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METAMATERIAL MECHANISM DESIGN BY TOPOLOGY OPTIMIZATION IN TRUSS GROUND STRUCTURE DOMAINS WITH LARGE DISPLACEMENTS

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Abstract. Metamaterials are artificial structures engineered to have extremal properties that are not found in naturally occurring materials, such as negative Poisson's ratio (auxetic behavior). These structures are obtained by repetitive cell patterns. Each cell of the metamaterial can be designed to have a controlled directional movement. This allows the creation of devices with a desired mechanical function. Compliant mechanisms perform certain functions from the elastic deformation of its body. The topology optimization (TO) technique has been shown to be the most generic and systematic for the design of compliant mechanisms. It consists of a method that distributes material within a domain in order to achieve the specified objective function, satisfying the imposed constraints. In this work, compliant mechanism is designed by using the Topology Optimization method to generate microstructure unit cells that simulate the effect of metamaterials that have negative Poisson's ratio (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. TO is performed in domains discretized by truss elements (ground structure), where the cross-sectional areas of the elements are the design variables. Large displacements are considered, which establishes a nonlinear relation between deformation and displacement and requires the use of nonlinear FEM. Computational simulations are presented to verify the results of the metamaterial design.

Keywords: Metamaterial, Topology Optimization, Compliant Mechanisms, Auxetic Structure, Ground Structure

1 Introduction

Metamaterials are artificial structures designed to have extreme properties that are not found in the natural form of materials, such as negative Poisson's ratio (auxetic behavior). These structures are obtained by repeating a cell pattern. Each metamaterial cell can be designed to have a directional controlled movement. This allows the creation of mechanisms with a desired mechanical function. Compliant mechanisms can be used to generate microstructures in unit cells that simulate the effect of metamaterials (auxetic materials). The metamaterial unit cell (microstructure) must have the same characteristics as the compliant mechanism, that is, a monolithic body that performs a desired movement from a load at a given point [1].

Common materials have positive ν, i.e. the material contracts transversely under uniaxial extension and expands laterally when compressed in one direction. For linear and isotropic elastic materials, the Poisson's ratio cannot be less than -1 or greater than 0.5. This is because of empirical considerations related to work and energy factors, so that the modulus of elasticity has positive values [2]. For auxetic materials, these limits are different. Auxiliary behavior can guarantee structural materials mechanical properties such as higher shear strength and higher energy absorption capacity [3].

Auxetic materials can be obtained by structural transformation of conventional materials such as polymers [4]. Another way to obtain this macrostructure is by designing a reentrant unit cell (microstructure) with auxetic behavior (Fig. 1) and applying the periodic repetition of this cell by a design domain. Thus, the auxetic behavior is obtained from the deformation of the mechanism that results from the geometric configuration of periodic reentrant unit cells [5].

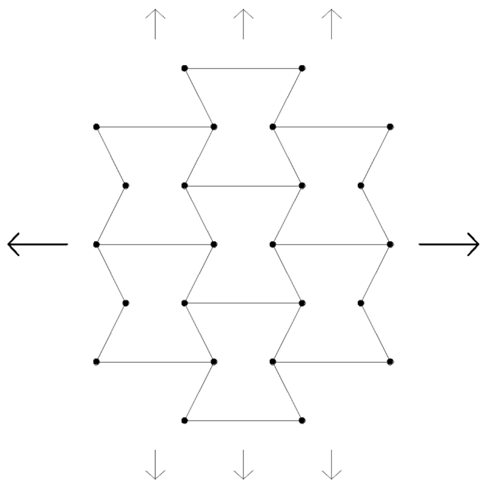

Figure 1. Reentrant unit cell

Through optimization methods, it is possible to design reentrant cells in a more systematic and improved way. The topology optimization method (TOM) is a powerful way for this purpose. In Sigmund [6], cells in truss shape are used to obtain materials with prescribed properties, such as negative Poisson's ratio.

