How does the initial cell configuration influence the final topology in a metamaterial generation process?

Jeffrey Guevara-Corzo* 0000-0002-8929-5903, Jesús García-Sánchezb 0000-0003-0806-1660, Carolina Quintero-Ramírezc 0000-0002-1993-2305, Oscar Begambre-Carrillod 0000-0002-2895-9374

a School of Mechanical Engineering, Universidad Industrial de Santander, Bucaramanga 680002, Santander, Colombia. Email: jeffrey.guevara1@correo.uis.edu.co
b Institute of Mechanical Engineering, Universidade Federal de Itajubá, Itajubá 37500-903, Minas Gerais, Brazil. Email: jesus@unidei.edu.br
c Department of Structural Engineering, Universidade de São Paulo, São Carlos 13566-590, São Paulo, Brazil. Email: carolqr@sc.usp.br
d School of Civil Engineering, Universidad Industrial de Santander, Bucaramanga 680002, Santander, Colombia. Email: ojbegam@uis.edu.co

* Corresponding author

Abstract
This research aims to evaluate the impact of the initial cell configuration and the limit volume fraction on the generation of mechanical metamaterial cells. The creation of the cell was achieved by integrating a robust topological optimization based on the solid isotropic material with penalization (SIMP) with a numerical homogenization process coded in Fortran. The procedure was developed using a three-stage methodology to facilitate fast exploration of metamaterial cell space design. The cell generation strategy involved defining finite elements and optimization parameters (pre-processing). Next, finite element calculations, sensitivity analysis, and the application of density filters (processing) were conducted. Finally, based on the objective function, the most suitable candidates were selected, and cells were smoothed (postprocessing). The analysis focused on 2D and 3D linear elastic design scenarios. The initial cell consisted of a square or cube of material with a central circular or spherical void of 10 mm, 20 mm, and 30 mm in diameter. In addition, the generation process employed three limit volume fractions (30%, 40%, and 50%) and eleven objective functions for 2D and 3D scenarios. These functions were intended to generate cells that maximize stiffness in one or multiple directions and cells with maximum compressibility or shear modulus. The tailored mechanical properties of some of the obtained cells are analogous to those described in the literature, while others exhibit novel geometrical configurations. The results highlight volume fraction as one of the most significant factors in the generation process. Well-defined metamaterial cells were generated using a volume fraction of 50%, the highest volume fraction investigated, and those with low to medium void diameters. The code used to generate the results presented in this work is available in the open-source GitHub repository.

Keywords
Mechanical metamaterials, topological optimization, numerical homogenization, cell configuration
1 INTRODUCTION

The metamaterials have gained significant attention in the scientific community due to their unique properties and versatile nature [1, 2, 3]. These artificial cellular structures exhibit behavior that deviates from their constituent materials, making them highly advantageous for applications in passive seismic protection [4, 2], non-reciprocal sound propagation [3], camouflage of objects from incident acoustic energy [5], vibration isolation [6, 7, 8], unidirectional motion guidance [9] and bioengineering and biomedical engineering [10]. In recent years, Kadlec et al. [11] and Fraternali et al. [12, 13] have successfully applied pentamode metamaterials to structural vibration isolation; Zheng et al. [14], present scalable metallic mechanical metamaterials that simultaneously exhibit high strength and low density, the approach to design these multiscale metamaterials was based on assembling microscale filaments following a trajectory defined by a larger length scale structure. Zheng et al. [15] present a material category that maintains nearly constant stiffness even at ultra-low densities. Jenett et al. [16] introduced a module-based approach for manufacturing heterogeneous metamaterials that exhibit properties comparable to certain previously reported metamaterials. Importantly, their innovative scalable system streamlines the production process. Finally, Zhang et al. [17] proposed a 3D metamaterial cell consisting of a hollow rhombic dodecahedron and six cylindrical tubes with shock resistance and vibration isolation capacity.

In this context, most studies [2, 3, 5, 10, 11, 12, 15, 17] have mainly employed pre-defined cell structures. In these approaches, the designer’s experience is decisive in generating the cell topology, or heuristic procedures have been used to design metamaterial cells. However, this has resulted in works focusing more on adapting existing rather than generating new structures through exhaustive and systematic exploration. Using inverse design, Sigmund et al. [18, 19, 20] looked at developing cellular networks with extreme properties. In another relevant study, Gibiansky and Sigmund [21] proposed analytical and numerical methods to obtain two-dimensional, three-phase materials exhibiting extreme conductivity. Milton and Cherkaev [22, 23] have conducted seminal research that allowed the creation of the theory of analytical materials. Moreover, Milton [23] achieved the first rigorous verification of the existence of auxetic materials without holes or sliding surfaces. He also highlighted the feasibility and potential of metasurfaces and planar lattice metamaterials for practical applications.

