Topology Optimization of Periodic Cellular Materials through the Progressive Directional Selection Method and the Finite-Volume Theory

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Abstract. This investigation presents the Progressive Directional Selection (PDS) method to optimize the topology of periodic cellular materials, achieving high performance and minimal weight. The homogenized elastic properties of cellular materials are determined using the homogenization method applied to periodic materials based on the unit cell concept as an intermediate step of the topology optimization procedure. The literature often constructs the design domain to conduct a finite element analysis. However, some problems are related to numerical issues, such as the checkerboard pattern and mesh dependence. The checkerboard effect is related to the assumptions of the finite element method, as the satisfaction of equilibrium and continuity conditions at the element nodes, particularly for linear triangular and quadrilateral discretization in the absence of regularization schemes. This problem can be overcome by the Finite-Volume Theory (FVT), which satisfies the equilibrium equations at the subvolume level, and the compatibility conditions are established through the adjacent subvolume interfaces. The PDS method is inspired by natural selection processes found in biology and employs a strategy to meet the objective function of a discretized analyzed domain subject to a volume constraint. Population selection is based on performance criteria specific to the problem through an iterative process that concludes when the optimized topology ceases to evolve. Numerical example of topology optimization for materials with periodic cellular microstructures are analyzed using PDS and FVT comparing with traditional Rational Approximation of Material Properties (RAMP) method.

Keywords: topology optimization, periodic cellular materials, progressive directional selection, finite-volume theory.

1 Introduction

Composite materials have gotten the interest of many researchers and found important applications in the more diverse modern industrial sectors because such materials generally present behavior quite different in comparison with traditional homogeneous materials (Santos Júnior et al. [1]). Materials with porous microstructures, such as honeycomb architecture, bone, and bamboo, correspond to a particular class of composite materials and are widely found in nature. The objective of the material design is to create a new microstructure that produces behavior similar to that of natural materials. Topology optimization (Bendøe and Kikuchi [2]) has become an interesting technique for designing microstructural topologies. Several studies have been developed to provide an efficient material layout that accounts for the required performance and employs less material. In that regard, Wang et al.

[3] provide a systematic and comprehensive review of educational articles and codes on structural and multidisciplinary optimization.

Originally presented by Bansal and Pindera [4], the finite-volume theory emerged as a powerful alternative to the established finite-element method for analyzing structures and materials. According to Cavalcante et al. [5], this technique employs the volume average of the many fields that define the material's behavior and applies boundary and continuity conditions between adjacent subvolumes in an average sense. In the context of designing optimal structures, this theory was first employed by Araujo [6] and Araujo et al. [7, 8].

Véras and Araujo [9] presented a new approach for Topology Optimization (TO) of two-dimensional continuum elastic structures through the Progressive Directional Selection (PDS) method, taking advantage of the simplicity of applying ESO and inspired by the natural directional selection observed in biology. This work presents a new approach for topology optimization of periodic cellular materials through the PDS comparing with RAMP method.

2 Finite-Volume Theory

The scientific community and engineers commonly employ the finite-volume method to simulate a wide range of physical problems. This method ensures the satisfaction of the governing field equations (transport or equilibrium) within the control volumes of the discretized domain of interest in an integral sense, resulting in strict conservation. Moukalled *et al.* [10] highlight that this essential feature, coupled with the method's simplicity and demonstrated stability, establishes the finite-volume method as a preferred choice in Computational Fluid Dynamics (CFD) simulations. On the other hand, the acceptance of the finite-volume theory by the mechanics of the heterogeneous media community has increased slowly, and it is usually confused with different versions of the finite-volume method traditionally employed in fluid mechanics problems (Cavalcante *et al*., [11]).

