Topology Optimization of a Transient Thermo-Mechanical Problem using Material Penalization

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1. Abstract

Designing transient thermal mechanical systems is a challenging task. Material can have many different functions: it can provide heat capacity, heat conduction, mechanical stiffness or even function as an actuator. Topology optimization can provide the engineer with valuable insight on such a problem. One of the most popular topology optimization approaches is the density method. This method is applied to a transient thermal mechanical problem. In order to ensure manufacturability, penalization is applied to suppress intermediate densities in the final design. However, for transient thermal mechanical optimization problems, conventional penalization does not work for most objective functions. A new penalization method, material penalization, is presented that does suppress intermediate densities in the transient thermal mechanical domain. Each element is given its own unique set of penalization parameters which are optimized to maximize the objective function for a minimization problem. By reusing sensitivity information from the density variables, the additional computational cost is limited. **2. Keywords:** Topology optimization, Penalization, Manufacturability, Transient thermo-mechanical.

3. Introduction

In the density method, the usually discrete material placement problem is relaxed, allowing for intermediate element densities. The material properties of the elements are scaled with these densities. To ensure manufacturability and to allow for interpretation, however, the final design of a topology optimization (TO) should not contain intermediate densities. In order to achieve an intermediate density free, or black-and-white, design with the density method, the intermediate material is penalized. SIMP (Simplified Isotropic Material with Penalization) is a common approach, but in this paper RAMP (Rational Approximation of Material Properties) [1] is used because of its reported superior performance on thermo-elastic problems [2]. For stiffness optimizations, SIMP and RAMP penalization are able to result in a black-and-white design. However, for transient thermal mechanical (TM) problems, SIMP or RAMP penalization is often not sufficient to result in a black-and-white design. Because of the complex relationship between element density and objective in transient TM problems, intermediate densities are in some places more optimal than a void or completely filled element, even in absence of a volume constraint. SIMP and RAMP are not able to change this, which is also apparent in literature. Most transient TM topology optimizations that utilize the density approach contain intermediate densities ([3], [4]). This is also the case for steady-state TM optimization problems ([5], [6]).

Besides penalization, there are other methods to suppress intermediate densities. Grey penalization is a widely applied method. The objective function is augmented with a term, that increases when intermediate densities are present. However, determining the scaling of this grey penalization term w.r.t. the original objective is cumbersome. By choosing it too high, the design will end up in an inferior local minimum. Too low, and final design will still contain intermediate densities. Grey penalization has been used in, for example, in [6]. Nonetheless, it was not able to produce a black-and-white design for every design case. Other methods that are available are projection methods. This has been used in [4] as a post-processing step, where a threshold was set at 0.5. However, the thresholded design had a much lower performance, because there is no guarantee that a post processed design is still an optimum. Projection during the optimization, as proposed in [7] has, by the author's best knowledge, not yet been applied to transient TM problems. This might create an intermediate density free design without deteriorating the performance, however, in this study a different approach has been chosen.

In this paper an extension to the conventional penalization method is presented that is able to create a blackand-white design for transient TM problems. This is done by assigning individual penalization parameters to every element, which are included in the optimization with very limited extra computational cost. In the following section, Section 4, background on penalization in transient TM systems is given. In Section 5 the new penalization method is presented and the resulting topology optimization problem is stated in Section 6. Finally, the new penalization method is applied to a transient TM problem in Section 7.



Figure 1: Standard RAMP penalization for different penalization parameters.

4. Background on penalization in TM systems

In density-based topology optimization involving solid mechanics, the Young's modulus is interpolated with the element densities. With RAMP penalization, the interpolated Young's modulus of an element is defined as:

$$E^{*}(\boldsymbol{\rho}) = E_{min} + \frac{\boldsymbol{\rho}}{1 + q(1 - \boldsymbol{\rho})} (E_0 - E_{min}), \qquad (1)$$

where E^* indicates the interpolated Young's modulus, E_0 the Young's modulus of the original material and E_{min} denotes a lower bound added for numerical reasons, chosen a factor 10^{-6} lower than E_0 . ρ is the virtual element density and q the penalization parameter. The effect of q on the interpolation can be observed in Figure 1. It is apparent that if an intermediate value of the Young's modulus is optimal, penalization will not prevent the optimizer from utilizing this intermediate density since all the intermediate values of the Young's modulus are still available after penalization, only with different corresponding density values.

