



Multiscale structural optimization for prescribed deformations in the nonlinear elastic regime

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Abstract

In this paper, a multiscale structural optimization framework capable of efficiently designing two-scale structures with prescribed displacements in the nonlinear elastic regime is presented. In contrast to previous multiscale structural optimization frameworks, which are founded upon the assumptions of linear elasticity, the present framework is capable of efficiently operating within the nonlinear elastic regime. At the core of the present framework is a parameterized microscale geometry, which through the straightforward manipulation of the microscale parameters provides direct access to both positive and negative Poisson's ratios. The microscale model is concurrently coupled to the macroscale model such that only the microscale parameter space traversed by the optimizer is resolved during the optimization procedure, leading to a significant reduction in the computational expense of analysis. To demonstrate the capability of this framework, three prescribed deformation profiles are targeted by three distinct optimization procedures. In all instances, the deformation profile is successfully targeted. To verify the accuracy of the optimized structures, high-fidelity single-scale simulations are performed. In each case, excellent agreement is noted between the high-fidelity simulations and the corresponding optimized macroscale displacement fields, with errors of less than 10%.

Keywords Nonlinear · Multiscale · Optimization · Auxetic · Mechanical cloaking

1 Introduction

Advances in additive manufacturing (AM) have enabled the fabrication of complex geometries previously inaccessible through traditional subtractive technologies (Attaran 2017; Prakash et al. 2018). This has prompted a revolution within the domain of structural design, as researchers seek to design frameworks capable of leveraging this new-founded design flexibility in the pursuit of enhanced structural performance (Plocher and Panesar 2019). This has catalyzed the development of multiscale topology optimization frameworks (MTOFs), which give rise to performant designs only manufacturable via AM techniques (Sivapuram et al. 2016; Imediegwu et al. 2019; Colabella et al. 2019; Liu et al. 2020; Murphy et al. 2021b, a; Thillaithevan et al. 2022).

Multiscale topology optimization frameworks permit the microscale description of a structure to be spatially optimized to fulfill functional objectives at the macroscale. In contrast to conventional topology optimization-based approaches (Bendsøe and Kikuchi 1988; Querin et al. 1998; Wang et al. 2003; Bendsøe and Sigmund 2004), this formulation facilitates direct access to extremal point properties (Wu et al. 2021), which would otherwise require the heterogeneous assembly of isotropic material, typically reliant on initialization conditions, optimization algorithm, mesh resolution, and regularization. This permits hierarchical structures with superior mechanical (Imediegwu et al. 2019; Murphy et al. 2021b), thermal (Imediegwu et al. 2021), and dynamic (Nightingale et al. 2021) performance to be generated relative to conventional topology optimization-based approaches.

Multiscale topology optimization frameworks are typically founded upon the assumptions of linear elasticity (Coman 2019), as this permits a significant reduction in the computational expense of analysis at both scales. This enables functional objectives cast exclusively as a function of infinitesimal displacements to be efficiently targeted without

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loss of accuracy (Christensen et al. 2023). However, these assumptions hinder the exploitation of these hierarchical frameworks within the large deformation regime (Thillaithevan et al. 2024) and consequently, their broader application within the domains of soft robotics (Schmitt et al. 2018; Chen and Wang 2020), crashworthiness (Isaac and Ezekwem 2021; Liang et al. 2023), and biomedical engineering (Bobbert et al. 2018; Manen et al. 2021), among others. Consequently, to permit application within these domains, it is necessary to extend the structural analysis at both scales to enable succinct operation within the materially and geometrically nonlinear regimes.

2 Overview

The primary objective of this paper is to present a multiscale structural optimization framework for the efficient design of hierarchical structures with targeted nonlinear mechanical behavior. This work is founded upon the MTOF detailed by Murphy et al. (2021b), which permits the efficient derivation of optimized hierarchical structures for infinitesimal displacement applications exclusively. Consequently, this paper presents extensions to the structural analysis at both the micro- and macroscales, which represents the principal novelty of this framework, and enables the efficient and precise optimization of functional objectives defined in the nonlinear elastic regime.

At the core of the present approach is a parameterization-based optimization strategy, where the parameters describing the microscale geometry are spatially optimized to fulfill functional objectives at the macroscale. As a consequence of extending this approach to the nonlinear elastic regime, the response of the microscale model is no longer invariant with respect to macroscale strain. This necessitates the inclusion of all unique elements of the macroscale strain tensor as additional input parameters to the microscale model. Each additional input parameter exponentially enlarges the microscale parameter space, which consequently increases the computational expense associated with assembling the microscale model. To mitigate this issue, the micro- and macroscale models are concurrently coupled (Abdulle et al. 2012), which enables only the microscale data needed to perform each iteration of macroscale structural analysis to be collected. In the context of multiscale nonlinear structural analysis, concurrent coupling restricts the exploration of the macroscale strain space to the physical strain space for an arbitrary microstructure, which helps to prevent the simulation of non-convergent strain combinations and represents a further point of novelty for this framework.

To demonstrate the efficacy of the present framework, three prescribed deformation cases are presented which exploit nonlinearities at both scales to satisfy the requisite functional

objectives. The accuracy of these results are verified using high-fidelity single-scale finite-element analysis. In addition, the computational benefits afforded by concurrently coupling the micro- and macroscale models are also presented. To reduce the computational cost of expensive nonlinear structural analysis, the present framework is restricted to two-dimensional space; however, only trivial modifications would be required to extend the present framework to the three-dimensional regime.

3 Methodology

The theory of nonlinear elasticity forms the foundation for the present framework, as it enables the accurate prediction of displacements in the large deformation regime. Large deformations introduce geometric nonlinearities due to alterations in the load path resultant from significant differences between the undeformed and deformed configurations (see Fig. 1). To accurately capture this phenomenon, strains are computed for the remainder of this paper using the Green–Lagrange strain tensor ($\mathbf{E}_{ij}$)

$$\mathbf{E}_{ij} = \frac{1}{2} (\mathbf{F}_{ij}^T \mathbf{F}_{ij} - \mathbf{I}) \quad (1)$$

where $\mathbf{I}$ denotes the identity matrix and $\mathbf{F}_{ij}$ denotes the deformation gradient

$$\mathbf{F}_{ij} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{I} + \frac{\partial \mathbf{u}}{\partial \mathbf{X}} \quad (2)$$

where $\mathbf{x}$ and $\mathbf{X}$ denote the deformed and undeformed position vectors respectively and $\mathbf{u}$ denotes displacement (see Fig. 1). Stresses are measured using the second Piola–Kirchhoff stress tensor ($\mathbf{S}_{ij}$)

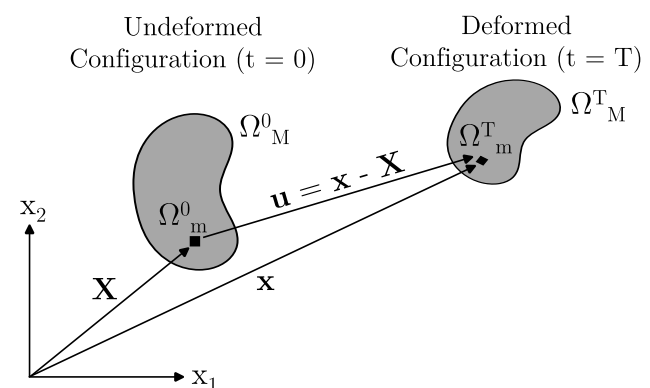


Fig. 1 The quasi-static deformation of a continuum body in the large deformation regime. Here, $\mathbf{x}$ and $\mathbf{X}$ denote the deformed and undeformed position vectors, respectively, $\mathbf{u}$ denotes the displacement, Ω denotes a control volume, and subscripts m and M denote micro- and macroscale control volumes respectively

$$S_{ij} = \frac{\partial W(E_{ij})}{\partial E_{ij}} \quad (3)$$

where W denotes the strain energy density, as this stress measure is conjugate to the Green–Lagrange strain tensor. Importantly, this representation of the second Piola–Kirchhoff stress tensor enables material nonlinearity to be introduced by tailoring the response of the strain energy density-functional (W) as a function of the Green–Lagrange strain tensor (Eq. 1).

All subsequent finite-element analyses presented within this paper have been conducted using *Firedrake* (Ham et al. 2023), an open-source and highly versatile Python package with robust capabilities for solving partial differential equations. In addition, *Firedrake*'s integration with sophisticated automatic differentiation capabilities facilitates the efficient computation of adjoint models for sensitivity analysis and subsequent optimization (Farrell et al. 2013; Mitusch et al. 2019).

3.1 Microscale model

The microscale model represents a data-driven continuous functional which relates geometric parameters and the local macroscale strain tensor to the local macroscale stress tensor for each element within the macroscale domain. This model is directly integrated within the macroscale model and permits the accurate computation of macroscale displacements for two-scale structures and is discussed in detail in Sect. 3.3.

The parameterized microstructural geometry used for the remainder of this paper is illustrated in Fig. 2. This geometry and parameterization (a_1 , a_2) is chosen as it enables direct access to both positive and negative Poisson's ratios. Individual amplitude parameters are afforded to the horizontal (a_1) and vertical (a_2) members respectively, as this enables enhanced control over the Poisson's ratio and the effective stiffness in each axis. Straightforward access to these material properties represents an advantage over classical topology optimization techniques, which would otherwise require the considerably more difficult heterogeneous assembly of isotropic material to achieve these properties. In combination, this geometry and parameterization provides a suitable foundation to succinctly target prescribed deformation functional objectives in the large deformation regime, while simultaneously abiding by the requirements of the heterogeneous multiscale method (Abdulle et al. 2012).

