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Two-scale topology optimization using homogenization theory

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Abstract

Homogenization theory forms the basis for solving the topology optimization problem (TOP) of composite structures. The simplest repeating unit of the microstructure, that if isolated represents exactly the macroscopic behavior of the structure, is called the *unit cell*. Scope of homogenization is to determine the macroscopic properties of the non-homogeneous unit cell. In this study, homogenization is implemented on a 3D lattice unit cell, with the radius of the unit cell being the varying parameter of the homogenization procedure. Different values of the radius result to different configurations, hence, to different equivalent properties of the unit cell. Therefore, a fitting process takes place in order to accurately model the variations of the obtained effective properties with respect to the design variable. The corresponding, homogenization-based TOP is posed and the resulting geometries for several case studies are presented.

Keywords: *Design of composite materials; topology optimization; homogenization approach; 3D lattice unit cell; fitting process; scale parameter.*

1. Introduction

The starting point of structural design is the selection of a suitable material. Criterion of the material's effectiveness is its specific properties, i.e. its strength to density and its stiffness to density quotients. Materials of high specific properties, are the composite materials. Their high specific properties along with the ability to tailor those in order to meet the structural requirements, makes them extremely attractive over the conventional bulk materials. The next step is to determine the type of the structural design required. Frequently, the main objective is to

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reduce the weight of the structure and make it as light as possible that is, to remove as much material as needed in order to come up with a final structure still capable of safely withstanding the loads imposed. The question of how the material can be effectively redistributed throughout the design domain, constitutes the objective of topology optimization. Topology optimization requests the optimal distribution of the density field that optimizes a certain physical quantity, called the *objective function*. The objective function whose value is to be optimized is accompanied with a certain set of constraints that the candidate optimal designs should satisfy. There is a great deal of studies published so far where different mathematical formulations and different approaches for dealing with TOP, such as Solid Isotropic Material with Penalization (SIMP), Bi-directional Evolutionary Structural Optimization (BESO) and Level Set [1]-[6] are implemented.

In this work, a *homogenization-based* methodology for approaching the TOP for the 3D case of composite structures, is proposed. The new methodology is divided in two successive procedures of different scale each. In the first one, the 3D homogenization theory is implemented and the equivalent mechanical properties of the composite unit cell are obtained while in the second one, the corresponding TOP is set up, i.e. the objective function along with the governing constraints of the TOP. Finally, the reliability of the proposed methodology is assessed on different case studies.

Nomenclature

V	Volume of the unit cell
C_{pqrs}	Varying elasticity tensor
$\varepsilon_{pq}^{0(ij)}$	Macroscopic strain fields applied on the unit cell
$\varepsilon_{pq}^{(ij)}$	Locally varying strain fields

2. Overview of the homogenization theory

Homogenization combines the properties of each discrete component that constitutes the composite material in order to determine its equivalent properties; isolating a unit cell from the composite's micro structure and "applying" the homogenization theory on it, the equivalent properties of the composite material are obtained. The theoretical background of the method is thoroughly presented in [7]-[9]. The numerical implementation of the homogenization theory, is provided in [10]-[11]. Frequently, the property of the composite material that is intended to be homogenized, is the elasticity tensor of the unit cell. According to the homogenization theory, the equivalent elasticity tensor is given by the following volume integral:

$$C_{ijkl}^{H} = \frac{1}{V}\int C_{pqrs}(\varepsilon_{pq}^{0(ij)} - \varepsilon_{pq}^{(ij)}) \cdot (\varepsilon_{rs}^{0(kl)} - \varepsilon_{rs}^{(kl)}) \cdot dV \tag{1}$$

The computationally calculated form of Eq. (1) is provided in Eq. (2).

$$C_{ij}^{H} = \frac{1}{V}\sum_{e=1}^{N}\int \left(\chi_e^{0(i)} - \chi_e^{(i)}\right)^T \cdot k_e \cdot (\chi_e^{0(j)} - \chi_e^{(j)}) \cdot dV_e \tag{2}$$

where *i, j* are indexes of the strain field applied (The vector format of the strain field is denoted as ε^i, where i=1, ...,6 for the 3D case), $\chi_e^{(i)}$ is the displacement vector of the element *e* corresponding to the application of the volumetric strain field ε^i and, $\chi_e^{0(i)}$ is the displacement vector of the *e* element corresponding to the macroscopic strain field ε^i.

