Inverse Design of Periodic Materials: Numerical Experiments using Finite Elements

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Abstract

In this paper, we study certain computational aspects of an inverse homogenization approach to the design of materials with prescribed constitutive properties. This approach assumes that the material consists of periodically repeated unit cells, and thus the problem of designing a material with prescribed properties is reduced to one of designing the unit cell. This problem of designing the unit cell is formulated as a layout optimization problem, where the objective is to minimize the weight of the unit cell subject to constraints on the effective properties of the unit cell. The effective properties of the unit cell are computed using asymptotic homogenization theory. Details of asymptotic homogenization theory are reviewed and the formulation of the inverse homogenization approach is discussed. Several numerical experiments involving the use of bilinear and biquadratic finite elements for the solution of the inverse homogenization are presented.

1 Introduction

In recent decades, there have been several advances in the area of computer simulations, particularly in the analysis of engineering materials. Given a material’s properties, it is now routine to predict its behavior under the actions of loads and forces using computer simulation. However, the reverse process, that of designing a material that has prescribed material properties (such as a negative Poisson’s ratio), is less well understood and mostly unexplored.
This article is aimed at studying certain aspects of a computational approach proposed by Sigmund [6, 7] for the design of materials with prescribed material properties. In the inverse homogenization approach proposed by Sigmund, the material to be designed is assumed to be periodic, i.e., the material is obtained by the periodic repetition of a unit cell. The overall properties of the material depend only on the unit cell, and thus the problem is one of designing the unit cell that results in prescribed effective properties. Of course, for a given design of the unit cell, the effective properties can be found easily, using the theory of asymptotic homogenization [1, 5].

Sigmund’s approach to designing the unit cell consists of posing a layout optimization problem: the goal is to find the unit cell layout that minimizes the weight, subject to equality constraints on the effective properties of the cell (found via asymptotic homogenization). This layout problem is discretized using either truss finite elements or continuum finite elements. For the case of truss finite elements, the lengths of the elements form the design variables. For the case of continuum elements, the relative densities of the elements are taken to be the design variables. In either case, the stiffness of each element is taken to be proportional to the design variable. The discrete layout optimization problem is then solved using an optimality criteria (OC) method [4].

In this work, we implement Sigmund’s inverse homogenization approach using the finite element software PIFED [8]. The procedure is tested for various prescribed properties including materials with Poisson’s ratio $\nu = -0.95$. Such materials are known as auxetic materials; they display superior resilience and toughness, are typically light in weight, and are ideal candidates for use as cores in composite sandwich panels [3, 2].

We study the effect of factors such as mesh size, order of approximation and the assumed initial distribution of the design variables. We restrict our attention to continuum elements in two dimensions.

The rest of this article is organized as follows: In Section 2, we review the basics of the asymptotic theory of homogenization of periodic materials. The inverse homogenization problem is formulated in Section 3, following the treatment by Sigmund [6]. We conclude the article with numerical experiments in Section 4, and some comments in Section 5.

2 Effective Properties of Periodic Materials

In this section, we briefly review the theory of asymptotic homogenization for computing the effective properties of materials with periodic microstructure.

Consider a domain $\Omega \subset \mathbb{R}^n$, $1 \leq n \leq 3$ occupied by a linearly elastic body. The domain is assumed to be composed of microscopic cells $Y_\epsilon$, each cell being the image of a unit cell $Y$ under a dilation $x = \epsilon y$ and a translation. We will use $x$ to denote the coordinate system at the macroscopic level and $y$ to denote the coordinate at the microscopic level. The scaling parameter $\epsilon$ provides an estimate of the ratio of the unit cell’s size to the domain’s size. In what follows, we will use $u^\epsilon$, $\epsilon^\epsilon$, $\sigma^\epsilon$ to denote the displacement, strain and stress fields,
respectively, in the body. The superscript $\epsilon$ indicates the dependence of the quantities on the mapping between the global and local scales.

\[ \Gamma_u \]

\[ \Omega \]

\[ Y \]

Figure 1: Schematic of a periodic domain $\Omega$.