For a defined array of microscale parameters (a_1 , a_2) and macroscale strains ($E_{M,11}$, $E_{M,22}$, $E_{M,12}$), the corresponding second Piola–Kirchhoff stress tensor is derived through the application of nonlinear finite-element

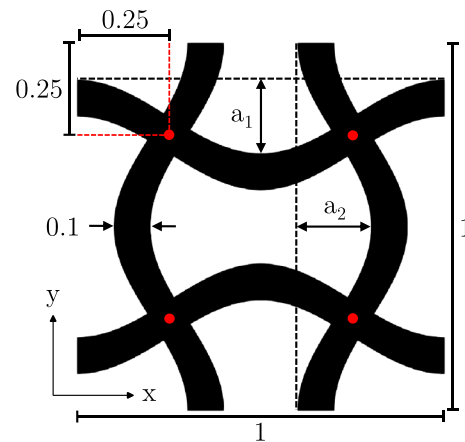


Fig. 2 The microscale geometry and parameterization applied within this paper, illustrated using non-dimensional lengths. The variables a_1 and a_2 denote the amplitude parameters for the horizontal and vertical members, respectively. All members are constructed from transformed cosine waves, with red dots marking the intersections of their midlines. The intersection points are fixed, causing the extremities of each member to move along the boundary in response to variations in the amplitude parameters

analysis. The output of this analysis is used to assemble the continuous microscale functional, which is discussed in Sect. 3.2. The second Piola–Kirchhoff stress tensor is calculated for each parameter configuration using Eq. 3. This calculation necessitates the prior computation of the strain energy density functional, which requires the application of periodically constrained nonlinear finite-element analysis to determine the microscopic displacement field. To ensure the validity of this analysis, the response of the microscale model needs to accurately reflect the behavior of a material point at the macroscale. Consequently, the microscale analysis is founded upon the Hill–Mandel condition, which guarantees that the energy transfer between scales is consistent (Murshed and Ranganathan 2017). This is equivalent to equating the virtual power at the micro- and macroscales

$$\mathcal{P}_m = \mathcal{P}_M \quad (4)$$

where $\mathcal{P}_m$ and $\mathcal{P}_M$ denote the virtual power at the micro- and macroscale respectively. The macroscale virtual power can be expressed as

$$\mathcal{P}_M = \mathbf{P}_{M,ij} : \nabla_{\mathbf{x}_M} \mathbf{u}_M \quad (5)$$

where $\mathbf{P}_{M,ij}$ denotes the macroscale first Piola–Kirchhoff stress tensor, $\mathbf{x}_M$ denotes the macroscopic undeformed position vector, and $\mathbf{u}_M$ denotes the macroscopic displacement. In contrast, the microscale virtual power is expressed using a volume-averaged homogenization formulation

$$\mathcal{P}_m = \frac{1}{\Omega_m} \int_{\Omega_m} \mathbf{P}_{m,ij} : \nabla_{\mathbf{x}_m} \mathbf{u}_m \, d\Omega_m \quad (6)$$

where Ω_m denotes the microscopic control volume, $\mathbf{P}_{m,ij}$ denotes the microscale first Piola–Kirchhoff stress tensor, $\mathbf{x}_m$ denotes the microscopic deformed position vector, and $\mathbf{u}_m$ denotes the microscopic displacement. To simplify subsequent analysis, the microscopic displacement field is expanded using the following identity (de Souza et al. 2015)

$$\mathbf{u}_m = \mathbf{u}_M + \nabla_{\mathbf{x}_M} \mathbf{u}_M \mathbf{x}_m + \mathbf{u}_m^* \quad (7)$$

which represents a summation of the local macroscopic displacement ($\mathbf{u}_M + \nabla_{\mathbf{x}_M} \mathbf{u}_M \mathbf{x}_m$) and the microscopic displacement fluctuation $\mathbf{u}_m^*$. Substituting Eq. 7 into Eq. 6 yields

$$\mathcal{P}_m = \frac{1}{\Omega_m} \int_{\Omega_m} \mathbf{P}_{m,ij} : [\nabla_{\mathbf{x}_M} \mathbf{u}_M + \nabla_{\mathbf{x}_m} \mathbf{u}_m^*] \, d\Omega_m \quad (8)$$

Then, by equating the virtual powers at both scales

$$\begin{aligned} \mathbf{P}_{M,ij} : \nabla_{\mathbf{x}_M} \mathbf{u}_M &= \\ \frac{1}{\Omega_m} \int_{\Omega_m} \mathbf{P}_{m,ij} : [\nabla_{\mathbf{x}_M} \mathbf{u}_M + \nabla_{\mathbf{x}_m} \mathbf{u}_m^*] \, d\Omega_m & \end{aligned} \quad (9)$$

and setting $\nabla_{\mathbf{x}_M} \mathbf{u}_M = 0$, which is valid only when there is a significant separation between the micro- and macroscale characteristic length scales, it is possible to derive a simplified equation

$$\int_{\Omega_m} \mathbf{P}_{m,ij} : \nabla_{\mathbf{x}_m} \mathbf{u}_m^* \, d\Omega_m = 0 \quad (10)$$

with only one unknown ($\mathbf{u}_m^*$). The microscale first Piola–Kirchhoff stress tensor in Eq. 10 is computed using

$$\mathbf{P}_{ij} = \frac{\partial W}{\partial \mathbf{F}_{ij}} \quad (11)$$

where a modified St. Venant–Kirchhoff (SVK) hyperelastic model is used to evaluate the strain energy density

$$W = \frac{1}{2} \lambda (J - 1)^2 + \mu \text{Tr}(\mathbf{E}_{ij}^2) \quad (12)$$

where λ and μ denote the Lamé parameters (Coman 2019) and J denotes an invariant equal to $\det(\mathbf{F}_{ij})$. The deformation gradient in Eq. 12, required to compute the invariant J , is calculated using

$$\mathbf{F}_{ij} = \mathbf{I} + \mathbf{E}_{M,ij} + \nabla_{\mathbf{x}_m} \mathbf{u}_m^* \quad (13)$$

where again for clarity $\mathbf{E}_{M,ij}$ denotes the macroscale strain tensor, which serves as an input parameter to the microscale model. The Green–Lagrange strain tensor in Eq. 12 is then calculated by substituting the result of Eq. 13 into Eq. 1. Initially, the standard SVK model was employed, however,

to counteract the well-documented limitation of the classical SVK hyperelastic model, which exhibits artificial softening during compression, a modified version of the SVK model is instead implemented (Sautter et al. 2022).

A unit-square domain ($[0, 1] \times [0, 1]$) and discretization is used for all permutations of the microscale geometry, with each permutation realized by spatially allocating either solid ($E = 1$ GPa, $\nu = 0.3$) or void ($E = 1$ kPa, $\nu = 0.3$) materials properties to each node within the set domain depending on whether it lies on the interior or the exterior of a structural member (see Fig. 3). For more details on nodal allocation and its validity, the reader is directed to Imediegwu et al. (2019). After conducting a mesh sensitivity study for both strain and geometric parameters, 300 divisions per axis were selected to discretize the set domain. This resolution, which equates to 90,000 quadrilateral elements, enables the computationally efficient derivation of the second Piola–Kirchhoff stress tensor with an error of less than 5% relative to the fully-converged discretization. Nodal allocation is used rather than body-fitted meshing-based approaches, as the unit-square domain enables the straightforward implementation of periodic boundary conditions due to identical node-sets on opposing sides and Firedrake’s topological periodicity capability.

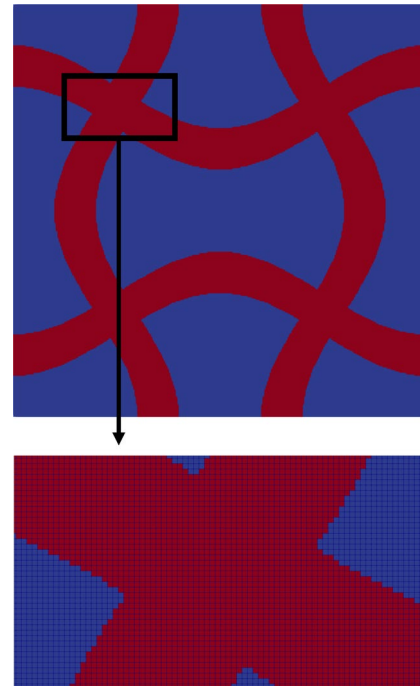


Fig. 3 Demonstration of nodal allocation applied to achieve the microstructure illustrated in Fig. 2, characterized by amplitude parameters a_1, a_2 set equal to 0.2. The rectangular domain is discretized into 300 divisions along each axis following the results of a mesh sensitivity study, with solid and void material depicted in red and blue, respectively. To illustrate this resolution, a magnified view with the quadrilateral elements highlighted is also presented

Together, Eq. 10 is solved over the periodically constrained set domain to compute the microscopic displacement fluctuation for a given configuration ($a_1, a_2, E_{M,11}, E_{M,22}, E_{M,12}$). During the solution procedure, additional constraints are imposed on the displacement field. These constraints restrict the space of kinematically admissible displacements by removing rigid body modes, to ensure that Eq. 10 is well posed and to improve the convergence properties. For brevity, further details are not included in this paper. However, for more comprehensive information, the reader is directed toward de Souza et al. (2015). Following the derivation of the microscopic displacement fluctuation, the second Piola–Kirchhoff stress tensor is computed by differentiating the strain energy density (evaluated using Eq. 12) with respect to the Green–Lagrange strain tensor (see Eq. 3) using Firedrake’s automatic differentiation capability.

3.2 Concurrent coupling

The microscale model is concurrently coupled to the macroscale model throughout the optimization procedure. This approach ensures that microscale data are only collected for the regions of the microscale parameter space that the optimizer traverses through. This is in contrast with prohibitively expensive sequentially coupled methods, where the microscale parameter space is resolved in its entirety prior to the commencement of the optimization procedure (Imediegwu et al. 2019; Colabella et al. 2019; Thillaithevan et al. 2022). In the context of the present work, concurrent coupling restricts the exploration of the macroscale strain space to the physical strain space, which helps to prevent the simulation of non-convergent strain combinations and represents a further point of novelty for this work.

This procedure is initiated by pre-populating the microscale parameter space with the simulation nodes of a full-factorial Design Of Experiments (DOE) (Antony 2023). The spatial distribution of nodes is derived using both the parameter bounds and the corresponding discretization resolution (levels) detailed in Table 1. In combination, this results in a total of 24, 880, 481 simulation nodes, with each configuration constituting a unique permutation of both geometrical parameters and macroscale strains. The geometrical parameter bounds are selected to facilitate access during the optimization procedure to significant variations in both Poisson’s ratio and axial stiffness.

