Multi-objective optimization of composite materials with negative Poisson ratio along several directions

Anca-Maria Toader
Cristian Barbarosie

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{amtan,barbaros}@ptmat.fc.ul.pt

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Abstract

The goal of this paper is the optimization of periodic microstructures for obtaining homogenized elastic tensors having negative Poisson ratio (so-called auxetic materials) using shape and/or topology variations in the model hole. In previous works of the same authors, anisotropic homogenized tensors have been obtained which exhibit negative Poisson ratio in a prescribed direction of the plane. In the present work, a new approach is proposed. Our approach emploies multi-objective optimization in order to minimize the Poisson ratio of the (possibly anisotropic) homogenized elastic tensor in two or more prescribed directions of the plane, in order to obtain a material having (the same) negative Poisson ratio in all directions. We generalize this approach by making use of a min-max algorithm in order to minimize the largest Poisson ratio of the homogenized elastic tensor among all possible directions of the plane.

Keywords : porous materials, microstructure, auxetic materials

1 Introduction

The main motivation of the present paper comes from the study of periodic microstructures and optimization of their macroscopic properties, in the context of linearized elasticity. A periodic microstructure is a body whose material coefficients vary at a microscopic scale, according to a periodic pattern. Homogenization theory allows one to accurately describe the macroscopic behaviour of such a microstructure by means of so-called cellular problems, which are elliptic

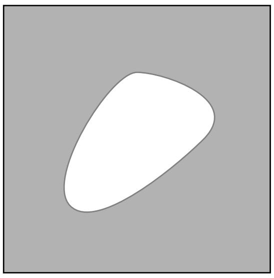

Figure 1: Periodicity cell with model hole (zoomed)

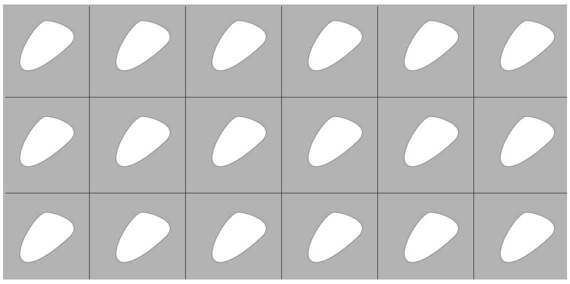

Figure 2: Periodically perforated plane $\mathbb{R}^2_{\text{perf}}$

PDEs subject to periodicity conditions. Porous materials, that is, bodies with periodic infinitesimal perforations, can be described in a similar manner.

The present study focuses on minimizing the Poisson ratio of the homogenized material, in the spirit of [1, Section 7] and [2, Subsection 6.6]

We shall consider a model hole, which is a compact set $T \subset Y$ (see Figure 1), where Y is the periodicity cell. Usually, Y is the unit cube in $\mathbb{R}^n$; see, however, [1] for a general notion of periodicity.

The perforated body is obtained by removing from $\mathbb{R}^n$ translations of the model hole. For a cubic cell Y, one has (see Figure 2)

$$\mathbb{R}^n_{\text{perf}} = \mathbb{R}^n \setminus \bigcup_{\vec{k} \in \mathbb{Z}^n} (T + \vec{k}) \tag{1}$$

The cellular problem describing the behaviour of such a porous material is:

$$\left\{ \begin{array}{rc} \text{find } u_{\mathbf{A}}(\vec{x}) & = \mathbf{A}\vec{x} + \phi_{\mathbf{A}}(\vec{x}), \\ \text{where } \phi_{\mathbf{A}} & \text{is a periodic function, and} \\ -\text{div}(\mathbf{C}\varepsilon(\vec{u}_{\mathbf{A}})) & = \vec{0} \text{ in } \mathbb{R}^n_{\text{perf}} \\ \mathbf{C}\varepsilon(\vec{u}_{\mathbf{A}})\vec{n} & = \vec{0} \text{ on } \partial T \end{array} \right. \tag{2}$$

