First Steps towards Topology Optimization of Nonlinear Structures using the One-Shot Approach

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Summary

The one-shot approach is traditionally used in the context of shape optimization with an underlying expensive partial differential equation constraint. If the solution process for the partial differential equation can be interpreted as a fixed point iteration, it can be augmented with an adjoint solver. Then, in the one-shot approach state and adjoint feasibility are pursued simultaneously with optimality using a suitable preconditioner. In the present work we transfer the ideas of one-shot optimization to the field of topology optimization. The structural analysis involving geometrical and material non-linearities is realized with a Newton-like solver, that can be augmented by an adjoint solver. Several new challenges for one-shot topology optimization like projection methods and filter methods are discussed. Results are presented for topology optimization of nonlinear elastic structures in a two-dimensional setting to minimize compliance.

Keywords: *one-shot optimization, topology optimization, minimum compliance*

1 Introduction

The one-shot approach, also referred to as simultaneous analysis and design,[1] can be applied for optimization problems involving the solution of an underlying partial differential equation. Especially for slowly converging Newton-like PDE solvers it is advantageous to make use of one-shot approaches instead of recovering state and adjoint feasibility in each optimization step in a nested fashion. The state solver can be interpreted as a fixed point solver and can be augmented by a corresponding discrete adjoint fixed point solver based on algorithmic differentiation. In a one-shot approach, the state and adjoint equation together with the design equation are iterated simultaneously, e.g. by using a design space preconditioner based on the doubly augmented Lagrangian.[2] A summary of one-shot approaches can be found in Bosse et al.[3]

So far, the one-shot approach has been mainly used for shape optimization problems, e.g. in aerodynamic applications.[4] The main bottleneck for shape optimization is the need to perform a mesh deformation or even remeshing in each optimization step, that might become overhead in the one-shot framework. For topology optimization this problem is not apparent which can be a high potential for one-shot optimization methods. A popular nested approach for topology optimization is the method of moving asymptotes.[5] Simultaneous analysis and design has been performed in the context of topology optimization of truss structures[6] and interior-point multi-grid methods have been applied for the topology optimization of linear elastic materials.[7]

We newly apply the one-shot approach based on Hamdi and Griewank for the topology optimization of nonlinear elastic materials. In this work we intend to formulate challenges and first ideas in the direction of one-shot topology optimization. Several concepts to project or filter obtained sensitivities or design variables, that are essential for topology optimization, have to be incorporated in the one-shot framework.

2 The Topology Optimization Problem

The structural analysis for the nonlinear material under large displacements is based on the principle of virtual work. The resulting weak form of the equilibrium equation in the current configuration V

$$R(u) := \int_V \sigma : \delta e dV - \left(\int_V f \cdot \delta u dV + \int_{\delta V} t \cdot \delta u da \right) = 0 \qquad (1)$$

with the Cauchy stress tensor σ, the rate of deformation tensor e, the virtual displacement field δu, the boundary element da, the volume force f and the surface traction t is discretized using a finite element approach and solved iteratively with a Newton-Raphson scheme. The nonlinear hyperelastic material is modeled as a Neo-Hookean solid.

For topology optimization we consider the mean compliance as an objective function to maximize the stiffness of the structure. Using the SIMP[8] (Solid Isotropic Material with Penalization) approach, the density ρ_e serves as a design variable and is used in each element e to model areas containing material ($\rho_e = 1$) and void areas ($\rho_e = 0$). The Young's modulus E_e of an element is given by $E_e(\rho_e) = E_{\min} + \rho_e^p(E - E_{\min})$, where $p > 1$ penalizes densities between 0 and 1 and $E_{\min} > 0$ is a very small value representing the void regions in the stiffness matrix. An additional constraint is imposed on the volume of the resulting structure by prescribing a volume fraction $f_v > 0$. The resulting optimization problem to be solved reads

$$\begin{aligned} \min_{u,\rho} \quad & c(u,\rho) := \textstyle\int_V f \cdot u dV \\ \text{s.t.} \quad & R(u,\rho) = 0, \\ & V(\rho)/V_0 = f_v, \quad 0 \le \rho \le 1. \end{aligned} \tag{2}$$

3 The One-Shot Approach

3.1 General Description

Problem (2) can be discretized and the PDE constraint can be written as a fixed point equation $G(u,\rho) = u$ with $\rho \in \mathbb{R}^n$, and $\lambda,\ u \in \mathbb{R}^m$. In the following analysis we neglect the additional constraints for the density, as these will be treated separately by a projection method. The Lagrangian for the discretized problem is $L(u,\rho,\lambda) = c(u,\rho) + (G(u,\rho) - u)^\top \lambda = N(u,\rho,\lambda) - u^\top \lambda$, where $N(u,\rho,\lambda)$ is the referred to as the shifted Lagrangian. Based on the first-order necessary optimality conditions and with a suitable chosen preconditioner B_k the one-shot strategy can be formulated as

$$\begin{aligned} u_{k+1} &= G(u_k,\rho_k) \\ \rho_{k+1} &= \rho_k - B_k^{-1} N_\rho(u_k,\rho_k,\lambda_k)^\top \\ \lambda_{k+1} &= N_u(u_k,\rho_k,\lambda_k)^\top. \end{aligned} \tag{3}$$