The method can be extended for metamaterial design in various applications such as thermoelastic microstructures with negative thermal expansion coefficient, electromagnetic etc. Using 3D printers, the design of auxetic structures can be put into practice and fabricated with the final material distribution [7].

In the topological optimization problem for auxetic structures, as input and output are considered a load F_{in} and a displacement u_{out}, respectively. Therefore, in order to obtain auxetic behavior, the domain of the mechanism structure must necessarily be designed to expand u_{out} perpendicular to the direction of the applied load F_{in}. Considering a small rectangular region of the structure domain, in the plane, the Poisson's ratio can be written as [8]:

$$\nu = -\frac{\Delta_y}{\Delta_x} = -\frac{u_{out}}{u_{in}} \quad (1)$$

Where u_{in} is the input displacement produced by the input force F_{in}. Δ_x and Δ_y are the axial and transverse elongations, respectively. Thus, to obtain an optimized compliant mechanism that reproduces the microstructure of an auxetic material, the topological optimization problem can be formulated to maximize ν from Eq. (1).

In this work, the objective is the design of a compliant mechanism that simulates the behavior of an auxetic metamaterial created in a MATLAB solver developed by the authors. Large displacements are considered, so nonlinear FEM is used to provide more accurate results.

In section 2, the optimization problem and its sensitivity analysis are presented. Section 3 shows flowcharts of the numerical implementation of the problem and its algorithms. Section 4 presents results and the final structure. Finally, section 5 gives the conclusion.

2 Topology optimization problem

One of the most important objectives in the synthesis of compliant mechanisms is to be able to control the ratio between input and output displacements and input and output forces, which are described by geometric and mechanical advantage, respectively. The TO of compliant mechanisms can be made from continuous or ground structure domains [9].

For mechanisms, it is important to model the problem using nonlinear finite element analysis. Structures with large displacements may or may not be subject to large strains. In this paper small strains are considered, so material nonlinearity can be ignored.

The optimization problem for compliant mechanisms aims to maximize the u_{out} displacement performed in a spring with k_{out} stiffness. By specifying different values of k_{out} we can control the range of displacement. If we specify a low value for k_{out} we get large output displacements and vice versa. An optimization problem incorporating these ideas can be written as

$$\max_{A} u_{out} = \boldsymbol{L}^T \boldsymbol{u}(A)$$

$$\begin{aligned} \text{Subject to:} \quad & \boldsymbol{R} = 0 && \text{(equilibrium equation)} \\ & \textstyle\sum_{i=1}^{n} A_i L_i \le V_{max} && \text{(volume constraint)} \\ & A_i^{min} \le A_i \le A_i^{max} && i = 1,2,\dots,n \end{aligned} \quad (2)$$

Where R is the residual of the finite element analysis problem with the applied load F_{in}.

The Green-Lagrange strain (nonlinear) is defined by

$$\eta_{ij} = \frac{1}{2}(u_{i,j} + u_{j,i} + u_{k,i}u_{k,j}) \quad (3)$$

where u is the displacement and the subscript "$,j$" means differentiation in relation to the coordinate j.

Variation in deformation is given by

$$d\boldsymbol{\eta} = \boldsymbol{B}(u)d\boldsymbol{u} \quad (4)$$

where $\boldsymbol{B}$ is the strain-displacement matrix.

Linear Hooke's Law for Piola-Kirchhoff stresses and Green-Lagrange strains is written as

$$s_{ij} = C_{ijkl}^{e}\eta_{kl} \quad (5)$$

where C_{ijkl}^{e} is the constitutive tensor of element e.

Residual is defined as the error in obtaining the equilibrium

$$\boldsymbol{R}(u) = \boldsymbol{f} - \int_V \boldsymbol{B}(u)^T \boldsymbol{s}(u)\, dV \tag{6}$$

where f is the external force vector and s is Piola-Kirchhoff stress written in vector form. The integration is done with the undeformed volume. Equilibrium is found when residual vector is equal to zero.