The behavior of periodic materials is described by analyzing a single-unit cell subjected to Periodic Boundary Conditions (PBC), and typically, such problems are addressed through asymptotic homogenization theory (Bensoussan *et al*., [12]). It's worth noting that periodic solutions have been successfully developed by employing the Fourier series expansion method for periodic mechanical fields with various unit cell architectures, as demonstrated recently by Ramírez-Torres *et al*. [13] and Lages and Marques [14]. The simplest homogenization approach introduced by Bensoussan *et al*. [12] employs a two-scale expansion. This representation incorporates both global (x) and local (y) coordinates, including macroscopic and microstructure-induced fluctuating components expressed as:

$$u_i^{(q)}(\boldsymbol{x},\boldsymbol{y}) = \bar{\varepsilon}_{ij} x_j + u_i'^{(q)}(\boldsymbol{y}) \tag{1}$$

where $u_i'^{(q)}$ denote fluctuating displacement components induced by the heterogeneous microstructure and $\bar{\varepsilon}_{ij}$ are the specified macroscopic (volume-averaged) strains applied to the entire material. Note that the subscripts are denoted as $i,j = 1,2$ for two-dimensional analysis. Following Drago and Pindera [15], we consider periodic materials characterized by the basic building block called a repeating unit cell (RUC) which is replicated to generate the periodically repeating material microstructure, see Fig. 1. Hence, the response of the periodic material is characterized by the response of a unit cell subjected to periodic boundary conditions.

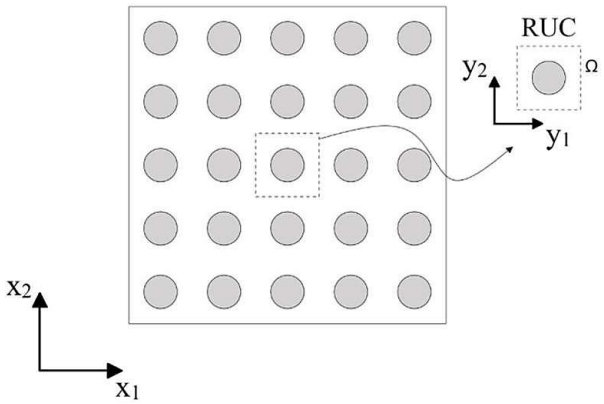


Figure 1. Periodic microstructure characterized by an RUC.

The formulation for two-dimensional problems in Cartesian coordinates involves analyzing a rectangular domain in the $y_1 - y_2$ plane of analysis, which spans the region $0 \leq y1 \leq L$ and $0 \leq y2 \leq H$ (Figure 2).

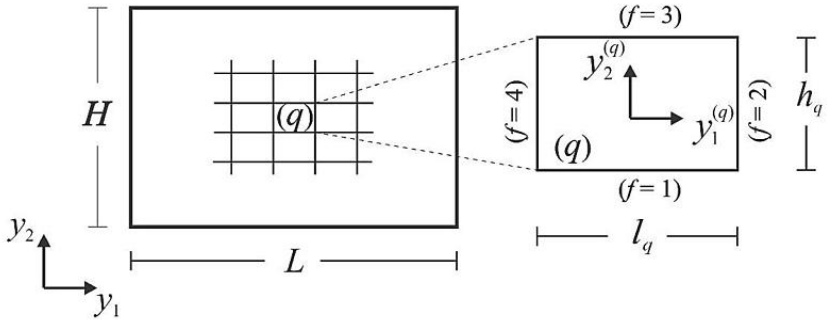


Figure 2. Discretized structure in rectangular subvolumes and local coordinate system of a generic subvolume *q*.

2.1 Zero-Order Finite-Volume Theory for Periodic Materials

Inside this domain are subvolumes with dimensions l_q and h_q along the y_1^q and y_2^q axes, respectively. These subvolumes may contain different elastic materials with uniform values inside each subvolume. In the present zeroth-order or standard finite-volume theory formulation, the components of the fluctuating displacements field ($u_i^{\prime(q)}$) in the local coordinates system are approximated by the second-order polynomial, as follows:

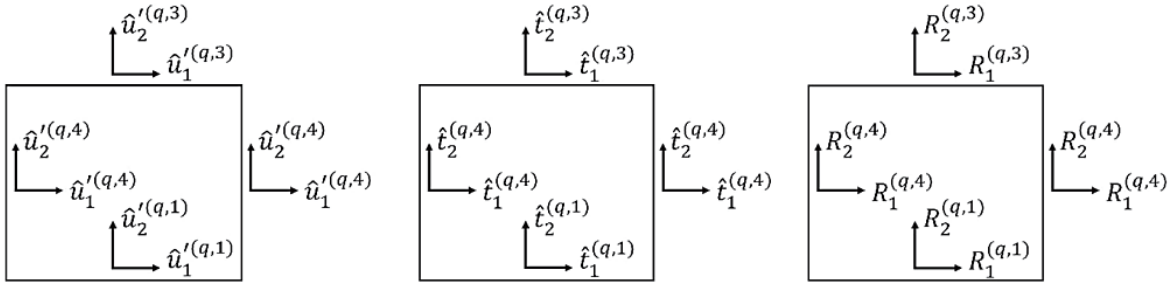
$$u_i^{\prime(q)} = W_{i(00)}^{(q)} + y_1^{(q)} W_{i(10)}^{(q)} + y_2^{(q)} W_{i(01)}^{(q)} + \frac{1}{2}\left(3{y_1^{(q)}}^2 - \frac{l_q^2}{4}\right) W_{i(20)}^{(q)} + \frac{1}{2}\left(3{y_2^{(q)}}^2 - \frac{h_q^2}{4}\right) W_{i(02)}^{(q)} \qquad (2)$$

where $i = 1,2$ and $W_{i(mn)}^{(q)}$ are the unknown coefficients.

The coefficients of the local displacement field can be expressed as a function of the surface-averaged displacements. The surface-averaged displacements are defined as

$$\begin{aligned} \hat{u}_i^{\prime(q,f=1,3)} &= \frac{1}{l_q} \int_{-\frac{l_q}{2}}^{\frac{l_q}{2}} u_i'\left(y_1^{(q)}, \mp\frac{h_q}{2}\right) dy_1^{(q)} \\ \hat{u}_i^{\prime(q,f=2,4)} &= \frac{1}{h_q} \int_{-\frac{h_q}{2}}^{\frac{h_q}{2}} u_i'\left(\pm\frac{l_q}{2}, y_2^{(q)}\right) dy_2^{(q)} \end{aligned} \qquad (3)$$

where $\hat{u}_i^{\prime(q,f)}$ is the surface-averaged fluctuating displacement components of a generic subvolume q in the respective face *f*, as illustrated in Figure 3(a).



a) *Averaged fluctuating displacements*

b) *Averaged tractions*

c) *Resultant of forces in the faces*

Figure 3. Surface kinematic and static quantities: (a) averaged fluctuating displacements; (b) averaged tractions; (c) resultant of forces in the faces.

Making use the Cauchy's relations, the surface-averaged tractions acting on the subvolume's faces can be defined as

$$\hat{t}_i^{(q,f=1,3)} = \mp\frac{1}{l_q}\int_{-\frac{l_q}{2}}^{\frac{l_q}{2}} \sigma_{2i}\left(y_1^{(q)}, \mp\frac{h_q}{2}\right) dy_1^{(q)}$$
$$\hat{t}_i^{(q,f=2,4)} = \pm\frac{1}{h_q}\int_{-\frac{h_q}{2}}^{\frac{h_q}{2}} \sigma_{1i}\left(\pm\frac{l_q}{2}, y_2^{(q)}\right) dy_2^{(q)} \tag{4}$$

Employing the equilibrium equation at level of the *qth* subvolume,

$$\int_S \boldsymbol{t}^{(q)}\, dS = \sum_{f=1}^{4}\int_{l_f^q} \boldsymbol{t}^{(q,f)} dl_f^{(q)} = \sum_{f=1}^{4} l_f \hat{\boldsymbol{t}}^{(q,f)} = \boldsymbol{0} \tag{5}$$

where $\hat{\boldsymbol{t}}^{(q)} = [\hat{t}_i^{(q,1)}, \hat{t}_i^{(q,2)}, \hat{t}_i^{(q,3)}, \hat{t}_i^{(q,4)}]$. In linear elastic analysis, this leads to the local stiffness matrix for each *qth* subvolume,

$$\hat{\boldsymbol{t}}^{(q)} = \boldsymbol{N}^{(q)}\boldsymbol{C}^{(q)}\bar{\boldsymbol{\varepsilon}} + \boldsymbol{K}^{(q)}\hat{\boldsymbol{u}}'^{(q)} \tag{6}$$

where $\hat{\boldsymbol{u}}'^{(q)} = [\hat{u}'^{(q,1)}_i, \hat{u}'^{(q,2)}_i, \hat{u}'^{(q,3)}_i, \hat{u}'^{(q,4)}_i]$ is the surface-averaged fluctuating displacement vector, $\boldsymbol{N}^{(q)}$ and $\boldsymbol{C}^{(q)}$ are the matrices containing components of the normal vectors at the subvolume faces and material constitutive matrix, respectively, $\bar{\boldsymbol{\varepsilon}}$ denotes the macroscopic strain, and $\boldsymbol{K}^{(q)}$ is the local stiffness matrix for a generic subvolume *q*.