The above problem models the microscopic behaviour of a microstructure with elastic tensor $\mathbf{C}$, occupying the domain $\mathbb{R}^2_{\text{perf}}$ and subject to the macroscopic strain $\mathbf{A}$. The homogenized elastic tensor $\mathbf{C}^H$, describing the effective (macroscopic) behaviour of this microstructure, is given by

$$\mathbf{C}^H\mathbf{A} = \frac{1}{|Y|}\int_{Y\setminus T}\mathbf{C}\varepsilon(\vec{u}_{\mathbf{A}}) \tag{3}$$

or

$$\langle\mathbf{C}^H\mathbf{A},\mathbf{B}\rangle = \frac{1}{|Y|}\int_{Y\setminus T}\langle\mathbf{C}\varepsilon(\vec{u}_{\mathbf{A}}),\varepsilon(\vec{u}_{\mathbf{B}})\rangle\,, \tag{4}$$

where $\mathbf{A}$ and $\mathbf{B}$ are given macroscopic strains.

The cellular problem (2) can be reformulated in stress, as follows (see [1]) :

$$\left\{\begin{array}{c} \vec{w}_\sigma \in LP_{\text{perf}}, \\ -\text{div}(\mathbf{C}\varepsilon(\vec{w}_\sigma)) = \vec{0} \text{ in } \mathbb{R}^n_{\text{perf}} \\ \mathbf{C}\varepsilon(\vec{w}_\sigma)\vec{n} = \vec{0} \text{ on } \partial T \\ \dfrac{1}{|Y|}\displaystyle\int_{Y\setminus T}\mathbf{C}\varepsilon(\vec{w}_\sigma) = \sigma\,, \end{array}\right. \tag{5}$$

where σ represents an applied macroscopic stress.

We shall denote by $\mathbf{D}^H$ the homogenized compliance tensor, that is, the inverse of $\mathbf{C}^H$.

2 Shape and topology derivatives

The effective elastic properties of the above described porous body can be optimized by varying the size and shape of existing holes in the periodicity cell Y, and also by creating new, infinitesimal, holes.

The first approach is called shape optimization (here applied at the cellular level). The shape derivative describes the variation of a certain objective functional when an infinitesimal deformation is applied to a given geometry. Consider $\vec{\theta} : \mathbb{R}^n \to \mathbb{R}^n$ a vector field defining the deformation; note that $\vec{\theta}$ itself should be periodic in order to preserve the periodic character of the microstructure under study. Then the variation induced by this deformation in the quantity $\langle\mathbf{C}^H\mathbf{A},\mathbf{B}\rangle$ is (see [3] and [1, Section 6])

$$D_S\langle\mathbf{C}^H\mathbf{A},\mathbf{B}\rangle = \frac{1}{|Y|}\int_{\partial T}\langle\mathbf{C}\varepsilon(\vec{u}_{\mathbf{A}}),\varepsilon(\vec{u}_{\mathbf{B}})\rangle\,\vec{\theta}\cdot\vec{n}$$

where $\vec{n}$ is the unit vector normal to the boundary of the hole T and pointing inside T. Assuming that $\mathbf{C}$ is a linear isotropic elastic tensor, $\mathbf{C}\xi = 2\mu\xi + \lambda(\text{tr}\xi)I$, the above formula becomes

$$D_S\langle\mathbf{C}^H\mathbf{A},\mathbf{B}\rangle = \frac{1}{|Y|}\int_{\partial T}\big[2\mu\langle\varepsilon(\vec{u}_{\mathbf{A}}),\varepsilon(\vec{u}_{\mathbf{B}})\rangle + \lambda\text{tr}(\varepsilon(\vec{u}_{\mathbf{A}}))\text{tr}(\varepsilon(\vec{u}_{\mathbf{B}}))\big]\,\vec{\theta}\cdot\vec{n}$$

In particular, this gives the shape derivative of the homogenized coefficients:

$$D_S C^H_{ij} = D_S\langle\mathbf{C}^H\mathbf{f}_i,\mathbf{f}_j\rangle = \frac{1}{|Y|}\int_{\partial T}\big[2\mu\langle\varepsilon(\vec{u}_{\mathbf{f}_i}),\varepsilon(\vec{u}_{\mathbf{f}_j})\rangle + \lambda\text{tr}(\varepsilon(\vec{u}_{\mathbf{f}_i}))\text{tr}(\varepsilon(\vec{u}_{\mathbf{f}_j}))\big]\,\vec{\theta}\cdot\vec{n} \tag{6}$$

where $(\mathbf{f}_i)_{i=1,2,3}$ is the following basis in the space of symmetric matrices

$$\mathbf{f}_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \ \mathbf{f}_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}, \ \mathbf{f}_3 = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

and $\vec{u}_{\mathbf{f}_i}$ are the corresponding solutions of the cellular problem (2) with effective strain $\mathbf{f}_i$.

