

COMPUTING THE EFFECTIVE HOMOGENIZED MECHANICAL PROPERTIES FOR TOPOLOGICAL STRUCTURAL OPTIMIZATION

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Abstract. The aim of this work is to present the results obtained from a Matlab code built for computing, in a fast and iterative manner, the effective mechanical properties of regular periodic microstructures consisting of a square unit base cell with rectangular void. Such a code is used as a function call in the topological optimization main algorithm, where the structure that is to be optimized is modeled by using finite elements, being adopted for it that periodic material model with rectangular holes. Each finite element has its own microstructure, which is defined by the base cell hole dimensions and orientation and whose effective elastic components are calculated by using first the homogenization theory, next a data fitting method and then the well-known truss rotation matrix. Dependency of the finite element mesh used for base cell discretization and homogenized elasticity tensor computation as well as the effect of the number of points used in the data fitting are studied, concerning optimal topologies obtained for a bidimensional linear elastic problem whose design criterion is minimum compliance.

Keywords: structural optimization, homogenization method, finite elements method.

1. Introduction

The classical topology optimization problem concerns two fundamental points: the first one is the delimitation of an extended fixed domain and the second one is the definition of a material model.

First, a fixed domain is defined for the structure that is to be minimized. It should be large enough in order to provide a considerable number of feasible solutions for the optimal structure, which will be obtained from it. This extended fixed domain has its boundary limited by the loadings applied to the structure and its supports. Finite elements are used for modeling the problem domain.

Then, a material model is defined for each finite element. This model should ensure that the density of each element can vary within the range from 0 (void) to 1 (full material). Thus, the optimization problem is relaxed, that is, intermediate values are allowed for the transition from a bound density value to the other, what facilitates the numerical problem approach.

There are several material models described in literature (see Fig. 1). The simplest one is the solid isotropic material with penalization, the well-known SIMP (Bendsøe and Sigmund, 2004). The material density, ρ , of each finite element is treated as the design variable and a relationship between the material density and its elastic tensor, E , is defined, as shown in Fig. 1, where n is an empiric exponent.

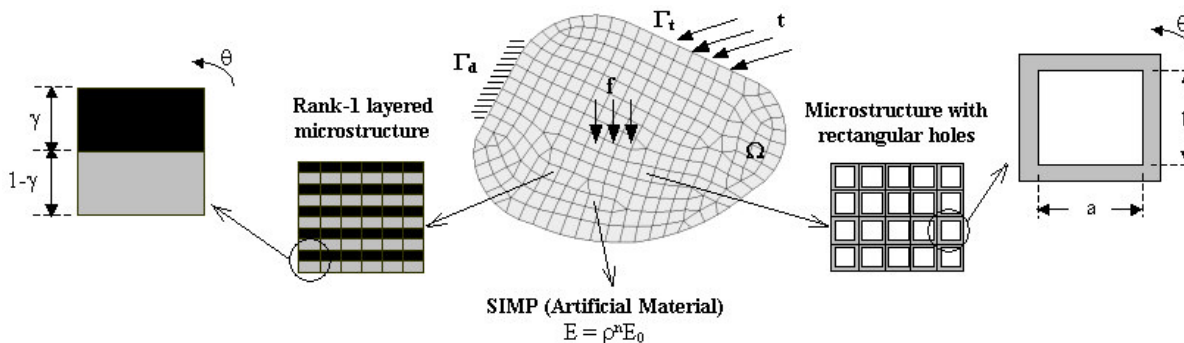


Figure 1. Types of material models used in topology optimization.

Ranked layered materials are another type of material model that can be applied in order to produce a relaxed form of the topological structural optimization problem (Hassani and Hinton, 1999). This model consists of a periodic microstructure whose unit base cell is formed by layers of different materials, for instance, a hard material with relative density γ and a soft one with relative density $1-\gamma$ (called rank-1 layered material, an anisotropic model), as depicted in Fig. 1.

