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Design of mechanical metamaterials using a level-set based topology optimization method

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Metamaterials are a family of artificially engineered materials consisting of an array of periodically arranged microstructures, offering unusual material properties that may not be easily found in nature. This paper will propose a new topological shape optimization method for the design of mechanical metamaterials with negative Poisson's ratios, by integrating the numerical homogenization method with a powerful level set method. The homogenization method is used to calculate the effective properties of the microstructure, and the level set method is utilized to implement shape and topology optimization of the microstructure until the desired material properties are obtained. The proposed method can retain the unique features of the level set methods, while avoid unfavourable numerical issues occurred in the conventional level set methods. Several typical numerical examples are used to showcase the effectiveness of the proposed design method.

1. Introduction

Metamaterials (Smith et al., 2004) are artificial materials engineered to have unconventional effective properties that cannot be easily obtained in nature. They are usually characterized by assemblies of a number of periodic microstructures fashioned with conventional materials, such as metals or plastics. Thus the layout of the microstructure has a great impact on the properties of metamaterials. In general, metamaterials gain extraordinary properties from their microstructures rather than from their material composition. Due to the exotic properties, metamaterials are experiencing popularity in a number of new and emerging areas. Over the past two decades, several types of metamaterials have been developed for a diverse of applications in science and engineering. However, this paper is focused on the design of a family of elastic metamaterials with negative Poisson's ratios (Lakes 1987; Milton 1992), also known as auxetic metamaterials.

The Poisson's ratio of a solid is defined as the ratio of transverse contraction strain to longitudinal stretching strain under uniaxial tension. It is a fundamental metric to measure the performance of elastic materials and facilitates the contemporary understanding of the mechanical properties of modern materials (Greaves at al., 2011). Although the classic theory of elasticity allows the Poisson's ratio to be negative, most conventional materials in nature possess positive values. In contrast to materials with positive Poisson's ratios, negative Poisson's ratio materials exhibit counter-intuitive properties: expanding laterally when stretched and contracting laterally when compressed. Since the work (Lakes 1987), the auxetic metamaterials have attracted increasing attention, due to their potential in a range of applications. However, the systematic design approaches are still in demand for creating novel auxetic metamaterials.

In the past two decades, topology optimization has been expanding as a powerful computational design tool for a broad range of structures and materials (Bensøe and Sigmund 2003). Essentially, topology optimization is a numerical iterative process that distributes a given amount of material inside a fixed design domain to seek the best material layout, such that the objective function is optimized subject to a set of constraints. So far, there have been several methods developed for topology optimization of structures, e.g., the homogenization method, the evolutionary structural optimization method, the element density SIMP method, the nodal density SIMP approach, and the level set based method (LSM). Amongst a number of applications of topology optimization, one of the most promising applications is the optimal design of micro-structured materials (Sigmund and Torquato 1996; Sigmund 1994, 2000; Guest and Prevost 2006).

The LSM (Sethian 1999; Osher and Fedkiw 2002) has recently emerged as a new method for shape and topology optimization of structures. After the pioneer's work of Sethian and Wiegmann (2000), several LSM-based topology optimization methods (Allaire et al., 2004; Wang et al., 2003) have been developed within the context of standard level set method (Osher and Sethian 1988; Sethian 1999). One of the major concepts behind these LSMs is to represent the design boundary of a structure implicitly as the zero level set of a higher dimensional level set function (LSF). Then, the motion of the design boundary is mathematically described as a Hamilton-Jacobi partial differential equation (H-J PDE) (Osher and Sethian 1988), in which the normal velocity field to enable the evolution of the design boundary is often obtained using the shape derivative method (Choi and Kim 2005).

