Project report: "Optimization driven design of materials with exotic properties"

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Abstract

In this project a topology optimization framework for designing periodic viscoplastic microstructures under finite deformation has been developed. Microstructures with tailored macroscopic mechanical properties, i.e. maximum viscoplastic energy absorption and prescribed Poisson's ratio, are designed by performing numerical tests of a single unit cell subjected to periodic boundary conditions. The applicability of the framework is demonstrated by several numerical examples of optimized two-dimensional continuum structures exposed to multiple load cases over a wide range of macroscopic strains. The results has been presented at "The 13th World Congress in Computational Mechanics, New York, July 2018" and the results are currently being prepared for journal publication.

1. Introduction

Since the work by [1], topology optimization has undergone rapid development and been applied to a variety of physical problems. Specifically, topology optimzation based material design methods based on the inverse homogenization approach have demonstated the possibility to create novel materials with enhanced properties, through optimal material distribution of the material microstructure. Examples of these include linear elastic materials with negative Poisson's ratio [2], negative thermal expansion [3].

In the design of such materials, a common simplification in the topology optimization formulation is to use linearized theory, e.g. linear elasticity and assume small strain structural response. This means that materials that exhibit irreversible processes and are exposed to large deformations cannot be designed. To specify, although linear assumptions suffice for many structural optimization problems of materials that are subject to moderate macroscopic strain levels, they may fail to accurately model the microstructural material response, as moderate macroscopic strains generally give much higher local strains at the microscopic scale. To predict microstructural response, nonlinear finite strain theory should therefore be incorporated in topology optimization.

When accounting for geometrical nonlinearities of the material microstructure, however, the evaluation of the homogenized material properties become more demanding. For

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these nonlinear cases, multiscale approaches are required to account for heterogeneity in the microstructure. Such multiscale homogenization methods are cumbersome due to the iterative nonlinear analyis and the extensive computational effort needed [4]. To solve coupled multiscale topology optimization problems for nonlinear elastic structures, one possibility is to apply efficient parallel programming, as presented in [5], but although efficient, this method is still computationally intense.

In recent works [6], alternatives to nonlinear homogenization methods has been proposed. These methods use numerical tensile experiments for calculating the effective material response, and use topology optimization to achieve prescribed nonlinear properties under finite deformation. In this way, the computational effort required for the analysis is significantly reduced, since the entire macroscopic structure is represented by a single representative volume element (RVE).

Of the developed topology optimization methods, few consider material design problems related to inelastic material response. Contributions incorporating small strain elastoplastic formulations include work that use topology optimization to obtain conceptual designs of energy absorbers for crashworthiness, modeled with 2D-beam elements [7]. Protective systems with maximum energy dissipation for structures subject to impact loading have also been designed by [8], where a transient elastoplastic topology optimization formulation is used. Elastoplastic material modelling has further been used in [9] for optimizing steel-reinforced concrete structures and in a recent study, [10] presents a topology optimization routine based on finite strain plasticiy. Thus, to date, most topology optimization frameworks on material nonlinearities focus on homogeneous materials, or heterogeneous materials with given micostructures, whereas research on topological material design for inelastic material properties remains scarce.

To generate optimal topologies of periodic microstructures, for maximum energy dissipation and for specific Poisson's ratio, we present a finite strain viscoplastic topology optimization framework. The constitutive model is based on finite strain isotropic hardening viscoplasticity. Macroscopic nonlinear material properties are evaluated by numerical tensile- and shear tests of a single unit cell that is subjected to periodic boundary conditions. Similar to the work in [11] we include rate-dependent finite strain effects into topology optimization, but we restrict ourselves by excluding dynamic inertial effects.

2. Problem formulation

The constitutive model is based on isotropic hyperelasticity and isotropic hardening viscoplasticity. Since we use finite strains, multiplicative split of the deformation gradient is employed. The specific viscoplastic power, $\dot{w}^{vp}$, is obtanied from thermodynamics and it can be integrated to yield the total plastic work, i.e.

$$W^{vp} = \int_0^{T^f} \int_{\Omega_o} \dot{w}^{vp} dV dt, \tag{1}$$

where T^f is the terminal time and Ω_o the design domain.