According to Cavalcante *et al*. [17], imposition of traction and displacement continuity between adjacent subvolumes in a surface-average sense, together with periodic boundary conditions, produces the global system of equations for the unknown fluctuating surface-averaged interfacial displacements, symbolically expressed in the form,

$$\widehat{\boldsymbol{K}}\widehat{\boldsymbol{u}}' = \widehat{\boldsymbol{F}} \tag{7}$$

where $\widehat{\boldsymbol{u}}'$ is the global surface-averaged fluctuating displacements, $\widehat{\boldsymbol{K}}$ is the global stiffness matrix, and $\widehat{\boldsymbol{F}}$ is the global load vector due to the heterogeneity and the macroscopic strain. This global load vector depends on the differences in the material stiffness matrices of adjacent subvolumes and vanishes if the analyzed model consists of homogeneous material. More details are presented for Santos Júnior and Cavalcante [17].

2.2 Strain energy-based approach

For evaluating effective elastic properties of two-dimensional cellular materials based on asymptotic homogenization theory, this work used a strain energy-based approach, through the satisfaction of the Hill-Mandel condition, which directly relates the strain energy in the heterogeneous microstructure with the strain energy in the equivalent. The homogenization can be interpreted as finding a homogeneous material energetically equivalent to a given material with a heterogeneous microstructure (Qu and Cherkaoui [18]).

Considering the zeroth-order formulation of the finite-volume theory, Araujo et al. [19] demonstrated the equivalence between the structural strain energy (U) and the work done by external forces (W), once the differential equilibrium equations are satisfied pointwise inside the subvolumes. Based on this observation and using the strain energy density definition ($\bar{U} = U/\Omega$),

$$\bar{U} = \frac{1}{\Omega}\sum_{q=1}^{N_q} W^{(q)} = \frac{1}{\Omega}\sum_{q=1}^{N_q}\frac{1}{2}\boldsymbol{R}^{(q)^T}\widehat{\boldsymbol{u}}^{(q)} = \frac{1}{\Omega}\sum_{q=1}^{N_q}\frac{1}{2}\widehat{\boldsymbol{u}}^{(q)^T}\widehat{\boldsymbol{K}}^{(q)^T}\widehat{\boldsymbol{u}}^{(q)} \tag{8}$$

where $\widehat{\boldsymbol{u}}^{(q)}$ corresponds to the total surface-averaged displacement field (macroscopic + fluctuating) of the

subvolume q, and Ω is the domain of a repeating unit cell (RUC). Making use of the micro-macro Hill's energy equivalence,

$$\frac{1}{2}\bar{\boldsymbol{\sigma}}^T\bar{\boldsymbol{\varepsilon}} = \frac{1}{2\Omega}\int_\Omega \bar{\boldsymbol{\sigma}}^T\bar{\boldsymbol{\varepsilon}}\, d\Omega = \frac{1}{\Omega}\sum_{q=1}^{N_q}\frac{1}{2}\hat{\boldsymbol{u}}^{(q)^T}\hat{\boldsymbol{K}}^{(q)^T}\hat{\boldsymbol{u}}^{(q)},$$
$$\bar{\boldsymbol{\varepsilon}}^T\boldsymbol{C}^*\bar{\boldsymbol{\varepsilon}} = \frac{1}{\Omega}\sum_{q=1}^{N_q}\frac{1}{2}\hat{\boldsymbol{u}}^{(q)^T}\hat{\boldsymbol{K}}^{(q)^T}\hat{\boldsymbol{u}}^{(q)} \tag{9}$$