3. Proposed Homogenization-based Theory

3.1. *Unit Cell Configuration*

In this work, a 3D lattice type unit cell is considered, as illustrated in Fig. *1*. For the sake of convenience, the dimensions of the unit cell are set equal to unit and the radius of the unit cell *r* is defined as the alternating

parameter. The elements whose center is located within the arc defined by the radius, constitute the 1st material of the composite unit cell and are assigned the index 1, while the remaining elements of the unit cell constitute the 2nd material and are assigned the index 2. The *lamé* and *mu* engineering constants of the unit cell materials are imported in a 1 by 2 vector format: $l = lamé[material_1, material_2]$, $mu = mu[material_1, material_2]$.

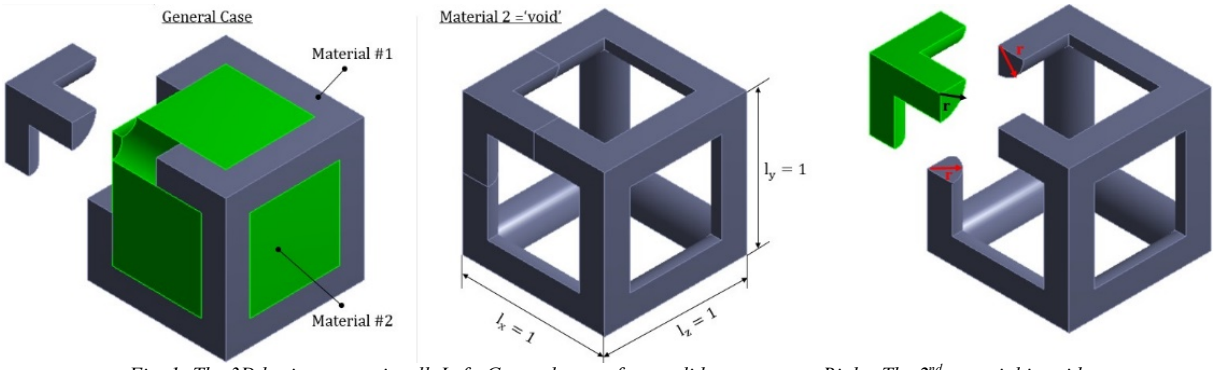

Fig. 1: The 3D lattice type unit cell. Left: General case of two solid components, Right: The 2nd material is void.

3.2. *Homogenization Process of the Unit Cell*

Each value of the radius corresponds to a unit cell of a particular equivalent elasticity tensor. Therefore, by constantly updating the unit cell radius, the corresponding equivalent elasticity matrices are obtained. In Fig. *2*, the iterative procedure applied, is illustrated. The procedure is terminated when the maximum value of the radius is reached; where the final equivalent property obtained coincides with that of the 1st material (i.e. $CH^H_{r=r_{max}} = CH_{material_1}$). *The homogenization code for the case of a 3D lattice unit cell is provided in* [10].