Today, the approach to metamaterial design has shifted from adapting or fine-tuning existing structures (cells) to a more pragmatic direction that combines topology optimization with the latest advances in additive manufacturing. In recent years, Andreassen et al. [24, 25] and Chatterjee et al. [26] have developed and applied robust topological optimization techniques mixed with numerical homogenization to obtain mechanical metamaterials. In addition, the performance of convolutional neural networks to get the optimal design of metamaterials with maximum compressibility or shear modulus was demonstrated by Kollmann et al. [27]. Using couple-stress homogenization techniques, Chen and Huang [28] reported the obtention of a new chiral metamaterial. The work of Wu et al. [29] and Li et al. [30] provide noteworthy examples of topology optimization for the creation of pentamodal cells using the ground structure technique. The former case employed topological optimization, whereas the latter used a multivariable optimization approach with a genetic algorithm. Although the results reported by Wu et al. [29] and Li et al. [30] differ from the original pentamodal cell proposed by Milton [22], both authors achieved 3D petamodal lattices from a ground structure evolution via genetic algorithms.

A recent study by Huang et al. [31], focused on generating metamaterials used the BESO approach to generate cells that maximized shear modulus and bulk modulus by varying the volume fraction. Although the examples were limited to a single base structure, reliable results were obtained. Other researchers have proposed alternative approaches to complement or improve upon the shortcomings of current methods. For instance, Ai et al. [32], used the parametric level set method (PLSM) in combination with the Meshfree method to generate cells with maxima in shear modulus, bulk modulus, and auxetic cells. This work extended the processes to cells with two phases. Finally, Wu et al. [33], proposed a Robust Topological Optimization (RTO), an improved version of PLSM, applied in the generation of auxetic structures. In this context, current generative processes focus on formulating topological optimization problems employing search procedures of local nature. It is evident that the initial point (to begin the search) or the configuration or parameters used in each optimization algorithm play a highly influential role in the final obtained topology.

In these circumstances, much of the research on the generative cell process rarely considers the influence that variations in the initial cell configuration, limiting volume fractions, approximation models, mutation rates, or the choice of different algorithms may have in obtaining a hands-on metamaterial. In this context, this research aims to investigate the generative process of mechanical metamaterials, focusing on the influence of the initial cell configuration on the generation of elastic mechanical metamaterials. Following a similar approach taken by Andreassen et al. [24, 25], Wu et al. [29] and Li et al. [30], the generative process developed was based on topological optimization and numerical homogenization for 2D and 3D solids in linear elasticity. The base solid used (as initial cell configuration) is represented.
by a square (2D) or cubic (3D) element of 50 mm side with an empty circular (2D) or spherical (3D) void inside. Void
diameter variation of 10 mm, 20 mm, and 30 mm was considered.

In addition, the optimization process was subjected to limit volume fractions of 30%, 40% and 50% of the initial solid
and, finally, eleven objective functions were studied. The optimization results were post-processed and filtered to
generate manufacturable cells without intermediate densities (i.e., more suitable for additive manufacturing). In
addition, for the 3D cases, due to the low voxel density, the surface was smoothed to ensure a better-defined cell
topology. Finally, the resulting metamaterial cells were idealized in a simpler model and then analyzed using ANSYS [34]
to validate the results of the generative process. This paper is organized as follows: Section 2 presents the generation
strategy used, Section 3 discusses the topological optimization strategy, Section 4 focuses on the numerical
homogenization process, Section 5 describes the initial cell configuration (base solid) and the objective functions
employed, Section 6 presents the results of the topological optimization and the developed idealization, and finally,
Section 7 provides the conclusions of this research and possible future works.

2 MECHANICAL METAMATERIAL CELL GENERATION STRATEGY

The proposed methodology for the generation of metamaterial cells follows similar schemes to those developed by
Esfarjani et al. [35] and Chatterjee et al. [26], which is organized into 3 stages: pre-processing, processing, and post-
processing (see Figure 1). In the pre-processing stage, all essential parameters and data for the numerical model are
defined. This involves setting the initial parameters for the finite element analysis (FEA), choosing the topological
optimization method, and specifying the study parameters, such as the search space and the objective functions used in
the optimization process. Further details are discussed in Section 5.

The processing stage is focused on the numerical process of metamaterial generation. The stage relies on the use
of the Solid Isotropic Material with Penalization (SIMP) technique. However, the objective function inherent in the SIMP
algorithm requires the integration of a numerical homogenization process leading to the evolution and creation of a
novel cell structure. Additionally, numerical homogenization necessitates an FEA to obtain the mechanical analysis of the
solid under multiple loading states.

Lastly, the post-processing stage involves selecting and treating the optimization results. This stage encompasses
four phases. Firstly, the selection phase focuses on choosing the best candidate based on superior mechanical behavior
and a clearly shape. Subsequently, the filtering phase aims to eliminate intermediate densities generated during the
topological optimization process. Surface smoothing is then applied (specifically in the 3D case) to improve the definition
of the model, particularly in instances where the voxel size is significant. Finally, the idealization phase simplifies the
previously treated result by establishing a manufacturable cell.

Figure 1 Flowchart of the proposed mechanical metamaterial cell generation strategy.
3 TOPOLOGICAL OPTIMIZATION STRATEGY

Topological optimization (TO) was initially developed by Bendsøe, Sigmund, and Suzuki for relatively simple solid structures with isotropy [36, 37, 38]. However, this line has evolved by developing multiple topological optimization approaches, such as the Evolutionary Structural Optimization (ESO) [39, 40], Bidirectional Evolutionary Structural Optimization (BESO) [41, 42], the Solid Isotropic Material with Penalization (SIMP) method [43, 36]. As well as combined approaches such as hybrid methods (HM) [44] or more complex approaches such as variational topology optimization (VARTOP) [45].