Finite element equilibrium is solved iteratively using Newton-Raphson method, which requires the determination of the tangent stiffness matrix

$$\boldsymbol{K}_T = -\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{u}} \tag{7}$$

The spring on the output node simulates the resistance of a part (Fig. 2). The goal of the problem is to maximize the work done on the spring. It is possible to design compliant mechanisms with emphasis on force (high spring stiffness) or mechanisms with emphasis on displacement (low spring stiffness) [10].

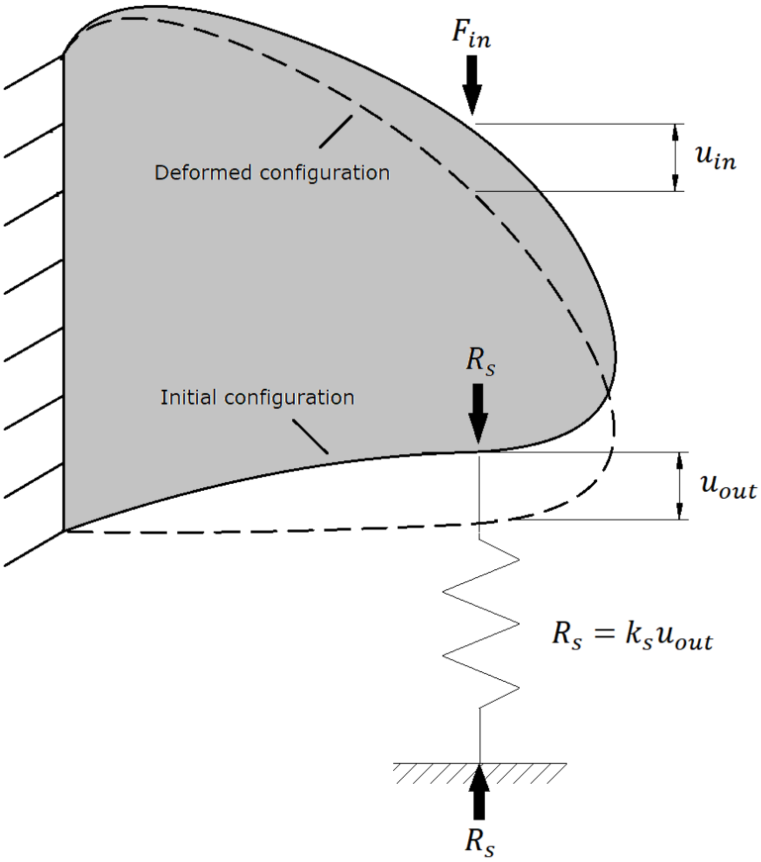

Figure 2. Compliant mechanism design with spring

W_{out} work on stiffness output spring k_s can be calculated by

$$W_{out} = \frac{1}{2} R_s u_{out} = \frac{1}{2} k_s u_{out}^2 \tag{8}$$

where R_s and u_{out} are the resistance force and the displacement at the output node, respectively.

2.1 Sensitivity analysis

All deterministic optimization methods (except zero-order methods) require the calculation of the first derivatives (or gradients) of the objective function or constraints that are also called sensitivities.

Sensitivity must be calculated accurately, otherwise the method will move in the wrong direction, not reaching the optimal solution [11].

The sensitivity analysis of the large displacements compliant mechanism problem is carried out as follows [10].

Displacement u_i of a prescribed degree of freedom i can be written as

$$u_i = \boldsymbol{L}^T \boldsymbol{U} \tag{9}$$

where L is a vector of zeros, except in i position, where its value is 1.

The sensitivity of the displacement u_i in relation with changes in the design variable e is

$$\frac{du_i}{dA_e} = \boldsymbol{L}^T \frac{d\boldsymbol{U}}{dA_e} \tag{10}$$

Adjoint method is used to determine the sensitivity $d\boldsymbol{U}/dA_e$.