Another anisotropic material that is commonly used is the periodic microstructure consisting of square solid unit base cell with rectangular void (Bendsoe and Kikuchi, 1988), as illustrated in Fig. 1. In the case of anisotropic material models, the geometric dimensions, a , b , γ and orientation, θ , of the microstructure base cell are considered as the design variables and each finite element has its own microstructure. The effective material properties are computed based on the homogenization theory (Bendsoe and Kikuchi, 1988)(Guedes and Kikuchi, 1990) (Allaire, 2002).

Since the goal of this work is to aid the optimal design of composite structures like the one illustrated in Fig. 2, consisting the metal sheet of solid material and holes, the material model with rectangular voids is here investigated.

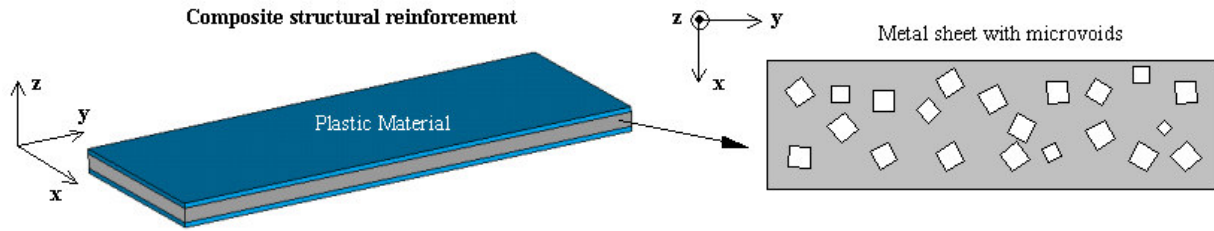


Figure 2. An example of a composite reinforcement consisting of a metal sheet with microvoids and a plastic coating.

Topology optimization problem can also be solved by other methods such as genetic algorithm (Goldberg, 1989), evolutionary method (Xie and Steven, 1993) and hybrid approach (Bulman *et al.*, 2001).

Topology optimization methods have been widely used in compliance minimization (Suzuki and Kikuchi, 1991), natural frequency maximization (Díaz and Kikuchi, 1992) and frequency response minimization (Ma *et al.*, 1995). However, recent works have been applied to other engineering branches rather than structural mechanics: piezoelectric actuators (Silva *et al.*, 1998), magnetic harmonic excitation (Yoo and Kikuchi, 2002), flexible mechanisms design, crashworthiness, wave propagation, and composite materials design (Bendsoe and Sigmund, 2003).

2. Homogenization theory

This section deals with the homogenization method. This method is here briefly commented and for further details about this theory we refer the reader to the works of Guedes and Kikuchi (1990), Hassani and Hinton (1999) and Allaire (2002). The homogenization method in optimal design was introduced by Murat and Tartar in the late 1970's. After the various contributions restricted to academic problems, the work of Bendsoe and Kikuchi (1989) was the first to demonstrate the efficiency of the method in solving shape optimization problems. In the following, the homogenization theory is shortly described.

Given a regular periodic heterogeneous medium, by using the homogenization method one can calculate its effective mechanical properties considering it as a homogeneous material. A heterogeneous medium that is said regular periodic has the following property:

$$F(\mathbf{x} + \mathbf{N}\mathbf{Y}) = F(\mathbf{x}), \quad (1)$$

where

$$\mathbf{x} = \{x_1 \quad x_2 \quad x_3\}^T, \quad \mathbf{N} = \begin{bmatrix} n_1 & 0 & 0 \\ 0 & n_2 & 0 \\ 0 & 0 & n_3 \end{bmatrix} \text{ and } \mathbf{Y} = \{Y_1 \quad Y_2 \quad Y_3\}^T.$$

In Eq. (1), \mathbf{x} is the position vector of a point in the heterogeneous material, where x_1 , x_2 and x_3 are its components; \mathbf{N} is a diagonal matrix, where n_1 , n_2 and n_3 are arbitrary integer number; \mathbf{Y} is a constant vector which determines the period of the regular structure; and F is a certain characteristic function that depends on the position vector, \mathbf{x} .