The body is in equilibrium under the action of body forces $f \in L^2(\Omega)$ and tractions $t \in L^2(\Gamma_t)$, where $\Gamma_t \subset \partial \Omega$ is the portion of the boundary under tractions. Essential boundary conditions $u = 0$ are prescribed on $\Gamma_u \subset \partial \Omega$. We assume $\Gamma_u \cap \Gamma_t = \emptyset$ and $\Gamma_u \cup \Gamma_t = \partial \Omega$. The boundary $\partial \Omega$ is assumed to be sufficiently smooth. The equations governing the equilibrium of the body are

\[ -\text{div}(\sigma^\epsilon) = f \quad \text{in } \Omega \]

\[ \sigma^\epsilon = E^\epsilon \epsilon^\epsilon \]

\[ \epsilon^\epsilon = \frac{1}{2} \left( \nabla u^\epsilon + (\nabla u^\epsilon)^T \right) \]

\[ \sigma^\epsilon \cdot n = t \quad \text{on } \Gamma_t \]

\[ u^\epsilon = 0 \quad \text{on } \Gamma_u \]

(1)

Here $n$ is the unit outward normal to $\partial \Omega$.

The body’s elasticity tensor $E^\epsilon$ is given by

\[ E^\epsilon(x) = E \left( \frac{x}{\epsilon} \right) \] (2)

where $E$ is the $Y$-periodic elasticity tensor on the unit cell $Y$. We assume $E$ is symmetric and elliptic.

We seek two-scale expansions of the form

\[ u^\epsilon(x, y) = u^0(x, y) + \epsilon u^1(x, y) + \epsilon^2 u^2(x, y) + \ldots \]

\[ \epsilon^\epsilon(x, y) = \epsilon^0(x, y) + \epsilon \epsilon^1(x, y) + \epsilon^2 \epsilon^2(x, y) + \ldots \]

\[ \sigma^\epsilon(x, y) = \sigma^0(x, y) + \epsilon \sigma^1(x, y) + \epsilon^2 \sigma^2(x, y) + \ldots \] (3)

where $u^i$, $\epsilon^i$ and $\sigma^i$ are $Y$-periodic. Introducing the expansions into the governing equations, equating terms of equal $\epsilon$ order, and noting that \[ \frac{d}{dx_i} = \frac{\partial}{\partial x_i} + \frac{1}{\epsilon} \frac{\partial}{\partial y_i} \], we obtain two sets of equations:
• The macro-scale equations:

At the macro-scale, the equations governing the equilibrium are:

\[-\text{div}_x (E^0 \nabla_x u^0) = f \text{ in } \Omega\]
\[u^0 = 0 \text{ on } \Gamma_u\]
\[E^0 \nabla_x u^0 \cdot n = t \text{ on } \Gamma_t\]  \hspace{1cm} (4)

where the subscript \(x\) denotes differentiation with respect to the macroscopic coordinate system.

• The micro-scale equations:

The homogenized elasticity tensor is given by

\[E^0_{ijkl} = \frac{1}{|Y|} \int_Y (\varepsilon^*_{kl} - \varepsilon(\chi^{kl})) : E : (\varepsilon^{*ij} - \varepsilon(\chi^{ij})) \, dy\]  \hspace{1cm} (5)

where the functions \(\chi^{kl}\) are solutions to the following periodic boundary value problem: Find \(\chi^{kl} \in V_Y\) such that \(\int_Y \chi^{kl} \, dy = 0\) and

\[\int_Y \varepsilon(\chi^{kl}) : E : \varepsilon(v) \, dy = \int_Y \varepsilon^*_{kl} : E : \varepsilon(v) \, dy \quad \forall \ v \in V_Y,\]  \hspace{1cm} (6)

where the strains are understood to be with respect to the microscopic coordinate system, and

\[V_Y = \{v : v \in [H^1_{\text{loc}}(\mathbb{R}^n)]^n, v_i \ Y - \text{periodic}\} .\]  \hspace{1cm} (7)