Introducing a vector of lagrangian multipliers λ, assuming the equilibrium in Eq. (6) was found, the term $\lambda^T \boldsymbol{R}$ is equal to zero and can be added to the displacement without changing nothing

$$u_i = \boldsymbol{L}^T \boldsymbol{U} + \lambda^T \boldsymbol{R} \tag{11}$$

The sensitivity of this modified function is

$$\frac{du_i}{dA_e} = \boldsymbol{L}^T \frac{d\boldsymbol{U}}{dA_e} + \lambda^T \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}} \frac{d\boldsymbol{U}}{dA_e} + \frac{d\boldsymbol{R}}{dA_e} \right) \tag{12}$$

As $\boldsymbol{R} = 0$, the lagrangian multiplier vector λ can be chosen freely. To eliminate the unknown term $d\boldsymbol{U}/dA_e$ of Eq. (12), λ is chosen as

$$(\boldsymbol{L}^T - \lambda^T \boldsymbol{K}_T) \frac{d\boldsymbol{U}}{dA_e} = 0 \tag{13}$$

That corresponds to the solution of the linear equations system

$$\boldsymbol{K}_T \lambda = \boldsymbol{L} \tag{14}$$

where the tangent matrix is considered symmetric ($\boldsymbol{K}_T^T = \boldsymbol{K}_T$). Inserting the solution of the system λ in Eq. (12), we come to the sensitivity

$$\frac{du_i}{dA_e} = \lambda^T \frac{\partial \boldsymbol{R}}{\partial A_e} \tag{15}$$

The gradient $\partial \boldsymbol{R}/\partial A_e$ is developed as follows [12]

].

$$\begin{aligned} \frac{\partial \boldsymbol{R}}{\partial A} &= \frac{\partial (\boldsymbol{K}(u, A)u - \boldsymbol{L})}{\partial A} \\ &= \frac{\partial (\boldsymbol{K}(u, A)u)}{\partial A} - \frac{\partial \boldsymbol{L}}{\partial A} \\ &= \left[\frac{\partial \boldsymbol{K}(u, A)}{\partial A} \right] u \end{aligned} \tag{16}$$

Substituting in Eq. (15)

$$\frac{du_i}{dA_e} = \lambda^T \left[\frac{\partial \boldsymbol{K}(u, A)}{\partial A} \right] u \tag{17}$$

3 Numerical implementation

3.1 Sequential linear programming

Sequential Linear Programming (SLP) is a robust and efficient way to solve constrained nonlinear optimization problems. It is a direct method for solving a nonlinear optimization problem by solving a series of linear programming (LP) problems. It has great applicability in structural optimization.

Using first order Taylor expansion for the design variable X_i, each LP problem is generated by the linear approximation of the objective function and constraints [13]. The LP problem is solved by using the simplex method to find the new vector X_{i+1}. If X_{i+1} does not meet the convergence criterion the problem is linearized again over the point X_{i+1} and the procedure continues until the optimal solution X^* is found.

The objective functions and constraints are approximated by expansion in Taylor series to first-order derivative terms and limiting the variation of each design variable in each linear subproblem trough moving boundaries.

As shown by the flowchart in Fig. 3, first, an initial value is determined for the design variable A_i. Then the sensitivities, the objective function gradients in relation to the design variable (df/dA), are calculated. If any of the areas violates the established boundaries, its value is changed to the minimum area if the value is smaller than the minimum area. If it is larger than the maximum area, its value is changed to the maximum area value. Finally, with the values of the areas that do not violate the boundaries, the final volume of the structure is calculated.