The mechanical balance laws are spatially discretized by means of the finite element method and the constitutive equations are integrated with the backward Euler scheme. The continuous non-dimensional volume fraction field $c \in [0, 1]$ is the design variable and it describes the amount of material for a material point, where regions filled with material are defined by $c = 1$ and void regions are identified by $c = 0$. The variation of the continuous volume fraction field c is reguralized through the Helmholtz' partial differential equation filtering technique which we solve using using finite elements.

3. Topology optimization

The objective is to design a material microstructure with maximum viscoplastic energy absorption capability, W^{vp}. We also consider constraints on the displacement during the loading. For a longitudinal loading test where $\bar{u}_{xx}$ is prescribed, the displacement constraint is imposed using a secant measure of Poisson's ratio, i.e.

The topology optimization problem is to find a design $\boldsymbol{\phi}$ that solves

$$\mathcal{O}: \begin{cases} \underset{\boldsymbol{\phi}}{max}\ W^{vp}, \\ \text{s.t.} \begin{cases} g_1 & = \sqrt{\dfrac{1}{T} \sum_{n=1}^{N} \left(\nu_{xy}^{(n)} - \nu_{xy}^{*}\right)^2 \Delta t_n} - \delta_\nu \leq 0, \\ g_2 & = V - V_{max} \leq 0, \end{cases} \end{cases} \tag{2}$$

where g_1 reprsents the constrain on the Poisson's ratio and where g_2 represents the volume constraint.

The optimization problem is solved using gradients of the objective function and the constraints to form a convex approximation of the optimization problem. We therefore perform a sensitivity analysis in each optimization iteration, and as the number of design variables outnumber the number of constraints, we use the adjoint method [12].

4. Numerical examples

To show the effectiveness of the presented framework, we present the solution of different topology optimization design problems. The primal viscoplasticity problem is solved with an adaptive time stepping where the time increments used to perform the sensitivity analysis are consistent with those used to solve the primal problem.

First, we consider a tensile loading scenario, where simultaneous longitudinal and transverse displacement boundary conditions are applied, i.e. $\varepsilon_{xx} = \varepsilon_{yy} = 1\%$. The volume fraction is 35%. Quarter symmetry within the design is enforced, ensuring zero shear forces. The performance of the four designs using different random initial conditions is compared in Fig. 1 which reveal that several local minima to this optimization problem exist. In Fig. 1, the energy absorption during the optimization is also shown, where it is clear that the four topological different designs have a similar performance, and that the objective function has been maximized.

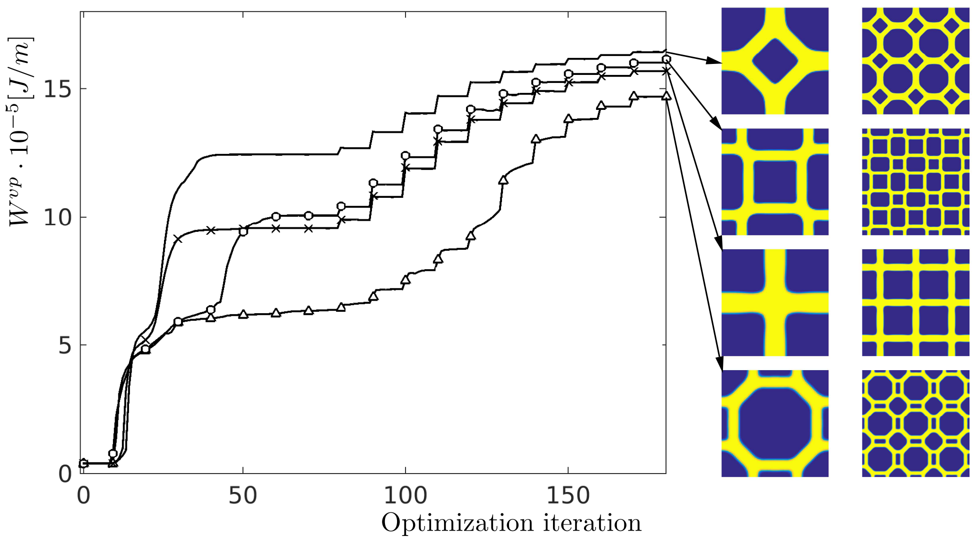

Figure 1: Viscoplastic work versus optimization iteration for different optimized designs.