The strains \(\varepsilon^*_{kl}\) are constant and are usually termed pre-strains. In component form, they are given by

\[\varepsilon^*_{pq} = \delta_{kp}\delta_{tq}.\]  \hspace{1cm} (8)

Typically, the equations (6) are solved first to find the array \(\chi^{kl}\), and equation (5) is then used to evaluate the homogenized coefficients \(E^0\). It is worth noting that since the array \(\chi^{mn}\) is symmetric, we need only compute \(\chi^{11}, \chi^{22}, \chi^{12}\) for two-dimensional problems. For three-dimensional problems, we need compute \(\chi^{11}, \chi^{22}, \chi^{33}, \chi^{12}, \chi^{13}, \chi^{23}\). For more details, see [5].

Our goal is to find unit cells \(Y\) that have prescribed homogenized properties \(E^0 = E^*\). We will restrict ourselves to orthotropic elasticity tensors. To facilitate a computational treatment, we modify the notation. For two-dimensional problems, we use: \(\chi^1 \leftarrow \chi^{11}, \chi^2 \leftarrow \chi^{22}, \chi^3 \leftarrow \chi^{12}\), and \(\varepsilon^* \leftarrow \varepsilon^{*11}, \varepsilon^{*2} \leftarrow \varepsilon^{*22}, \varepsilon^{*3} \leftarrow \varepsilon^{*12}\). For components of the homogenized elasticity tensor, we use the simplified notation \(E^0_1 \leftarrow E^{0\,1111}, E^0_2 \leftarrow E^{0\,2222}, E^0_3 \leftarrow E^{0\,1122}\).
resulting in:

\[
E_1^0 = \frac{1}{|Y|} \int_Y (\varepsilon^{s_1} - \varepsilon(\chi^1)) : \mathbf{E} : (\varepsilon^{s_1} - \varepsilon(\chi^1)) \, dy
\]

\[
E_2^0 = \frac{1}{|Y|} \int_Y (\varepsilon^{s_2} - \varepsilon(\chi^2)) : \mathbf{E} : (\varepsilon^{s_2} - \varepsilon(\chi^2)) \, dy
\]

\[
E_3^0 = \frac{1}{|Y|} \int_Y (\varepsilon^{s_1} - \varepsilon(\chi^1)) : \mathbf{E} : (\varepsilon^{s_2} - \varepsilon(\chi^2)) \, dy
\]

\[
E_4^0 = \frac{1}{|Y|} \int_Y (\varepsilon^{s_3} - \varepsilon(\chi^3)) : \mathbf{E} : (\varepsilon^{s_3} - \varepsilon(\chi^3)) \, dy
\]

(9)

in place of (5). For three-dimensional problems, similar notation is used.

3 Formulation of the Optimization Problem

The inverse homogenization problem is solved by posing it as a layout optimization problem, where the objective is to minimize the weight of the unit cell \( Y \), subject to equality constraints on the desired constitutive properties. It is assumed that the unit cell’s elasticity tensor is given by

\[
\mathbf{E}(y) = (\rho(y))^p \cdot \mathbf{E}
\]

(10)

where \( \rho \in L^\infty(Y) \), \( p \geq 1 \), and \( \mathbf{E} \) is constant. The function \( \rho \) represents the relative density of the material in the unit cell. The exponent \( p \) represents a penalization parameter that is commonly used in layout optimization problems to suppress intermediate values of \( \rho \). The problem of determining \( \mathbf{E} \) is now reduced to that of finding \( \rho(\cdot) \). In this paper, we will restrict the discussion to two-dimensional problems, and the treatment of three-dimensional problems is analogous. Also, without any loss of generality, it will be assumed that \( |Y| = 1 \).