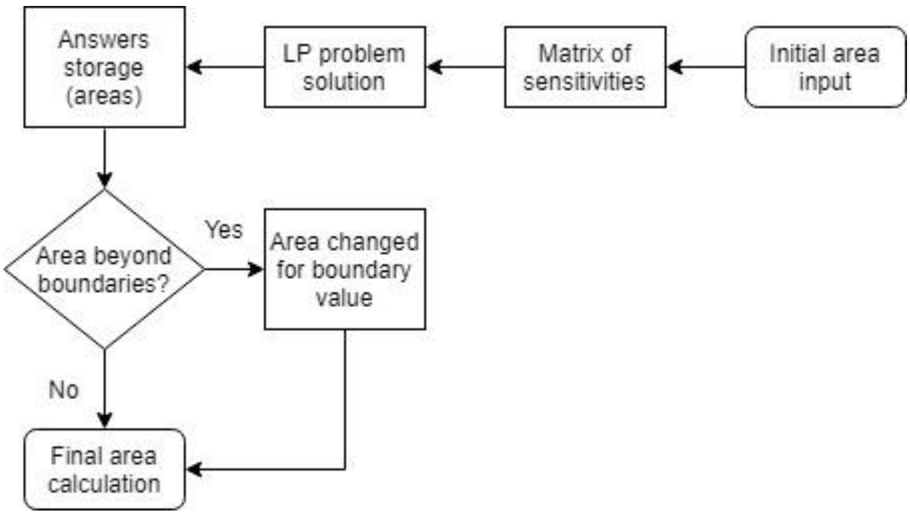

Figure 3. SLP flowchart

3.2 Modified Newton-Raphson Method

First, we must consider the equilibrium equation between internal and external forces given by the following system of nonlinear equations

$$\boldsymbol{P}(u) = \boldsymbol{F} \tag{18}$$

where $\boldsymbol{u} = \{u_1, u_2, \dots, u_n\}^T$ is a vector of unknowns, $\boldsymbol{F} = \{F_1, F_2, \dots, F_n\}^T$ is a vector of known values and $\boldsymbol{P}(u) = \{P(u)_1, P(u)_2, \dots, P(u)_n\}^T$ is a vector of nonlinear functions of u. In structural applications, u is the displacement vector, $\boldsymbol{F}$ is the applied force vector and $\boldsymbol{P}(u)$ is the internal force vector. In a linear problem, the internal force vector is a linear function of u such that $\boldsymbol{P}(u) = \boldsymbol{K} \cdot \boldsymbol{u}$, where K is the constant stiffness matrix.

Nonlinear analysis searches the solution of Eq. (18) effectively through iterative methods. Starting with an initial estimate u^0, the increment Δu is obtained by solving a system of linear equations. After obtaining the increment, the solution is updated iteratively until a certain convergence criterion is met [14].

In this work, to solve the nonlinear optimization problem, the Newton Raphson method (NR) and the modified Newton Raphson method (MNR) were used. MNR was up to 56% faster than NR, converging on the same results. This is because in NR the tangent stiffness matrix is generated at each iteration and in MNR it is generated only once. The generation of tangent stiffness matrix has a high computational cost, so the solution converged in shorter times with the use of MNR.

3.3 Topology optimization solver algorithm

The program implemented in MATLAB to design compliant mechanisms aims to maximize the displacement in a given node under certain boundary conditions and an external force applied in another node. The domain is discretized in bars and the design variable is the area of each bar and may vary within a given range. When the convergence criterion is met, the program stops and the results are plotted.

The flowchart of the program's algorithm is shown in Fig. 4.