In transient TM problems, four material properties can be penalized: the Young's modulus E, the coefficient of thermal expansion (CTE) α , the heat capacity c and the heat conductivity k. In this study, instead of the CTE, the thermal stress coefficient (TSC) β is penalized, defined as $\beta = E\alpha$, as advised in [2]. Little research has been conducted on how to penalize the material properties, often they are all penalized with the same penalization factor. By the author's knowledge, the possibility of penalizing the material properties by different factors for TM problems is first mentioned in [8]: "In principle, the power p [the penalization parameter] could take different values for each physical property. However, for simplicity and to avoid having to choose multiple parameters, the same power is selected for all material interpolations.". The latter is common practice in TM optimizations. Gao and Zhang [2] explored the effect of different penalizations, but only on an optimization of a mechanical system with a given temperature rise. Outside of the TM field, some research has been done on the effect of different penalization parameters. For piezoelectric systems, [9] pose a set of rules for different penalization parameters. In [9], different penalization rules are found for different types of piezoelectric systems. The effect of different penalization parameters on a piezoelectric energy harvesting device under static and dynamic loading is investigated in [10]. They find that different sets of penalization parameters produce different layouts. Because these papers employ the electro-mechanical domain it is hard to draw quantitative conclusions for the TM domain. However, as in the electro-mechanical domain, it is likely that different penalization parameters have an influence on the final layout of TM optimization problems.

5. Material penalization

When all the material properties are penalized by the same factor, the material behavior at intermediate densities will be similar to the original material, except it will behave as if there is less material (for example, a less thick plate in 2D). However, when the penalization parameters are changed relative to each other, the material behavior at intermediate densities will change. Let q_c , q_k , q_E and q_β be the penalization parameters for the heat capacity, heat conduction, Young's modulus and TSC respectively. An element with, for example, $q_c = 0$, $q_k = 5$, $q_E = 0$ and $q_\beta = 0$, will have a much lower heat conduction in relation to the change of the other material properties at intermediate densities, because the conduction. On the other hand, an element with $q_c = 0$, $q_k = 0$, $q_E = 5$ and $q_\beta = 0$ has a much lower stiffness in relation to the other material properties. The intermediate material could represent a type of copper wire connection. Thus, by changing the penalization parameters relative to each other, a range of material behaviors can be generated.

The basic idea of the new penalization method, material penalization, is: find a set of penalization parameters, that gives the material at intermediate densities adverse behavior for the optimization problem. This will prevent the optimizer from using intermediate densities as design elements. For example, when high conduction is optimal,

the intermediate material should behave insulating. However, the adverse behavior is often not easily selected and depends on different aspects. At first, different objectives benefit from other sets of penalization parameters, as shown in [9]. It is, therefore, not possible to find a single set of penalization parameters that gives a black-and-white design for all transient TM TO problems. Secondly, within one problem, intermediate material that is adverse at one location can have favorable behavior at other locations. Thus, in order to ensure a black-and-white design, each element needs its *individual set of penalization parameters* that creates intermediate material that behaves adversely. Thirdly, as the design evolves during optimization, the function of an element may also evolve and therefore, the penalization parameters need to be altered. Concluding, because the adverse behavior depends on the design problem, element location and function, the penalization parameters of each element are included as design variables.

The penalization parameters are optimized simultaneously with the density variables, but the penalization parameters are optimized to maximize the objective function, whereas the density variables minimize the objective function. Maximizing will provide the set of penalization parameters for each element that gives intermediate material adverse behavior. Keep in mind that these parameters will not change the material properties of the final design, as it should consist of only black or white elements, which are not affected by the material penalization. The new optimization problem can be stated as a continuous min-max problem.

6. Topology optimization

6.1 Problem formulation

As stated, the focus of this study is on TM problems. Mechanical coupling to the thermal domain is neglected, and therefore a one-way coupled system of equations has to be solved to get the system response. Furthermore, the mechanical behavior is considered to be quasi-static compared to the thermal dynamics. The finite element method (FEM) is used to discretize the thermal and mechanical equilibrium equations in space. This gives the following initial value problem:

$$\mathbf{C}_{\mathbf{T}}\dot{\mathbf{T}}(t) + \mathbf{K}_{\mathbf{T}}\mathbf{T}(t) = \mathbf{Q}(t), \tag{2}$$

$$\mathbf{K}_{\mathbf{U}}\mathbf{u}(t) = \mathbf{A}\mathbf{T}(t),\tag{3}$$

$$\mathbf{T}(0) = \mathbf{T}_{ambient},\tag{4}$$

where C_T and K_T denote the heat capacitance- and conduction-matrix, respectively, T and Q indicate the nodal temperature- and the thermal loading-vector, K_U denotes the mechanical stiffness matrix, A denotes the thermalmechanical coupling matrix and u indicates the nodal displacement vector. These equations are solved by Euler backward time integration with an initial temperature field which is given in Equation 4. For the example in this study, the objective is only a function of displacements and time. The optimization problem can thus be written as:

$$\min_{\rho_i} \max_{s_{i,j}} \left(f = \int_0^{t_f} p(\mathbf{u}(t), t) dt \right), \tag{5}$$

subject to:
$$\mathbf{C}(\boldsymbol{\rho}_i, s_{i,j})\dot{\mathbf{T}} + \mathbf{K}_{\mathbf{T}}(\boldsymbol{\rho}_i, s_{i,j})\mathbf{T} = \mathbf{Q},$$
 (6)

$$\mathbf{K}_{\mathbf{U}}(\boldsymbol{\rho}_{i}, \boldsymbol{s}_{i,j})\mathbf{u} = \mathbf{A}(\boldsymbol{\rho}_{i}, \boldsymbol{s}_{i,j})\mathbf{T},\tag{7}$$

$$0 \le \rho_i \le 1,\tag{8}$$

$$-1 \le s_{i,j} \le 1, \qquad i \in [1,N], \qquad j \in [1,4],$$
(9)

where *f* is the objective, *p* a chosen function of the displacements and time, *N* the total number of elements and t_f the end time. ρ_i is the virtual density of element *i*, and $s_{i,j}$ is the penalization parameter design variable of property *j* and element *i*. Since there are four penalized material properties per element, there are 4*N* penalization parameters in total. Note that all the system matrices are dependent on the element densities ρ , as well as on the penalization parameters design variables *s*.