The optimization problem can be stated as: Find \( \rho(y) \) such that \( W(\rho) = \int_Y \rho \, dy \) is minimized, subject to the constraints

\[
\rho(y) \geq \underline{\rho} > 0 \ a.e \ in \ Y
\]

\[
\rho(y) \leq \bar{\rho} < \infty \ a.e \ in \ Y
\]

(11)

where \( E_k^0 \) are defined by (9) and \( E_k^* \) are the desired effective properties.

A discrete formulation of the above problem is obtained using the finite element method. The domain \( \Omega \) is discretized in \( NE \) non-overlapping finite elements \( \Omega_i \). We approximate \( \rho(\cdot) \) by a piecewise constant function \( \rho^h = \{\rho^{h,i}\}_{1 \leq i \leq NE} \) and the functions \( \chi^k \) by piecewise polynomial functions \( \chi^{k,h} \).
The discrete optimization problem is now given by: Find \( \{ \rho^{h,i} \} \) such that

\[
W(\rho^h) = \sum_{i=1}^{NE} \rho^{h,i} A^i
\]

is minimized, subject to

\[
\begin{align*}
\rho^{h,i} & \geq \rho, \quad 1 \leq i \leq NE \\
\rho^{h,i} & \leq \bar{\rho}, \quad 1 \leq i \leq NE \\
\sum_{i=1}^{NE} Q^{h,i}_k & = E_k^0, \quad 1 \leq k \leq 4,
\end{align*}
\]

where \( A^i \) is the area of element \( i \), and \( Q^{h,i}_k \) is the contribution of element \( i \) to the effective property \( E_k^0 \). For instance,

\[
Q^{h,i}_1 = \int_{\Omega_i} (\varepsilon^{*1} - \varepsilon(\chi^{1,h})) : E : (\varepsilon^{*1} - \varepsilon(\chi^{1,h})) \, dy, \quad \text{and} \quad E_1^0 = \sum_{i=1}^{NE} Q^{h,i}_1.
\]

The inverse homogenization problem can now be solved using an optimality criteria (OC) method [9, 4]. OC methods are iterative methods that seek to find a solution to the optimization problem by updating the design variables at each iteration based on problem-dependent optimality criteria. To derive the optimality criteria for the problem at hand, the Lagrangian for the problem is first written as:

\[
\mathcal{L}(\rho^h) = \sum_{i=1}^{NE} \rho^{h,i} A^i + \sum_{k=1}^{4} \lambda_k \left( E_k^* - \sum_{i=1}^{NE} Q^{h,i}_k \right) + \sum_{i=1}^{NE} \Lambda_i (-\rho^{h,i} + \rho) + \sum_{i=1}^{NE} \Gamma_i (\rho^{h,i} - \bar{\rho})
\]

where \( \lambda_k \) are the Lagrange multipliers for the equality constraints, \( \Lambda_i \) and \( \Gamma_i \) are the Lagrange multipliers for the lower and upper bounds on \( \rho^{h,i} \), respectively.

Equating the first derivative of the Lagrangian with respect to \( \rho^{h,i} \) to zero,

\[
\frac{\partial \mathcal{L}}{\partial \rho^{h,i}} = A^i - \sum_{k=1}^{4} \lambda_k \frac{Q^{h,i}_k}{\rho^{h,i}} - \Lambda_i + \Gamma_i = 0,
\]

where \( \frac{\partial Q^{h,i}_k}{\partial \rho^{h,i}} = \frac{Q^{h,i}_k}{\rho^{h,i}} \) at constant strains.