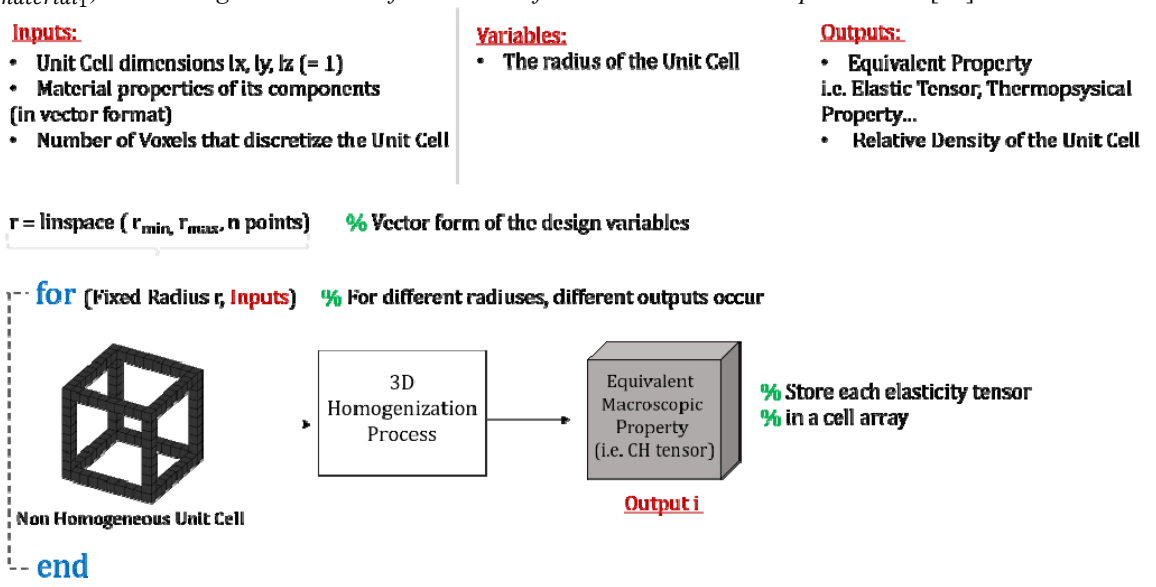

Fig. 2: The iterative procedure applied for the determination of the unit cell equivalent properties.

3.2.1. Fitting of the elasticity tensor terms

The following step is to collect the same terms of the equivalent elasticity tensors obtained that correspond to the different radius values and choose the most appropriate model type that best fits the data. The suitability of the fitting is indicated by the adjusted R-square value. In Fig. *3*, a second order polynomial fit type is chosen for the

CH_{ij} terms and the R-square value of each fit is displayed along. For illustration purposes of the methodology proposed, the case study of a unit cell consisting of a *solid* material of $E = 1$ and $v = 0.3$ and a *void* is considered from now on.

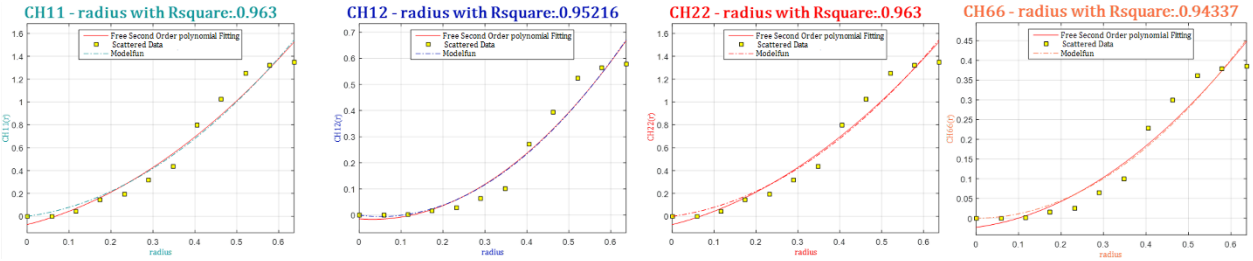

Fig. 3: Second order polynomial fitting of the elasticity tensor terms.