Importantly, a full-factorial DOE is selected for this application, as the uniform distribution of simulation nodes affords a number of advantages. The primary benefit of this uniformity is the existence of rotational and reflectional symmetries, which enables up to eight unique-second Piola–Kirchhoff stress tensors to be derived from a single parent simulation. Symmetries are identified within the DOE by applying

Table 1 The full-factorial DOE is constructed using the bounds and levels detailed for both geometrical parameters and macroscale strains in this table. By discretizing the microscale parameter space using these values, a total of 24, 880, 481 unique permutations are generated

Microscale Parameters	Levels	Lower bound	Upper bound	Level increment
a_1	19	− 0.36	0.36	0.04
a_2	19	− 0.36	0.36	0.04
$E_{M,11}$	41	− 0.25	0.25	0.0125
$E_{M,22}$	41	− 0.25	0.25	0.0125
$E_{M,12}$	41	− 0.25	0.25	0.0125

combinations of two-dimensional transformation matrices to a series of points representing all four structural members and all four strain direction vectors. The transformed set of points is then inspected to determine how each parameter is permuted during the transformation procedure. This process is systematically repeated until a parent microstructure is identified for each one of the 24, 880, 481 unique permutations. This enables the derivation of all permutations from 6, 380, 010 unique combinations of geometrical parameters and macroscale strains. Furthermore, in order to minimize the storage overhead, microscale data are stored exclusively for parent microstructures. Transformations matrices are then applied on-the-fly during the optimization procedure to recover the corresponding second Piola–Kirchhoff stress tensors.

For the purpose of evaluating the second Piola–Kirchhoff stress tensor at points in the microscale parameter space in between DOE nodes, piecewise continuous linear interpolants are constructed. A local response surface-based approach is selected as this facilitates the implementation of concurrently coupling the micro- and macroscale models. Prior to the construction of these interpolants, it is first necessary to define the design variable matrix

$$\mathbf{X}_{ij} = \begin{bmatrix} a_{1,1} & a_{2,1} \\ a_{1,2} & a_{2,2} \\ \vdots & \vdots \\ a_{1,n} & a_{2,n} \end{bmatrix} \quad (14)$$

and the macroscale strain matrix

$$\mathbf{Y}_{ij} = \begin{bmatrix} E_{M,11,1} & E_{M,22,1} & E_{M,12,1} \\ E_{M,11,2} & E_{M,22,2} & E_{M,12,2} \\ \vdots & \vdots & \vdots \\ E_{M,11,n} & E_{M,22,n} & E_{M,12,n} \end{bmatrix} \quad (15)$$

where n denotes the number of elements in the macroscale domain. Importantly, the concatenation of rows $\mathbf{X}_i$ and $\mathbf{Y}_i$, hereby denoted as $\mathbf{Z}_i$, define the inputs to the macroscale model for element $\mathbf{e}_i$. For each configuration ($\mathbf{Z}_i$), a hypercube interpolant (n -dimensional extension of linear

interpolation) is constructed. This approach is selected, as it enables the assembly of piecewise linear response surfaces with C^0 continuity. Moreover, the response is bounded by the nodal values and the prediction error tends to zero as the DOE discretization resolution is increased. This is in contrast to popular global response surface-based approaches, such as least-squares polynomial regression, where the addition of data points does not necessarily improve the accuracy or boundedness of the predictions.

To initiate this procedure, the vertices which constitute the nodes of the enclosing hypercube are computed for each configuration, hereby denoted $\mathbf{A}_{n,ij} \in \mathbb{R}^{n \times 2^m \times m}$, where m denotes the number of input parameters to the microscale model. This is achieved by initially identifying two specific values for each parameter within its respective dimension: the largest DOE parameter value ($\mathbf{A}_{n,i}^-$) that is less than or equal to the given parameter, and the smallest DOE parameter value ($\mathbf{A}_{n,i}^+$) that is greater than the given parameter. Combining the associated parameter values for each dimension enables the two extremities of each respective hypercube ($\mathbf{A}_n^- \in \mathbb{R}^{n \times m}$, $\mathbf{A}_n^+ \in \mathbb{R}^{n \times m}$) to be determined. Using these extremal vertices as reference points, all 2^m vertices of each hypercube can be efficiently generated through an n -bit binary search method. This approach effectively navigates the binary sequence space, allowing for the systematic enumeration of all possible vertices. After deriving all vertices for each configuration, the corresponding parent configurations are identified. Configurations without existing data are then submitted to the microscale model, which is utilized to derive the corresponding second Piola–Kirchhoff stress tensors.

After all the necessary microscale data have been collected and transformed, a continuous hypercube interpolant is generated for the second Piola–Kirchhoff stress tensor for all n configurations

$$\check{\mathbf{S}}_{n,ij}(\mathbf{Z}_n) = \sum_{k=1}^{2^m} \mathbf{S}_{ij}(\mathbf{A}_{n,k}) \prod_{l=1}^m \begin{cases} \frac{\mathbf{Z}_{n,l} - \mathbf{A}_{n,l}^-}{\mathbf{A}_{n,l}^+ - \mathbf{A}_{n,l}^-}, \mathbf{A}_{n,kl} = \mathbf{A}_{n,l}^- \\ \frac{\mathbf{A}_{n,l}^+ - \mathbf{Z}_{n,l}}{\mathbf{A}_{n,l}^+ - \mathbf{A}_{n,l}^-}, \mathbf{A}_{n,kl} = \mathbf{A}_{n,l}^+ \end{cases} \quad (16)$$

and provides a direct link between the micro- and macroscale structural mechanics. This approach permits the generation of piecewise linear response surfaces, limited exclusively to the regions of the microscale parameter space traversed by the optimizer. Furthermore, the underlying microscale data are efficiently stored in an indexed database, which can be reused during subsequent iterations or entirely new optimization problems.

3.3 Macroscale model

This section presents an outline of the macroscale model, which is designed to enable the accurate computation of macroscale displacements for the parameterized microscale geometry applied within this paper (see Fig. 2). To derive this model, the principle of minimum potential energy is employed to enable the precise computation of displacements within the nonlinear elastic regime. The total potential energy (Π) of the system can be expressed as

$$\Pi(\mathbf{u}) = \int_{\Omega_M} W(\mathbf{E}_{ij}(\mathbf{u})) \, d\Omega_M - \int_{\Omega_M} \mathbf{B} \cdot \mathbf{u} \, d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot \mathbf{u} \, d\Gamma \quad (17)$$

where $\mathbf{B}$ and $\mathbf{T}$ denote body forces and surface tractions, respectively, and Γ denotes the surfaces on which the tractions are applied. To compute the displacement field which corresponds to the minimum potential energy, a test function ($\hat{\mathbf{u}}$), representing a small and arbitrary variation in the displacement field, is introduced, as it enables variations in the potential energy to be calculated. This enables the directional derivative of the potential energy, taken in the direction of the test function, to be derived, which quantifies how the potential energy varies with changes in displacement

$$D\Pi(\mathbf{u}; \hat{\mathbf{u}}) = \left. \frac{d}{dh} \Pi(\mathbf{u} + h\hat{\mathbf{u}}) \right|_{h=0} \quad (18)$$

where h denotes an infinitesimal perturbation. To compute the minimum potential energy, Eq. 18 is set equal to zero for any variation

$$\frac{d\Pi(\mathbf{u} + h\hat{\mathbf{u}})}{dh} = \frac{d}{dh} \left[\int_{\Omega_M} W(\mathbf{E}_{ij}(\mathbf{u} + h\hat{\mathbf{u}})) \, d\Omega_M - \int_{\Omega_M} \mathbf{B} \cdot (\mathbf{u} + h\hat{\mathbf{u}}) \, d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot (\mathbf{u} + h\hat{\mathbf{u}}) \, d\Gamma \right] = 0 \quad (19)$$

This can be simplified to

$$\int_{\Omega_M} \frac{dW(\mathbf{E}_{ij}(\mathbf{u} + h\hat{\mathbf{u}}))}{dh} \, d\Omega_M - \int_{\Omega_M} \mathbf{B} \cdot \hat{\mathbf{u}} \, d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot \hat{\mathbf{u}} \, d\Gamma = 0 \quad (20)$$

It is then possible to expand the derivative of strain energy density using the chain rule and the Green–Lagrange strain tensor as the intermediate variable

$$\int_{\Omega_M} \frac{dW}{d\mathbf{E}_{ij}} : \frac{d\mathbf{E}_{ij}(\mathbf{u} + h\hat{\mathbf{u}})}{dh} d\Omega_M - \int_{\Omega_M} \mathbf{B} \cdot \hat{\mathbf{u}} d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot \hat{\mathbf{u}} d\Gamma = 0 \quad (21)$$

Importantly, the term ‘ $dW/d\mathbf{E}_{ij}$ ’ in Eq. 21 represents the second Piola–Kirchhoff stress tensor (see Eq. 3), which permits the substitution of this term with the continuous hypercube interpolants constructed for the second Piola–Kirchhoff stress tensor (Eq. 16) in Sect. 3.2

$$\int_{\Omega_M} \check{\mathbf{S}}_{ij}(\mathbf{Z}_{ij}) : \hat{\mathbf{E}}_{ij} d\Omega_M - \int_{\Omega_M} \mathbf{B} \cdot \hat{\mathbf{u}} d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot \hat{\mathbf{u}} d\Gamma = 0 \quad (22)$$

where $\hat{\mathbf{E}}_{ij}$ denotes the variational Green–Lagrange strain tensor. It is then possible to solve Eq. 22 to accurately compute the macroscale displacement field of a spatially varying two-scale structure, so long as a clear separation of scales exists between the micro- and macroscopic characteristic length scales. During the solution procedure, constraints are again imposed to restrict the space of kinematically admissible displacements to improve the convergence properties by removing rigid body modes (de Souza et al. 2015). After each iteration of the solution procedure, the resultant strain field is inspected to ensure that it remains within the strain bounds outlined in Table 1, otherwise, the optimization procedure is terminated. Moreover, all enclosing hypercubes are updated after each iteration and convergence is only realized once two consecutive numerically converged iterates are obtained with identical sets of enclosing hypercubes.