More recently, several alternative LSMs (e.g., Belytschko et al., 2003; Haber 2004; Luo et al., 2008; Luo et al., 2009) have been developed for topological shape optimization of structures, to avoid the above numerical issues in the conventional LSMs. In particular, Luo et al. (2007, 2008) have proposed a parametric level set method (PLSM) for topological shape optimization of continuum structures. In this method, the compactly supported radial basis function (CS-RBF) (Wendland 2005) was utilized to achieve the interpolation of the implicit LSF, and then the design boundary was advanced by iteratively updating a set of unknown expansion coefficients of the interpolant. The PLSM has shown its ability as a powerful topological shape optimization method for structures (Luo et al., 2007, 2008), which can remain the favorable while avoid unfavorable numerical issues of the conventional LSMs. Particularly, many well-established optimization algorithms, including the optimality criteria (OC) (Luo et al., 2007) and mathematical programming methods (Haber 2004; Luo et al., 2008) an be directly applied.

This paper will develop a new systematic design method for auxetic metamaterials by using a level set-based topological shape optimization approach. Here, the numerical homogenization method is used to predict the material effective properties, while the PLSM is employed to optimize the shape and topology of the unit cell. The proposed method is a general methodology, which can be applied to the design of not only auxetic metamaterials, but also other metamaterials. Although the PLSM has been applied to the design of structures, this paper is the first time to extend the PLSM to the design of periodic metamaterials. Several numerical examples will be presented to demonstrate the effectiveness of the proposed method.

2. Level set-based parametric method

As mentioned above, in the level set-based topological shape optimization methods, the first element is to implicitly represent the design boundary of a structure by the zero level set of a higher dimensional LSF with Lipschitz continuity (Osher and Sethian 1988). For instance, Figure 1 shows the representation of a two-dimensional boundary with a three-dimensional level set surface, where φ is used to denote different parts of the reference domain, as follows:

$$\begin{cases} \varphi(\mathbf{x}) > 0 & \forall \mathbf{x} \in \Omega \setminus \Gamma & \text{(solid region)} \\ \varphi(\mathbf{x}) = 0 & \forall \mathbf{x} \in \Gamma & \text{(design boundary)} \\ \varphi(\mathbf{x}) < 0 & \forall \mathbf{x} \in D \setminus (\Omega \cup \Gamma) & \text{(void region)} \end{cases} \tag{1}$$

where D is the reference domain containing all admissible shapes of Ω, i.e. ($\Omega \subset D$), and Ω is the solid region. Γ is the design boundary located at the zero level-set.

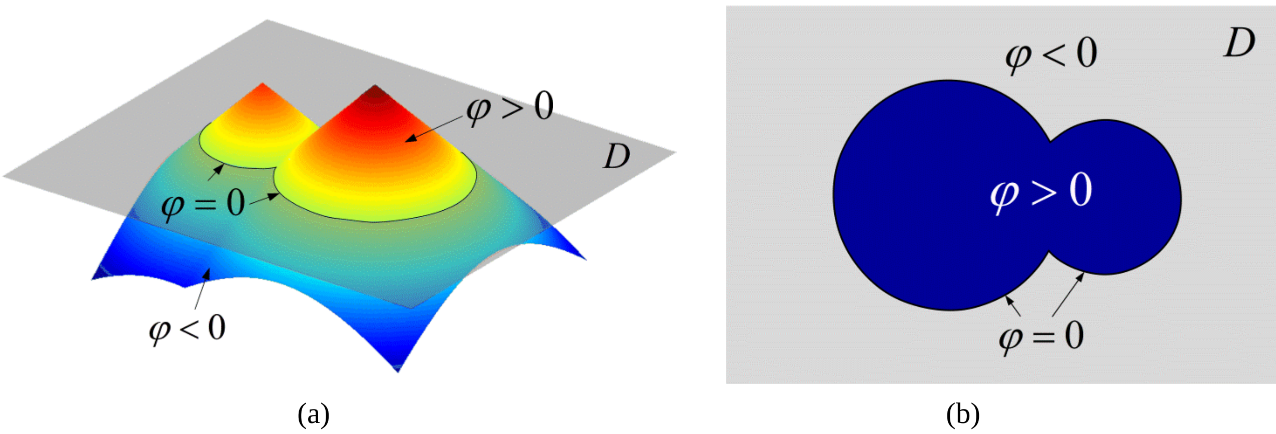


Fig. 1. (a) Three-dimensional LSF; and (b) Design domain with the zero level set.