If one assumes the constraints on the bounds on \( \rho^i \) to be inactive, i.e., \( \Lambda_i = \Gamma_i = 0 \), then

\[
\rho^{h,i} = \sum_{k=1}^{4} \lambda_k Q^{h,i}_k / A^i.
\]
Based on (17), Sigmund [6] suggests the following scheme to update the design variables \( \rho^{h,i} \) at each iteration of the OC scheme:

\[
\rho^{h,i} = \begin{cases} 
\rho & \text{for } \sum_{k=1}^{4} \frac{\lambda_k Q_k^{h,i}}{A^i} \leq \rho \\
\sum_{k=1}^{4} \frac{\lambda_k Q_k^{h,i}}{A^i} & \text{for } \rho < \sum_{k=1}^{4} \frac{\lambda_k Q_k^{h,i}}{A^i} < \bar{\rho} \\
\bar{\rho} & \text{for } \sum_{k=1}^{4} \frac{\lambda_k Q_k^{h,i}}{A^i} \geq \bar{\rho}.
\end{cases}
\]  

(18)

At each iteration of the OC method, the Lagrange multipliers \( \lambda_k \) are computed using a Newton-Raphson algorithm. For this, the equality constraints (13) are written as:

\[
\phi_k = \sum_{i=1}^{NE} \frac{\rho_{h,i} Q_k^{h,i}}{\rho_0^{h,i}} - E_k^{*} = 0, \quad 1 \leq k \leq 4,
\]  

where \( \rho_0^{h,i} \) is the value of the design variable from the previous iteration. The rationale is that the ratio \( \rho^{h,i}/\rho_0^{h,i} \) is unity when the procedure converges and thus the original equality constraints are recovered. To minimize the functions \( \phi = \{ \phi_k \} \), the Lagrange multipliers \( \lambda = \{ \lambda_k \} \) are computed iteratively using the formula

\[
\lambda_{l+1} = \lambda_l - (\nabla \phi)^{-1}_l \phi_l.
\]  

(20)

The outer OC iterations are continued till the change in the objective function is below a preset tolerance. The overall flowchart is shown in Fig. 2.

4 Numerical Experiments

The inverse homogenization procedure described in the previous section is used to generate various microstructures with prescribed properties \( E^* \). Our goal is to study the effect of factors such as mesh size, order of approximation and the (assumed) initial conditions for the design variables on the outcome of the procedure. In particular, because the solution to the inverse homogenization procedure is non-unique, we are interested in the effect of the initial distribution of the design variables (element densities \( \rho^{h,i} \)).

The algorithm is implemented in two spatial dimensions using the public-domain finite element package PIFED [8]. In the experiments that follow, the unit cell \( Y \) is taken to be the unit square and is discretized using a 20 \( \times \) 20 or 40 \( \times \) 40 mesh of equal-sized finite elements. Two types of initial conditions are assumed for the design variables \( \rho^{h,i} \). The two distributions, referred to as IC1 and IC2, are shown in Fig. 3, and feature radially varying distributions.
Figure 2: Overall flowchart for the inverse homogenization procedure.

Each combination of mesh discretization and initial distribution is tested for three different target prescribed elasticity tensors. For the case of a 20x20 mesh, we also use an enriched
mesh that employs biquadratic elements. Thus, for each target elasticity tensor, six numerical experiments are performed: three for distribution IC1 and three for IC2. This information is summarized in Table 1.

Table 1: Summary of parameters used for each target elasticity tensor.

<table>
<thead>
<tr>
<th>Case</th>
<th>Number of Elements</th>
<th>Initial Density Distribution</th>
<th>Degree of Approximating Polynomial</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>20×20</td>
<td>IC1</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>40×40</td>
<td>IC1</td>
<td>1</td>
</tr>
<tr>
<td>3</td>
<td>20×20</td>
<td>IC1</td>
<td>2</td>
</tr>
<tr>
<td>4</td>
<td>20×20</td>
<td>IC2</td>
<td>1</td>
</tr>
<tr>
<td>5</td>
<td>40×40</td>
<td>IC2</td>
<td>1</td>
</tr>
<tr>
<td>6</td>
<td>20×20</td>
<td>IC2</td>
<td>2</td>
</tr>
</tbody>
</table>

We assume that the base elasticity tensor $\mathbf{E}$ (recall (10)) is that of an isotropic material with Poisson’s ratio 0.3 and Young’s Modulus 0.91 GPa, and that the unit cell is under plane stress conditions. The exponent $p$ in (10) is taken to be 1. The maximum and minimum values for the design variable are taken to be $\underline{\rho} = 0.01$ and $\bar{\rho} = 20.0$.