A second approach for the optimization of a structure is topology variation (here applied at the cellular level). It consists in drilling an infinitesimal circular hole and imposing zero Neumann condition on the newly created boundary. The topological derivative describes the infinitesimal variation thus induced in the functional $\langle \mathbf{C}^H \mathbf{A}, \mathbf{B} \rangle$, and depends on the location x of the new hole. It can be proven (see [1, Section 5] and [4]) that the topological derivative is given by

$$\begin{aligned} D_T \langle \mathbf{C}^H \mathbf{A}, \mathbf{B} \rangle (x) \qquad &= -\frac{\pi}{|Y|} \frac{\lambda + 2\mu}{\lambda + \mu} \Big[4\mu \varepsilon(\vec{u}_{\mathbf{A}}) \varepsilon(\vec{u}_{\mathbf{B}}) + \\ &+ \frac{\lambda^2 + 2\lambda\mu - \mu^2}{\mu} \operatorname{tr} \varepsilon(\vec{u}_{\mathbf{A}}) \operatorname{tr} \varepsilon(\vec{u}_{\mathbf{B}}) \Big] (x) \end{aligned} \tag{7}$$

In [2], an algorithm was proposed for optimizing the microgeometry of the hole(s) in the cellular problem, with the goal of improving certain macroscopic properties of the porous microstructure (which is a body with periodically distributed infinitesimal perforations). The algorithm alternates shape variations with topology variations until a certain convergence criterion is fulfilled. The properties to be optimized include the effective bulk modulus, the effective response to shear and the effective Poisson coefficient (see [2, Section 6]).

Both shape and topology derivatives of the homogenized compliance tensor $\mathbf{D}^H$ are obtained from the derivatives of the homogenized tensor $\mathbf{C}^H$ by :

$$D_S \mathbf{D}^H_{ijkl} = -D^H_{ij\alpha\beta}\, D_S \mathbf{C}^H_{\alpha\beta\gamma\delta}\, D^H_{\gamma\delta kl}, \quad D_T \mathbf{D}^H_{ijkl} = -D^H_{ij\alpha\beta}\, D_T \mathbf{C}^H_{\alpha\beta\gamma\delta}\, D^H_{\gamma\delta kl}. \tag{8}$$

3 Poisson ratios and the min-max technique

This work focuses on the search of two-dimensional periodic microstructures exhibiting negative Poisson ratio at the macroscopic level (so-called auxetic materials). In previous works of the same authors [1], [2], anisotropic effective elastic tensors have been obtained which exhibit negative Poisson ratio in a prescribed direction of the plane (the horizontal direction), see Figure 3. In the present work, we look for periodic microstructures with the same negative Poisson ratio among all directions in the plane. This is done by combining the technique described in the previous section (for shape optimization at the cellular level) with a min-max algorithm which ensures that the largest Poisson ratio among all the directions in the plane is being minimized.