In the homogenization theory, the period \mathbf{Y} is considered very small compared to the dimensions of the overall domain, in such a way that if one look at the neighborhood of a given point of the heterogeneous material the

characteristic functions will vary fast. In this sense, the homogenization theory considers two different scales for all (physical or mechanic) quantities: one on the macroscopic (or global) level, \mathbf{x} , and the other on the microscopic (or local) level, \mathbf{y} . The former describes slow oscillations, and the latter fast ones (see Fig. 3). These two scales are related by the parameter, δ , called characteristic inhomogeneity dimension, so that $\delta \mathbf{y} = \mathbf{x}$ or $\mathbf{y} = \mathbf{x}/\delta$. This parameter provides an indication of the proportion between the dimensions of the base cell of a composite and the overall domain. And the quantity $1/\delta$ can be also thought of as a magnification factor that enlarges the dimensions of the base cell in order to make it comparable with the dimensions of the whole material. The two-scale technique is illustrated in Fig. 3, where $\phi(\mathbf{x})$ is a given quantity of a regular periodic heterogeneous medium.

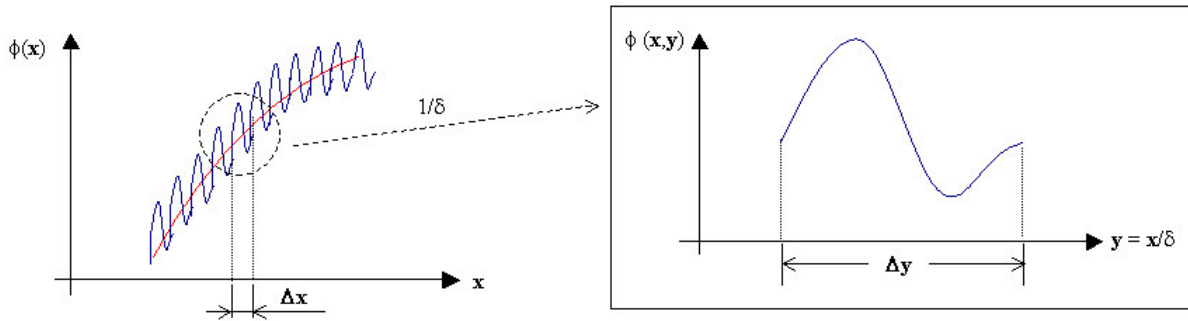


Figure 3. Illustration of the two-scale technique.

The two-scale technique has already proved to be useful in the analysis of slightly perturbed periodic processes in the theory of vibrations and the same principle is extendible to processes occurring in composite materials with a regular structure (Hassani and Hinton, 1999).

With regard to the boundary value problem in cellular heterogeneous bodies, it may be treated by asymptotically expanding the solution in powers of the parameter δ , where the partial differential equations of the problem have coefficients of the form $A(\mathbf{y} = \mathbf{x}/\delta)$, which are \mathbf{Y} -periodic of their arguments. If we consider a coordinate system \mathbf{x} in \mathbb{R}^3 space that defines the domain of the composite material problem, assuming periodicity, the domain can be defined as a collection of parallelepiped cells of identical dimensions $\delta Y_1, \delta Y_2, \delta Y_3$, where Y_1, Y_2 and Y_3 are the sides of the base cell \mathbf{Y} in a local coordinate system $\mathbf{y} = \mathbf{x}/\delta$. So, for a fixed \mathbf{x} in the global level, any dependency on \mathbf{y} can be considered \mathbf{Y} -periodic. In addition, it is assumed that the form and composition of the base cell vary in a smooth way with the macroscopic variable \mathbf{x} , that is, the structure of the composite for different points may vary, but if one looks at a point at \mathbf{x} , a periodic pattern can be found.