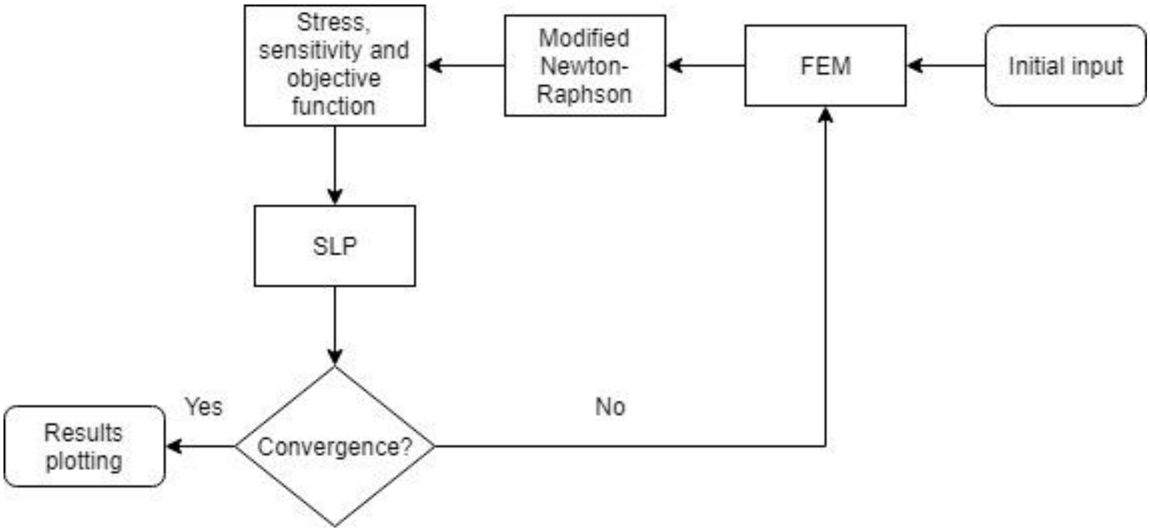

Figure 4. Optimization program flowchart

4 Results

The ground structure domain was generated by GRAND software [15], that is a MATLAB implementation for this purpose. The initial mesh configuration is a *10x10* square domain divided in 10 elements in each axis, as shown in Fig. 5.

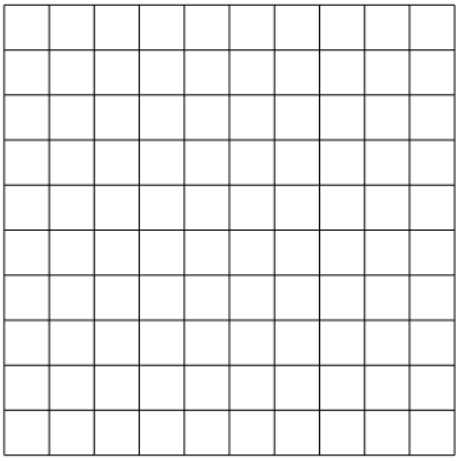

Figure 5. Initial 10x10 mesh, discretized in 10x10 elements

GRAND's connectivity level determines the level of inter-connectedness. If the connectivity level is sufficiently high, the algorithm will interconnect all nodes. In the 10×10 domain, total connectivity is obtained in level 10.

In connectivity level 1 (nodes are connected by bars to its neighbors) the mesh has 121 nodes and 420 bars. In level 10 (total connectivity), the mesh has 4492 bars (Fig. 6).

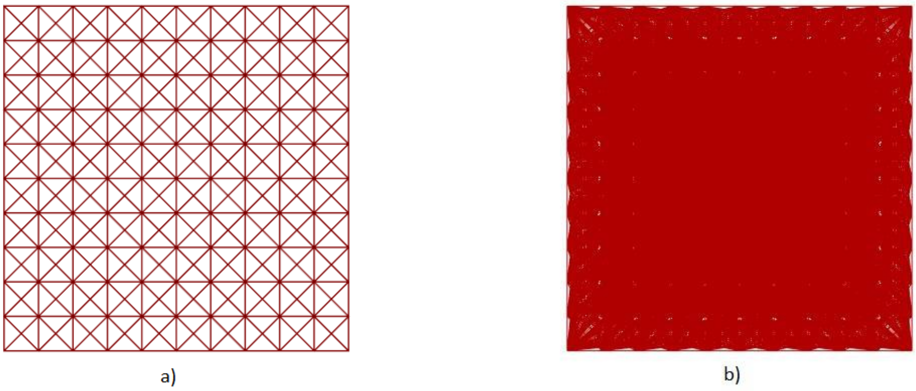

Figure 6. 10x10 elements a) reduced connectivity b) total connectivity

The purpose of this problem is to design a material of artificial properties, that is, properties that are not found in its natural form. The aim here is to obtain an auxetic structure, a structure whose Poisson ratio is negative. The design of compliant mechanisms is very suitable for this purpose, because they are monolithic bodies that perform a certain displacement from a force applied in another point of the structure.

A force was applied in the x direction in the positive orientation, aiming to cause a displacement in the y direction, also in a positive orientation, as indicated in Fig. 7, along with the design domain and boundary conditions.

