COMPUTATIONAL MECHANICS 2023
38th conference with international participation
Srní
October 23 - 25, 2023

Periodic homogenization of structural metamaterials

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1. Introduction

This paper focuses on the periodic homogenization of structural metamaterials and methods of parametric control of the geometry of individual patterns. Based on the selection of 6 parameters, it will be possible to create a wide range of derived shapes of the original geometry and then continue to homogenize these patterns. The upcoming task will be based on the implementation of this method using neural networks. Homogenization of structural materials is a process that aims to simplify the description of their complex structure into efficient continuous material models.

2. Formulation of liner elasticity for pattern

In this section, we formulate the equations governing linear elasticity for single pattern with conventional material (metal, polymer). The governing equations are as follows:

$$-\nabla \cdot \boldsymbol{\sigma} = \mathbf{0} \quad \text{in } \Omega, \tag{1}$$

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{0} \quad \text{on } \Gamma, \tag{2}$$

where $\boldsymbol{\sigma}$ is the stress tensor, $\mathbf{n}$ is the outward unit normal vector on the boundary Γ, and Ω represents the spatial domain.

The strain tensor $\boldsymbol{\varepsilon}(u)$ is defined as:

$$\boldsymbol{\varepsilon}(u) = \hat{\boldsymbol{\varepsilon}} + \frac{1}{2}\left(\nabla u + \nabla u^T\right), \tag{3}$$

where $\hat{\varepsilon}$ denotes the given macroscopic strain, and u represents the micro displacement field.

The stress-strain relationship is given by

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = \lambda \cdot \mathrm{tr}(\boldsymbol{\varepsilon} + \hat{\boldsymbol{\varepsilon}}) \cdot \mathbb{I} + 2\mu(\boldsymbol{\varepsilon} + \hat{\boldsymbol{\varepsilon}}) = \bar{\boldsymbol{\sigma}}(\boldsymbol{\varepsilon}) + \hat{\boldsymbol{\sigma}}(\hat{\boldsymbol{\varepsilon}}), \tag{4}$$

where λ and μ are the Lamé parameters, and $\mathbb{I}$ is the identity tensor. Periodic conditions admit rigid translation, therefore, an additional constraint on fluctuation field was imposed

$$\int_\Omega u \,\mathrm{d}\Omega = 0. \tag{5}$$

To obtain the weak form of the equations together with constraints above satisfied, we can use either Lagrange multipliers or a penalty method [1]. Using Lagrange multipliers g (and test function δg), we arrive at the following variational formulation:

$$\int_\Omega \boldsymbol{\varepsilon}(v) : \bar{\boldsymbol{\sigma}}(u)\,\mathrm{d}\Omega + \int_\Omega g \cdot v\,\mathrm{d}\Omega + \int_\Omega \delta g \cdot u\,\mathrm{d}\Omega = -\int_\Omega \hat{\boldsymbol{\sigma}} : \boldsymbol{\varepsilon}(v)\,\mathrm{d}\Omega. \tag{6}$$

We discretized this scheme with mixed finite elements with linear basis functions for both displacement and multipliers and their test functions v and δg. Alternatively, employing a penalty method, we have

$$\int_\Omega \boldsymbol{\varepsilon}(v) : \bar{\boldsymbol{\sigma}}(u)\,\mathrm{d}\Omega + \int_\Omega u \cdot v\,\mathrm{d}\Omega = -\int_\Omega \hat{\boldsymbol{\sigma}} : \boldsymbol{\varepsilon}(v)\,\mathrm{d}\Omega. \tag{7}$$

It is worth noting that a necessary condition for applying periodic boundary conditions is the requirement for identical node positions on opposite periodic boundaries.

3. Homogenization

In the study of homogenization, we establish the relation between macroscale ($\hat{\boldsymbol{\sigma}}$, $\hat{\boldsymbol{\varepsilon}}$) and microscale ($\boldsymbol{\sigma}$, $\boldsymbol{\varepsilon}$) quantities. The relationships are defined as follows:

$$\hat{\boldsymbol{\sigma}} = \frac{1}{\Omega}\int_\Omega \boldsymbol{\sigma}\,\mathrm{d}\Omega, \qquad \hat{\boldsymbol{\varepsilon}} = \frac{1}{\Omega}\int_\Omega \boldsymbol{\varepsilon}\,\mathrm{d}\Omega. \tag{8}$$

Here, $\hat{\sigma}$ represents the macroscopic stress averaged over the entire domain Ω and $\hat{\varepsilon}$ represents the prescribed macroscopic strain. The connection between macroscopic stress $\hat{\sigma}$ and macroscopic strain $\hat{\varepsilon}$ is expressed as

$$\hat{\boldsymbol{\sigma}} = \mathbb{C}^{hom} : \hat{\boldsymbol{\varepsilon}}. \tag{9}$$

In this context, tensor $\mathbb{C}^{hom}$ is formed by elastic constants characterizing the homogenized medium. The components of the tensor $\mathbb{C}^{hom}$ can be determined through the solution of standardized strain $\hat{\boldsymbol{\varepsilon}}$ load cases (six load cases).