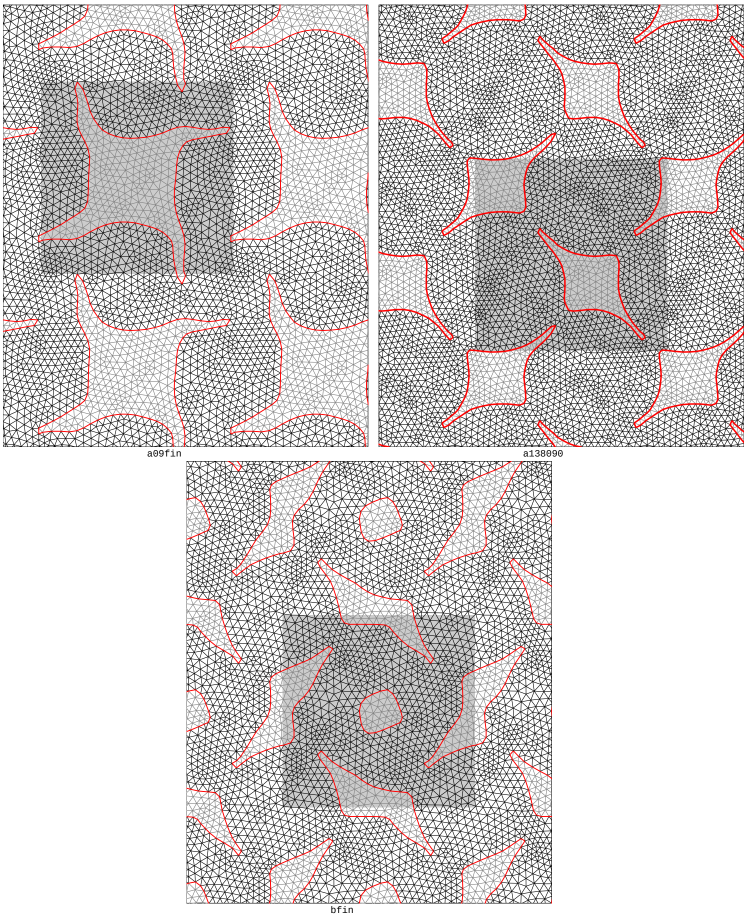

Figure 3: Optimized microstructures with one, two and three holes, respectively

3.1 The Poisson coefficient

Note that the effective elastic tensor resulting from the homogenization technique, defined by (3) or (4), is not isotropic in general. Thus, the notion of Poisson coefficient must be defined with care : it is minus the ratio between the transverse strain and the axial strain when the material is stretched or compressed along the axial direction, see [5]. In the two dimensional case under consideration, the Poisson ratios to be used are: for a unit vector $\vec{v} = (v_1, v_2)$, arbitrarily fixed in the plane, a stretching stress is applied along the direction of $\vec{v}$; in the frame $\{\vec{v}, \vec{v}^\perp\}$ the stress writes $\sigma = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$. Then the Poisson ratio ν_v in the direction $\vec{v}$ is defined as $\nu_v = -\dfrac{\varepsilon_{\perp\perp}}{\varepsilon_{vv}}$, where $\varepsilon_{\perp\perp}$ is the strain in the direction $\vec{v}^\perp$ and ε_{vv} is the strain in the direction $\vec{v}$. The above defined stress σ expressed in cartesian coordinates has the form

$$\sigma = \begin{pmatrix} v_1^2 & v_1 v_2 \\ v_1 v_2 & v_2^2 \end{pmatrix} \tag{9}$$

and the associated strain matrix is $\varepsilon = \mathbf{D}^H \sigma$ (recall that $\mathbf{D}^H$ is the homogenized compliance tensor). Then the axial strain is $\varepsilon_{vv} = \mathbf{D}^H \sigma\, \vec{v} \cdot \vec{v}$ and the transverse strain is $\varepsilon_{\perp\perp} = \mathbf{D}^H \sigma\, \vec{v}^\perp \cdot \vec{v}^\perp$. The Poisson ratio writes as $\nu_v = -\dfrac{\mathbf{D}^H \sigma\, \vec{v}^\perp \cdot \vec{v}^\perp}{\mathbf{D}^H \sigma\, \vec{v} \cdot \vec{v}}$ and introducing the stress corresponding to a stretch in the direction $\vec{v}^\perp$, denoted by

$$\sigma^\perp = \begin{pmatrix} v_2^2 & -v_1 v_2 \\ -v_1 v_2 & v_1^2 \end{pmatrix}, \tag{10}$$

it becomes :

$$\nu_v = -\frac{\langle \mathbf{D}^H \sigma, \sigma^\perp \rangle}{\langle \mathbf{D}^H \sigma, \sigma \rangle}. \tag{11}$$