3.4 Optimization formulation

During the optimization procedure, macroscale functional objectives are targeted by spatially optimizing the continuous microscale parameters ($\mathbf{X}_{ij}$). This enables the efficient derivation of spatially varying two-scale structures with prescribed nonlinear mechanical behavior. To ensure that the structures derived through this framework are smoothly varying, which is a fundamental requirement of the heterogeneous multiscale method (Abdulle et al. 2012), the design variables are parsed through a Helmholtz PDE filter prior to the computation of the continuous hypercube interpolants. The weak variational form of the Helmholtz PDE (Lazarov and Sigmund 2011) is defined as

$$\int_{\Omega_M} R^2 \nabla \tilde{\mathbf{X}}_j \cdot \nabla \boldsymbol{\nu} + \tilde{\mathbf{X}}_j \boldsymbol{\nu} d\Omega_M = \int_{\Omega_M} \mathbf{X}_j \boldsymbol{\nu} d\Omega_M \quad (23)$$

where R denotes the filter length, $\tilde{\mathbf{X}}_j$ denotes the filtered design variables and $\boldsymbol{\nu}$ denotes a test function which

represents arbitrary variations in the design variables. Importantly, the filter length is set equal to a conservative value of three times the length of an element for all results presented within this paper, as this strongly promotes smoothly varying parameter fields.

All optimization problems presented within this paper are structured as

$$\begin{aligned} \min_{\mathbf{X}_{ij}} \quad & J(\tilde{\mathbf{X}}_{ij}) \\ \text{s.t.} \quad & \int_{\Omega_M} \check{\mathbf{S}}_{ij}(\tilde{\mathbf{X}}_{ij}, \mathbf{Y}_{ij}) : \hat{\mathbf{E}}_{ij} d\Omega_M - \\ & \int_{\Omega_M} \mathbf{B} \cdot \hat{\mathbf{u}} d\Omega_M - \int_{\Gamma} \mathbf{T} \cdot \hat{\mathbf{u}} d\Gamma = 0 \\ & \mathbf{X}_{\min,j} \leq \mathbf{X}_j \leq \mathbf{X}_{\max,j} \end{aligned} \quad (24)$$

where $J(\tilde{\mathbf{X}}_{ij})$ denotes the objective functional cast as a function of the filtered design variables, the first constraint denotes the satisfaction of the nonlinear elastic PDE constraint, and $\mathbf{X}_{\min,j}$, $\mathbf{X}_{\max,j}$ denote the lower and upper bounds outlined for the amplitude variables in Table 1, respectively. Sensitivities of the objective functional with respect to the design variables are computed using Firedrake’s automatic differentiation capability, which enables the efficient derivation and solution of adjoint PDEs. The sensitivities derived from these adjoint models have been extensively verified using finite-difference methods. Optimization is executed utilizing the open-source optimizer Ipopt (Wächter and Biegler 2006). This optimizer employs the interior-point method, enabling the efficient resolution of large and complex nonlinear optimization problems. The optimization process is terminated when the objective function exhibits a change of less than 0.01% across five consecutive iterations.

4 Results

In this section, the framework outlined in Sect. 3 is applied to solve three prescribed deformation problems. In addition, the computational benefits afforded by concurrently coupling the micro- and macroscale models in the context of multiscale nonlinear elasticity is also presented. Furthermore, the optimized macroscale displacement fields generated during the optimization procedure are verified using single-scale finite-element analysis, to demonstrate the validity of the present framework.

Importantly, the displacement field is uniformly initialized for all cases with the vector $[0, 0]\text{m}$. Moreover, to minimize strain overshoot and consequently exceeding the strain bounds (see Table 1), five intermediate uniformly spaced load steps are employed in all cases.

4.1 Strain space exploration

To demonstrate the benefits afforded by concurrently coupling the micro- and macroscale models, a single execution of the macroscale model is performed, and the resultant exploration of the strain space is presented. The geometry, boundary conditions, and discretization used for this case are outlined in Fig. 4. To restrict this study to the strain space

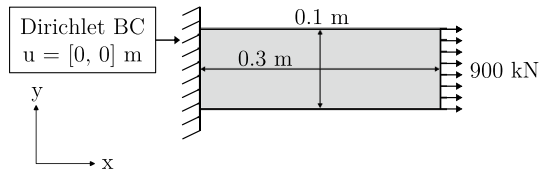
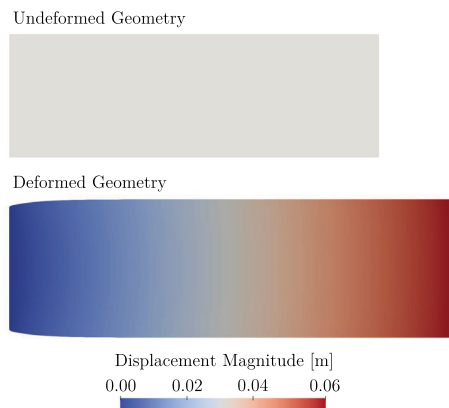
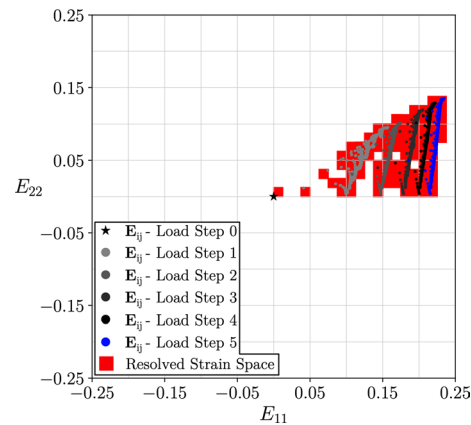


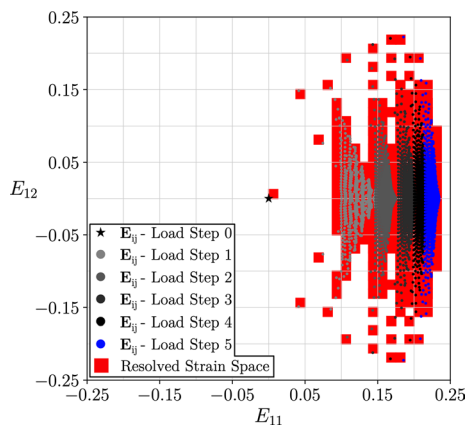
Fig. 4 The cantilever beam geometry and boundary conditions used to execute a single iteration of macroscale analysis. A total of 150×50 elements are used to discretize this geometry



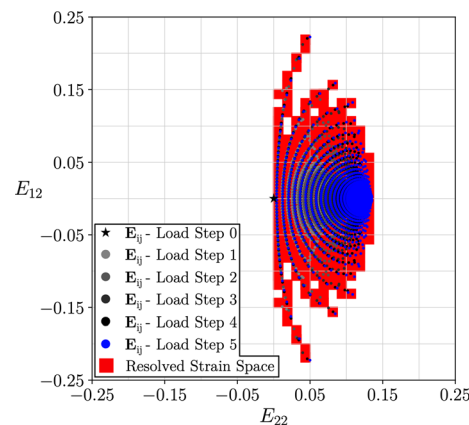
(a) Comparison between the undeformed and deformed geometries



(b) E_{11} vs E_{22}



(c) E_{11} vs E_{12}



(d) E_{22} vs E_{12}

Fig. 5 The displacement field and the corresponding macroscale strain fields derived from a single execution of the macroscale model for the geometry, boundary conditions, and discretization outlined in Fig. 4. Strain is plotted using two-dimensional projections to aid visualization. Moreover, each load step corresponds to the respective force value in the vector $[0, 180, 360, 540, 720, 900]$ kN

only, the amplitude parameters a_1 and a_2 are set uniformly equal to 0.36, which corresponds to the extreme auxetic configuration.

The results of this study are illustrated in Fig. 5, which depicts the macroscale strains that correspond to the minimum potential energy for each load step, superimposed on the resolved design space. In Fig. 5b–d, it is clearly demonstrated that only a small proportion of the permissible macroscale strain space has been resolved in order to derive the displacement field illustrated in Fig. 5a. The proportion of the resolved strain space amounts to 1.45% of the total strain space.

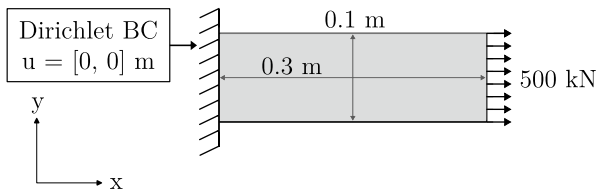
The strain distributions illustrated in Fig. 5b–d depict clear patterns, which represents the physical strain space for this specific geometry, boundary conditions and microstructure. Significantly, as the exploration of the strain space is directed by sensitivities with respect to the minimum potential energy, concurrent coupling helps to eliminate

the simulation of unphysical and/or non-convergent strain combinations. This is in contrast to sequentially coupled frameworks, which necessitate the complete resolution of the microscale parameter space prior to the evaluation of the macroscale model. Consequently, a concurrent approach reduces the difficulty associated with assembling a nonlinear microscale model. In addition, for a fixed computational budget, concurrent coupling enables the exploration of a larger strain space or an increase in the fidelity of microscale simulations.

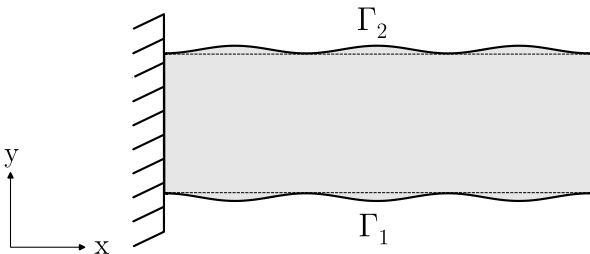
4.2 Prescribed displacement: Case 1

In this section, the prescribed auxetic deformation illustrated in Fig. 6b is targeted through optimization of the continuous microscale parameters. The geometry, boundary conditions, and discretization used for this case are outlined in Fig. 6a. The deformation profile targeted exclusively on the lower (Γ_1) and upper (Γ_2) edges is expressed as follows:

$$\check{\mathbf{u}}_{\Gamma_1,y}^1(\mathbf{x}) = -3 \times 10^{-3} \left[\frac{1 - \cos\left(\frac{6\pi x}{l_x}\right)}{2} \right] \quad (25)$$



(a) The cantilever-beam geometry and boundary conditions used to target the prescribed deformation detailed in Fig. 6b. A total of 150×50 elements are used to discretize this geometry.