To resolve the components of the effective constitutive matrix $\boldsymbol{C}^*$, it is required previously to apply three linearly independent cases of unit strain to calculate the corresponding total surface-averaged displacements. In the plane stress state, the independent strain cases can be $\bar{\boldsymbol{\varepsilon}}|_{(1)} = \{1,0,0\}^T$, $\bar{\boldsymbol{\varepsilon}}|_{(2)} = \{0,1,0\}^T$ *and* $\bar{\boldsymbol{\varepsilon}}|_{(3)} = \{0,0,1\}^T$, that involve two cases of normal strains, occurring in orthogonal directions, and a pure shear strain, respectively. Therefore, the effective constitutive matrix components are evaluated as follows:

$$C_{ij}^* = \frac{1}{\Omega}\sum_{q=1}^{N_q}\frac{1}{2}\hat{\boldsymbol{u}}^{(q)^T}|_{(i)}\ \hat{\boldsymbol{K}}^{(q)^T}\ \hat{\boldsymbol{u}}^{(q)}|_{(j)} \tag{10}$$

with i, j = 1, 2, 3 and $\hat{\boldsymbol{u}}^{(q)}|_{(i)}$representing the total surface-averaged displacement field for the qth subvolume, due to the application of macroscopic strain case (i). In Eq. (10), the calculation of total surface mean displacement vectors involves the combination of different macroscopic strain cases. This method is based on the Maxwell-Betti reciprocal work theorem, where for linear elastic analysis, the work done by the macroscopic stress associated with the macroscopic strain case (i) through the macroscopic strain case (j) is equal to the work done by the macroscopic stress related to the macroscopic strain case (j) through the macroscopic strain case (i).

3 Progressive Directional Selection Method

Topological optimization methods generally seek the best structure design that produces the stiffest response with a given volume of material. In the traditional ESO method, a structure can be optimized by removing elements, and if the correct parameters are provided, the solution can be achieved. Although it is difficult to define these parameters, several preliminary analyses must occur until an engineer decides which solution to adopt. To overcome this problem, the Progressive Directional Selection method, inspired by Darwin's natural selection theory, specifically directional selection, takes a discrete problem as a discretized structure in a "population" of structural elements. The selection can be made progressively by eliminating the individuals least contributing to the structure's stiffness.

In nature, when directional selection acts on a population, a specific characteristic can guarantee these individuals' survival. Thus, the PDS method optimizes the structure by minimizing the objective function and defining which structural elements will remain at the end of the selection. The process is simple because, once the desired final volume of the structure is known, the main idea is to gradually remove the elements from an initial configuration, as many times as necessary, wherein each stage increases the number of removals and decreases the number of removed elements by removing, until verifying whether the process leads to the same solution.

3.1 Numerical implementation of PDS

Based on the performance criteria adopted for the problem, the selected population is reached through an iterative process that converges when the optimal topology does not evolve anymore, i.e., there is no change in the final set of selected elements. The proposed PDS technique applies a strategy to maximize the objective function. Unlike the structural optimization problem with a prescribed boundary load, setting periodic boundary conditions on the repeated unit cell implies maximizing the complementary strain energy ($\overline{U}$) and effective constitutive matrix components along the optimization process.

The optimization problem in their standard form can be expressed mathematically as:

$$\begin{gathered}\text{maximizing } \overline{U} = \frac{1}{2}\sum_{q=1}^{N} \boldsymbol{u}_q^t \boldsymbol{k}_q \boldsymbol{u}_q \\ \text{subject to: } \widehat{\boldsymbol{K}}\widehat{\boldsymbol{u}}' = \widehat{\boldsymbol{F}} \\ \frac{V}{V_0} = f\end{gathered} \tag{11}$$

$\boldsymbol{k_q}$ is local stiffness matrix, V and V_0 are the material volume and design domain volume, respectively, and f is the prescribed volume fraction.

The procedures for running PDS are the following:

1. Initialize an original model (assemble the stiffness matrix and initial parameters) and determine boundary and loading conditions.
2. Assemble an array that identifies the elements.
3. Start the stage of the selection loop.
4. For the actual stage, specify the number of steps and the number of removed elements for each step.
5. Solve the problem and specify the optimization criterion.
6. Ranking individuals according to the optimization criterion.
7. For each step, remove the elements that contribute the least to the structure.
8. Save the identities of the selected individuals.
9. Repeat the procedure steps from 4 to 8 until the current stage's selected individuals are the same as one or more previous stages.

