DESIGNING MICROSTRUCTURES FOR DESIRED FUNCTIONAL MATERIALS AND LOCAL FIELDS

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Summary An inverse approach is presented to address the problem of designing microstructures/structures for desired functional materials and local fields. Motivated by many convenient properties of ellipsoids, we define innovative geometric concepts such as (periodic) E-inclusions and polynomial inclusions, and construct analytic solutions which are then used to produces designs for desired functionalities and local fields.

INTRODUCTION

The invention of new technologies depends critically on new multifunctional materials and innovative structures generating desired local fields. The requirements on these new materials or structures are often given in terms of a desired effective property, e.g., a maximum magnetoelectric coupling coefficient, or a desired local field, e.g., a minimum stress concentration. Therefore, there is a pressing need to relate directly microstructures/structures with effective properties and local fields and be able to find microstructures/structures for desired functionalities and local fields. The forward problem of predicting effective properties and local fields is straightforward and can be achieved by solving boundary value problems, e.g., the Maxwell equations in electromagnetics or the equilibrium equations in elasticity. However, there is no efficient method to solve the problem backward: to find microstructures/structures for desired functionalities or local fields. The conventional method relies heavily on the brute-force computational method which may be successful for particular applications but yields little systematic insight. In this paper we present an inverse approach to the problem.

METHODOLOGY AND EXAMPLES OF APPLICATIONS

In many modeling and design problems of physics, mechanics and materials, the mathematical problem eventually amounts to solving a simple scalar potential problem:

$$\Delta u = \sum_{i=0}^{N} p_i \chi_{\Omega_i} \quad \text{on } D, \tag{1}$$

where D is the domain of interest in the model, p_i are constants, Ω_i $(i = 0, \cdots, N)$ are a mutual disjoint subdivision of D and will be referred to as the microstructures or structures subsequently, χ_{Ω_i} $(= 1 \text{ on } \Omega_i, \ = 0$ otherwise) is the characteristic function of Ω_i, and $\xi : D \to I\!R$ is the scalar potential to be determined. Also, equation (1) shall be supplemented with appropriate boundary conditions on ∂D. Moreover, we remark that considerable amount of non-trivial arguments are necessary for converting the original problem in the model to the above simple potential problem, as one may observe from the classic works of Eshelby (1957 [1]) and Hashin-Strikman (1963 [3]). Conventionally, the above problem is addressed in a forward manner: the potential u is solved for specified microstructures/structures Ω_i, e.g., ellipsoids and polygons. In contrast, the new approach is to *seek* special microstructures/structures Ω_i for desired potential u. The first or second gradients of potential u correspond to the physical fields such as strain and magnetic fields which are of crucial importance in physical models. By studying these special microstructures/structures, we are able to solve the original problems analytically, make consistent and closed-form predictions, and construct optimal microstructures/structures for a variety of modeling and design problems. Below we briefly present two examples of special microstructures/structures: E-inclusions and polynomial inclusions and their applications. The interested reader is invited to check out detailed calculations and proofs in publications of the author and coworkers [9, 8, 5, 6, 7].

E-inclusions and their uniformity and optimality properties

E-inclusions are geometric shapes which are natural generalizations of ellipsoids in the context of second-order linear partial differential equations. Specifically, an E-inclusion is such that the solution to (1) with D being the entire space and appropriate decay boundary conditions at the infinity, satisfies the overdetermined conditions:

$$\nabla\nabla u(\mathbf{x}) = \mathbf{Q}_i \qquad \text{on } \Omega_i, \ i = 1, \cdots, N, \tag{2}$$