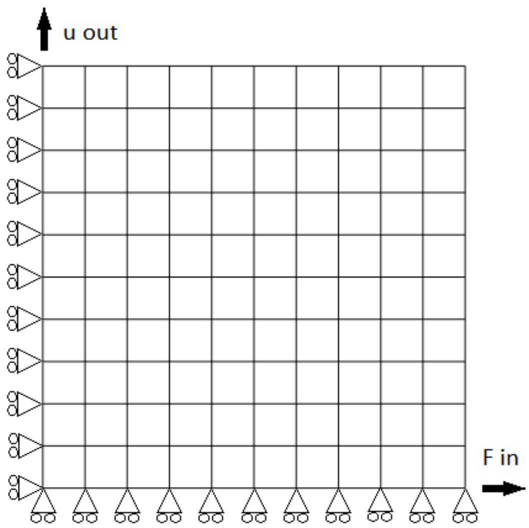

Figure 7. Initial metamaterial domain

Due to symmetry, only a quarter of the domain is used in the topology optimization problem to save computational time.

Parameters used in metamaterial problem are shown in Table 1.

Table 1. Metamaterial parameters

E	F_{in}	A_{min}	A_{max}	A_{init}	k_s^{in}	k_s^{out}	$Cutoff$
$1.4\ GPa$	$100\ kN$	$10^{-5}\ m^2$	$10^{-3}\ m^2$	$2.5 \times 10^{-4}\ m^2$	$20\ kN/m$	$10\ kN/m$	$> 5 \times 10^{-4}\ m^2$

Where k_s is the stiffness of the spring and $Cutoff$ represents which bars are going to be plotted depending on their areas.

The optimal topology was found in connectivity level 1 and volume restriction of 25% of the initial domain.

Results are shown in Table 2.

Table 2. Metamaterial results

lvl	V^*	V_f	$n\ of\ bars$	u_{in}	u_{out}	ν
1	25%	$0.116\ m^3$ (23.15%)	91	$1.9065\ m$	$0.8706\ m$	-0.4566

Where lvl is the level of connectivity of the ground structure and V^* is the volume constraint of the optimization problem.

The optimized domain and its deformed configuration is shown in Fig. 8.

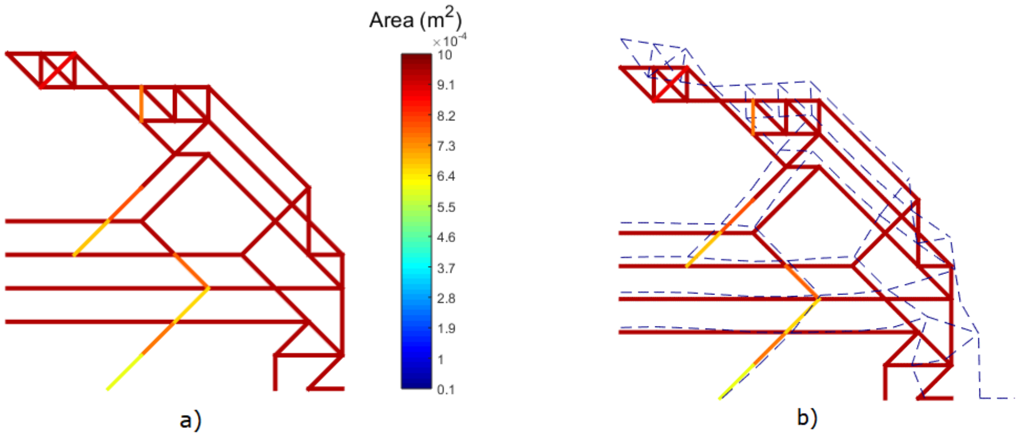

Figure 8. a) optimized topology b) deformed configuration

A negative Poisson ratio is obtained ($\nu = -0.4566$), which means that the structure becomes laterally thinner when compressed and thicker when stretched.

The behavior of the objective function can be seen in Fig. 9.