Functions determining the behavior of the composite can be expanded as follows:

$$\phi^\delta(\mathbf{x}) = \delta^0 \phi^0(\mathbf{x}) + \delta^1 \phi^1(\mathbf{x}) + \delta^2 \phi^2(\mathbf{x}) + \dots, \quad (2)$$

where δ tends to zero and functions $\phi^i(\mathbf{x})$, $i = 0, 1, 2, \dots$, are smooth with respect to \mathbf{x} and \mathbf{Y} -periodic in \mathbf{y} , what means that they take equal values on the opposite sides of the parallelepiped base cell. The superscript δ indicates the dependency of the quantity to the length of periodicity.

3. Homogenization equations

Let us again consider the linear elasticity problem depicted in Fig. 1 and the regular periodic microstructure with rectangular voids. Body forces, f , and surface forces, t , are applied to the structure. The domain Ω corresponds to the overall domain in \mathbb{R}^3 space and Γ is the smooth boundary of the structure. It comprises the boundaries Γ_d , where the displacements are prescribed, and Γ_t , on which are applied the surface forces. The unit base cell is assumed \mathbf{Y} -periodic in \mathbb{R}^3 . Forces acting inside the cell are neglected, since they are not considered in topology optimization approach.

For a given neighborhood of an arbitrary point \mathbf{x} of the linear elastic structure, the non-homogenized elasticity tensor, D , is given in the form

$$D^\delta_{ijkl}(\mathbf{x}) = D_{ijkl}(\mathbf{x}, \mathbf{x}/\delta) = D_{ijkl}(\mathbf{x}, \mathbf{y}) \quad (3)$$

Once the body and surfaces loads are applied to the structure, from Eq. (2), the resulting displacement field can be written as

$$u^\delta(\mathbf{x}) = u_0(\mathbf{x}) + \delta u_1(\mathbf{x}) + \dots, \quad (4)$$

where u_0 represents the macroscopic mechanical behavior and u_1 the microscopic one.

And the homogenized effective elastic tensor is given by

$$D_{ijkl}^H(\mathbf{x}) = \frac{1}{|\mathbf{Y}|} \int_Y \left[D_{ijkl}(\mathbf{x}, \mathbf{y}) - D_{ijpq}(\mathbf{x}, \mathbf{y}) \frac{\partial \mu_q^{kl}}{\partial y_q} \right] dy \quad (5)$$

In Eq. (5), μ^{kl} refers to the microscopic displacement field, which is considered as the Y -periodic solution of the cell-problem (weak form):

$$\int_Y D_{ijpq}(\mathbf{x}, \mathbf{y}) \frac{\partial \mu_p^{kl}}{\partial y_q} \frac{\partial v_i}{\partial y_j} dY = \int_Y D_{ijkl}(\mathbf{x}, \mathbf{y}) \frac{\partial v_i}{\partial y_j} dY \quad \forall v \in U_Y, \quad (6)$$

where U_Y denotes the set of all Y -periodic virtual displacement fields.

4. Solution of the homogenization formulas for topology optimization

For 2D problems, which are studied in this work and where $i, j, k, p, q = 1, 2$, the cases $(k = l = 1)$, $(k = l = 2)$ and $(k = 1, l = 2)$ are sufficient to find the homogenized elastic matrix, D^H , from Eq. (5) and Eq. (6):

Case (a): $k = 1, l = 1$

Using a compact notation and assuming orthotropy for the material, Eq. (6) can be rewritten as

$$\int_Y \boldsymbol{\varepsilon}^T(v) \mathbf{D} \boldsymbol{\varepsilon}(\mu) dy = \int_Y \boldsymbol{\varepsilon}^T(v) \mathbf{d}_1 dy \quad \forall v \in U_Y, \quad (7)$$

where

$$\boldsymbol{\varepsilon}(v) = \begin{Bmatrix} \partial v_1 / \partial y_1 \\ \partial v_2 / \partial y_2 \\ \partial v_1 / \partial y_2 + \partial v_2 / \partial y_1 \end{Bmatrix}, \quad \boldsymbol{\varepsilon}(\mu) = \begin{Bmatrix} \partial \mu_1 / \partial y_1 \\ \partial \mu_2 / \partial y_2 \\ \partial \mu_1 / \partial y_2 + \partial \mu_2 / \partial y_1 \end{Bmatrix} \quad \text{and} \quad \mathbf{d}_1 = \begin{Bmatrix} D_{11} \\ D_{12} \\ 0 \end{Bmatrix}.$$