In our implementation, we use a loose tolerance on the Newton-Raphson loop (see Fig. 2) to allow the iterations to continue in case of convergence difficulties. Thus, the actual effective properties of the microstructure $\mathbf{E}^0$ determined by the inverse homogenization procedure may be slightly different from the prescribed material properties $\mathbf{E}^*$. Also, for the outer OC loop, the maximum change in the design variables $\rho^{h,i}$ is limited to 1% of the value in the previous iteration. This has the effect of stabilizing the iterations, but the total number of
iterations increases.

4.1 Experiment 1: Material with $\nu = 0.99$

Our first experiment involves the design of a material with Poisson’s ratio $\nu = 0.99$. Thus, we have $E^* = [1.00 \ 1.00 \ 0.99 \ 0.02]$ GPa. The results from the three cases corresponding to the initial distribution IC1 are shown in Fig. 4, and the results from the three cases corresponding to the initial distribution IC2 are shown in Fig. 5.

For this experiment, the resulting unit cell topologies are essentially black and white topologies, with some “gray” areas seen in Fig. 5. For the distribution IC1, it is seen that refining the mesh or increasing the order of approximation does not alter the basic topology of the unit cell. For the sake of comparison, the topology obtained by Sigmund [6] for this target elasticity tensor is also shown in the figure. For the distribution IC2, however, there is a change in the basic topology of the unit cell when the initial 20×20 mesh is either refined or enriched: each ligament extending from the center of the cell to the corners is split into two ligaments. This signals a dependence of the solution on the mesh, an undesirable effect. The obvious dependence of the result on the initial distribution of the design variables is due to the non-uniqueness of the solution.

The actual effective properties of the microstructures and the number of OC iterations are listed in Table 2.

<table>
<thead>
<tr>
<th>Case</th>
<th>OC iterations</th>
<th>Actual $E^*$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>860</td>
<td>[1.04 1.04 0.97 0.09]</td>
</tr>
<tr>
<td>2</td>
<td>860</td>
<td>[1.07 1.07 0.99 0.07]</td>
</tr>
<tr>
<td>3</td>
<td>540</td>
<td>[1.24 1.24 1.02 0.21]</td>
</tr>
<tr>
<td>4</td>
<td>880</td>
<td>[1.02 1.00 0.91 0.21]</td>
</tr>
<tr>
<td>5</td>
<td>980</td>
<td>[1.07 1.07 1.05 0.28]</td>
</tr>
<tr>
<td>6</td>
<td>700</td>
<td>[1.12 1.11 1.03 0.17]</td>
</tr>
</tbody>
</table>

Table 2: Summary of results for Experiment 1: Material with $\nu = 0.99$.

4.2 Experiment 2: Anisotropic Material with $\nu = 0.48$

Here, our goal is to design an anisotropic nearly-incompressible material with the effective elasticity tensor $E^* = [1.00 \ 0.25 \ 0.48 \ 0.02]$ GPa. As in the previous example, the inverse homogenization procedure is used and all six cases listed in Table 1 are considered.