In LSMs, the second element is to mathematically represent the motion of the design boundary, which is a first-order H-J PDE (Sethian 1999; Osher and Fedkiw 2002):

$$\frac{\partial \varphi(\mathbf{x},t)}{\partial t} + \mathbf{v} \cdot \nabla \varphi(\mathbf{x},t) = 0 \tag{2}$$

Where **v**=dx/dt is the velocity field at the design boundary. The velocity field $\mathbf{v}$ actually includes two components: normal velocity field and tangent velocity field. However, since the only normal velocity component v_n contributes to the shape evolution of the design boundary (Wang et al., 2003; Allaire et al., 2004), the above H-J PDE can be rewritten as

$$\frac{\partial \varphi(\mathbf{x},t)}{\partial t} - v_{\mathrm{n}} \left|\nabla \varphi(\mathbf{x},t)\right| = 0 \text{, where } v_{\mathrm{n}} = \mathbf{v}\cdot\mathbf{n} = \left(\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\right)\cdot\left(-\frac{\nabla\varphi}{\left|\nabla\varphi\right|}\right) \tag{3}$$

Hence, moving the boundary Γ of a structure is equivalent to propagating the LSF φ by numerically finding the steady-state solution of the H-J PDE.

In the PLSM, the LSF is determined by the interpolation of the CS-RBFs (Wendland 2005) at a set of knots fixed in the design domain, as expressed in a summation form by

$$\varphi(\mathbf{x},t) = \omega_i(\mathbf{x})\alpha_i(t) \quad (i = 1,2,\dots,N) \tag{4}$$

where N is the total number of the knots in the design domain, α_i is the expansion coefficients for the ith knot, and $w(x)$ is the CS-RBF of the ith knot evaluated at the computational point $\mathbf{x}$, which are

$$\omega_i(\mathbf{x}) = \left(1 - r_i(\mathbf{x})\right)_+^4 \left(4r_i(\mathbf{x}) + 1\right) \quad (i = 1,2,\dots,N) \tag{5}$$

Thus, the decoupling of the time and space terms of the H-J PDE, when the expansion coefficient α_i is time-dependent:

$$\omega_i(\mathbf{x})\dot{\alpha}_i(t) - v_{\mathrm{n}}\left|\nabla\omega_i(\mathbf{x})\alpha_i(t)\right| = 0, \quad \text{where} \quad \dot{\alpha}(t) = \frac{\mathrm{d}\alpha(t)}{\mathrm{d}t} \quad \text{and} \quad v_{\mathrm{n}} = \frac{\omega_i(\mathbf{x})\dot{\alpha}_i(t)}{\left|\nabla\omega_i(\mathbf{x})\alpha_i(t)\right|} \tag{6}$$

3. Design of metamaterials by using PLSM

In the proposed method, the micro-structured material is constructed by repeating a unit cell in all spatial directions, because the design is periodic. The effective material properties are obtained by using the numerical homogenization method. In order to achieve metamaterials with prescribed effective properties, the PLSM is employed to optimize the shape and topology of the unit cell with a given amount of conventional materials. This section will introduce the numerical homogenization method, and then present the mathematical formulation of the optimization problems.

In this study, the material is assumed to consist of periodically-arranged unit cells, as shown in Fig. 3. The topological shape optimization will then be performed within a unique cell Y, which is the design domain.

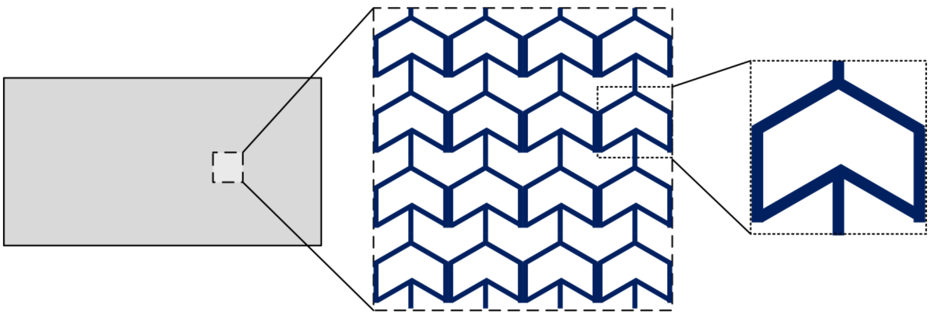


Fig. 3. A schematic illustration of periodic-arranged unit cells.