Recent studies by Yago et al. [45] and Shao [44], highlight key aspects, such as the computational efficiency and stability of the SIMP method, which is recognized for its popularity and versatility. The ability to generate clearly defined topologies (without intermediate densities) of the ESO/BESO approaches, as well as the efficiency and robustness of the VARTOP [45] and HM [44] methods. Despite the advantages of these approaches, some of them may have inherent limitations due to the nature of their algorithms. For instance, when using discrete design spaces in ESO/BESO, stability issues may arise, leading to the creation of disconnected zones in the solid structure. Additionally, the SIMP method necessitates the use of filters to guarantee a well-defined solution. In contrast, the level set (LS) method may exhibit an over-dependence on contour controls.

In this context, the SIMP approach was chosen for this research because of its conceptual simplicity, ease of implementation and the computational stability of the algorithm. The SIMP method aims to find an optimal distribution of material within a pre-defined design space, considering specific load cases, boundary conditions, manufacturing constraints, and performance requirements. Unlike shape and size optimization, topological optimization heavily relies on FEA, which enables the division of the design space (domain) into isotropic solid microstructures.

During the TO, the objective is to determine the optimal material state (filled or void) in each finite region or element. The material density distribution within the design domain, denoted as \( \rho \), is typically represented discretely using binary values, where one (1) represents a filled state and zero (0) represents an empty state. However, it can also be treated continuously, allowing for the consideration of intermediate densities. This continuous approach helps to avoid issues arising from the binary nature of the problem. A minimum value, \( \rho_{\text{min}} \), is often assigned to represent an empty state to prevent the development of singularities in the modeling, while a value of 1 represents a filled state.

Using a relative density of the material that can change continuously allows the material’s mechanical properties to vary always. In this sense, the property that is penalized by \( \rho \) would be the Young’s modulus. The equation expressing the penalty is as follows:

\[
E(\rho) = \rho^p E_0
\]

where \( p \) is the penalty factor and \( E_0 \) is Young’s modulus. This penalty allows avoiding intermediate densities, forcing a full or empty distribution. In general, TOs follows the standard formulation as presented by Andreassen et al. [25]:

\[
\text{Min} \rightarrow F(x),
\]

\[
\text{St.}
\]

\[
E(\rho_i) = \rho_i^p E_0, \quad e = 1, 2, \ldots, n
\]

\[
[K]\{x_i\} = \{f_i\},
\]

\[
g_j(x) \geq 0, \quad j = 1, 2, \ldots, J
\]

\[
\frac{1}{n} \sum_{e=1}^{n} (v_e \rho_e) \geq V,
\]

\[
\rho_{\text{min}} \leq \rho_e \leq 1, \quad e = 1, 2, \ldots, n
\]

where \( [K] \) is the stiffness matrix, \( \{x_i\} \) is the displacement vector, \( \{f_i\} \) is the load case, \( E_0 \) is the Young modulus of the material and finally the design variable \( \rho_e \) represents the state in which the material is found which is restricted between two values \( (\rho_{\text{min}} \leq \rho_e \leq 1) \) during the optimization process. In the case of the SIMP algorithm, it relies heavily...
on the application of the penalty factor, which is reflected in the calculation of the global stiffness matrix, which is modulated by the function:

\[ K(\rho) = \sum_{e=1}^{n} [\rho_{\min} + (1 - \rho_{\min})\rho_e^p]K_e \]

Additionally, the SIMP algorithm performs a sensitivity analysis to evaluate the impact of varying material densities on the objective function. Mathematically, the sensitivity analysis is expressed as the derivative of the objective function concerning the densities, resulting in:

\[ \frac{dC}{d\rho_e} = -P(\rho_e)^{P-1}C \]

\( C \) is the Compliance, which is usually set as a measure of the overall flexibility or softness of a structure, usually set as the deformation energy, \( P \) is the penalty factor (usually 3 for 2D and 5 for 3D), which helps to push intermediate densities to extreme values. The TO code used in this research was developed in FORTRAN [46] based on the work developed by Andreassen et al. [47] and Liu and Tovar [48]. In this work, the optimality criterion (OC) was used in most of the generative processes, as illustrated in Figures 4, 8 and 9. In addition, in specific cases where isotropy conditions needed to be considered, the method of moving asymptotes (MMA) was implemented according to the proposal of Svanberg [49] as shown in Figure 10. Finally, to solve the system of equations, we chose to use the HSL MA87 library [50] and the visualization of results was done using the software Paraview [51]. The FORTRAN routines and the Makefile for the compilation are available in the GitHub repository [52].