This homogenization process (Fig. 1) enables us to bridge the gap between the macroscopic behavior of a material and its underlying microstructure, allowing for the characterization of effective properties on a larger scale [2].

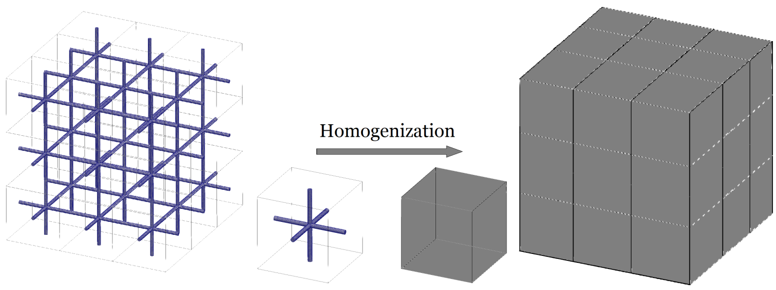


Fig. 1. Structural homogenization scheme

4. Geometry control

Our research focuses on parametric control of explicit geometries using two methods: numerical and analytical. In the numerical approach, we assign structural properties to the original model and induce controlled deformations by rotation and translation along specified axes. The resulting deformed mesh is homogenized. In the analytical approach, we use transformation functions to project nodes from the original mesh into the new coordinates, ensuring that there is no overlapping of nodes or violation of mesh connectivity. We use the following function for the translational transformation:

$$f_i(x,y,z) = T_i\,\frac{(K^2-x^2)(K^2-y^2)(K^2-z^2)}{2K^4}\left[e^{\left(\frac{-x^2}{1+K}\right)} + e^{\left(\frac{-y^2}{1+K}\right)}\right],\ \mathrm{i}\ \in \{\mathrm{X},\mathrm{Y},\mathrm{Z}\}, \tag{10}$$

where T_i are three control parameters for analytical transformation in the axis direction. For rotational transformation, the following function was chosen:

$$f_{\varphi Z}(x, y) = \frac{(K - |x|)(K - |y|)(x + y)}{K^3}, \tag{11}$$

$$Rot_Z = \begin{bmatrix} x - [x \cdot cos(R_Z \cdot f_{\varphi Z}) - y \cdot sin(R_Z \cdot f_{\varphi Z})] \\ y - [y \cdot sin(R_Z \cdot f_{\varphi Z}) + y \cdot cos(R_Z \cdot f_{\varphi Z})] \\ z \end{bmatrix}, \tag{12}$$

where R_Z is control parameter for analytical rotation by corresponding axis. The remaining 2 parameters (R_X, R_Y) are similarly defined. Figs. 2–3 show the behavior of the functions for a particular case.

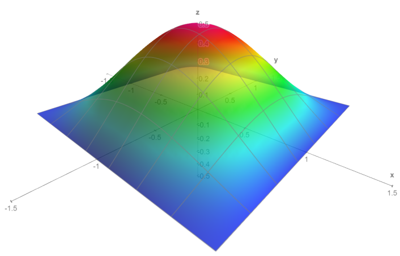


Fig. 2. Translation function

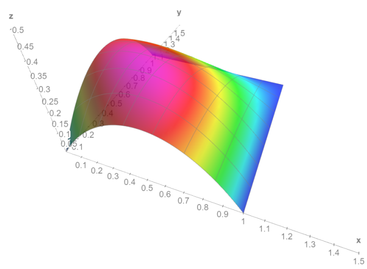


Fig. 3. Rotation function

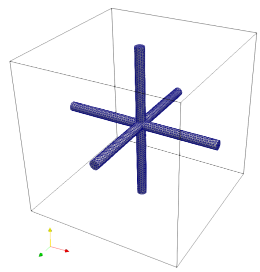
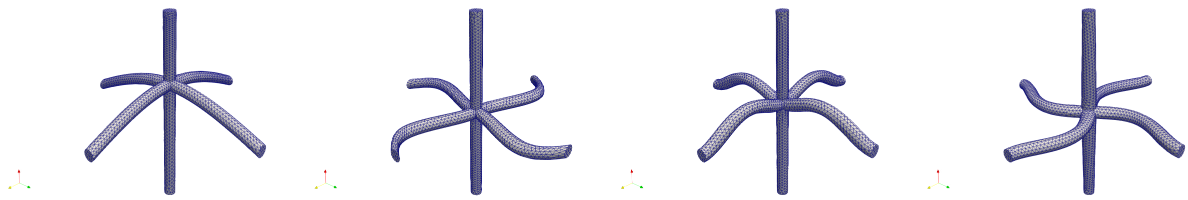