(b) The auxetic deformation field generated using Eqs. 25 and 26 on the lower and upper edges respectively. The dashed lines represent the lower and upper edges of the undeformed geometry for comparison.

Fig. 6 The problem setup and target deformation field targeted in Sect. 4.2

$$\check{\mathbf{u}}_{\Gamma_2,y}^1(\mathbf{x}) = 3 \times 10^{-3} \left[\frac{1 - \cos\left(\frac{6\pi x}{l_x}\right)}{2} \right] \quad (26)$$

where $\check{\mathbf{u}}_{\Gamma_1,y}^1$ and $\check{\mathbf{u}}_{\Gamma_2,y}^1$ denote the target displacements for the y -component of displacement on the lower and upper edges, respectively, and l_x denotes the length of the geometry in the x -direction. The deformation profile represents a three-period cosine wave with an amplitude of 3×10^{-3} m or equivalently 3% of the vertical length of the geometry. The objective function is formulated as

$$J(\tilde{\mathbf{X}}_{ij}) = \left\| \mathbf{u}_{\Gamma_1,y}(\tilde{\mathbf{X}}_{ij}) - \check{\mathbf{u}}_{\Gamma_1,y}^1 \right\|_2^2 + \left\| \mathbf{u}_{\Gamma_2,y}(\tilde{\mathbf{X}}_{ij}) - \check{\mathbf{u}}_{\Gamma_2,y}^1 \right\|_2^2 \quad (27)$$

where $\mathbf{u}_{\Gamma_1,y}(\tilde{\mathbf{X}}_{ij})$ and $\mathbf{u}_{\Gamma_2,y}(\tilde{\mathbf{X}}_{ij})$ denote the subset of macroscale displacements on the lower and upper edges, respectively. Importantly, the microscale parameters are uniformly initialized with an amplitude of zero at the beginning of the optimization procedure. The convergence plot for this case is illustrated in Fig. 7. In addition, the optimized microscale parameters, displacement field, and geometry reconstruction are illustrated for this case in Fig. 8.

It is clearly depicted in Fig. 8c that the prescribed deformation field has been successfully obtained following the optimization of the continuous microscale parameters. The amplitude parameters are distributed such that auxetic configurations, where $\text{sgn}(a_1) = \text{sgn}(a_2)$ are allocated in regions that are vertically aligned with the maxima (negative $\mathbf{u}_y$ on Γ_1 and positive $\mathbf{u}_y$ on Γ_2) of the cosine wave. In contrast, amplitudes approximately equal to zero are allocated in regions vertically aligned with the minima of the cosine wave. These combinations exhibit a relatively high axial stiffness and consequently restrict the displacement

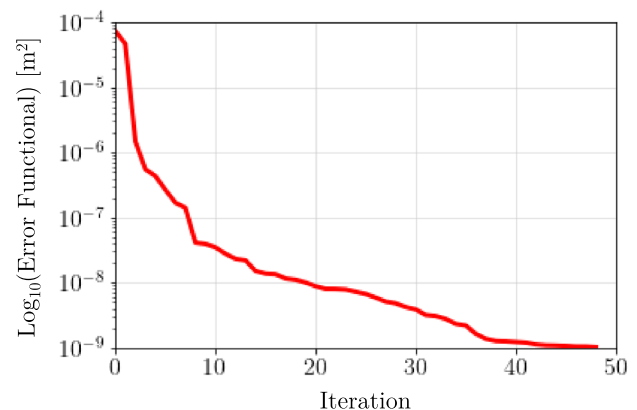


Fig. 7 The convergence of the objective functional as a function of iteration number

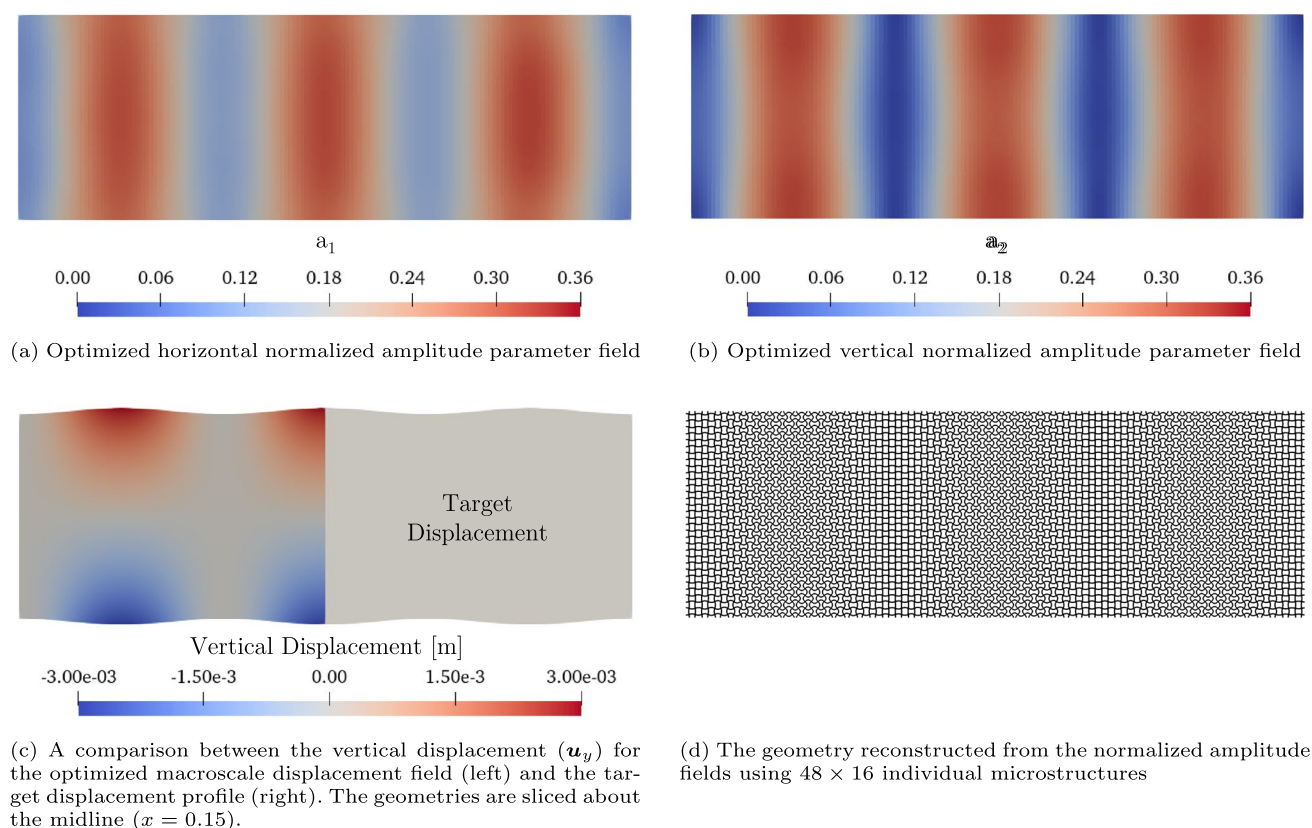


Fig. 8 The optimized microscale parameter fields, displacement field, and geometry reconstruction for the case presented in Sect. 4.2

in these regions as necessitated by the objective functional. Furthermore, the effectiveness of this framework is clearly evidenced by the straightforward minimization of the error functional depicted in Fig. 7.

In order to verify the accuracy of the optimized macro scale displacement field, the geometry reconstructed from the normalized amplitude fields (see Fig. 8d) is used to perform a single high-fidelity finite-element analysis. The mesh used for this analysis is created by first converting the normalized amplitude fields into volumetric data, which is then parsed to a marching squares algorithm using 50^3 division per microstructure to reliably generate the mesh. The results of this analysis are presented alongside the optimized macro scale displacement field for comparison in Fig. 9. It is clearly illustrated in Fig. 9 that the high-fidelity analysis demonstrates excellent agreement with the optimized macro scale displacement field in both the horizontal and vertical directions, despite the multiscale structural analysis taking over two orders of magnitude less time to execute. Importantly, the largest errors in displacement occur at the maxima of the cosine wave with an error of just under 10% in the vertical direction. However, errors of only 0.1% are noted in the horizontal direction. The difference in errors between the

vertical and horizontal directions is as expected, with the displacements being over an order of magnitude smaller in the vertical direction. Considering the errors inherent in the discretization of the microscale model and the assumptions underlying multiscale analysis, which collectively facilitate substantial computational savings, the observed displacement error is deemed to be more than acceptable. The necessity of nonlinear analysis in this context is verified by performing an identical simulation using the reconstructed geometry and linear elastic assumptions. In comparison, the errors noted in the vertical and horizontal directions are 127% and 59%, respectively, demonstrating the inability of linear analysis to accurately capture the extension and stiffening effects inherent in the present microstructure.

The benefits afforded by concurrently coupling the micro- and macro scale models are again demonstrated for this case, as only 4,465 parent microscale simulations are required to complete the optimization procedure. This represents only 0.070% of the total parent microscale database and only 0.018% of all possible permutations, despite strains aligned to the x -axis (E_{11}) surpassing 18%. In combination, this clearly demonstrates the efficiency of

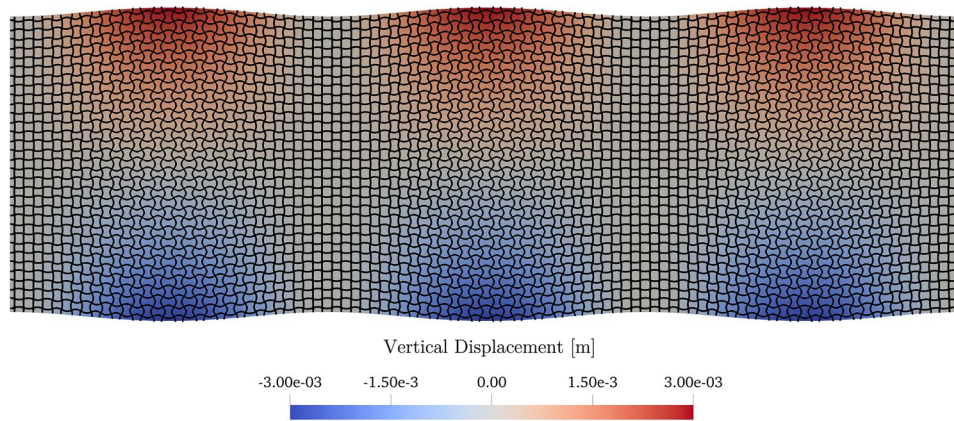


Fig. 9 A comparison between the optimized macroscale displacement field (see Fig. 8c), obtained from the multiscale structural analysis, and the displacement field derived from a high-fidelity structural analysis of the reconstructed geometry illustrated in Fig. 8d. The displacement fields are warped in both the horizontal and vertical directions

this framework and its ability to operate in the nonlinear elastic regime.