4 NUMERICAL HOMOGENIZATION PROCEDURE

Numerical homogenization processes have been used in the generation of cellular structures by Andreassen et al. [25] or Wu et al. [29]. According to the theory used to develop the homogenization process, as presented by Andreassen et al. [25] and Yvonnet [53], the homogenized stiffness tensor \( E_{ijkl}^H \) of a periodic material is calculated by the equation:

\[ E_{ijkl}^H = \frac{1}{V} \int_0^V E_{pqrs} \left( \varepsilon^{(ij)}_{pq} - \varepsilon^{(ij)}_{pqr} \right) \left( \varepsilon^{(kl)}_{rs} - \varepsilon^{(kr)}_{rs} \right) dV \]

where \( E_{pqrs} \) the local tensor, \( \varepsilon^{(ij)}_{pq} \) the preset macroscopic displacement field and \( \varepsilon^{(ij)}_{pq} \) the local variation of displacements. The latter is calculated by the equation:

\[ \varepsilon^{(ij)}_{pq} = \varepsilon_{pq} (\chi^{(ij)}) = \frac{1}{2} (\chi^{(ij)}_{pq} - \chi^{(ij)}_{qp}) \]

where \( \chi^{(ij)} \) is the displacement field obtained by solving the system of equations with a prescribed macroscopic strain Writing the process in a way that facilitates its implementation. The homogenised stiffness tensor is also presented in simplified form in terms of the mutual energy of the element [26]. Using Voigt notation (e.g., for 2D we write 11 ← 1, 22 ← 2 and 12 ← 3) the stiffness tensor can be expressed as [26]:

\[ E_{ijkl}^H = \begin{bmatrix} E_{1111}^H & E_{1122}^H & E_{1112}^H \\ E_{2211}^H & E_{2222}^H & E_{2212}^H \\ E_{1211}^H & E_{1222}^H & E_{1212}^H \end{bmatrix} = \begin{bmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{bmatrix} \]

Where the sum of the mutual energies of the elements \( Q_{ij} \) can be calculated with the equation:

\[ Q_{ij} = \frac{1}{V} \sum_{e=1}^{n} U_i^T K_e U_j \]
Where $K_e$ is the stiffness matrix for each element and $U$ is a matrix containing the displacement field for the different states of deformation (as shown in the example in Fig. 2). The displacement fields are obtained by solving the equilibrium for the multiple deformation states.

$$f^i = \sum_{i=1}^{n} \int_{V_e} B_e^T C_e \varepsilon^i dV_e$$

Where the matrix $B_e$ is the strain–displacement matrix, $C_e$ is the constitutive matrix for the element and $\varepsilon^i$ is the strain state vector (see Fig. 2).

5 MODELING: INITIAL CELL CONFIGURATION (BASE SOLID) AND OBJECTIVE FUNCTIONS

The proposed base solids are a 2D square cell and a 3D cubic cell, both with 50 mm sides. The void within these structures is either circular or spherical in shape depending on the dimensionality of the structure. The void diameter (VD) was varied to analyze the TO behavior, performing analyses for structures with VD of 10 mm, 20 mm, and 30 mm (See Fig. 3). Finally, the initial cell was assigned the mechanical properties of structural steel, with a Young’s modulus of $E = 2.1 \times 10^5$ MPa and a Poisson’s ratio of $\nu = 0.3$.

In the TO process, a penalty factor $P$ of 3.0 and 5.0 was used for the 2D and 3D cases, respectively. A limit volume fraction (VF) of 30%, 40% and 50% was set for all analyses, and no stress constraints were applied. Additionally, all TO processes were limited to a maximum of one hundred (100) iterations to ensure stability and a density vector change limit of 1E-3, which does not significantly affect the result. A filter radius of 1.5 times the full element size was employed, and the maximum finite element size was set to 1.0 mm (2D) and 2.0 mm (3D) for pixels and voxels, respectively (see Fig. 3). A classical finite element analysis formulation based on the displacement approximation was used. The meshing was performed using ANSYS [34] and subsequently exported to the developed FORTRAN code [52].
Eleven objective functions were used to evaluate the influence of initial configuration and VF on the cell generation process in multiple cases. The choices of these functions were focused to generate cells with maximum stiffness in one or more directions (i.e., functions F1 and F2 in the 2D scenario and functions F1, F2, F3, F5 and F6 in the 3D scenario) and generating structures that maximize shear or bulk modulus, represented by functions F3 and F4 in 2D and functions F4 and F7 in the 3D scenarios, respectively. These approaches were taken from the work of Chatterjee et al. [26] and Kollmann et al. [27]. The objective functions used in the TO are presented in Table 1.

<table>
<thead>
<tr>
<th>Table 1 Objective Functions used for 2D and 3D scenarios. OF: objective function</th>
</tr>
</thead>
<tbody>
<tr>
<td>2D OF</td>
</tr>
<tr>
<td>$F_1 = E_{1111}^H$</td>
</tr>
<tr>
<td>$F_2 = E_{1111}^H + E_{2222}^H$</td>
</tr>
<tr>
<td>$F_3 = E_{1111}^H + E_{2222}^H + E_{1122}^H + E_{2211}^H$</td>
</tr>
<tr>
<td>$F_4 = E_{1212}^H$</td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td></td>
</tr>
<tr>
<td>$F_5 = E_{1212}^H$</td>
</tr>
<tr>
<td>$F_6 = E_{1212}^H + E_{2323}^H$</td>
</tr>
<tr>
<td>$F_7 = E_{1212}^H + E_{2323}^H + E_{3131}^H$</td>
</tr>
</tbody>
</table>

### 6 Optimization and Idealization Results

The results from the processing and post-processing stage are presented below. The final cell topology from the processing stage is presented in Figure 4 for 2D and 8 for 3D, as well as the final values of the objective function for each optimization process in Figure 5 and 12. Also, the results from the post-processing stage (idealization, optimization performance and validation) are shown in Figure 6 and 7 and Table 2 and 3 for the 2D cases and in Figure 13 and 14 and Table 4 and 5 for the 3D scenarios.