The derivative of ν_v with respect to $\mathbf{D}^H$ is given by :

$$\frac{\partial \nu_v}{\partial \mathbf{D}^H_{ijkl}} = -\frac{\sigma_{ij} \sigma^\perp_{kl}}{\langle \mathbf{D}^H \sigma, \sigma \rangle} + \frac{\langle \mathbf{D}^H \sigma, \sigma^\perp \rangle}{\langle \mathbf{D}^H \sigma, \sigma \rangle^2} \sigma_{ij} \sigma_{kl} \tag{12}$$

The above formulae (11) and (12) are suitable for implementation since they can actually be seen as depending on the homogenized tensor $\mathbf{C}^H$, see (8).

3.2 The min-max algorithm

The min-max algorithm proposed in [6] and mentioned in [7, Section 8] considers a family of functionals to minimize in simultaneous. More precisely, the goal is to minimize the maximum of several different functionals :

$$\min_s \max\{f_1(s), f_2(s), \ldots, f_m(s)\}.$$

This approach is based on the notion of active indices, which refer to functionals f_j that attain the maximum in the formula above.

In the present case, this family consists of all Poisson ratios associated to the effective elasticity tensor $\mathbf{C}^H$ in many different directions of the plane. Specifically, we consider a (large but finite) set of directions $\vec{\mathrm{v}}$ in the plane and for each direction we associate the respective Poisson ratio ν_v defined by (11), (9) and (10). Each Poisson ratio ν_{v} is a functional of $\mathbf{D}^H$ which is the inverse tensor of $\mathbf{C}^H$ which in turn is function of the shape and topology of the perforations denoted by T in Section 1. The respective derivatives of these dependencies have been presented in Section 2, formula (8) and subsection 3.1 formula (12). Each Poisson ratio ν_v depends on the unit vector $\vec{v}$ as a parameter, fixed during the optimization process.

Here is a sketch of the min-max algorithm :

- `start with some initial guess` s
- `consider a set of active indices (initially empty)`
- `repeat until convergence :`
  - `compute` $\max\{f_1(s), f_2(s), \ldots, f_m(s)\} = f_i(s)$
  - `add` i `to the set of active indices`
  - `call the routine for` $\min_s f_i(s)$ `under the constraints` $f_j(s) - f_i(s) \leq 0$ `(`j `active,` $j \neq i$`)`

The constrained minimization routine, refered in the last step of the algorithm, has the following scheme :

`Goal :` $\min_s f(s)$ `subject to` $g_1(s) \leq 0, g_2(s) \leq 0, \ldots, g_n(s) \leq 0$

- `consider a step` δs `of the form` $\delta s = -\eta \nabla f(s) - \sum_{j \ active} \lambda_j \nabla g_j(s)$
- `compute` λ_j `by imposing the Newton conditions` $\delta s \cdot \nabla g_j(s) = -g_j(s)$ `with` j `active`
- `if` $\lambda_j < 0$ `then the index` j `should become inactive`

The directions corresponding to the largest Poisson ratios are chosen and those ratios are minimized in simultaneous. This ensures that, after convergence, the effective elastic tensor thus obtained has the same Poisson ratio in all directions of the plane; also, if the process is successful, this Poisson ratio will be negative. Note, however, that this does not ensure that $\mathbf{C}^H$ is isotropic.

4 Numerical implementation and numerical results

The algorithm used in this work is an improved version of our home-made code, presented in [2, Section 4]. The improvement consists in the addition of a min-max routine which handles the optimization of the worst case among several functionals, see Section 5.

As explained in [2, Section 4], in order to discretize problem (2), the microstructure is meshed with triangular finite elements of Lagrange type of degree two. Some of the triangles are marked as “full”, corresponding to the elastic material, while other triangles are marked as “empty”, corresponding to the hole T. The interface between material and hole is marked in red (see Figure 3). Note that, although for graphical purposes several contiguous cells are represented, the mesh covers only one cell Y and is “closed” in itself, having no boundary. It can be described as a mesh on the two-dimensional torus; the graphical representation in Figure 3 refers to an unfolded mesh where vertices, segments and triangles are drawn more than once.