In Eq. (7) the vector \mathbf{d}_1 is the first column of the elastic matrix, \mathbf{D} . And from Eq. (7), we can rearrange Eq. (5) as

$$D_{11}^H = \frac{1}{|\mathbf{Y}|} \int_Y (D_{11} - \mathbf{d}_1^T \boldsymbol{\varepsilon}(\mu)) dy \quad (8)$$

Now applying the finite elements method (Reddy, 1987)(Bathe, 1996) to Eq. (7), we can write that

$$\mathbf{K}\mathbf{U} = \mathbf{F}, \quad (9)$$

where

$$\mathbf{k}^e = \int_{Y^e} \mathbf{B}^{eT} \mathbf{D} \mathbf{B}^e dy^e \quad \text{and} \quad \mathbf{f}^e = \int_{Y^e} \mathbf{B}^{eT} \mathbf{d}_1 dy^e.$$

The superscript e refers to element quantities. Matrix \mathbf{k}^e and vector \mathbf{f}^e will form, respectively, the global quantities \mathbf{K} (stiffness matrix) and \mathbf{F} (nodal forces vector). \mathbf{B} is the displacement-strain matrix and \mathbf{U} the nodal solution.

Therefore, solving Eq. (9) we find the displacement vector, μ , and then substituting it in Eq. (8) we obtain the homogenized modulus D_{11}^H .

Case (b): $k = 2, l = 2$

Following the same procedure as for case (a), we have

$$D_{12}^H = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} (D_{12} - \mathbf{d}_1^T \boldsymbol{\varepsilon}(\mu)) dy \quad (10)$$

$$D_{22}^H = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} (D_{22} - \mathbf{d}_2^T \boldsymbol{\varepsilon}(\mu)) dy \quad (11)$$

Case (c): $k = 1, l = 2$

And similarly, from case (c) one finds the elastic modulus D_{66}^H :

$$D_{66}^H = \frac{1}{|\mathbf{Y}|} \int_{\mathbf{Y}} (D_{66} - \mathbf{d}_6^T \boldsymbol{\varepsilon}(\mu)) dy \quad (12)$$

Once the stiffness matrix and the nodal forces are already known, in order to solve Eq. (9) completely the boundary conditions have to be defined. Figure 4 illustrates the boundary conditions derived from periodicity (Hassani and Hinton, 1999), which are applied to the cell problem.

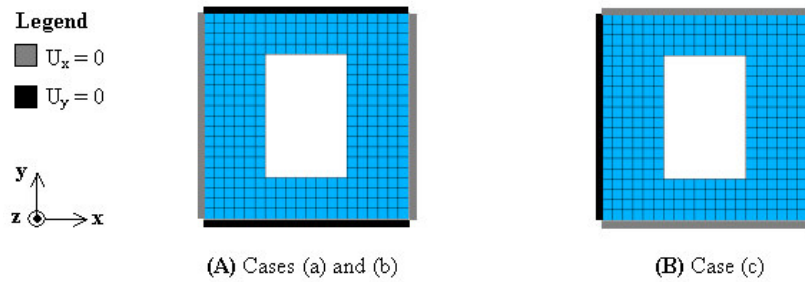


Figure 4. Boundary conditions for cases (a), (b) and (c).

Figure 5 illustrates the deformations of the unit cell depicted in Fig. 4 ($a = 0,4$ and $b = 0,6$) for the cases (a), (b) and (c) mentioned above.