![Figure 4 Final Topology for 2D Cases. VD: void diameter; VF: volume fraction; OF: objective function.](image)

According to the results for the 2D cells (see Figure 4), for the F1 function all final topologies developed a double bar pattern in the X-direction which depending on the available volume fraction, the bars can be either slender (for low VF) or robust (for high VF). For the F2 function, a crossbar topology was obtained in the X and Y direction, where it was one bar in each direction for the cells of 10 mm VD with 30% VF; 20 mm VD with 30% VF and 30 mm VD with 30% and 40% VF and double cross-bars for the remaining cases. For the F3 function, the cases (apart from three) developed a
rhomboid pattern. However, as exceptions, the final topologies with 30 mm VD and 30% VF generated a double diagonal bar pattern and the topologies with 10 mm and 20 mm VD and 50% VF generated a circular topology. Finally, the function F4 also developed a rhomboid pattern, highlighting that the topology with 10 mm VD and a VF of 50% set a double bar rhomboidal material distribution; the exception was the topology resulting from 30 mm VD with 30% VF which generated a double diagonal bar.

Note that some results obtained with the F2, F3, and F4 functions are consistent with works by Huang et al. [31] or Chatterjee et al. [26] who studied the generation of cellular structures with a different approach to the one used in this research. In addition, the TO employed in this work has generated topologies not reported in the literature as those obtained with the F3 function with a VF of 50% and a VD of 10 mm and 20 mm.

On the other hand, according to Figure 5, it is observed that the value of the OF is directly proportional to VF. However, the OF is inversely proportional to VD (in most cases). A 10% variation of the VF (i.e., growth from VF of 30% to 40%) can lead to an increase between 8% to 45% in the value of the OF analyzed. For a variation of VD, a maximum decrease of 17% can be achieved. Though, cases where an increase in the OF value were presented are VF of 40% for F2, VF of 30% for F3 and VF of 30% and 50% for F4, achieving a maximum OF increase of 6%.

For this first 2D instances, all the TO processes developed generated clearly defined topologies that have the potential to be applied as microgrid-like metamaterials. On the other hand, although all results were consistent, only those with a VF of 50% with a VD of 20 mm were selected to continue with the post-processing stage (see Figure 6). In addition, Figure 7 shows the behavior of the selected cases during the optimization process. It starts with the initial solid, followed by a stage of reduction of the VF until the assigned limit is reached. At this point, the TO process begins the generation of a clearly defined solid and finally the process stabilizes generating the final topology. In all cases a stable behavior is observed, reaching the final topology in less than 30 iterations. This pattern is also repeated in the 3D case, as can be seen in Figure 14.

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Finally, the idealized cases (see Figure 6) were loaded into the Material Designer module of ANSYS [34] to obtain the homogenized elasticity tensor. Unfortunately, this module does not allow the study of 2D cellular structures, so an idealized surface extrusion was performed, the numerical homogenization was done using the designer material and finally the tensor values related to the extrusion direction were omitted. The results are presented in the tables 2 and 3.

**Table 2** Value of the ANSYS Homogenized Elastic Tensor (HET) for 2D Cases. HET is in Pa

<table>
<thead>
<tr>
<th>HET</th>
<th>F₁</th>
<th>F₂</th>
<th>F₃</th>
<th>F₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>E[1,1]</td>
<td>8.89E+10</td>
<td>4.60E+10</td>
<td>2.53E+10</td>
<td>1.75E+10</td>
</tr>
<tr>
<td>E[2,1]</td>
<td>4.14E+09</td>
<td>4.75E+09</td>
<td>2.02E+10</td>
<td>1.68E+10</td>
</tr>
<tr>
<td>E[2,2]</td>
<td>2.24E+10</td>
<td>4.60E+10</td>
<td>2.53E+10</td>
<td>1.75E+10</td>
</tr>
<tr>
<td>E[3,3]</td>
<td>3.73E+08</td>
<td>9.76E+08</td>
<td>4.16E+09</td>
<td>1.48E+10</td>
</tr>
</tbody>
</table>

**Table 3** Elastic Tensor Values Normalized (TVN) for 2D Cases. TVN was calculated with respect to the highest tensor value for each case.

<table>
<thead>
<tr>
<th>HET</th>
<th>F₁</th>
<th>F₂</th>
<th>F₃</th>
<th>F₄</th>
</tr>
</thead>
<tbody>
<tr>
<td>E[1,1]</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>E[2,1]</td>
<td>0.05</td>
<td>0.10</td>
<td>0.80</td>
<td>0.96</td>
</tr>
<tr>
<td>E[2,2]</td>
<td>0.25</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>E[3,3]</td>
<td>0.00</td>
<td>0.02</td>
<td>0.16</td>
<td>0.85</td>
</tr>
</tbody>
</table>