In order to implement the periodicity condition in (2), linear+periodic functions are considered on this mesh (they can be identified with multi-functions on the torus). This is done by keeping track of segments crossing the boundary of the cell Y and by taking into account the jump of the function along those segments.

Along the optimization process, the mesh deforms in order for the holes to change their shape. The deformation of the mesh is accomplished by simply moving the vertices. However, this implies a gradual loss in the quality of the mesh : sharp angles appear eventually, as well as too long or too short sements. At some point, certain triangles may even become flat or be reversed. Of course this must be prevented, since it turns the process of solving problem (2) by the finite element method ill posed and consequently unstable. With this end in view, the program improves frequently the quality of the mesh, either by moving the vertices (equilibrating the mesh) or by changing the elements of the mesh (flipping segments, adding/eliminating vertices). See [2, Section 5] for details.

For shape optimization, the integrands in (6) are computed. These are scalar functions defined on the boundary of the holes and depending on the solutions $u_{\mathbf{f}_j}$ of three cellular problems ($j = 1, 2, 3$). A functional J is chosen which depends on the homogenized coefficients C^H_{ij} (here, the Poisson ratio – see Section 5). The shape derivative of J is computed as

$$D_S J = \sum_{ij} \frac{\partial J}{\partial C^H_{ij}} D_S C^H_{ij} = \int_{\partial T} \gamma\, \vec{\theta} \cdot \vec{n}$$

where γ is a scalar function defined as a linear combination of the integrands in (6). In accordance with a steepest descent method, one chooses a deformation equal to $-\gamma\vec{n}$ (multiplied by some positive constant which controls the speed of the process) on the interface ∂T in order to decrease the value of J. This provides a deformation of the interface ∂T, which is then propagated into the whole mesh by means of an averaging process (see [2, Section 5]).

Topology optimization can be performed by simply changing the triangles neighbour to a certain vertex from material to void. However, in the present paper we focus only on shape optimization, which means that we begin the optimization process with a certain number of holes in the periodicity cell, and this number is going to remain constant up to the end of the optimization process.

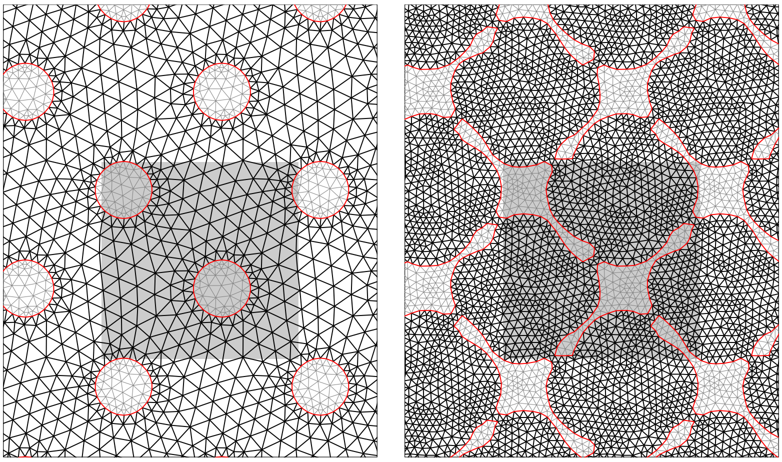

Figure 4: Initial guess and final microstructure for square periodicity

In the first example we optimize the Poisson ratios along ten directions in the plane, at angles uniformly distributed between 0 and 180 degrees. The largest Poisson ratio among those ten directions is minimized. The initial microstructure (initial guess), see Figure 4, has a square periodicity, property that does not vary during the optimization process. It presents two model holes that repeat periodically. The algorithm, after 54 iterations, produced the microstructure on the right in Figure 4, still with square periodicity and still presenting two model holes. At iteration 47 the Poisson ratios became negative and the final design presents Poisson ratios less then -0.7. In the history of convergence, see Figure 5, one can observe that in the first iterations the algorithm makes the ten Poisson ratios as close as possible and afterwards it decreases them all together.