However, in the case of continuous two-dimensional elastic structures, applying a penalty factor (PF) to the stiffness of the eliminated elements of the discretized analyzed domain is necessary to avoid the re-meshing and singularity of the global stiffness matrix. Particular attention should be given to the classification of the individuals. Convergence criteria are named depending on the number of repetitions desired for the selected individuals. For example, the C7 criterion refers to selecting individuals from a population repeated in the seven consecutive stages. To achieve a good ranking that overcomes some numeric imprecisions, for each removal step, a selection tolerance (ST) is applied to the ranked array (Figure 3). This procedure can add an individual with a value of the objective function significantly closer to the last selected element at the ranked array. This procedure directly interferes with the optimal topology, especially in analyzing two-dimensional continuous structures.

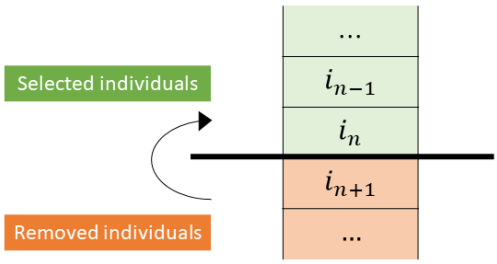


Figure 3. Selection tolerance scheme applied to the ranked array.

Another aspect of the procedure is to define the number of removed individuals (NR^{step}) in each removal step. The *i-th* selection stage is initially proportional to the final number of removed individuals (NS), which refers to the final volume desired for the structure in continuous problems. Thus, $NR^{step} = NS/i$, which must be an integer to access an array by index. When this does not occur, the NR^{step} must be adjusted, redistributing the decimal part among the other steps. The problem is treated as essentially it is, a discrete problem, differently of the approaches based on the concept of material density and penalization method.

3.2 Filtering scheme

A simple filtering technique can be adopted using a scheme based on the weight factors for subvolumes in the neighborhood. Depending on the position of the subvolume in the mesh, the contribution of the neighboring subvolumes must be adjusted, as illustrated in Figure 4. Only three cases are considered: internal, edge, and corners subvolumes, and the dark blue ones are the main subvolumes for each case.

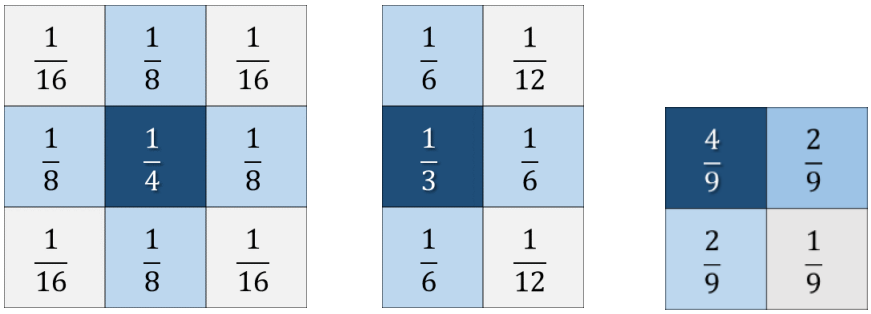


Figure 4. Filtering scheme: weight factors for internal, edge and corners subvolumes, respectively.

The filter is limited to calculating the objective function during ranking. Once the selected population is defined, the value of the objective function is calculated as the response without employing the filter. Véras and Cavalcante [20] employed this filtering scheme in the context of structures, confirming the reduction of mesh dependence and the decrease in the appearance of thin bars in the optimized topologies.

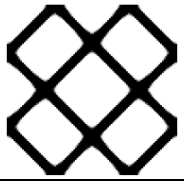
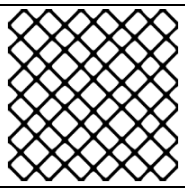
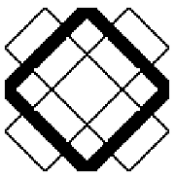
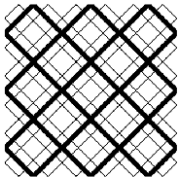
4 Numerical examples