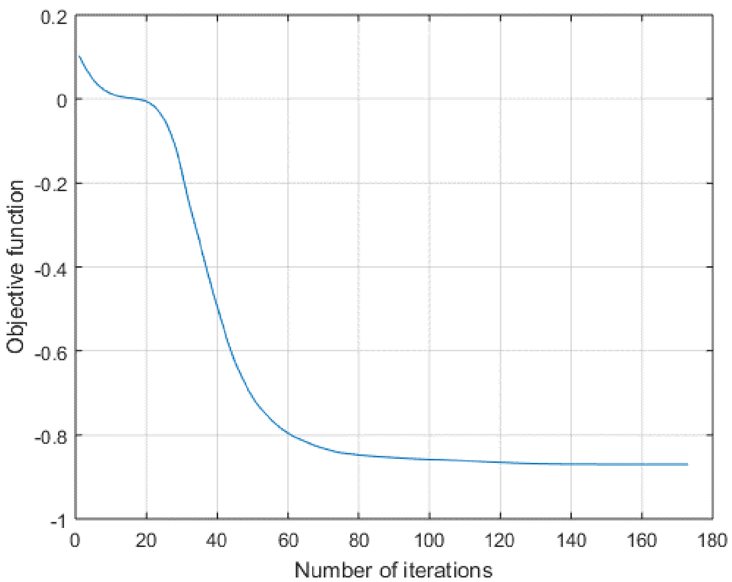

Figure 9. Convergence graph of metamaterial's objective function

The initial domain can be mirrored to generate the auxetic microstructure shown in Fig. 10:

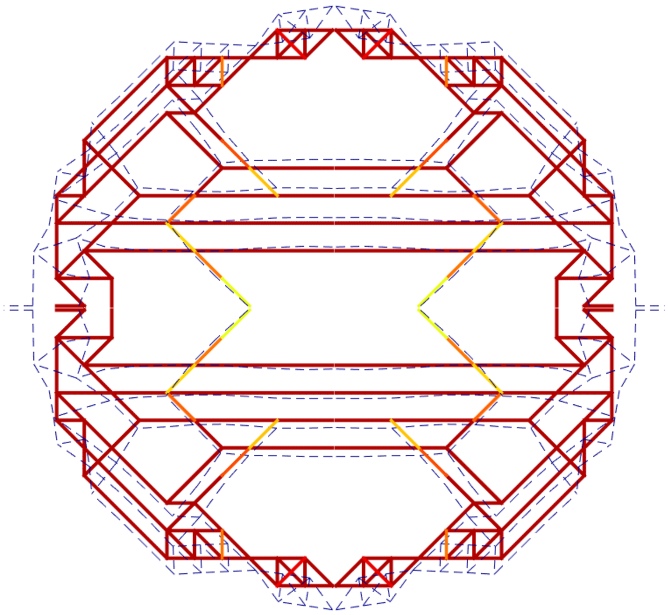

Figure 10. Auxetic Microstructure and its deformation

Thus, this microstructure (Fig. 10) can be repeated many times inside a domain to form a macrostructure that simulates the properties of an auxetic metamaterial.

5 Conclusion

In this work a software in MATLAB was developed to design compliant mechanisms with large displacements, using topology optimization and solving the mathematical programming problem by Sequential Linear Programming. Discrete bar domains were used, where the design variable is the area of each bar, which may vary within pre-established values.

Within the program it is possible to use different levels of domain discretization and, according to the results obtained, it was concluded that the best way to discretize a domain in bars for the objective function that tries to maximize the displacement in a given node of the structure is the reduced connectivity.

It was possible to obtain convergence in the results through iterative methods for the nonlinear finite element analysis. The Modified Newton-Raphson method proved to be the fastest form.

Through the design of compliant mechanisms it was also possible to develop a microstructure with negative Poisson's ratio. This structure can be replicated multiple times in the domain of a macrostructure, simulating the effect of a metamaterial.

The program proved to be generic and efficient for designing compliant mechanisms in different geometries and domains and could be useful in the design and research of this type of mechanism.

Acknowledgements

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