Having expressed the elasticity tensor as a function of the unit cell radius, the stiffness matrix of the element takes the form:

$$K_{e(r)} = \int_{V_E} B_e^T \cdot CH_{(r)} \cdot B_e \cdot |J| \cdot dV \tag{3}$$

and its derivatives with respect to the design variable:

$$\frac{d^n K_{e(r)}}{dr^n} = \int_{V_E} B_e^T \cdot \frac{d^n dCH_{(r)}}{dr^n} \cdot B_e \cdot |J| \cdot dV \tag{4}$$

where, B_e is the 6 by 24 matrix of the partial derivatives of the linear shape functions with respect to the natural coordinates of the element, $CH_{(r)}$ is the elasticity tensor as predicted by the fitting process, $|J|$ is the determinant of the Jacobean matrix and V_E is the volume of the macro scale element. Since all the elasticity tensor terms are a second-order fit of the design variable, the derivatives of the stiffness matrix higher than the order of the fitting model, will equal to zero, i.e. $\frac{d^n K_{e(r)}}{dr^n} = 0 \; \forall \; \mathrm{n} >$ order of polynomial fitting. It is pointed out that through the volume integral of (3) the connection between the two scales is accomplished.

3.2.2. Relative Density of the First Component

Since the unit cell is considered to be of unit dimensions, its volume will equal to unit. The radius value determines the volume of the 1st material within the unit cell, therefore, only the relative density of the 1st material is calculated. By utilizing the element indexing process mentioned in (Sec. *3.1*) the relative density of the 1st material is calculated as follows:

$$Rel.Dens._1 = \frac{Number\ of\ Solid\ Elements\ (index\ i = 1)}{Number\ of\ Total\ Elements\ (Unit\ Cell\ Volume)} \tag{5}$$

Different values of the radius define different relative densities of the 1st material. The variation of the relative density of the 1st material with the radius is approximated by a linear regression model as shown in Fig. 4. The suitability of the fitting is once again quantified by the adjusted R-square value. For a relative density equal to one, that is the unit cell consists solely of the 1st material, the maximum value of the radius is obtained. Thus, the maximum value of the radius equals to: $r_{max} = \frac{1}{grd}$, where *grd* is the slope of the fitting line.

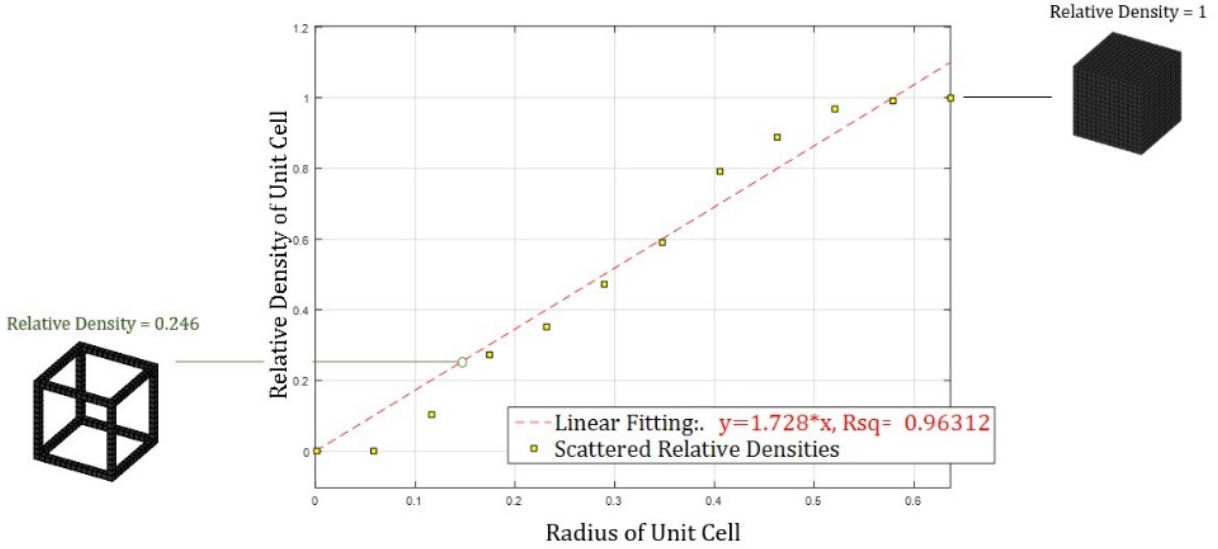

Fig. 4: Linear fitting of the relative density. The goodness of fit is denoted by the Rsq index.