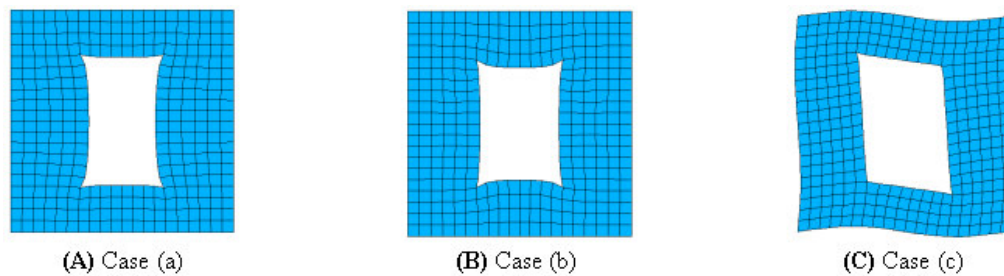


Figure 5. Base cell deformations for cases (a), (b) and (c).

5. Effect of the base cell mesh density on homogenized elasticity components

In order to study the effect of the unit base cell mesh discretization, two different settings are considered. In the first case a base cell with a $0,8 \times 0,8$ void is analyzed, whereas in the second one a base cell with $0,4 \times 0,6$ hole is studied. The solid isotropic part of the unit base cell is characterized by Young's modulus = 26,6672 MPa and Poisson's ratio = 0,33333. The following mesh densities were adopted, using 4-node identical isoparametric finite elements: 10×10 , 20×20 , 40×40 , 80×80 and 100×100 . The convergence results for the homogenized effective moduli are shown in Fig. 6.

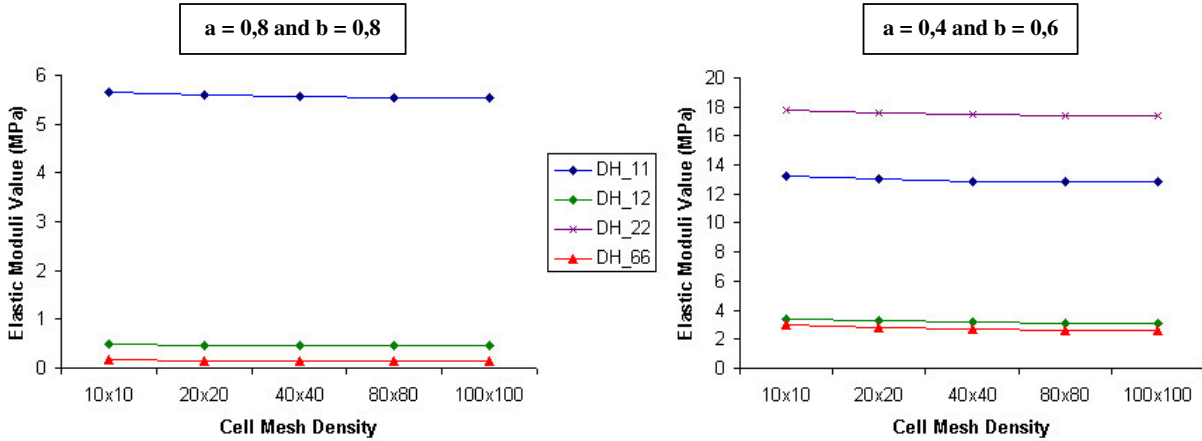


Figure 6. Effect of the cell discretization on the homogenized elastic moduli.

The obtained results for the case of base cell with 0,4 x 0,6 void are compared to those obtained by Hassani and Hinton (1999) and by Bendsoe and Kikuchi (1989) in their works. Results are presented in Tab. 1.

Table 1. Comparison between Matlab and literature results.

FE Mesh	D^H_{11} (MPa)	D^H_{12} (MPa)	D^H_{22} (MPa)	D^H_{66} (MPa)	Obtained by
20 x 20 (4-node)	13,015	3,241	17,552	2,785	Bendsoe and Kikuchi (1989)
1 st adapt.	12,910	3,178	17,473	2,714	Bendsoe and Kikuchi (1989)
2 nd adapt.	12,865	3,146	17,437	2,683	Bendsoe and Kikuchi (1989)
3 rd adapt.	<u>12,844</u>	<u>3,131</u>	<u>17,421</u>	<u>2,668</u>	Bendsoe and Kikuchi (1989)
436 (8-node)	12,839	3,139	17,422	2,648	Hassani and Hinton (1999)
305 (8-node)	<u>12,820</u>	<u>3,124</u>	<u>17,407</u>	<u>2,634</u>	Hassani and Hinton (1999)
40 x 40 (4-node)	12,896	3,174	17,465	2,691	Matlab
80 x 80 (4-node)	12,842	3,138	17,424	2,650	Matlab
100 x 100 (4-node)	<u>12,832</u>	<u>3,131</u>	<u>17,416</u>	<u>2,643</u>	Matlab