The first iteration is the primal iteration solving the PDE constraint. The second iteration is the design update and the third iteration is the iteration procedure for the adjoint vector λ. For a particular choice of penalty parameters α and β it can be shown, that the doubly augmented Lagrangian

$$L^a(u,\rho,\lambda) = \frac{\alpha}{2}\|G(u,\rho) - u\|^2 + \frac{\beta}{2}\left\|N_u(u,\rho,\lambda)^\top - \lambda\right\|^2 + N(u,\rho,\lambda) - u^\top\lambda$$

is a suitable penalty function and that the update in (3) is a descent direction for L^a for a large enough symmetric positive definite preconditioner B. As a result, the one-shot iteration can be used together with an appropriate line search in a descent algorithm to find a stationary point of the augmented Lagrangian.

It can be shown, that the preconditioner B is strongly related to the Hessian $\nabla_{uu}L^a$. In practice it is not computed exactly but its inverse is approximated by means of a BFGS update. If one identifies H with the approximated inverse of B, the secant equation is given as $H_{k+1} r_k = \Delta\rho_k$ with $r_k := \nabla_\rho L^a(u_k, \rho_k + \Delta\rho_k, \lambda_k) - \nabla_\rho L^a(u_k,\rho_k,\lambda_k)$. It is important to apply this update only if the positive definiteness of H is maintained, which is guaranteed when using a line search to satisfy the second Wolfe condition. For reasons of efficiency we use a backtracking line search in the following and set $B = I$ when the curvature condition $r_k^T \Delta\rho_k > 0$ is not fulfilled, which is a common practice. We obtain

$$\nabla_\rho L^a = \alpha G_\rho^\top(G-u) + \beta N_{u\rho}^\top(N_u^\top - \lambda) + N_\rho^\top \tag{4}$$

with the reverse mode of algorithmic differentiation.

3.2 Challenges in Topology Optimization

There are several challenges inherent to topology optimization, among them the following:

- The constraints for the density have to be fulfilled at least for the optimal design. We propose to use a projection step, that can be applied separately from the updating scheme.
- The number of design variables is large which makes the approximation of the design space preconditioner very difficult. Additionally, the preconditioner itself or an additional preconditioning step has to serve as a filter to ensure mesh-independency and prevent checkerboard patterns. We will investigate on the potential of B and pursue two different approaches to prevent checkerboard patterns.
- For the structural analysis of nonlinear materials undergoing large displacement it can be advantegeous to apply the load in an incremental fashion making the underlying problem instationary. We do not consider instationary problems in this context. There exists a one-shot strategy for instationary PDE constraints.[9]
- As it is the case in nested approach, the found local minimum depends highly on the chosen starting value. This issue will not be treated in the following, but in future work strategies like the continuation method have to be adjusted to the one-shot framework.

3.3 Projection and Helmholtz Filtering

For fulfilling the volume constraint and the box constraints in 2 we make use of a projection method proposed by Tavakoli and Zhang.[10] Let

$$\mathscr{D} := \{\rho \in \mathbb{R}^n \ ;\ 1^\top \rho = f_v \cdot V_0,\ 0 \le \rho \le 1\}$$

be the feasible set if all additional constraints are incorporated in the Lagrangian and let $\bar{\rho}$ be the density after applying the one-shot update, then the projection of $\bar{\rho}$ into the feasible set is the unique minimizer of the box constrained Lagrangian for $0 \le z \le 1$

$$\mathscr{L}(z,\mu) := \frac{1}{2}\|z\|_2^2 - \bar{\rho}^\top z + \frac{1}{2}\|\bar{\rho}\|_2^2 + \mu\left(1^\top z - f_v \cdot V_0\right),$$

that can be found using a root finding method for μ. The projection step is applied as a last optimization step.

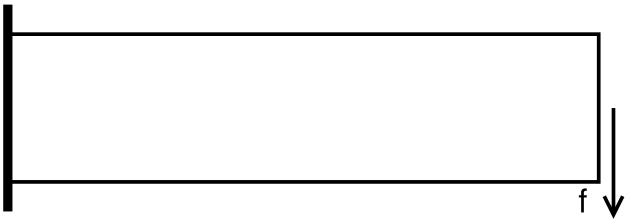

Figure 1: Numerical test case: Tip-loaded cantilever beam.