4. Formulation of the homogenization based TOP

4.1. *Formulation of the TOP*

In the case of the homogenization-based TOP, the design variables refer to the microstructure of the design domain. Each finite element bares its own microstructure, thus, the number of design variables of the TOP equals to the number of the finite elements that discretize the design domain. Since the stiffness matrix of each finite element is a dependent function of its microstructure (function of the unit cell radius), each element contributes to the total stiffness of the structure proportionally to its unit cell "*solidity*", i.e. $K_{all} = \sum_{i=1}^{N} K_e(r_{ei})$. The first step in the formulation of the TOP is the computation of the objective function (i.e. the compliance of the structure) along with the constraints imposed, all expressed in terms of the design variables. The corresponding homogenization-based TOP is posed as follows:

$$min\ C(r_{e1}, r_{e2}, \dots, r_{eN}) = min \sum_{i=1}^{N} U_{ei}^{T} \cdot K_e(r_{ei}) \cdot U_{ei} \tag{6}$$

s.t.

$$K_{all} \cdot U_{all} = F_{all} \ \ or \ \ \sum_{i=1}^{N} K_e(r_{ei}) \cdot U_{ei} = F \tag{7}$$

$$\frac{V_{wanted}}{V_0} = f_{VolFrac} \tag{8}$$

$$\{r_{min}\} \leq \{r_e\} \leq \{r_{max}\} \tag{9}$$

The volume restriction (8) is not directly expressed as a function of the design variables. To do so, a series of simple operations should take place; consider a randomly chosen finite element i of volume V_{Ei} and its corresponding periodic unit cell of volume $V_{ei} = grd \cdot r_{ei}$. The volume of the finite element V_{Ei} equals to:

$$V_{Ei} = V_{ei} \cdot \prod_{j=1}^{3} \frac{L_{Ej}}{l_{ej}} = grd \cdot r_{ei} \cdot \prod_{j=1}^{3} \frac{L_{Ej}}{l_{ej}} \tag{10}$$

where, L_{Ej} denotes the dimensions of the finite element at each direction j and l_{ej} are the corresponding dimensions of the unit cell, which are considered unary, i.e. $l_{ej} = 1\,,\ \ j = 1,2,3$. Substituting Eq. (10) to Eq. (8), the volume constraint given in Eq. (8) is modified to Eq. (11):

$$\frac{V_{wanted}}{V_0} = grd \cdot \frac{\sum_{i=1}^{N} r_{ei}}{N} = f_{volfrac} \tag{11}$$

Through Eq. (11), the expression of the volume constraint from the macroscopic level to the microscopic level is accomplished. Theoretically, the minimum value every design variable r_{ei} can receive is zero, however in order to avoid any singularity issues, the minimum value is set equal to a relatively small value. The maximum value of the radius is reached when the relative density of the 1st material becomes equal to one. By means of the fitting process described in (Sec. *3.2.2*), the maximum value of the radius becomes equal to: $r_{max} = \frac{1}{grd}$. Thus, the constraint concerning the upper and lower bounds of the design variables is set as follows:

$$r_{min} = 10^{-6} \leq r_{ei} \leq \frac{1}{grd}, \qquad i = 1,2,\cdots,N \tag{12}$$