6. Use of a scale factor for calculating the homogenized elastic moduli

Regarding the homogenized components of the elasticity tensor, they are first computed for a few certain hole sizes of the unit base cell. Next, based on those components, mechanical properties for the other possible cell hole sizes are then calculated from interpolation techniques or a data fitting. Bendsoe and Kikuchi (1989) employed Legendre polynomials and Fujii and Kikuchi (2000) Lagrange ones. In this work, the conventional least squares method is used following Hassani and Hinton (1999). And finally, the well-known truss rotation matrix is applied in order to taken into account the base cell orientation (Bendsoe, 1989). See Eq. (13). Once completed these steps, a form of continuous function of hole sizes and cell orientation is obtained for the elasticity matrix.

$$\mathbf{R}(\theta) = \begin{bmatrix} \cos^2 \theta & \sin^2 \theta & \cos \theta \sin \theta \\ \sin^2 \theta & \cos^2 \theta & -\cos \theta \sin \theta \\ -\sin 2\theta & \sin 2\theta & \cos 2\theta \end{bmatrix} \quad (13)$$

For every different Young's modulus and/or Poisson's ratio, new calculations need to be performed in order to find the new homogenized mechanical properties of the microstructure. However, when only the elasticity modulus changes, from E_{old} to E_{new} , the new effective elastic components, D^H_{new} , can be found by multiplying the previous homogenized elastic tensor, D^H_{old} , by a scale factor as follows:

$$D^H_{new} = \frac{E_{new}}{E_{old}} D^H_{old} \quad (14)$$

The artifice of Eq. (14) is possible because the Young's modulus appears in the isotropic plane elasticity tensor as a multiplication factor, as shown in Eq. (15).

$$D = \frac{E}{(1-\nu^2)} \begin{bmatrix} 1 & \nu & 0 \\ \nu & 1 & 0 \\ 0 & 0 & (1-\nu)/2 \end{bmatrix} \quad (15)$$

Figure 7 compares the results obtained by using the scale factor of Eq. (14), $E_{\text{new}} = 1,0\text{E}5$ MPa, to the original ones, $E_{\text{old}} = 0,91$ MPa, for a unit base cell with a $0,4 \times 0,6$ hole.

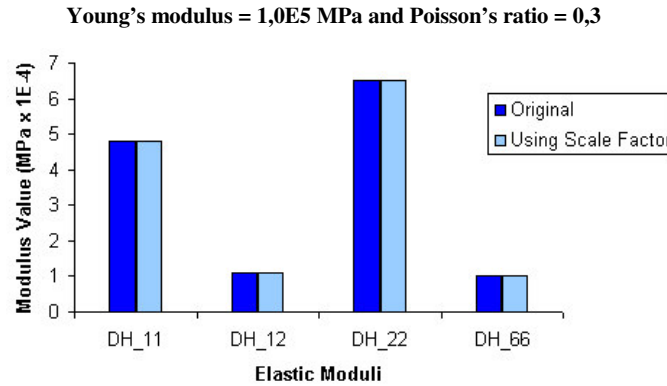


Figure 7. Use of the scale factor for computing the homogenized moduli (base cell with $0,4 \times 0,6$ void).