According to the results obtained by ANSYS [34] (see Table 2) it is evident that the tensor values influenced by each OF are higher with respect to the other tensor components, except for the result with the OF F4, where E[3,3] was not the highest tensor value, but it was the highest E[3,3] of all results by far. In addition to the normalized values (see Table 3) it is possible to visualize that the components with the highest ratio are indeed the homogenized components. The results for the case of 3D structures are presented below.
The topologies obtained with F1 developed a similar cylindrical pattern, six being hollow and three solids; however, the cases with a VF of 40% with a VD of 30 mm and a VF of 30% with VDs of 20 mm and 30 mm developed a separate structure. With F2, a dual plane pattern was obtained which, depending on the VF, could be either slender or robust, except for the topology obtained with 30% VF and 10mm VD which only developed one plane. F3 generated a topology characterized by a robust plane in one direction. However, the structures with a VF of 40% and 50% with a VD of 10 mm and 20 mm as well as the structure with a VF of 30% with a VD of 30 mm developed transverse elements, in some cases flat and in others following a cylindrical pattern. With F4 a similar topology was generated for all cases with the shape of 3 hollow cylinders in the 3 axes, this pattern is quite close to that obtained by Huang et al. [31] or to the Pshape reported by Lu et al. [54]. However, in the structures with a 50% VF with a VD of 10 mm and 20 mm and with a 40% VF with a VD of 20mm the topology was generated with a reinforcement-like plane. The topologies generated with F5 (similar to the F2) are essentially the same as those generated by F2 in that a double plane develops, with the exception of those generated with the 30% VF with a VD of 10mm, which were only 1 structure, and with VDs of 20mm and 30mm which developed a marked cross-shaped pattern in the plane. F6 generated well-defined topologies in all cases but different according to their initial configuration. The topologies generated with the 10 mm VD generated elements supported in the center of the cell, the 50% VF and 20mm VD generated a topology similar to the empty octet and the remaining topologies are close to the octahedron (also reported by Lu et al. [54]) but omitting the horizontal elements. Finally, with the F7 function varied according to their initial configuration. For the 20 mm and 30 mm VD, A truncated octahedron or P shape cells were generated for the 20 mm and 30 mm VD initial cells. The structures with VD of 10 mm and VFs of 40% and 50% yielded a design with a central support and an octet, respectively, and the remaining cells generated a cross-shaped topology.

In cases such as with F3 or F7 functions, it may be necessary to apply additional constraints. For example, the isotropy constraint proposed by Andreassen et al. [25] or the use of the Zener ratio as proposed by Wu et al. [29] can be employed. These constraints limit the search space of the optimization algorithm to favor the generation of symmetric cells. The optimization model can implement this constraint by adding a penalty factor to the objective function or incorporating an inequality function in the model. By repeating the search indicated in figure 7, for the cases where F3 and F7 were employed, and using the isotropy constraint proposed by Andreassen et al. [25], the results obtained were as follows (figure 9 and 10):
The additional constraints were successful in achieving their objective in all evaluated scenarios with F7, except for the case of 10 mm DV and 40% VF, where symmetric cell formation was observed. However, this strategy was inadequate when the F3 function was used; satisfactory results were only achieved with 10 mm VD. This finding emphasizes the significance of the initial conditions and the optimization algorithm used. It is important to note that when using the MMA algorithm, which is more robust but slightly more computationally expensive, satisfactory results were obtained in all cases. This resulted in the formation of symmetrical cells, although with less well-defined structures at 30 mm VD.

The cells obtained from the 3D TO process were clearly defined, and even unreported cases were brought, such as the reinforced P-shape obtained with F4 and 10 mm and 20 mm VD or the pattern generated with the F6 function with a VD of 20 mm and a VF of 50%. Additionally, it is evident that the proposed methodology is effective in the generation process, since structures close to the Hashin-Shtrikman limits are obtained, as reported by Berger et al. [55]. In Figure 11, we present some of the final cells obtained in this work with the OFs F3, F4 and F7 together with idealized topologies reported by Lu et al. [54] and Huang et al. [31].

According to Figure 12 and in the same way as in the 2D case, the VF is directly proportional to the OF value, obtaining even more marked increases ranging from 23% to 82% of OF value. However, for the 3D case, the OF Values does not present a clear tendency variation with VD where each case must be analyzed independently (Figure 12).
Figure 12 Value of the OFs (F1 to F7) and VF (30% to 50%) for the 3D Cells: a) VD of 10 mm; b) VD of 20 mm, and c) VD of 30 mm.

From the sixty-three generated topologies (see Figure 8), the following seven cases were considered for the post-processing stage: The structure with VF of 50% with 20 mm VD with OF F1, with 10 mm VD with OFs F2, F3, F4, F5 and F7 and finally with VF of 40% with 20 mm VD with OF F6. The results of the post-processing stage can be seen in the Figure 13.

<table>
<thead>
<tr>
<th>F1</th>
<th>F2</th>
<th>F3</th>
<th>F4</th>
<th>F5</th>
<th>F6</th>
<th>F7</th>
</tr>
</thead>
<tbody>
<tr>
<td>Filtering</td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Smoothing</td>
<td></td>
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<td></td>
<td></td>
</tr>
<tr>
<td>Idealization</td>
<td></td>
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<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Figure 13 Selection and Post-Processing for the 3D Results.

Figure 14 Evolution of the OF during the 3D TO process. a) F1 (VF=50%, VD=20mm). b), c), d), e) and g) F2 to F5 and F7 (VF=50%, VD=10mm). f) F6 (VF=40%, VD=20mm).