4.2. *Solving the TOP - Application of the OC method*

A rather simple and fast technique to solve the optimization problem of Eq. (6) is to apply the OC method. In order to implement OC, the Lagrangian function of the optimization problem must be defined first. For the TOP studied herein, the Lagrangian L is defined as follows:

$$L(r_{e1},\dots,r_{eN}) = C(r_{e1},\dots,r_{eN}) + \lambda \cdot \left(V - f_{volfrac} \cdot V_0\right) + \lambda_1^T \cdot (K \cdot U - F) + \sum_{i=1}^{N} \lambda_{3e} \cdot rei - rmax + \ i{=}1N\lambda 2e \cdot rmax - rrei \tag{13}$$

where, λ and λ_1 are the global Lagrange multipliers, while λ_{2e} and λ_{3e} refer to the Lagrange multipliers for the box constraints of the design variables. The lower and upper bound constraints of the design variables are usually considered inactive, therefore the two latter terms of (13) are absent (i.e. $\lambda_{2e} = \lambda_{3e} = 0$), while the values of design variables obtained during the OC iterations are examined if they lie within the permissible range. Optimality is achieved when the derivatives of the Lagrangian function of (13) with respect to the design variables are set equal to zero i.e. $\frac{dL}{dr_{ei}} = 0$, *i=1, 2, ...N.* Subsequently, the design variables are updated through the iterative process described in Eq. (14).

$$\{r_e^{\kappa+1}\} = \{r_e^{\kappa}\} \cdot \left(\frac{-\left\{\frac{\widehat{dC}}{dr_{el}}\right\} \cdot f_{volfrac} \cdot N}{\lambda \cdot grd} \right)^{\varsigma} = (B_e^{\kappa})^{\varsigma} \tag{14}$$

where, $\{\cdot\}$ denotes the column vector format of the design variables, ς is the damping factor varying from zero to 1 (usually is set equal to 0.5). The *filtered* derivative vector of the objective function $\left\{\frac{\widehat{dC}}{dr_{el}}\right\}$, calculated at the current iteration κ, along with the current design variable vector $\{r_e^{\kappa}\}$, constitute the input arguments of the solution algorithm. A new design variable vector $\{r_e^{\kappa+1}\}$ is the output argument of the method, which constitutes the input to the next iteration, $\kappa + 1$.

5. Numerical Example

In this section a 3D test example is presented. Inter alia, the computational implementation of the optimization problem studied is provided in [12] with the obtained optimal geometries, resulting from the application of the SIMP method.