4.3 Prescribed displacement: Case 2

In this section, a further prescribed deformation case is solved; however, in this instance, the target deformation profile requires a positive Poisson's ratio. The geometry, boundary conditions and discretization used for this case are outlined in Fig. 10a. The deformation profile is again targeted exclusively on the lower (Γ_1) and upper (Γ_2) edges and is expressed as

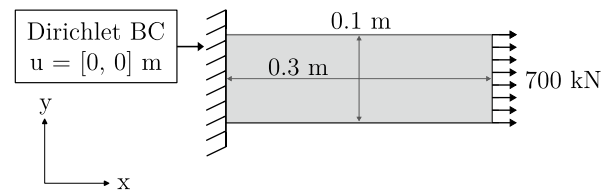
$$\check{\mathbf{u}}_{\Gamma_1,y}^2(\mathbf{x}) = 5 \times 10^{-3} \left[\frac{1 - \cos\left(\frac{4\pi x}{l_x}\right)}{2} \right] \quad (28)$$

$$\check{\mathbf{u}}_{\Gamma_2,y}^2(\mathbf{x}) = -5 \times 10^{-3} \left[\frac{1 - \cos\left(\frac{4\pi x}{l_x}\right)}{2} \right] \quad (29)$$

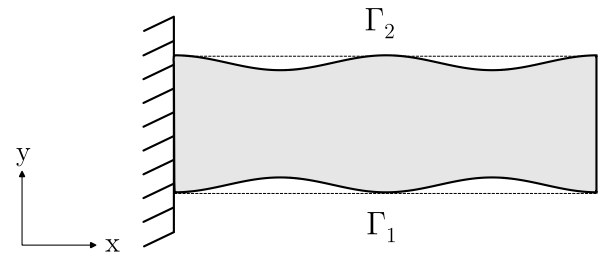
where $\check{\mathbf{u}}_{\Gamma_1,y}^2$ and $\check{\mathbf{u}}_{\Gamma_2,y}^2$ denote the target displacements for the y-component of displacement on the lower and upper edges, respectively. The deformation profile represents a two-period cosine wave with an amplitude of 5×10^{-3} m or equivalently 5% of the vertical length of the geometry. The objective function is formulated as

$$J(\tilde{\mathbf{X}}_{ij}) = \left\| \mathbf{u}_{\Gamma_1,y}(\tilde{\mathbf{X}}_{ij}) - \check{\mathbf{u}}_{\Gamma_1,y}^2 \right\|_2^2 + \left\| \mathbf{u}_{\Gamma_2,y}(\tilde{\mathbf{X}}_{ij}) - \check{\mathbf{u}}_{\Gamma_2,y}^2 \right\|_2^2 \quad (30)$$

where $\mathbf{u}_{\Gamma_1,y}(\tilde{\mathbf{X}}_{ij})$ and $\mathbf{u}_{\Gamma_2,y}(\tilde{\mathbf{X}}_{ij})$ denote the subset of macroscale displacements on the lower and upper edges, respectively. Importantly, the microscale parameters are uniformly



(a) The cantilever-beam geometry and boundary conditions used to target the prescribed deformation detailed in Fig. 10b. A total of 150×50 elements are used to discretize this geometry.



(b) The deformation field generated using Eqs. 28 and 29 on the lower and upper edges respectively. The dashed lines represent the lower and upper edges of the undeformed geometry for comparison.

Fig. 10 The problem setup and target deformation field targeted in Sect. 4.3

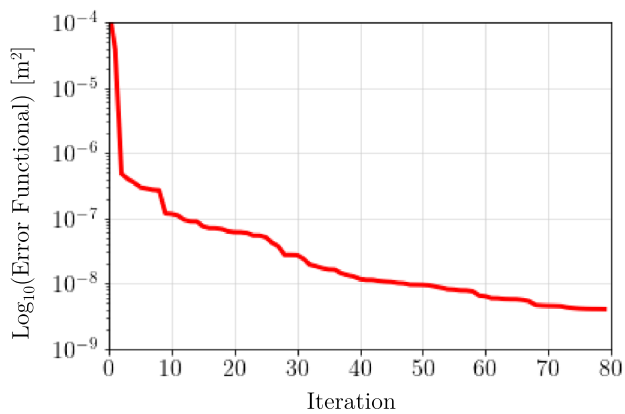


Fig. 11 The convergence of the objective functional as a function of iteration number

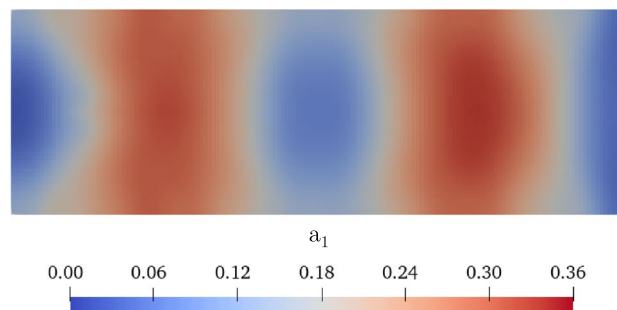
initialized with an amplitude of zero at the beginning of the optimization procedure. The convergence plot for this case is illustrated in Fig. 11. In addition, the optimized microscale parameters, displacement field, and geometry reconstruction are illustrated for this case in Fig. 12.

As illustrated in Fig. 12c, the continuous microscale parameters have once again been optimized to successfully

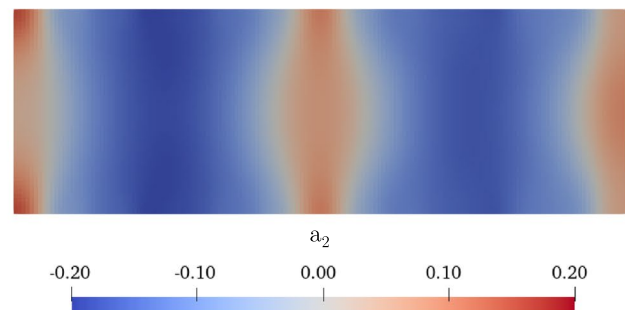
target the prescribed deformation field. This is achieved by allocating positive Poisson's ratio configurations, where $\text{sgn}(a_1) \neq \text{sgn}(a_2)$, in the regions vertically aligned to the minima (positive $\mathbf{u}_y$ on Γ_1 and negative $\mathbf{u}_y$ on Γ_2) of the cosine wave. In regions where the prescribed displacement is set approximately equal to 0 m, auxetic configurations with relatively small amplitudes are allocated. This permits the allocation of relatively larger positive Poisson's ratio configurations at the minima of the cosine wave, while still maintaining a displacement approximately equal to 0 m near to the maxima of the cosine wave. In combination, this succinctly demonstrates the direct access provided to the optimizer for both negative and positive

Poisson's ratio configurations. This is further evidenced by the straightforward minimization of the error functional depicted in Fig. 11.

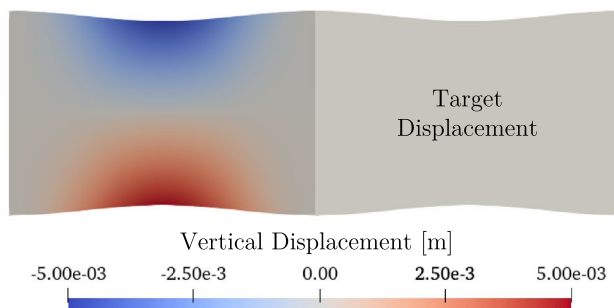
The accuracy of the optimized macroscale displacement field is once again tested using a single high-fidelity simulation of the reconstructed geometry (see Fig. 12d). An identical procedure to the one detailed in Sect. 4.2 is applied to generate the corresponding mesh. The results of this study are illustrated in Fig. 13. Once more, the high-fidelity analysis demonstrates excellent agreement with the optimized macroscale displacement field derived from the multiscale



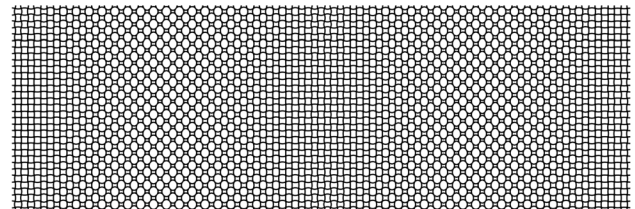
(a) Optimized horizontal normalized amplitude parameter field



(b) Optimized vertical normalized amplitude parameter field



(c) A comparison between the vertical displacement ($\mathbf{u}_y$) for the optimized macroscale displacement field (left) and the target displacement profile (right). The geometries are sliced about the midline ($x = 0.15$).