Next, we increase the load magnitude and consider two separate load cases; longitudinal and transverse tensile loading, prescribing the macro strain levels $\varepsilon_{xx} = 5\%$ and $\varepsilon_{yy} = 5\%$, respectively. The aim is now to maximize the total energy W absorbed due to the external load. As shown in the previous examples, the optimized designs are symmetric in the axial and diagonal directions due to the initial design. To ease the computational effort, we enforce symmetry along the axial and diagonal axes.

Four designs are shown in Fig. 2, optimized for maximum total energy absorption W, where the target Poisson's ratio is $\nu^* = 0$. The optimization problems are initiated with the same random design and are subjected to the prescribed macroscopic strain $\varepsilon_{xx} = 5\%$. The results are obtained using increasing filter length scale.

Conclusions

We have established a topology optimization framework for designing periodic microstructural materials with maximum viscoplastic energy absorption. Materials that possess near strain-independent Poisson's ratio have been designed. Sensitivities required to solve the optimization problem are obtained using the adjoint method. The finite strain viscoplastic effects on the designs are shown by simulation of several macroscopic load cases.

The unit cell that characterizes the design domain has been discretized with 3D finite elements. This formulation enables a smooth transition to large-scale 3D problems by relaxation of the plane strain assumption. In future work, we will apply parallel programming to the framework to efficiently solve such large-scale problems.