After the post-processing stage, the numerical analysis was performed using the ANSYS [34]. The results of the numerical analysis (homogenized elasticity tensor and normalized values) are presented in the tables 4 and 5. Similarly to the 2D case, the values of the tensor influenced by each objective function are larger with respect to the other tensor components. For the structures with OFs F5, F6 and F7, where the shear related components are sought to be maximized, these are not the largest in magnitude within the element, but they stand out when compared to the other structures.
In addition, when examining the ratios, the influence of the objective function can be appreciated; it is also highlighted that the optimization of these functions, which are related to the tensor components related to shear, indirectly influences the tensor components related to compression.

### Table 4
Value of the ANSYS Homogenized Elastic Tensor (HET) for 3D Cases. HET is in Pa.

<table>
<thead>
<tr>
<th></th>
<th>$F_1$</th>
<th>$F_2$</th>
<th>$F_3$</th>
<th>$F_4$</th>
<th>$F_5$</th>
<th>$F_6$</th>
<th>$F_7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E[1,1]$</td>
<td>1.07E+11</td>
<td>1.00E+11</td>
<td>6.80E+10</td>
<td>2.42E+10</td>
<td>1.00E+11</td>
<td>3.58E+09</td>
<td>7.42E+09</td>
</tr>
<tr>
<td>$E[2,1]$</td>
<td>1.77E+10</td>
<td>2.79E+10</td>
<td>1.54E+10</td>
<td>1.17E+10</td>
<td>2.79E+10</td>
<td>3.38E+09</td>
<td>3.59E+09</td>
</tr>
<tr>
<td>$E[3,1]$</td>
<td>1.77E+10</td>
<td>7.96E+09</td>
<td>1.54E+10</td>
<td>1.17E+10</td>
<td>7.96E+09</td>
<td>7.03E+07</td>
<td>3.59E+09</td>
</tr>
<tr>
<td>$E[2,2]$</td>
<td>3.30E+10</td>
<td>8.89E+10</td>
<td>6.80E+10</td>
<td>2.38E+10</td>
<td>8.89E+10</td>
<td>7.16E+09</td>
<td>7.42E+09</td>
</tr>
<tr>
<td>$E[3,2]$</td>
<td>2.61E+10</td>
<td>4.14E+09</td>
<td>1.54E+10</td>
<td>1.15E+10</td>
<td>4.14E+09</td>
<td>3.38E+09</td>
<td>3.59E+09</td>
</tr>
<tr>
<td>$E[3,3]$</td>
<td>3.30E+10</td>
<td>2.24E+10</td>
<td>6.80E+10</td>
<td>2.38E+10</td>
<td>2.24E+10</td>
<td>3.58E+09</td>
<td>7.42E+09</td>
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<tr>
<td>$E[4,4]$</td>
<td>2.25E+10</td>
<td>3.09E+10</td>
<td>1.41E+10</td>
<td>9.10E+09</td>
<td>3.09E+10</td>
<td>2.81E+09</td>
<td>3.29E+09</td>
</tr>
<tr>
<td>$E[5,5]$</td>
<td>1.42E+10</td>
<td>3.74E+08</td>
<td>1.41E+10</td>
<td>9.04E+09</td>
<td>3.74E+08</td>
<td>2.81E+09</td>
<td>3.29E+09</td>
</tr>
<tr>
<td>$E[6,6]$</td>
<td>2.25E+10</td>
<td>8.42E+09</td>
<td>1.41E+10</td>
<td>9.06E+09</td>
<td>8.42E+09</td>
<td>9.28E+07</td>
<td>3.29E+09</td>
</tr>
</tbody>
</table>

### Table 5
Elastic Tensor Values Normalized (TVN) for 3D Cases. TVN was calculated with respect to the highest tensor value for each case.

<table>
<thead>
<tr>
<th></th>
<th>$F_1$</th>
<th>$F_2$</th>
<th>$F_3$</th>
<th>$F_4$</th>
<th>$F_5$</th>
<th>$F_6$</th>
<th>$F_7$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E[1,1]$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>0.50</td>
<td>1.00</td>
<td></td>
</tr>
<tr>
<td>$E[2,1]$</td>
<td>0.17</td>
<td>0.28</td>
<td>0.23</td>
<td>0.48</td>
<td>0.28</td>
<td>0.47</td>
<td>0.48</td>
</tr>
<tr>
<td>$E[3,1]$</td>
<td>0.17</td>
<td>0.08</td>
<td>0.23</td>
<td>0.48</td>
<td>0.08</td>
<td>0.01</td>
<td>0.48</td>
</tr>
<tr>
<td>$E[2,2]$</td>
<td>0.31</td>
<td>0.89</td>
<td>1.00</td>
<td>0.98</td>
<td>0.89</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$E[3,2]$</td>
<td>0.24</td>
<td>0.04</td>
<td>0.23</td>
<td>0.48</td>
<td>0.04</td>
<td>0.47</td>
<td>0.48</td>
</tr>
<tr>
<td>$E[3,3]$</td>
<td>0.31</td>
<td>0.22</td>
<td>1.00</td>
<td>0.99</td>
<td>0.22</td>
<td>0.50</td>
<td>1.00</td>
</tr>
<tr>
<td>$E[4,4]$</td>
<td>0.21</td>
<td>0.31</td>
<td>0.21</td>
<td>0.38</td>
<td>0.31</td>
<td>0.39</td>
<td>0.44</td>
</tr>
<tr>
<td>$E[5,5]$</td>
<td>0.13</td>
<td>0.00</td>
<td>0.21</td>
<td>0.37</td>
<td>0.00</td>
<td>0.39</td>
<td>0.44</td>
</tr>
<tr>
<td>$E[6,6]$</td>
<td>0.21</td>
<td>0.08</td>
<td>0.21</td>
<td>0.37</td>
<td>0.08</td>
<td>0.01</td>
<td>0.44</td>
</tr>
</tbody>
</table>