In the framework of the LSM, based on the small parameter perturbation of the displacement, the effective elasticity tensor D_{ijkl}^{H} is computed by

$$D_{ijkl}^{\mathrm{H}} = \frac{1}{|Y|}\int_D \left(\varepsilon_{pq}^0 - \varepsilon_{pq}^*\left(\chi^{ij}\right)\right) D_{pqrs} \left(\varepsilon_{rs}^0 - \varepsilon_{rs}^*\left(\chi^{kl}\right)\right) H(\varphi)\,\mathrm{d}\Omega \quad (i,j,k,l = 1,2,\dots,d) \tag{7}$$

where D_{pqrs} is the elasticity tensor of the solid material that composes the unit cell, $|Y|$ is the area (volume) of the unit cell, $H(\bullet)$ is the Heaviside function, d is the spatial dimension, ε_{pq}^{0} is the applied unit strain fields, consisting of three components (horizontal, vertical and shear unit strains) in 2D, and ε_{pq}^{*} is the strain field obtained by solving the equilibrium equation as

$$\int_D \left(\varepsilon_{pq}^{0} - \varepsilon_{pq}^{*}\left(\chi^{ij}\right)\right) D_{pqrs} \varepsilon_{rs}^{*}\left(v^{kl}\right) H(\varphi)\,\mathrm{d}\Omega = 0 \quad \forall v^{kl} \in \overline{U}(Y) \tag{8}$$

where χ^{ij} is the displacement field in the unit cell, which is Y-period and $\overline{U}$ is the kinematically admissible displacement space with Y-period.

(3.1) Design of metamaterials using PLSM

In order to generate metamaterials with desired effective properties, typically, the objective function is defined as the minimization of the sum of squared difference between the homogenized property and the desired elasticity tensor. The optimization problem can thus be formulated as follows:

$$\begin{cases} \text{find} & \alpha_i \quad (i = 1, 2, \ldots, N) \\ \min & J = \dfrac{1}{2} \displaystyle\sum_{i,j,k,l=1}^{d} \eta_{ijkl} \left(D_{ijkl}^{\mathrm{H}} - D_{ijkl}^{*}\right)^2 \\ \text{s.t.} & a(\boldsymbol{\chi}, \mathbf{v}, \varphi) = l(\mathbf{v}, \varphi) \quad \forall \mathbf{v} \in \overline{U}(Y) \\ & V = |Y|\, f_{\mathrm{v}} \\ & \alpha^{\mathrm{L}} \le \alpha_i \le \alpha^{\mathrm{U}} \end{cases} \tag{9}$$

where η_{ijkl} is the weighting factor associated with corresponding component of elasticity tensor, α^{L} and α^{U} are the lower and upper bounds of the design variables to guarantee a stable iteration, f_{v} is the allowable material volume fraction of the unit cell.

(3.2) Sensitivity analysis

The "size" optimization problem (10) after the parameterization can be solved by the mathematical programming methods, which requires the first-order derivatives of the objective function and constraints with respect to the design variables (coefficients of the interpolant).

In this paper, the Method of Moving Asymptotes (MMA) (Svanberg 1987) will be employed. MMA has been widely recognized as an efficient optimization algorithm for topology optimization problems. It is easily to get the derivative of D_{ijkl}^{H} with respect to α_i, which can be computed by

$$\frac{\partial D_{ijkl}^{\mathrm{H}}}{\partial \alpha_m} = \frac{1}{|Y|} \int_D \left(\varepsilon_{pq}^{0} - \varepsilon_{pq}^{*}\left(\chi^{ij}\right)\right) D_{pqrs} \left(\varepsilon_{rs}^{0} - \varepsilon_{rs}^{*}\left(\chi^{kl}\right)\right) \omega_m(\mathbf{x})^{\mathrm{T}} \delta(\varphi)\,\mathrm{d}\Omega \quad (m = 1, 2, \ldots, N) \tag{10}$$