(d) The geometry reconstructed from the normalized amplitude fields using 48×16 individual microstructures

Fig. 12 The optimized microscale parameter fields, displacement field, and geometry reconstruction for the case presented in Sect. 4.3

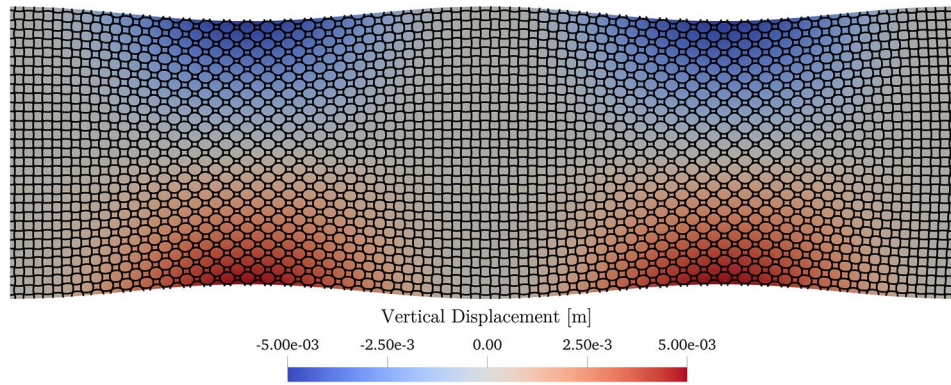


Fig. 13 A comparison between the optimized macroscale displacement field (see Fig. 12c), obtained from the multiscale structural analysis, and the displacement field derived from a high-fidelity structural analysis of the reconstructed geometry illustrated in Fig. 12d. The displacement fields are warped in both the horizontal and vertical directions

analysis. In this instance, errors of less than 7% are noted in the vertical direction and 2% in the horizontal direction. As previously outlined in Sect. 4.2, this magnitude of error is deemed to be more than acceptable, given the number of assumptions made in the derivation of this framework. Once more, the necessity of nonlinear analysis is verified by performing an identical simulation using the reconstructed geometry and linear elastic assumptions. In comparison, the errors noted in the vertical and horizontal directions are 39% and 52%, respectively, demonstrating the inability of linear analysis to accurately capture the extension and stiffening effects inherent in the present microstructure.

The benefits afforded by concurrently coupling the micro- and macroscale models are demonstrated by this case, as only 5,612 parent microscale simulations are required to reach convergence of the optimization procedure. This number of parent microscale simulations represents only 0.088% of the total parent microscale database and only 0.023% of all possible permutations, in spite of the strains aligned to the x-axis ($\mathbf{E}_{11}$) exceeding 20%.

4.4 Prescribed displacement: Case 3

In this section, a mechanical cloaking case is solved. Mechanical cloaks are structures specifically engineered to replicate the global elastic response of a homogeneous structure, despite the inclusion of void that are not present in the base structure (Wang et al. 2022). The geometry used for this case replicates the Imperial College London logo (Imperial College London 2024) and it is illustrated in Fig. 14, alongside the boundary conditions and discretization. The associated homogeneous structure used to generate the target deformation profile for this case is illustrated in Fig. 15. The objective function is formulated as

$$J(\tilde{\mathbf{X}}_{ij}) = \left\| \mathbf{u}_{\Gamma_1}(\tilde{\mathbf{X}}_{ij}) - \tilde{\mathbf{u}}_{\Gamma_1}^3 \right\|_2^2 + \left\| \mathbf{u}_{\Gamma_2}(\tilde{\mathbf{X}}_{ij}) - \tilde{\mathbf{u}}_{\Gamma_2}^3 \right\|_2^2 + \left\| \mathbf{u}_{\Gamma_3}(\tilde{\mathbf{X}}_{ij}) - \tilde{\mathbf{u}}_{\Gamma_3}^3 \right\|_2^2 \quad (31)$$

where $\mathbf{u}_{\Gamma_1}(\tilde{\mathbf{X}}_{ij})$, $\mathbf{u}_{\Gamma_2}(\tilde{\mathbf{X}}_{ij})$, and $\mathbf{u}_{\Gamma_3}(\tilde{\mathbf{X}}_{ij})$ denote the subset of macroscale displacements on the upper, left, and right edges, respectively, and similarly $\tilde{\mathbf{u}}_{\Gamma_1}^3$, $\tilde{\mathbf{u}}_{\Gamma_2}^3$, and $\tilde{\mathbf{u}}_{\Gamma_3}^3$ denote the target displacements on the upper, left, and right edges, respectively. In contrast to the two previous cases, the displacement is now targeted in both the x and y directions. The microscale parameters are uniformly initialized with an amplitude of zero at the beginning of the optimization procedure. The

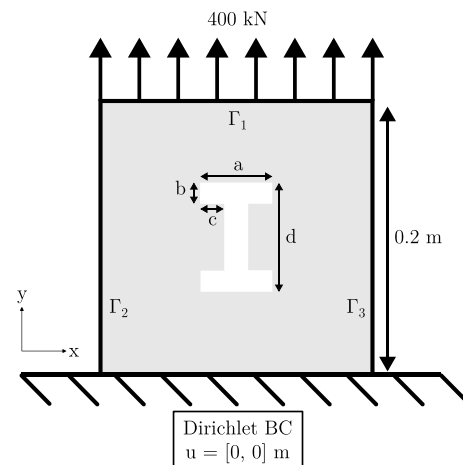


Fig. 14 The square geometry and boundary conditions used to target the deformation case detailed in Fig. 15. A total of 100×100 elements are used to discretize this geometry. The geometry is configured to represent the Imperial College London logo (Imperial College London 2024). The capital 'I' is centrally located and the interior denotes void space. The 'I' is constructed using the following constants: $a = 0.053\text{m}$, $b = 0.013\text{m}$, $c = 0.033\text{m}$, and $d = 0.08\text{m}$

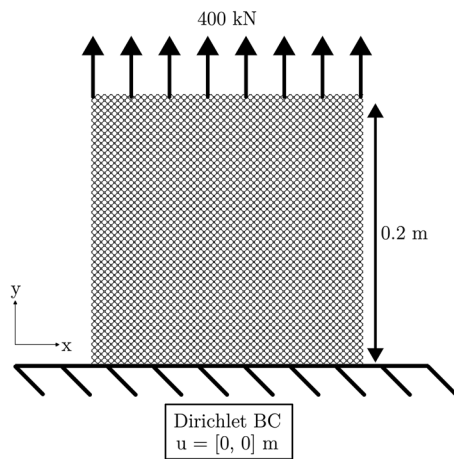


Fig. 15 The homogeneous structure and boundary conditions used to generate the deformation profile targeted in this section. The square structure is generated by setting the amplitude parameters uniformly equal to $a_1 = 0.15$ and $a_2 = -0.15$, which defines a microstructure with a positive Poisson's ratio. The geometry is constructed using 40×40 individual microstructures

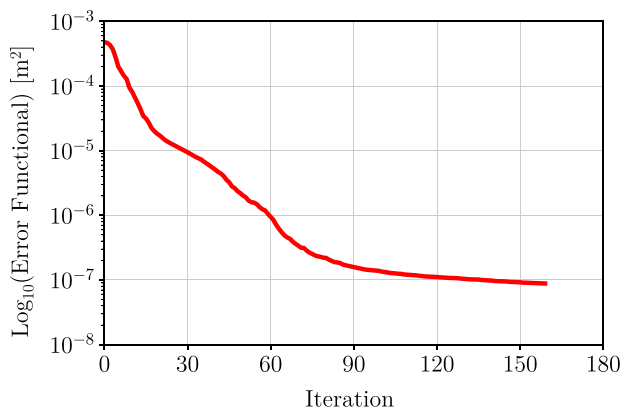


Fig. 16 The convergence of the objective functional as a function of iteration number

convergence plot for this case is illustrated in Fig. 16. In addition, the optimized microscale parameters, optimized displacement field, and geometry reconstruction are illustrated for this case in Fig. 17.

As illustrated in Fig. 17c, the continuous microscale parameters have been optimized to successfully target the prescribed deformation field for both components of displacement. The inclusion of a void space reduces the relative stiffness of the structure, particularly at the centerline of the geometry ($x = 0.1$ m). To recover the properties of the homogeneous structure (see Fig. 15), high stiffness microstructures are distributed ($a_1 = 0$ m, $a_2 = 0$ m) in the shape of a 'V' at the base of the optimized structure.

These microstructures compensate for the loss in stiffness and when loaded in tension, compress laterally, pulling the left and right surfaces toward the centerline, as mandated by the target deformation profile. Interestingly, to further compensate for the reduced centerline stiffness, auxetic microstructures ($\text{sgn}(a_1) = \text{sgn}(a_2)$) are distributed in the space between the 'V' and the base of the 'I'. These microstructures compress vertically when compressed laterally, pulling down the base of the 'I' to further reduce the vertical displacement along the centerline. The vast majority of the remaining structure is allocated a microstructure with a positive Poisson's ratio ($\text{sgn}(a_1) \neq \text{sgn}(a_2)$). This again demonstrates the direct access provided to the optimizer for both negative and positive Poisson's ratio configurations, which is further evidenced by the straightforward minimization of the error functional depicted in Fig. 16.

The accuracy of the optimized macroscale displacement field is once again tested using a single high-fidelity simulation of the reconstructed geometry (see Fig. 17d). An identical procedure to the one detailed in Sect. 4.2 is applied to generate the corresponding mesh. The results of this study are illustrated in Fig. 18a. Once more, the high-fidelity analysis demonstrates excellent agreement with the optimized macroscale displacement field derived from the multiscale analysis. In this instance, errors of less than 3% are noted in the vertical direction and 5% in the horizontal direction. As previously outlined in Sect. 4.2, this magnitude of error is deemed to be more than acceptable, given the number of assumptions made in the derivation of this framework. Once more, the necessity of nonlinear analysis is verified by performing an identical simulation using the reconstructed geometry and linear elastic assumptions. In comparison, the errors noted in the vertical and horizontal directions are 25% and 17%, respectively, demonstrating the inability of linear analysis to accurately capture the extension and stiffening effects inherent in the present microstructure.

A further comparison is made in Fig. 18b between the displacement fields derived from the high-fidelity simulation of the reconstructed geometry and a corresponding high-fidelity simulation of the homogeneous target structure illustrated in Fig. 15. Once more, excellent agreement is noted in the displacement fields between the two structures, and this case clearly illustrates the suitability of this framework to generate mechanical cloaks.

The benefits afforded by concurrently coupling the micro- and macroscale models are demonstrated by this case, as only 19,654 parent microscale simulations are required to reach convergence of the optimization procedure. This number of parent microscale simulations represents only 0.31% of the total parent microscale database and only 0.079% of all possible permutations, despite both shear and direct strains exceeding 22%.