For the initial distribution IC1, a reasonably converged topology is achieved only for case 1. For cases 2 and 3, the procedure does not converge. The result for case 1 is shown in Fig. 6. The result shows a significant amount of “gray” material, also an undesirable feature.
Figure 4: Experiment 1: Material with \( \nu = 0.99 \). Results obtained using initial distribution IC1 for (a) Case 1: 20\times20 mesh, bilinear elements, (b) Case 2: 40\times40 mesh, bilinear elements, (c) Case 3: 20\times20 mesh, biquadratic elements, and (d) Comparable result obtained by Sigmund [6].
Figure 5: Experiment 1: Material with $\nu = 0.99$. Results obtained using initial distribution IC2 for (a) Case 1: 20×20 mesh, bilinear elements, (b) Case 2: 40×40 mesh, bilinear elements, (c) Case 3: 20×20 mesh, biquadratic elements.
Figure 6: Experiment 2: Anisotropic material with \( \nu = 0.48 \). Results obtained using initial distribution IC1 for Case 1: \( 20\times20 \) mesh, bilinear elements. For the other two cases, the procedure does not converge.

Results from the three cases corresponding the initial distribution IC2 are shown in Fig. 7 and compared to Sigmund’s result for this problem [6]. The actual effective properties of the microstructures and the number of OC iterations are listed in Table 3. The procedure has difficulty converging, and the actual effective properties of the unit cells are not sufficiently close to the prescribed effective properties in all cases. Again, the results indicate that the solution is sensitive to both the mesh and the initial distribution.

<table>
<thead>
<tr>
<th>Case</th>
<th>OC iterations</th>
<th>Actual ( E^0 ) (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3200</td>
<td>[1.02 0.27 0.52 0.09]</td>
</tr>
<tr>
<td>2</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>2800</td>
<td>[1.12 0.28 0.53 0.09]</td>
</tr>
<tr>
<td>5</td>
<td>700</td>
<td>[1.21 0.35 0.58 0.23]</td>
</tr>
<tr>
<td>6</td>
<td>500</td>
<td>[1.59 0.55 0.73 0.27]</td>
</tr>
</tbody>
</table>

Table 3: Summary of results for Experiment 2: Material with \( \nu = 0.48 \).

4.3 Experiment 3: Material with \( \nu = -0.95 \)

In the last experiment, we seek to find microstructures with negative Poisson’s ratios. Such materials are also called auxetic materials or dilatational materials [3, 2]. Here, \( E^* = [1.00 1.00 -0.95 0.02] \) GPa. The inverse homogenization procedure converges only for
Figure 7: Experiment 2: Anisotropic material with $\nu = 0.48$. Results obtained using initial distribution IC2 for (a) Case 1: $20\times20$ mesh, bilinear elements, (b) Case 2: $40\times40$ mesh, bilinear elements, (c) Case 3: $20\times20$ mesh, biquadratic elements, and (d) Comparable result obtained by Sigmund [6].
case 4, and the resulting unit cell is shown in Fig. 8. Even for this case, the actual properties of the unit cell are not close to the desired material properties, as can be seen from Table 4.

![Image of the unit cell for case 4]

Figure 8: Experiment 3: Material with $\nu = -0.95$. Results obtained using initial distribution IC2 for Case 4: 20×20 mesh, bilinear elements. For the other cases, the procedure does not converge.

<table>
<thead>
<tr>
<th>Case</th>
<th>OC iterations</th>
<th>Actual $E''$ (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>2</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>4</td>
<td>3000</td>
<td>[1.41 1.51 -0.78 0.26]</td>
</tr>
<tr>
<td>5</td>
<td>No convergence</td>
<td>-</td>
</tr>
<tr>
<td>6</td>
<td>No convergence</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 4: Summary of results for Experiment 3: Material with $\nu = -0.95$.

5 Concluding Remarks

In this paper, we study a computational approach to the design of materials with prescribed material properties, based on Sigmund’s inverse homogenization procedure [6, 7]. Extensive numerical experiments show that while the procedure is successful for some target material properties, it has significant convergence difficulties for other target material properties, particularly when the target material has a negative Poisson’s ratio. Numerical experiments also show that the result of the inverse homogenization procedure is sensitive to factors such as mesh size and approximation order, as well as the initial distribution of the design.
variables. Future efforts in this area should focus on developing formulations that lead to convergent and mesh-independent solutions.

References