In the numerical implementation, the standard finite element method (FEM) is usually used to discretize the unit cell and obtain the displacement field. However, standard FEMs are difficult to accurately capture the strain for those elements crossed by the boundary, as the material distribution within such an element is not uniform. There have been several methods developed to solve this problem. For instance, the simple but efficient "ersatz" model (Allaire et al., 2004) has been frequently used to compute the strains of the elements cut by the moving boundary. We will consider geometrical symmetries of the unit cell to achieve orthotropic or square symmetric materials. For instance, single-axis symmetry (half symmetry) or bi-axis symmetry (quadrate symmetry) can be utilized to design orthotropic materials for a 2D problem. More details of applying the symmetric boundary conditions can be found in (Sigmund 1994, 1996).

For simplicity but without losing any generality, this paper focuses on the design of metamaterials subject to the plane stress condition. By following the scheme in (Sigmund 1994, 1996), the elasticity tensor can be written in the following matrix form:

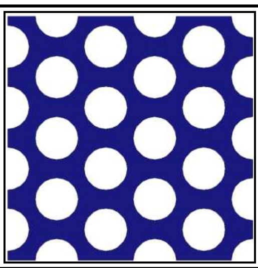
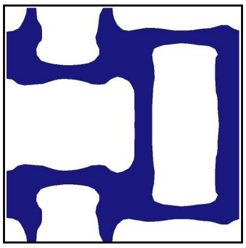
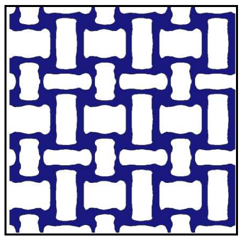
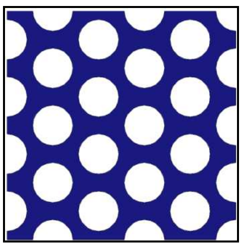
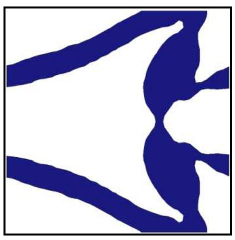
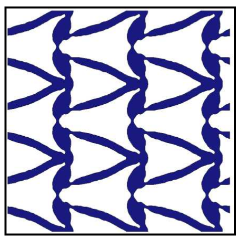
$$[D]=\begin{bmatrix} D_{1111} & D_{1122} & 0 \\ D_{1122} & D_{2222} & 0 \\ 0 & 0 & D_{1212} \end{bmatrix}=\frac{E}{1-\mu^2}\begin{bmatrix} 1 & \mu & 0 \\ \mu & 1 & 0 \\ 0 & 0 & G \end{bmatrix}, \text{ where } G=\frac{E}{2(1+\mu)} \tag{11}$$

where E is the Young's modulus, μ is Poisson's ratio and D is the matrix form of the elasticity tensor.

