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Topology optimization of binary microstructures involving various non-volume constraints

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ABSTRACT

In this paper, we use the Topology Optimization of Binary Structures (TOBS) method recently developed by Sivapuram and Picelli (2018) for microstructural optimization. This is the first work in topology optimization addressing various non-volume microstructural constraints with discrete (0/1) design variables. The objective and constraint functions are linearized at each iteration, and the obtained linear problem is solved through Integer Linear Programming (ILP) using sensitivities computed from asymptotic homogenization. A periodic filter is used to make the optimized solutions checkerboard-free and mesh-independent. Volume minimization problems subject to elastic and thermal constraints are considered. The examples consider different sets of constraints, including bulk and shear moduli, square/cubic symmetry, isotropy, thermal conductivity and a combination of them in two and three dimensions. The non-volume constraints are treated explicitly, i.e., without the use of Lagrange multiplier/penalty as used in conventional gradient-based binary topology optimization methods (Huang and Xie, 2010). The resulting microstructures are observed to be convergent in all the examples presented and in agreement with the Hashin–Shtrikman bounds.

1. Introduction

Many naturally occurring materials exhibit outstanding mechanical properties while being light-weight because of the presence of cellular microstructures. Gibson et al. [3] analyzed the microstructures in wood, palms and bamboo for their high-performing materials and also described the fabrication of model materials inspired from these microstructures. The material property charts for natural materials with microstructures like cellulose, keratin, collagen, etc. are given in [4]. These charts identify the extreme properties of materials which suggest the evolution of materials for specific modes of loading. Such materials with remarkable tensile or flexural properties motivate us to design similar or superior materials artificially using numerical algorithms.

Topology optimization is a tool for designing a structure with optimized distribution of material so as to maximize the structure's performance, subject to some constraints. Topology optimization has been used to solve various problems including compliant mechanisms' design [5], design of pressure-load bearing structures [6,7], acoustic design [8,9], etc. The material microstructures can also be systematically designed using topology optimization to create light-weight materials with enhanced properties.

The seminal paper by Bendsøe and Kikuchi [10] used the homogenization method through sizing optimization of material microstructures at various locations in the structure so as to optimize its topology. As a density-baed approach, the Solid Isotropic Material with Penalization (SIMP) method uses continuous ($[0, 1]$) density design variables and material interpolation using penalization to optimize for continuum structures [11,12]. Sigmund [13] used SIMP and an inverse homogenization approach to design 2D material microstructures with prescribed constitutive tensors. The SIMP method has also been used in the design of microstructures with optimized thermal expansion and piezoelectric coefficients [14,15] and in the design for maximum fluid permeability [16]. The SIMP method features the presence of gray regions (intermediate densities) in the optimized solution because of the continuous design variables. The gray regions are difficult to be minimized even by increasing penalty, which poses a challenge for specific problems, e.g., in thermoelastic design [17]. The final solution can be driven to a 0/1 design by using filtering or projection schemes [18]. The projected structures, however, might potentially be in the infeasible region of constraint space. The existence of intermediate densities during optimization motivates binary methods to be created for a series of applications.

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Some methods like the level-set topology optimization use an implicit description of the structural boundary using a level-set function, which is iteratively updated by solving a Hamilton–Jacobi (HJ) equation so as to improve the performance of the structure [19,20]. The exact location of the boundary is approximated using interpolation of the level-set function values defined over a grid. Using the level-set method, [21] presented the Pareto fronts that estimate the upper bound of bulk modulus and fluid permeability cross-property space. Structures with multiple materials have been designed using a parametric level-set topology optimization in [22]. Wang et al. [23] used parametrized level-set method and numerical homogenization to design metamaterials where the objective function is a measure of mismatch between the optimized and target constitutive tensors. Challis et al. [24] presented a method to design isotropic 3D microstructures optimized for a weighted combination of effective elastic and thermal properties using level-set method. They used two phases of materials, the stiff, insulating phase and the compliant, conductive phase. A review of level-set methods and the challenges faced by them are described in [25].

Another major class of topology optimization methods uses a discrete 0/1 set of design variables. The most established discrete topology optimization method is the Bidirectional Evolutionary Structural Optimization (BESO) [26]. The method uses binary design variables in the structure which are updated using rules based on the gradients of objective function towards satisfying a required volume constraint. Any non-volume constraint is dealt with using Lagrange multipliers so as to convert the original problem into an optimization problem with only volume constraint. Huang and Xie [2] show the usage of Lagrange multipliers to deal with the displacement constraint. In microstructural optimization, Xia and Breitkopf [27] developed a multiscale framework for concurrent design of material microstructures and macrostructure using FE^2 scheme, using the BESO method at both the micro and macro scales. In [28,29], BESO is used to obtain optimized isotropic microstructures where the isotropy constraint is again handled using Lagrange multipliers. The setting and updating of Lagrange multipliers is not trivial, especially in case of multiple non-volume constraints. The convergence of non-volume constraints is potentially affected when enforcing them via Lagrange multipliers. In Sivapuram and Picelli [1], we developed the TOBS (Topology Optimization of Binary Structures) method using Integer Linear Programming (ILP). Since mathematical programming is used to update the design variables, the non-volume constraints can be dealt explicitly. The working of the method in the presence of compliance and displacement constraints is demonstrated in [1]. This paper extends the TOBS method to microstructural optimization problems with multiple non-volume constraints.