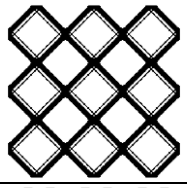
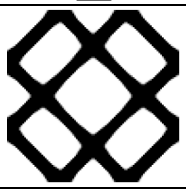
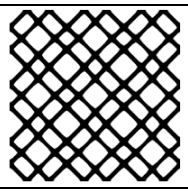
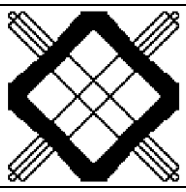
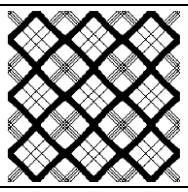
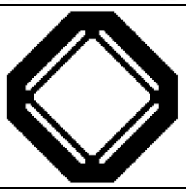
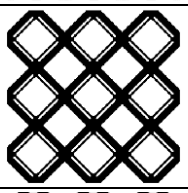
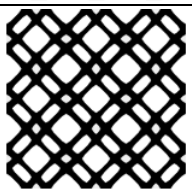
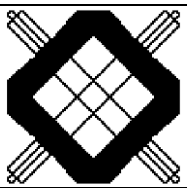
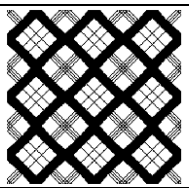
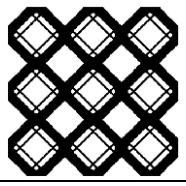
To validate the PDS method based on the finite-volume theory for designing periodic cellular materials with extreme elastic properties, a numerical example was analyzed to maximize the strain energy, which implies maximizing the shear modulus. This was done by considering only the macroscopic angular strain $\bar{\boldsymbol{\varepsilon}}|_{(3)}$ different from zero in Eq. 10. The adopted initial design domain for the periodic cellular material in the PDS method based on the finite-volume theory has a hole with 8x8 central subvolumes.

The following example adopts a solid material with Young's modulus $E = 1$ and Poisson's ratio $\nu = 0.3$, and the Repeating Unit Cell (RUC) discretized into 100x100 subvolumes. Tree cases of desired volume fraction are tested: 30%, 40%, and 50%. The results obtained using the PDS method are compared with the RAMP method presented by Santos Júnior and Cavalcante [17]. The PDS method optimized topologies were obtained employing the parameters $ST = 10^{-6}$ and $PF = 10^{-6}$ and the C7 convergence criterium.

Table 1 shows the shear modulus results for the optimized topologies obtained using the PDS and RAMP methods. Without filtering, the optimized topologies from the PDS method have similar shear moduli to those from the RAMP method. As expected, a decrease in shear modulus was observed with a reduction in volumetric fraction due to the higher presence of voids. The filtering scheme effectively reduced the presence of thin bars in the optimized topologies from the PDS method. Furthermore, the filtering technique improved the PDS method's performance, resulting in an increase in shear moduli of approximately 2% compared to the optimized topologies from the RAMP method.

Table 1. Optimized topologies with maximized shear modulus, considering tree levels of volume fraction constraints.

Volume fraction	**TO methods**	**Shear modulus**	**Unit Cell**	**3 × 3 cells**
30%	RAMP	0.0716		
	PDS	0.0660		

	PDS + Filter	0.0729		
40%	RAMP	0.1006		
	PDS	0.0914		
	PDS + Filter	0.1027		
50%	RAMP	0.1313		
	PDS	0.1223		
	PDS + Filter	0.1327		

5 Conclusions

This study presented the Progressive Directional Selection (PDS) method, integrated with Finite-Volume Theory (FVT), for the topology optimization of periodic cellular materials. The PDS method iteratively removes structural elements that contribute least to the material's stiffness, progressively refining the topology until the optimized configuration is reached. The homogenization method, based on the unit cell concept, was employed to calculate the effective elastic properties of the periodic materials. Compared to the Rational Approximation of Material Properties (RAMP) method, PDS achieved competitive results, especially when combined with filtering techniques, reducing the presence of thin bars and producing optimized topologies with improved mechanical performance.

In conclusion, the PDS method, coupled with FVT, offers a promising approach for the topology optimization of periodic cellular materials. The method effectively balances material usage and mechanical performance without requiring extensive parameter adjustments. Future studies should explore the method's applicability to three-

dimensional problems, nonlinear material behavior, and further comparisons with other state-of-the-art optimization methods to broaden its potential in advanced material design.

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