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Topology optimization of multiple anisotropic materials, with application to self-assembling diblock copolymers

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Abstract

We propose a solution strategy for a multimaterial minimum compliance topology optimization problem, which consists in finding the optimal allocation of a finite number of candidate (possibly anisotropic) materials inside a reference domain, with the aim of maximizing the stiffness of the body. As a relevant and novel application we consider the optimization of self-assembled structures obtained by means of diblock copolymers. Such polymers are a class of self-assembling materials which spontaneously synthesize periodic microstructures at the nanoscale, whose anisotropic features can be exploited to build structures with optimal elastic response, resembling biological tissues exhibiting microstructures, such as bones and wood. For this purpose we present a new generalization of the classical Optimality Criteria algorithm to encompass a wider class of problems, where multiple candidate materials are considered, the orientation of the anisotropic materials is optimized, and the elastic properties of the materials are assumed to depend on a scalar parameter, which is optimized simultaneously to the material allocation and orientation. Well-posedness of the optimization problem and well-definition of the presented algorithm are narrowly treated and proved. The capabilities of the proposed method are assessed through several numerical tests.

Keywords: Topology optimization; Anisotropy; Self-assembly; Diblock copolymers; Homogenization; Finite element

1. Introduction

The geometry and the topology of structures have a great impact on their performances. Therefore, the efficient use of material is crucial in many fields of application, from automotive industry, to bioengineering or MEMS industry. This explains the great interest towards topology optimization recorded in the past decades, both in the academic and in the industrial world. The classical topology optimization (TopOpt) problem looks for the optimal distribution of a given amount of isotropic material inside a prescribed domain, in order to optimize the mechanical response of the body to a given load. The performance of the design is measured by means of the so-called compliance, to be minimized, defined as twice the elastic energy computed at equilibrium [1–3].

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To overcome the computational complexity of large 0–1 type integer programming problems, the shape of the body is typically tracked by a density variable taking values in [0, 1], and a suitable interpolation scheme penalizing densities different from 0 and 1 is employed, one of the most popular being the SIMP (Solid Isotropic Material with Penalization) formulation [4,1]. An efficient algorithm to solve the minimum compliance problem is the OC (Optimality Criteria) method, a fixed point algorithm based on the optimality conditions [5]. In alternative, methods of sequential convex programming can be employed, like CONLIN (CONvex LINearization, see [6]) and MMA (Method of Moving Asymptotes, see [7,8]).

Alternative approaches for TopOpt are the level-set method and the phase-field method. With the first one, the borders of the body are determined as level-sets of a scalar function defined over the domain [9]. With the second approach, the TopOpt process is interpreted as a phase transition process, where a functional made of two contributions is minimized: the first term is an Allen–Cahn/Cahn–Hilliard type energy, which penalizes intermediate densities by means of a double well potential as well as the mean curvature of the border of the body, and the second term is proportional to the compliance [10–12].

1.1. Multimaterial TopOpt

It is well known that bodies exhibiting microstructures can be very efficient from the structural perspective. As a matter of fact nature exhibits plenty of examples of elastic bodies that, having to resist to mechanical loadings, present a fine-scale structure: bones, for instance, exhibit a sponge structure, and wood reveals a quasi-periodic microstructure. In fact, given a structure, it is always possible to enhance its stiffness with a refinement of the topology, i.e. by introducing holes without changing the total volume; by iterating this process one ends up with a microstructure [13]. Moreover, a microscopic structure can endow the medium with anisotropic properties at the macroscopic level. In this way the material is made lighter, enhancing at the same time its stiffness in the direction of the load, and making it more compliant in the other directions. Therefore, anisotropy is a key feature to build structures optimized for a prescribed purpose.

Most of the TopOpt formulations and algorithms are well suited for anisotropic materials: the SIMP formulation itself, in spite of its name, can be applied to this case by simply replacing the isotropic constitutive law with an anisotropic one. However, there is few sense in optimizing the distribution of a single anisotropic material, since the optimal level and type of anisotropy may depend strongly from point to point of the domain. This observation leads in a natural way to the problem of finding the optimal distribution of a given amount of material, with the possibility of choosing in each point of the domain among void and a certain number of candidate anisotropic materials, featuring different properties.

A multimaterial TopOpt has been formulated in a SIMP framework in [14] and [15]. In these works periodic microstructures made of two isotropic phases and void are optimized at the microscopic level, employing one design variable to track the topology of the structure, and one design variable to control the balance between the two phases. A constraint on the total amount of material was set independently for each phase.

The formulation was generalized in [16–18], under the name of DMO (Discrete Material Optimization), to encompass an arbitrary number of phases. In these works the resource constraint is set on the total mass, rather that on mass of the single phases. For the numerical resolution of the optimization problem MMA was employed. In this formulation the interpolation between phases is such that the increase of the density associated with one phase automatically penalizes other phases. A different generalization of the SIMP (and RAMP) formulation was given in [19]. Also in this case the optimization problem was solved by means of the MMA.

In [20] an ordered SIMP interpolation was proposed to solve multimaterial TopOpt problems without the introduction of new variables. With this formulation however, since the choice among the candidate materials is determined by a single variable, gradient-based update schemes are somehow short-sighted, making the numerical solution very likely to fall into local minima which may be far from the global minimum, as shown by the numerical results reported in the paper.

In [21] a multimaterial TopOpt problem is solved by means of a peak functions interpolation schemes. The interpolation of different phases is obtained by means of Gaussian peaks, which are gradually made sharper to steer the solution towards the selection of a pure phases. The advantage of this approach is that the number of phases can be increased without changing the number of design variables.