As a preconditioner of the design update we test the one-shot preconditioner based on the doubly augmented Lagrangian as explained in Section 3.1 and a preconditioner similar to the Helmholtz-type preconditioners[11] based on the design update using the doubly augmented Lagrangian. Let p present the unfiltered field and let $\tilde{p}$ present the filtered field. We obtain the filtered design field by solving the Helmholtz-type PDE with homogeneous Neumann boundary conditions

$$-r^2\nabla^2\tilde{p}+\tilde{p}=p$$
$$\frac{\partial\tilde{p}}{\partial n}=0,$$

where r is the filter radius. We apply the filtering for the reduced gradient of the doubly augmented Lagrangian given in (4), such that $p=-\nabla_\rho L^a$.

4 Numerical Example

We consider an example for stiffness optimization in a two-dimensional setting assuming plane stress. The solution procedure for the structural analysis is provided in the open-source framework SU2,[12,13] that also provides the basis for the discrete adjoint iteration based on algorithmic differentiation. The finite element analysis is performed using 4-node elements.

The material is modeled with a Young's modulus of 2GPa and a Poisson ratio of 0.4. We consider the minimization of end compliance for a tip-loaded cantilever beam presented in Figure 1. The results are presented for a load of 100N. The domain of 100 cm $\times$ 25 cm is discretized using 80 by 20 finite elements.

We make use of the volume projection method presented above to avoid the occurrence of checkerboard patterns. The volume fraction f_v is chosen to have a value of 0.4. Furthermore, we choose the factors $\alpha=2$ and $\beta=10^{-4}$ for the doubly augmented Lagrangian and a penalty factor $p=3$. It is common to choose α greater than β, but the parameter β found with the help of manual tuning is very small in comparison to one-shot shape optimization test cases. Using the one-shot preconditioner presented in Section 3.1 we obtain a design with grey areas, which represents densities between 0 and 1. Additionally, the convergence history shows a staircase profile which shows that the preconditioner tends to choose primal and dual convergence over design convergence and still needs tuning.

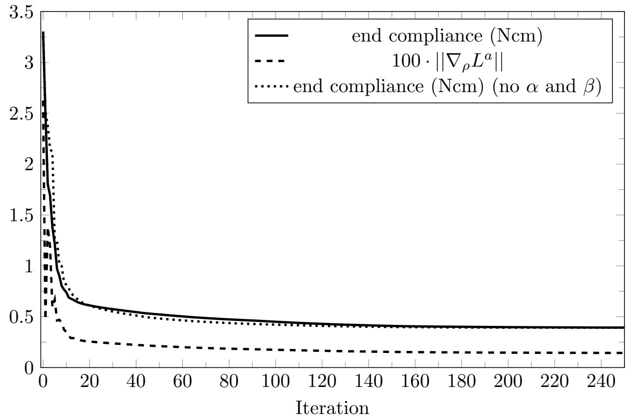

Figure 2: Optimization history for the minimization of end-compliance.

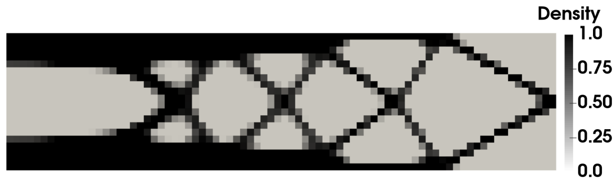

Figure 3: Optimized design after 250 iterations.

As grey areas are not admissible for the optimization, we do not stick to the classical approach.

Instead, in the following we will use the Helmholtz-type filtering method presented in Section 3.3 with a filter radius of $r=2$ and the same values for α and β. A backtracking line search using the reduced gradient of the doubly augmented Lagrangian is employed. The convergence history is shown in Figure 2 and the resulting optimized design is given in Figure 3.

The obtained design is a typical end-compliance design for a small load. The primal solution converges in 25 iterations. The used method needs around 200 outer iterations and 200 inner iterations to converge. As the material does not exhibit a highly nonlinear behavior under the given load, the method will also converge for $\alpha=0$ and $\beta=0$. The corresponding convergence history presented by the dotted line is very similar, but the method will need and additional number of around 150 inner iterations. This shows, that the use of the doubly augmented Lagrangian speeds up the convergence of the optimization.

5 Summary and Outlook

We have formulated challenges for one-shot topology optimization and have applied a one-shot approach based on Helmholtz filtering and a volume projection to a numerical test case. The method has proven to be feasible for the given topology optimization problem. For the conference we will present further results for nonlinear materials. As under the currently used load the material does not show the typical nonlinear behavior, we plan to increase the load or use different material properties. Especially, we will compare our results to classical topology optimization approaches. Further work will include the investigations on a suitable preconditioner. The long-term objective is to apply the presented approach to multiphysics real-world applications.

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