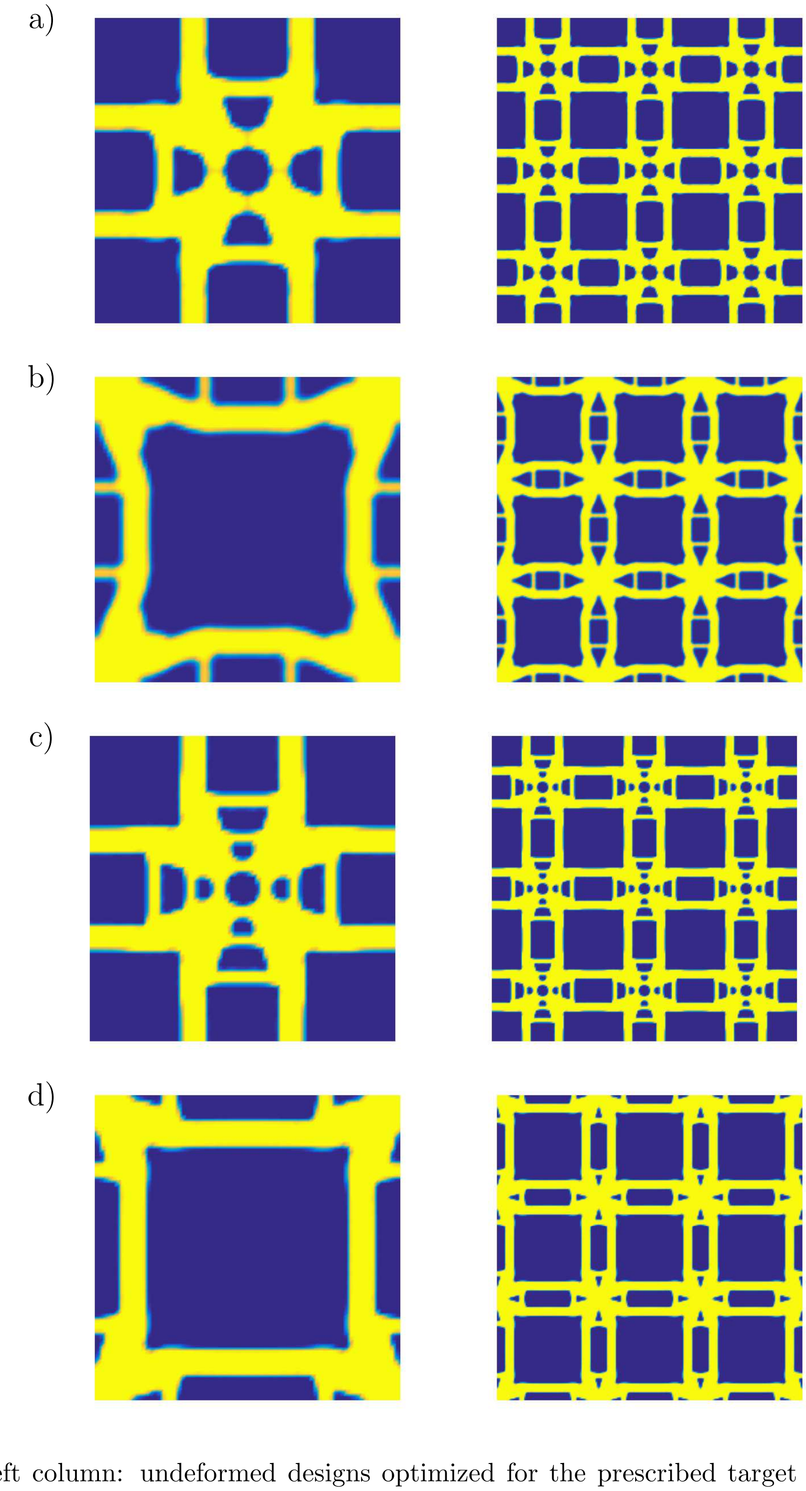

Figure 2: Left column: undeformed designs optimized for the prescribed target $\nu^* = 0$ with axial and diagonal symmetry enforced, and 5% prescribed macroscopic strain. Right column: arary of 3×3 unit cells. The filter length scale is a) $l_o = 0.0175$, b) $l_o = 0.0200$ c) $l_o = 0.0210$, d) $l_o = 0.0250$.

References

[1] Bendsøe MP, Kikuchi N. Generating optimal topologies in structural design using a homogenization method. *Comput. Methods Appl. Mech. Engng.* 1988; **71**:197–224.

[2] Sigmund O. Tailoring materials with prescribed elastic properties. *Mechanics of Materials* 1995; **20**(4):351 – 368.

[3] Sigmund O, Torquato S. Design of materials with extreme thermal expansion using a three-phase topology optimization method. *Journal of the Mechanics and Physics of Solids* 1997; **45**(6):1037 – 1067.

[4] Yvonnet J, Gonzalez D, He QC. Numerically explicit potentials for the homogenization of nonlinear elastic heterogeneous materials. *Computer Methods in Applied Mechanics and Engineering* 2009; **198**(33):2723 – 2737.

[5] Nakshatrala P, Tortorelli D, Nakshatrala K. Nonlinear structural design using multiscale topology optimization. part i: Static formulation. *Computer Methods in Applied Mechanics and Engineering* 2013; **261-262**:167 – 176.

[6] Wang F, Sigmund O, Jensen J. Design of materials with prescribed nonlinear properties. *Journal of the Mechanics and Physics of Solids* 2014; **69**:156 – 174.

[7] Pedersen CB. Crashworthiness design of transient frame structures using topology optimization. *Computer Methods in Applied Mechanics and Engineering* 2004; **193**(6):653 – 678.

[8] Nakshatrala P, Tortorelli D. Topology optimization for effective energy propagation in rate-independent elastoplastic material systems. *Computer Methods in Applied Mechanics and Engineering* 2015; **295**:305 – 326.

[9] Bogomolny M, Amir O. Conceptual design of reinforced concrete structures using topology optimization with elastoplastic material modeling. *Int. J. Numer. Meth. Engng* 2012; **90**(13):1578–1597.

[10] Wallin M, Jönsson V, Wingren E. Topology optimization based on finite strain plasticity. *Structural and Multidisciplinary Optimization* 2016; :1–11.

[11] Ivarsson N, Wallin M, Tortorelli D. Topology optimization of finite strain viscoplastic systems under transient loads. *International Journal for Numerical Methods in Engineering* ; :n/a–n/aNme.5789.

[12] Michaleris P, Tortorelli DA, Vidal CA. Tangent operators and design sensitivity formulations for transient non-linear coupled problems with applications to elastoplasticity. *Int. J. Numer. Meth. Engng* 1994; **37**(14):2471–2499.