In the second example eighteen directions in the plane are chosen, at angles uniformly distributed between 0 and 180 degrees. The largest Poisson ratio among those directions is minimized. The initial guess has a hexagonal periodicity and presents one model hole repeated periodically (with respect to the hexagonal periodicity), see Figure 6. After 60 iterations the algorithm produces the microstructure presented in Figure 6, on the right. The history of convergence in shown in Figure 7, with two zoom in views. The final design has Poisson ratios arround -0.9 in all eighteen directions.

5 Conclusions

An algorithm for optimization of periodic microstructures for obtaining homogenized elastic tensors with negative Poisson ratio, is presented. It uses shape and/or topology variations in the model hole that characterizes the microstructure. Multi-objective optimization is emploied in order to minimize the Poisson ratio of the homogenized elastic tensor in several prescribed directions of the

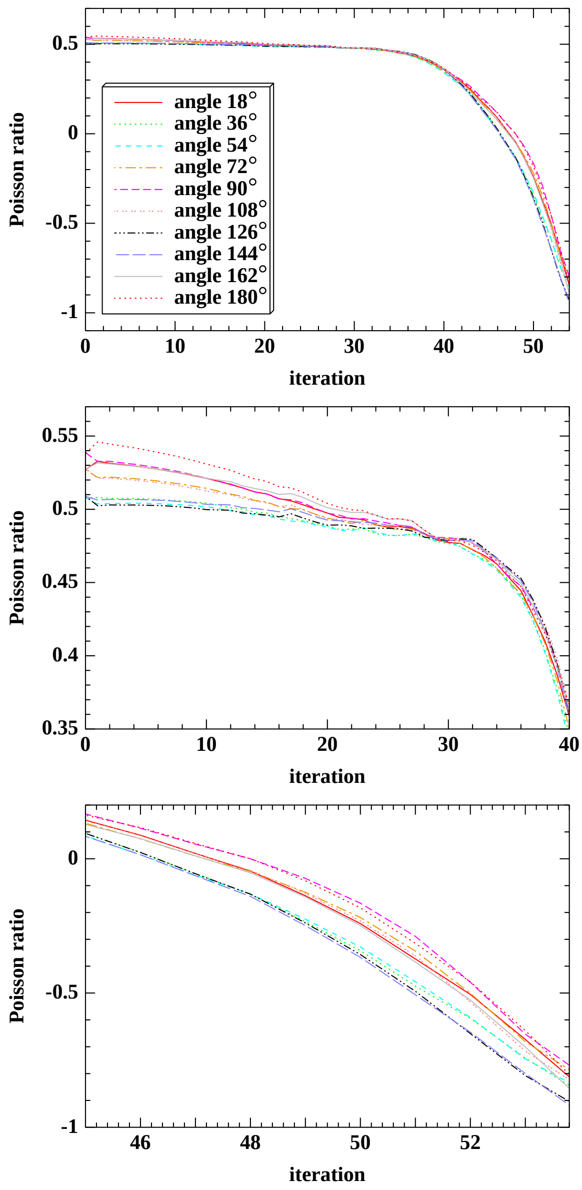

Figure 5: History of convergence, zoom of the first 40 iterations and zoom of the last 6 iterations

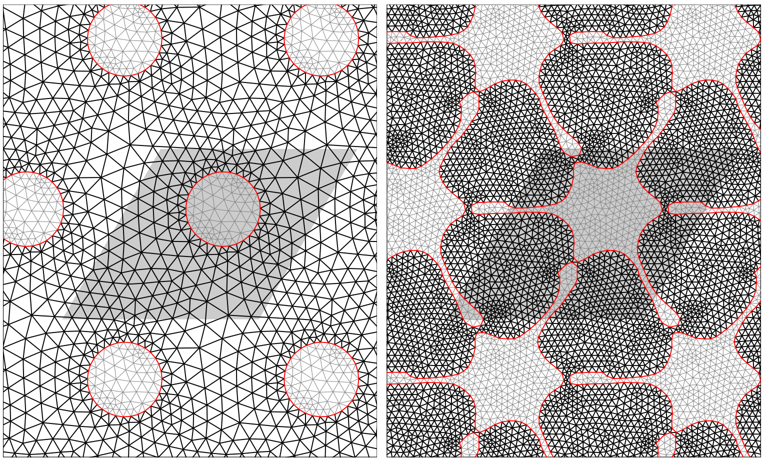

Figure 6: Initial guess and final microstructure for hexagonal periodicity

plane, in order to obtain a material having the same negative Poisson ratio in all directions. The algorithm is based on a min-max procedure in order to minimize the largest Poisson ratio of the homogenized elastic tensor among all possible directions of the plane.