7. Numerical examples

The purpose of this section is to present the numerical results obtained from the Matlab code, which calls the implemented homogenization function and uses an optimizer based on the optimality criteria (Haftka and Gürdal, 1999) for finding optimal topologies that minimize the compliance of a given linear elastic structure in plane stress state. The classical SBC beam problem is solved (Suzuki and Kikuchi, 1991), considering a force of 1 N applied, a 32×20 mm structure and 60% of mass reduction. 64×40 identical isoparametric 8-node finite elements are used for modeling the beam. Young's modulus is $1,0\text{E}5$ MPa and Poisson's ratio is 0.3. It is adopted a 40×40 base cell discretization.

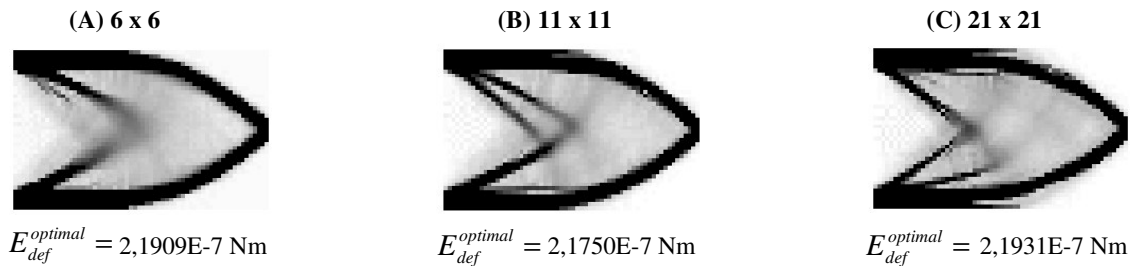


Figure 8. Effect of the number of fitted points of a and b in the final optimal topology and deformation energy.

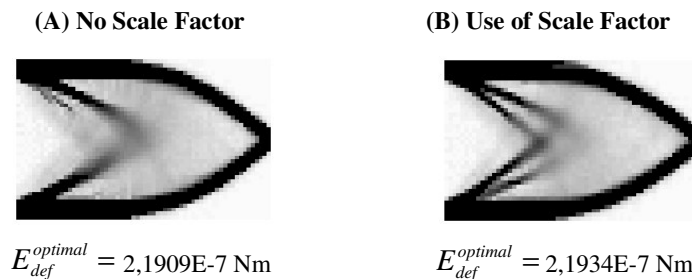


Figure 9. Effect of the use of a scale factor for finding new homogenized moduli from previous ones.

Figure 8 shows the influence of the number of fitted points on optimal results. Suzuki and Kikuchi (1991) used 6 x 6 sampling points of a and b , Hassani and Hinton (1999) 11 x 11 and Fuji and Kikuchi (2000) 51 x 51. Figure 9 presents the optimal topology obtained by using the scale factor of Eq. (14) for the case of 6 x 6 sampling points ($E_{\text{new}} = 1,0\text{E}5$ MPa and $E_{\text{old}} = 0,91$ MPa). In both Fig (8) and Fig. (9) the final optimal deformation energy, $E_{\text{def}}^{\text{optimal}}$, is also depicted.

8. Conclusions

This work has demonstrated the use of an implemented Matlab code for computing the effective homogenized elasticity moduli for topology structural optimization, concerning stiffness linear elastic problems in plane stress state. With regard to the effect of the mesh discretization of the unit base cell on homogenization results, reasonable values of the elasticity moduli can be obtained by using a 40 x 40 mesh of identical 4-node quadrilateral finite elements. With respect to the influence of the number of sampling points of design variables a and b on final optimal topologies, it is verified that the results tend to similar topologies with optimal deformation energies very close one another. The same occurs when using a scale factor for calculating new homogenized mechanical properties from previous ones. However, the use of 6 x 6 sampling points without scale factor application provides the smoothest and simplest topology among them. The difference between the optimal topologies found with and without scale factor can be explained by the fact that when using this multiplier in the case of a single base cell (for a single element), there is an insignificant error, which increases and becomes evident with the number of elements employed in structure discretization.

An extension of the present code to three-dimensional microstructures as well as its implementation in a visual programming environment are intended as further studies in order to extend its applicability to real-world problems.

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