The TOBS method is a discrete optimization method and conceptually simple. The optimization problem is converted into an integer linear program by linearization at each iteration using Taylor's first order approximation. An extra constraint is added to restrict dramatic changes in the structure at each iteration, thus keeping in check the truncation error due to linearization. The constraints are relaxed to ensure a feasible solution at every iteration and ILP can be used to solve the linear subproblem using branch-and-bound method. The design variables are then updated to obtain the new (micro) structure. Since we are using mathematical programming, the use of Lagrange multipliers is not necessary. This gives the method an advantage over the BESO method in dealing with non-volume constraints. Svanberg and Werme [30] also use ILP for a hard-kill topology optimization without the use of any filtering. However, they use hierarchical mesh refinement to achieve the optimized solution, therefore, making the problem mesh dependent. In this work, standard asymptotic homogenization is used to compute the material properties and characteristic displacements each iteration. The sensitivities are then computed and filtered for mesh-independency and to avoid checkerboards. In this paper, some volume-constrained problems from literature are solved to demonstrate that TOBS produces similar or improved solutions. We also solve volume minimization of 2D and 3D microstructures with constraints on bulk modulus, shear modulus, thermal conductivity and additional constraints for achieving square/cubic symmetry, orthotropy and isotropy. Several examples are presented to demonstrate the effectiveness of the TOBS method in dealing with multiple non-volume constraints for microstructures. Some of the problems solved consist of constraints related to both thermal and elastic properties thereby designing multifunctional materials.

This paper is organized as follows. Section 2 describes the TOBS method and the improvements of the technique from [1]. The standard asymptotic homogenization to compute material properties is briefly outlined in Section 3. Section 4 describes the objective and constraint functions used in the paper and their sensitivities. The filtering of sensitivities for microstructures is described in Section 5. Several 2D and 3D examples for microstructure design are shown in Section 6, and the results are discussed. Section 7 summarizes the work and presents the key conclusions.

2. Topology Optimization of Binary Structures (TOBS)

The TOBS method involves linearization of the objective and constraint functions at each iteration, and the subproblems created are solved using integer programming. The design variables of the optimization are binary, 1 for solid and 0 for void finite elements in the mesh of design domain. A generic topology optimization problem with objective function $f(\mathbf{x})$, constraints $g_i(\mathbf{x}) \leqslant \overline{g}_i$, where $\mathbf{x}$ are the design variables is given by:

$$\begin{aligned} \underset{\mathbf{x}}{\text{Minimize}} \quad & f(\mathbf{x}) \\ \text{Subject to} \quad & g_i(\mathbf{x}) \leqslant \overline{g}_i \quad i \in [1, N_g] \\ & x_j \in \{0, 1\} \quad j \in [1, N_d] \end{aligned} \tag{1}$$

where N_d is the number of design variables. Taylor's first order approximation is used to create the linearized subproblem given by Eq. (2).

$$\begin{aligned} \underset{\Delta\mathbf{x}^k}{\text{Minimize}} \quad & \left.\frac{\partial f}{\partial \mathbf{x}}\right|_{\mathbf{x}^k} \Delta\mathbf{x}^k \\ \text{Subject to} \quad & \left.\frac{\partial g_i}{\partial \mathbf{x}}\right|_{\mathbf{x}^k} \Delta\mathbf{x}^k \leqslant \Delta g_i^k \quad i \in [1, N_g] \\ & \Delta x_j^k \in \{-x_j^k, 1-x_j^k\} \quad j \in [1, N_d] \end{aligned} \tag{2}$$

where Δg_i^k is the right hand side of the i^{th} constraint at the k^{th} iteration, and $\Delta\mathbf{x}^k$ represents the change in design variables. At the end of each iteration, the design variables are updated using Eq. (3).

$$\mathbf{x}^{k+1} = \mathbf{x}^k + \Delta\mathbf{x}^k \tag{3}$$

The truncation error involved in approximation of the functions is $O(||\Delta\mathbf{x}||_2^2)$. In order to maintain the validity of this approximation, an additional constraint is imposed on the change in design variables $\Delta\mathbf{x}$ at every iteration. The extra constraint is given by Eq. (4).

$$||\Delta\mathbf{x}^k||_1 \leqslant \beta N_d \tag{4}$$

This equation implies that the number of flips between solid to void and vice versa is constrained to be a fraction β of the total number of flips possible, which is the number of design variables N_d. We used Eq. (4) in place of the two constraints used in [1] for keeping a check on the truncation error.

The gradient-based optimization requires an initial solution to start with, which might lie in the infeasible space of optimization problem. Thus, it can happen that the solution at the current iteration is infeasible, and far from being feasible. In such a case, it is difficult to satisfy the linearized constraints in the next iteration because the structure is allowed to have only small changes each iteration to keep the truncation error low. To address this issue, the constraints are relaxed, i.e, the values of Δg_i^k are chosen such that the linearized problem has a feasible solution. The relaxation for a constraint g at iteration k is given in Eq. (5).