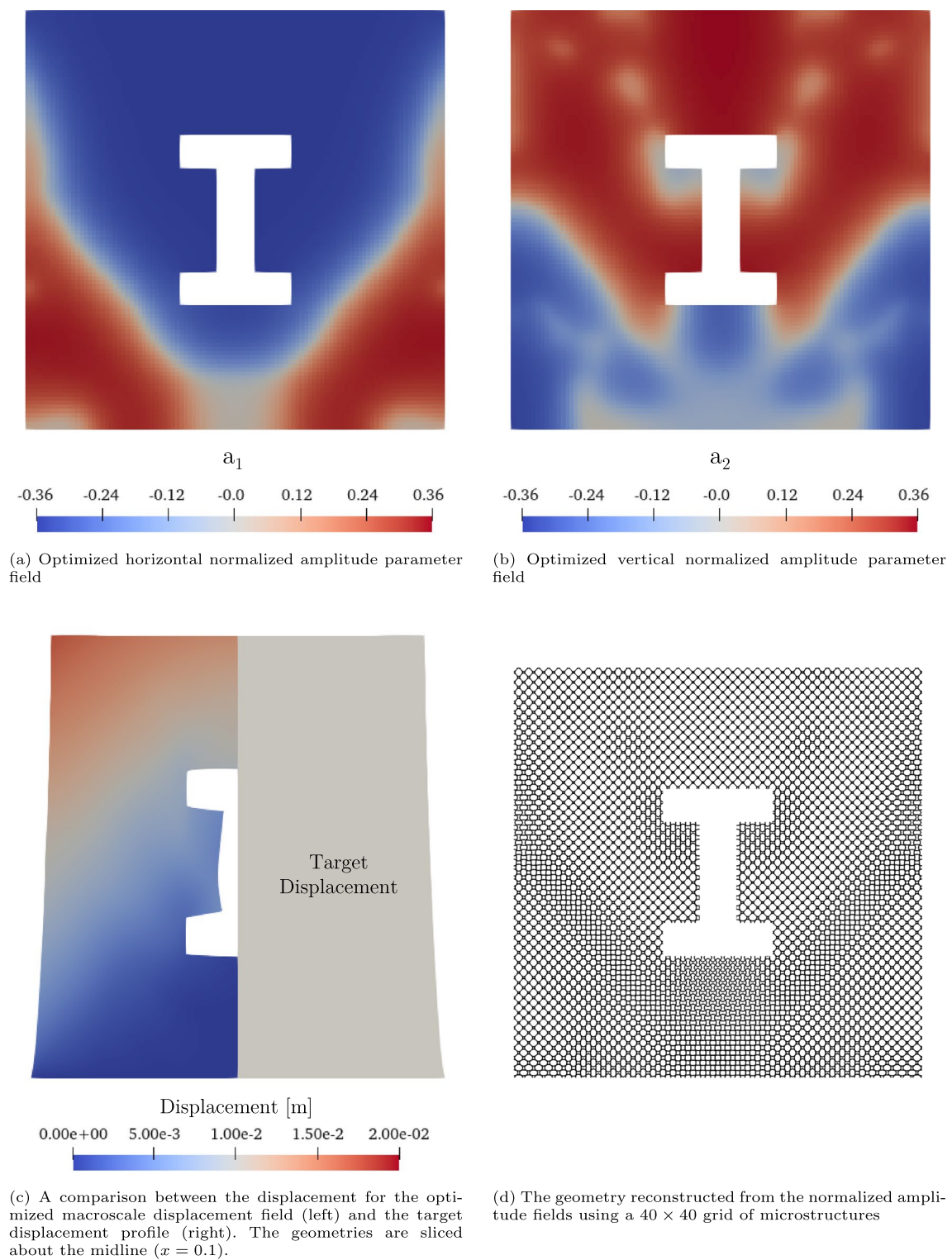


Fig. 17 The optimized microscale parameter fields, displacement field, and geometry reconstruction for the case presented in Sect. 4.4

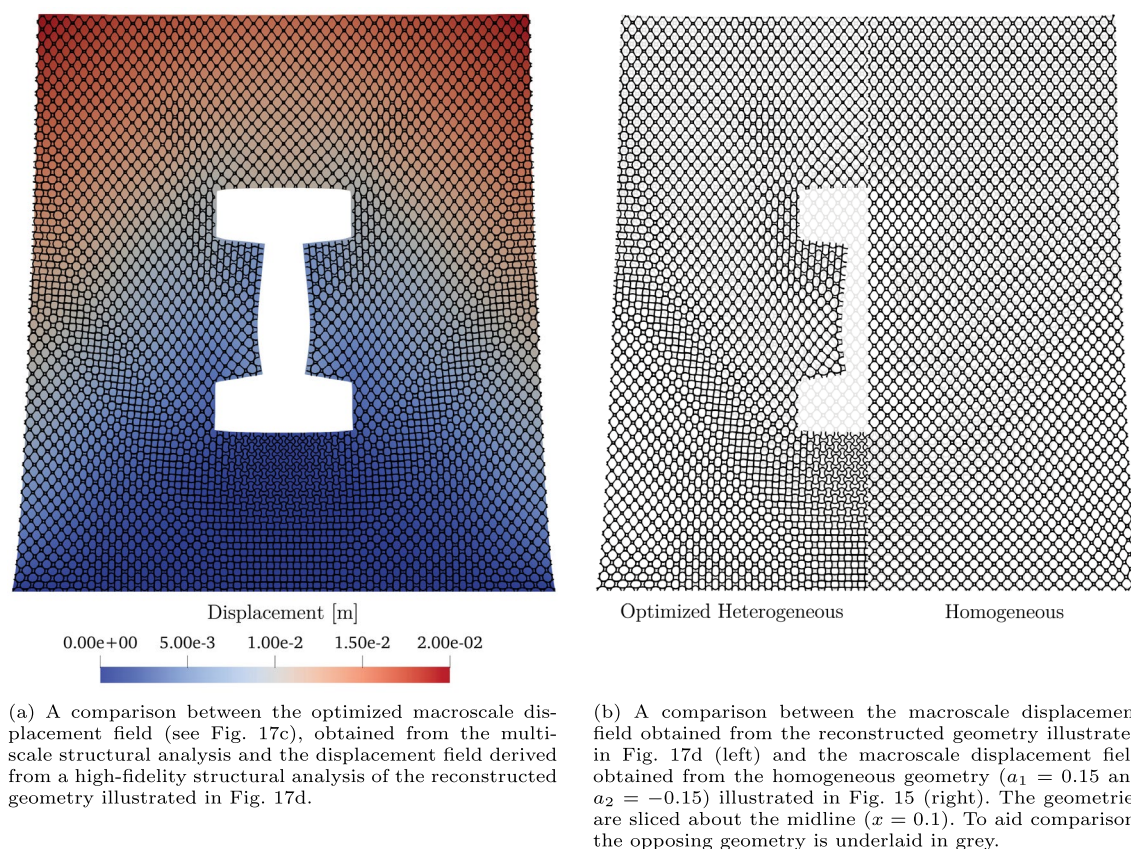


Fig. 18 Comparing the displacement field derived from the reconstructed geometry illustrated in Fig. 17d against both the optimized macroscale displacement field and the targeted homogeneous displacement field. The displacement fields are warped in both the horizontal and vertical directions

5 Conclusion

In this paper, a multiscale structural optimization framework capable of efficiently designing two-scale structures with prescribed displacements in the nonlinear elastic regime is presented. In contrast to previous multiscale topology optimization frameworks, which are founded upon the assumptions of linear elasticity, the present framework is capable of efficiently operating within the nonlinear elastic regime which represents the principal novelty of this paper. At the core of this framework is a parameterized microscale geometry, which through the straightforward manipulation of the associated amplitude parameters provides direct access to both positive and negative Poisson's ratios. The microscale model is concurrently coupled to the macroscale model such that only the microscale parameter space traversed by the optimizer is resolved during the optimization procedure. This is achieved by constructing a series of piecewise continuous linear interpolants as a function of the continuous microscale parameters and represents a further point of novelty for this framework. Significantly, as the exploration of the strain space is directed by sensitivities with respect to

the minimum potential energy, concurrent coupling helps to eliminate the simulation of unphysical and/or non-convergent strain combinations.

To demonstrate the capability of this framework, three prescribed deformation profiles are targeted by three distinct optimization procedures. In all instances, the deformation profile is successfully obtained through continuous optimization of the amplitude parameters. To verify the accuracy of the optimized macroscale displacement fields predicted by the multiscale structural analysis, high-fidelity simulations of the reconstructed geometries are performed. In each case, excellent agreement is noted between the high-fidelity simulations and the corresponding optimized macroscale displacement fields, with errors of less than 10% noted in all instances. Significantly, strains exceeding 18%, 20%, and 22% are observed in each respective case, which considering the excellent agreement with high-fidelity simulations, demonstrates this framework's capability to function effectively in the nonlinear elastic regime. The necessity of nonlinear analysis at both scales is verified by comparing the results of the high-fidelity simulations against identical simulations performed using linear elasticity. In all instances, the error

in displacement significantly increases, with some over an order of magnitude larger.

Concurrently coupling the micro- and macroscale models offers significant benefits, as evidenced by a single execution of the macroscale model. In this instance, only 1.45% of the total strain space is resolved to compute the macroscale displacement field, even though the direct strains exceed 24%. For the prescribed displacement optimizations, only 0.070%, 0.088%, and 0.31% of the parent database, equivalent to 0.018%, 0.023%, and 0.079% of all permutations, are required to derive the optimized amplitude fields. Given that the microscale model takes on average 6 seconds to execute on an Apple M1 Max CPU, the optimized structures are derived using only 7.4, 9.4, and 32.8 core-hours, as opposed to the 10, 633 core-hours that would be required to simulate the entire parent database in sequentially coupled frameworks.

Future studies should seek to experimentally validate the multiscale geometries presented within this paper. In addition, it would be interesting to explore higher-order homogenization schemes for the multiscale structural analysis, with the aim to exploit instabilities such as buckling at both scales to realize larger deformations. Higher-order homogenization schemes would necessitate the inclusion of further deformation-related design variables within the macroscale model; however, as proven within this paper, concurrently coupling the micro- and macroscale models provides a means to mitigate a significant proportion of the increased computation expense.

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Declarations

Conflict of interest The authors declare that they have no conflict of interest.

Replication of Results The authors wish to withhold the code for commercialization purposes. This includes the database of microscale simulations and a Python code implementing the optimization.

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