction (f_r) is 50% and distribution of homogeneous material is adopted at the start of the topology optimization process. Figure 7 shows the result (entire domain) obtained from topology optimization of compliant mechanism with pattern repetition constraint (3x3 patterns), considering R = 0.01 to the minimum member size constraint.

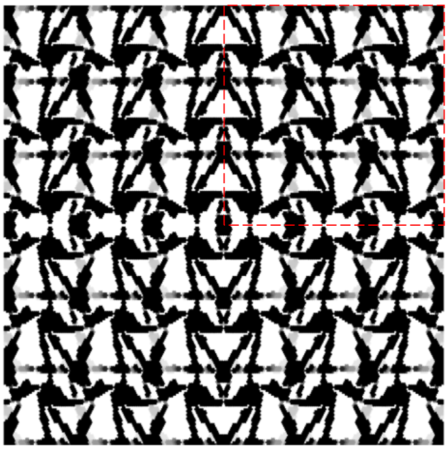


Figure 7. Auxetic macrostructure obtained by TO algorithm (3x3 patterns)

In this example, the volume constraint has been increased, since more than one cell and small relevance regions into the domain need to be filled with mass. The macrostructure obtained (Fig. 7) has auxetic behavior with Poison's ratio of $\nu = -0.090$, which can be improved by controlling the work performed by the output force (or k_{out}) on the compliant mechanism design.

5 CONCLUSION

A topology optimization algorithm is implemented to handle compliant mechanism design in order to create auxetic structures (metamaterials). Polygonal finite elements are employed, improving the topology optimization process to avoid the formation of one-node connections in the compliant mechanism design, as well the checkerboard problem. Moreover, a minimum member size constraint has been included in the topology optimization problem. Pattern repetition constraint is employed to generate in a straightforward manner macrostructures that presents auxetic behavior (negative Poisson's ration). Computational simulations using commercial FE software are carried out to verify the auxetic behavior of the topology optimization results. The results are focused on bidimensional (2D) metamaterial mechanisms under the linear elasticity assumption. Thus, a natural extension for this work is to implement tridimensional (3D) models that can be handling computationally at a low cost. Moreover, nonlinear finite elasticity may be considered to topology optimization, in order to obtain more accurate models to the structural response of compliant mechanisms under large deformation. Finally, the auxetic structure behavior may be improved by extending this work to multimaterial compliant mechanism design.

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