Fig. 4. Basic pattern

A simple cross-patern was chosen for development purposes, Fig. 4. Numerical and analytic methods guide this mesh in the following way, the resulting geometry of which can be seen in Fig. 5.



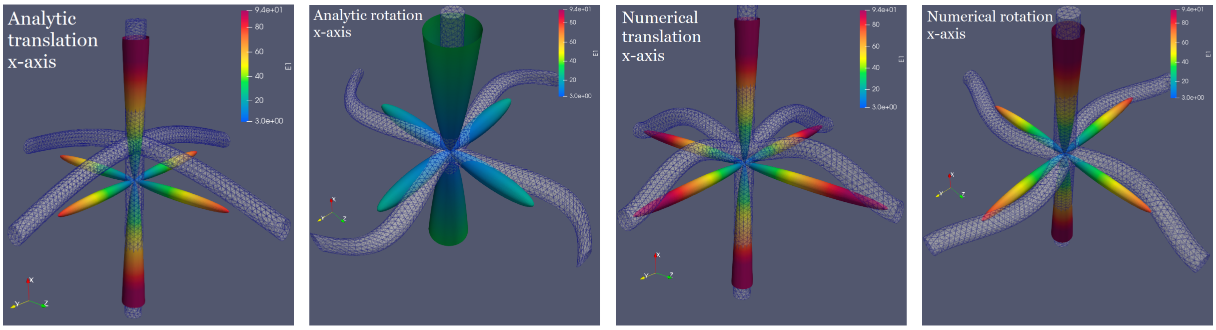
(a) Analytic translation (b) Analytic rotation (c) Numerical translation (d) Numerical rotation

Fig. 5. Deformation of basic pattern by individual methods

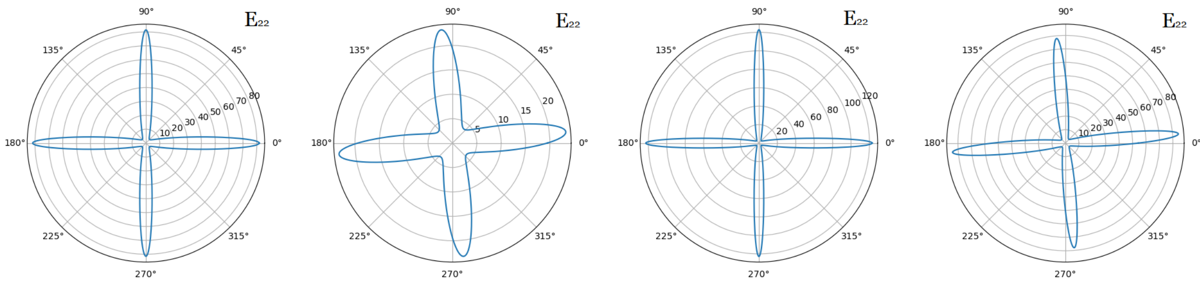
5. Results

Homogenized values obtained for specific geometries using different methods. Fig. 6 illustrates the homogenized values of E_{22} for 4 different types of transformation: analytic (translation and rotation), see Fig. 6a,b,e,f, and numerical (translation and rotation), see Fig. 6c,d,g,h.

We obtained similar homogenized results by analytical and numerical methods, but the analytical approach provides a wider range of geometry control and is less computationally intensive. The results show that using the developed methods we are able to control the material properties of the metastructures using 6 parameters.



(a) Analytic translation (b) Analytic rotation (c) Numerical translation (d) Numerical rotation



(e) Analytic translation (f) Analytic rotation (g) Num. translation (h) Num. rotation

Fig. 6. Homogenised values of E_{22} for the corresponding geometries (spherical and polar)

6. Conclusions

Appropriate methods have been developed to quantify the elastic constants of the designed metamaterials and an effective method to control their geometry. These assumptions are essential for further optimization of metamaterials using neural networks.

Acknowledgements

This work was supported by the Student Grant Competition (SGS) at the Technical University of Liberec in 2023. I thank TOPTEC, CAS IPP for supporting this research and look forward to future collaborations.

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