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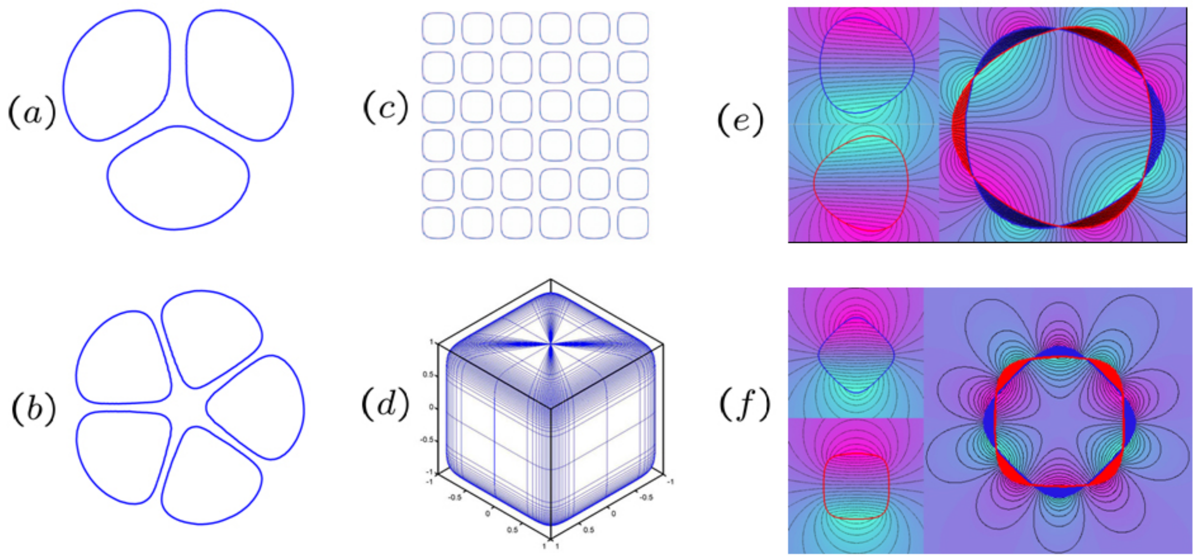

Figure 1. Examples of special shapes: (a) & (b) E-inclusions, (c) & (d) periodic E-inclusions, (e) & (f) polynomial inclusions.

where $\mathbf{Q}_1, \cdots, \mathbf{Q}_N$ are symmetric matrices. A periodic E-inclusion is defined similarly by imposing periodic boundary on ∂D with D being the periodic unit cell. These new shapes of E-inclusions (cf. Fig. 1 (a)&(b)) and periodic E-inclusions (cf. Fig. 1 (c)&(d)) are important for applications since they enjoy the following remarkable uniformity and optimality properties [8]: (i) they are optimal microstructures for minimizing field concentration, e.g., stress concentration, and the field inside the inclusions is uniform [9, 8]; (ii) effective properties of composites with microstructure of periodic E-inclusions can be calculated in a closed-form which allows for simple predictive models of multiphase multifunctional composites [8, 5]; (iii) they are optimal microstructures for maximum (or minimum) effective electric and thermal conductivity, effective dielectric constants, effective bulk elastic modulus, etc, among all microstructures with fixed volume fractions [7].

Polynomial inclusions and their applications

A polynomial inclusion of degree k is such that the solution to (1) with $N = 1$ and $p_0 = 0$, satisfies the overdetermined conditions: $u = p_k \quad \text{on} \quad \Omega_1$, where p_k is a polynomial of degree k. Examples of polynomial inclusions of degree three and degree four are shown in the left panels of Fig. 1 (e) & (f), respectively. Polynomial inclusions furnish a systematic design method to achieve arbitrary desired fields in a subdomain. For example, by overlapping two different polynomial inclusions of degree three, we obtain a design of magnet which generates a precise quadrupole field as shown in Fig. 1(e), whereas by overlapping two different polynomial inclusions of degree four, we obtain a design of magnet which generates a precise sextupole field as shown in Fig. 1(f) [6].

Finally, we remark that the overdetermined conditions in the definitions of E-inclusions and polynomial inclusions places strong restrictions on the geometry of the unknown domain Ω_i. The existence of (periodic) E-inclusions and polynomial inclusions is achieved by solving variational inequalities [4, 2, 8].

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