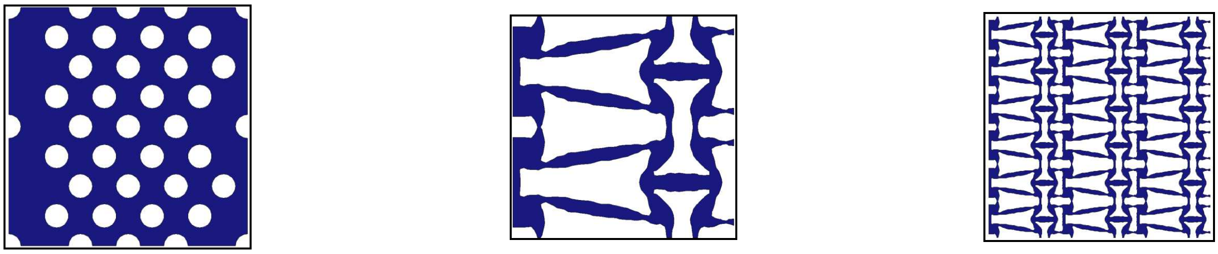
4. Numerical Examples

In this section, typical numerical examples are presented to demonstrate the effectiveness of the proposed method for the design of auxetic metamaterials. All the optimal results are limited to plane orthotropic materials, by making use of their geometric symmetries. However, it is straightforward to extend the present method to design other anisotropic and orthotropic materials. All numerical cases are performed without applying the re-initiations and the velocity extension. In all the examples, the Young's moduli for the solid material and void phase are $E^s=0.91$ and $E^v=0.001$, respectively, both with the same Poisson's ratio $\mu=0.3$. The unit cell is discretized by four-node square elements (Q4) with unit edge length, and each element contains 4×4 Gauss points. To obtain the materials with extreme Poisson's ratio $\mu=-1$, the optimization is performed from different initial guesses, weighting factors, geometric symmetries and volume fractions. Here, the total numbers of the elements used to discretize the unit cell are 40×40 for the cases 1 and 2, 60×60 for the case 3 and 80×80 for the case 4.

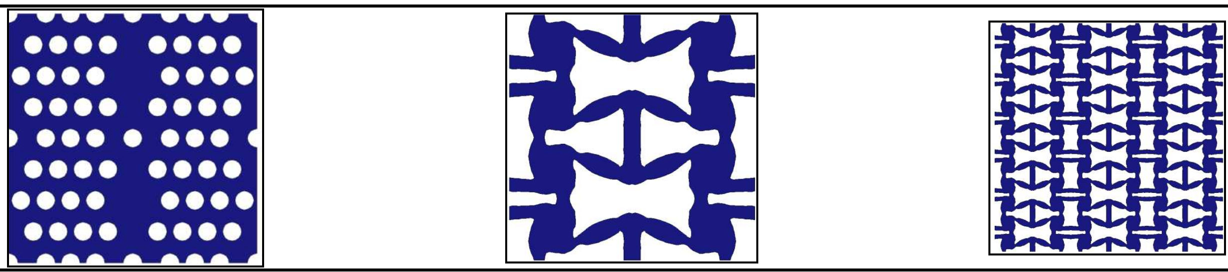
The optimal solutions for different cases are given in Fig. 4, and the corresponding effective matrices for the optimal designs are from -0.791 to -0.857. It can be seen that these different cases generate different topological shapes of the unit cell. This is reasonable as all the solutions exhibit negative Poisson's ratios. However, the Poisson's ratios of these optimal results do not reach $\mu=-1$.

Initial design	**Optimal design of unit cell**	**Repetitive unit cells**
		
Case 1		
		

Case 2



Case 3



Case 4

Fig. 4. Initial designs, optimal designs of unit cell, and 3×3 repetitive array of unit cells, for different cases

From these numerical results, we can carefully come to the conclusion that the metamaterials with Poisson's ratio -1 are hard to be obtained, if the topology optimization of continuum structures is used (Bendsøe and Sigmund 2003). This is consistent with the similar observations reported in the relevant literatures (Sigmund 1994, 2000; Sigmund and Torquato 1996). The effective properties of auxetic metamaterials are not only determined by the geometry (e.g. shape and topology) of the internal structure of the unit cell, but also dependent on the way the internal structure deforms when the unit cell is loaded.

As a result, if the bounds of extreme negative Poisson's ratios are expected, it is necessary to let the design generate rotating rigid mechanisms locally. However, the topology optimization is typically tailored as a specific method for continuum structures, and it generally does not allow the generation of rigid-link mechanisms to enable the rotating deformation. Hence, it is difficult to create auxetic metamaterials that can exactly reach the extreme bounds by using the continuum topology optimization formulation. However, the proposed method has provided a systematic design method for the creation of a range of new auxetic metamaterials.

5. Conclusions

This paper proposes a new topological shape optimization method for the design of elastic metamaterials, by systematically integrating the numerical homogenization approach with a level set method that is a more effective and efficient. In the method, the effective material properties are obtained by using the homogenization method, and the shape and topology changes of the unit cell are achieved by using the PLSM. In this setting, the proposed method can not only well retain the merits but also avoid numerical issues in the conventional LSMs. Several numerical examples have been applied to showcase the potential of the proposed method in the design of metamaterials.

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