Additionally, an ANOVA analysis was performed using Minitab software [56] with the data obtained at the end of the optimization process (presented in Figures 5 and 12) to determine the influence of the factors studied. The analysis was considered separately for 2D and 3D, taking FO, VD and VF as factors. An analysis of terms of up to second order (interaction of two (2) factors) was considered in the response with a significance level of 0.05. The results are presented in Figure 15.

**Figure 15** Pareto Diagrams of standardized effects. a) 2D cases; b) 3D cases.

The factor with the greatest influence (in both the 2D and 3D cases) on the value of the OF are the functions used (Table 1), followed by the VF and the OF-VF interaction. The behavior of the remaining terms varies depending on the case. In the 2D case the term with the greatest influence is the VD, ending with OF-VD and VD-VF which are below the threshold cutoff line of 2.18 (being interactions not significant on the final response). Finally for the 3D case the terms
that follow are the OF-VD, VD-VF interactions and, finally, the VD that have little influence as they are under the threshold limit line of 2.06.

The results presented here are validated by comparison with previous studies by Huang et al. [31], Yu et al. [10], Vangelatos et al. [57], Wang et al. [58, 59]. Specifically, in 3D for the solution of the F7 OF, the octet-tissue unit cell [60, 57, 59] or stretch-dominated octet-truss unit cell [10], known as a high strength-to-weight ratio cell [10, 57] was obtained. For the solution of the 3D F4 OF, a cell similar to the Schwars P-shell [59] was found; also reported by [31] as a cell material design for maximum bulk. However, the collected literature does not report cases such as the cell obtained from the OFs F3 (see Figure 13), F4 and F6 (see Figure 6).

8 CONCLUSIONS

Based on the results obtained, the following conclusions can be inferred.

1. The influence of the initial cell configuration was evident, since both the VF and the VD affect most of the resulting topologies, as well as the values of the OFs, which are directly proportional to the value of the VF; however, certain cases stand out, such as the F1 for the 2D case and the F2 and F5 OFs for the 3D cases, the influence of VD and VF was almost null, generating topologies with little variation. The influence of the initial configuration is more noticeable when working with more complex functions, such as those where the bulk modulus and the shear modulus are maximized, even generating a topology not reported in the literature reviewed in this research.

2. The use of an initial cell with a central void to generate metamaterial cells is an effective and robust approach that provides a good starting point for developing well-defined cells topologies, while maintaining reliable performance for both low and high VF. However, the best results were obtained at high VFs (50%) for 2D and 3D models and low and medium VDs (10mm and 20mm).

3. The TO process developed ran automatically with minimum user intervention and allowed generating, in a systematic, rapid, and stable way, topologies comparable to those reported in the literature (see Figure 8). New cells were obtained from the post-processing stage with the OFs F3 (see Table Figure6), F4 and F6 (see Figure10), which are not reported in the collected literature. However, cells with exceptionally low densities are obtained during the TO process (see Table 6 with OFs F2 and F5 for any VD and VF), leading to idealized cells that appear to be disconnected and remain disconnected during the filtering process, but their mechanical performance is not affected.

4. For objective functions F3, F4, and F7, the implementation of additional constraints is required to obtain results consistent with the problem. However, for these functions, which are the most complex, the OC method also proves to be inadequate for structure generation, so the use of more robust algorithms such as MMA, GCMMA or similar is highly recommended. Although these algorithms may be more computationally expensive, they provide accurate and reliable results.

Although the research was limited to a linear elastic approach, it is important for future research to extend the optimization/generation to more complex models, such as geometric nonlinearity with or without physical linearities. Additionally, it would be important to extend the process to metamaterials focused on manipulating dynamic properties, because pre-established forms are often used, but its generation is not delved into. For the latter, one could focus on phenomena such as the manipulation of natural frequencies, forcing the generation of specific bands gaps, to cite two examples.

Finally, it would be important to evaluate the behavior of the structures generated in experimental tests and to explore potential applications. For the latter, the potential of the 3D results stands out, where the results obtained are structures clearly constituted by planes, so it could have a potential exploration and application for origami or kirigami type structures that have been successfully used in impact absorption.

Acknowledgements: All authors would like to thank the Universidad Industrial de Santander-UIS, to the INME-UIS and the MSU-UNIFEI research groups for the technical support during the development of this research. Additionally, the first author is grateful for the financial support provided by the Universidad Industrial de Santander.

Declaration: The authors declare that there is no conflict of interest.
Author's Contributions: Conceptualization, investigation, writing and coding, Jeffrey Guevara-Corzo; Writing, review, editing, Carolina Quintero-Ramírez and Jesus Garcia-Sánchez; Review, resources, supervision and writing Oscar Begambre-Carrillo.

Editor: Marco L. Bittencourt

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