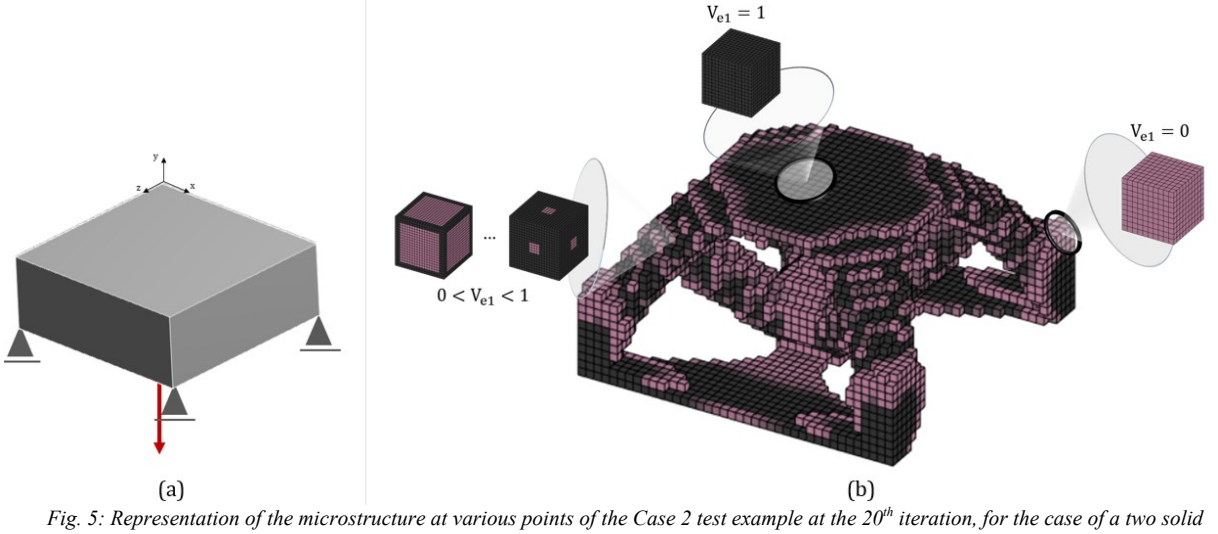

Fig. 5: Representation of the microstructure at various points of the Case 2 test example at the 20th iteration, for the case of a two solid components unit cell.

In (Sec. 3), a solid – void component unit cell was considered. In this section, the case of a two solid components unit cell is examined. In the example being studied, the 1st material of the unit cell is assumed to have a Young's modulus of *E=1* and Poisson ratio of *v=0.3*, while the 2nd material is considered *100* times "*weaker*" with a Young's modulus of *E=0.01* and the same Poisson ratio with the first. The *lamé* and *mu* engineering constants of each material are displayed in Fig. *6*. In this case, the radius value defines the relative density of the 1st material within the unit cell. A 3D plate test case is examined with the guiding mesh discretization along the x and z axis being equal to *40* elements respectively and *20* elements along the y one. The loading conditions refer to a single concentrated load along the y axis in the middle of the xz plane and the boundary conditions refer to fixed support in the all four edges of the design domain (Fig. *5*(a)). The optimized geometry presented in Fig. *5*(b) corresponds to the *20th* out of *100* iterations of the TOP. The volume fraction is set equal to *20%* of the initial domain ($f_{volfrac} = 0.2$) and the display threshold of the optimized structure is set equal to *0.5*. In Fig. *5*(b), for several random elements of the optimized structure selected, their microstructure is displayed along.

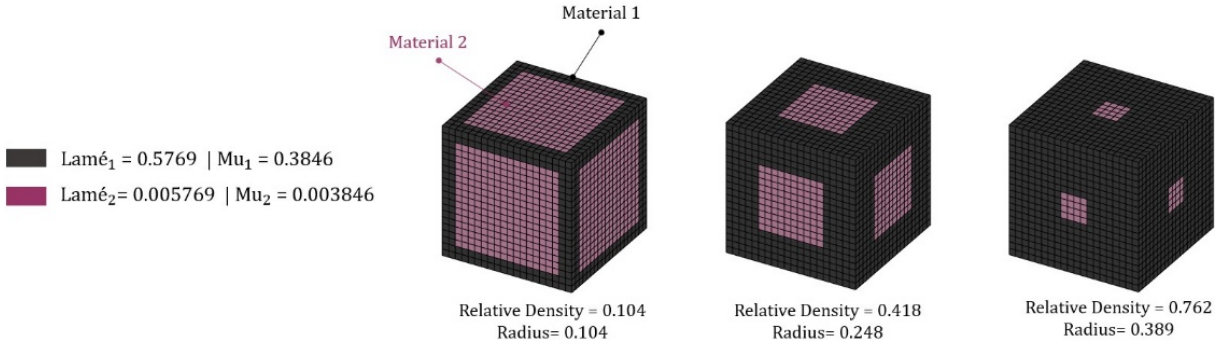

Fig. 6: Unit cell of two solid components.

6. Conclusions

Scope of this work is to propose a new methodology for the TOP of composite structures consisting of two distinct components. The proposed methodology is implemented in two steps of different scale each. In the first step, which takes place at the microstructural level, the homogenization theory is applied on the non-homogeneous unit cell and the obtained elasticity tensor terms of the *equivalent*, *pseudo-homogeneous* unit cell are polynomially expressed in terms of its design variable. In the latter step, the corresponding TOP is set up and applications of the proposed methodology are presented.

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