It is possible to obtain periodic 2D microstructures with Poisson ratio close to -1 and roughly the same in all directions of the plane. The algorithm is effective also for 3D microstructures. The examples show that the algorithm tends to "cut" the structure, so the bulk modulus approaches zero.

6 Acknowledgements

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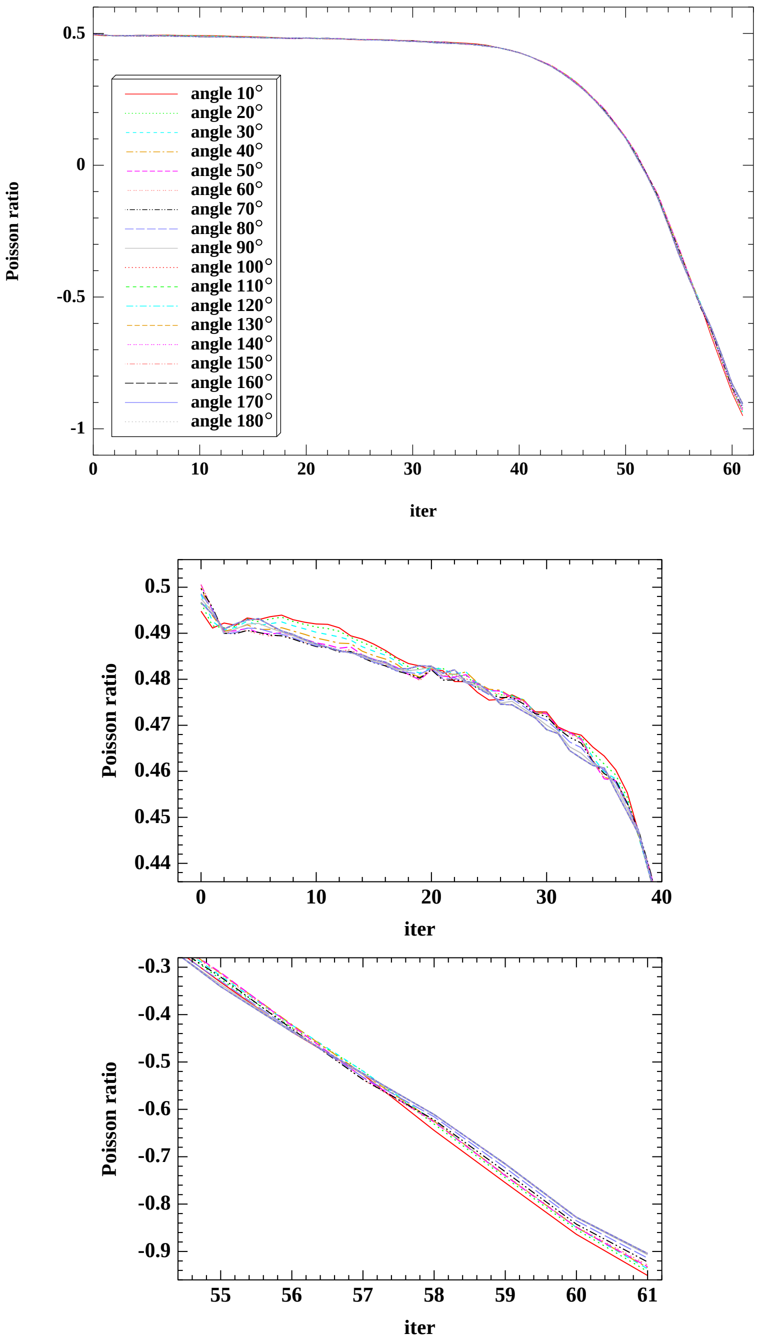

Figure 7: History of convergence, zoom of the first 40 iterations, zoom of the last 8 iterations

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