In order to normalize the penalization parameters and to smoothen the variation of the RAMP curve over the domain of s, a mapping has been applied that maps the domain of the design variables s onto the domain of the actual penalization parameters q which are input to the RAMP equation (Equation 1):

$$s^* = c_1 s^3 + c_2 s, \tag{10}$$

$$q = \begin{cases} s^* & s^* \ge 0\\ \frac{s^*}{1-s^*} & s^* < 0 \end{cases},$$
(11)

where the constants c_1 and c_2 are chosen as 13 and 2 respectively. Now, the design variables range from -1 to 1, which is handled better by the optimizer than the penalization parameters which range from -15/16 to 15. The



Figure 2: RAMP extended to also promote besides of penalizing properties. Design variable s varies from -1 to 1 and the RAMP curve changes roughly at the same rate over the complete range of s.

course of the RAMP curve for different values of the design variables s can be seen in Figure 2.

λ

6.2 Sensitivity analysis

Since the topology optimization contains many design variables and few constraints, adjoint sensitivities are used to calculate the sensitivities in order to save computational time compared to direct sensitivities [11]. By augmenting the objective with the governing equations (Equation 2 and 3), each multiplied with an adjoint variable, the following equations for the sensitivities can be derived [12]:

$$\frac{\mathrm{d}f}{\mathrm{d}v_i} = \int_0^{t_f} \left[\boldsymbol{\lambda}^T(t) \left(\frac{\mathrm{d}\mathbf{K}_{\mathbf{U}}}{\mathrm{d}v_i} \mathbf{u}(t) - \frac{\mathrm{d}\mathbf{A}}{\mathrm{d}v_i} \mathbf{T}(t) \right) + \boldsymbol{\mu}^T(t) \left(\frac{\mathrm{d}\mathbf{C}_{\mathbf{T}}}{\mathrm{d}v_i} \dot{\mathbf{T}}(t) + \frac{\mathrm{d}\mathbf{K}_{\mathbf{T}}}{\mathrm{d}v_i} \mathbf{T}(t) - \frac{\mathrm{d}\mathbf{Q}(t)}{\mathrm{d}v_i} \right) \right] \mathrm{d}t$$
(12)

$$^{T}(t)\mathbf{K}_{\mathbf{U}} = \frac{\mathrm{d}p(t)}{\mathrm{d}\mathbf{u}}$$
(13)

$$-\dot{\boldsymbol{\mu}}^{T}\mathbf{C}_{\mathbf{T}} + \boldsymbol{\mu}^{T}(t)\mathbf{K}_{\mathbf{T}} = \boldsymbol{\lambda}^{T}(t)\mathbf{A}$$
(14)

$$\boldsymbol{\mu}(t=t_f) = 0 \tag{15}$$

where λ and μ denote the adjoint vectors, independent of the design variables to which the objective is derived. Note that the numerator-layout notation has been used. The adjoint (Equation 14) is discretized in time using an Euler forward interpolation scheme. Since the adjoint problem is a terminal value problem (Equation 15), integration is done backwards in time, causing the Euler forward scheme to become implicit. In equation 12, the objective function is derived w.r.t. a yet to be defined parameter v_i . This can be both the element density as well as one of its penalization parameters. Note that for both cases the same adjoint variables can be used since no definition of v_i is needed in their calculation. This implies that the sensitivity information of the penalization parameters comes at little extra cost once the density sensitivities have been determined. Only the derivatives of the system matrices, which are known exactly, differ between the densities and the penalization parameters. The interpolated material property needs to be derived to either the density or the penalization parameter.

6.3 Optimization procedure

Linear programming with adaptive move limits is used as optimization algorithm. Every iteration the density variables are moved in the direction in which their derivatives w.r.t. the objective function is negative. Simultaneously, the penalization variables are moved in the direction in which their derivatives are positive, in order to maximize the objective function. The move limits determine the step size. The ratio between the size of the move limits of the density and penalization variables determines how fast the one can change with respect to the other. This has a large influence on the result. It was observed that when the density variables have much larger move limits than the penalization variables, the chance of ending up in an inferior local minimum is the lowest. However this also increases the number of iterations because the penalization variables change slowly due to their small move limits. Equal move limits for the penalization and density variables have been used as this already gave satisfactory results.

7. Transient TM demonstrator

In this section, the material penalization method presented in the previous sections will be applied on a transient TM case, as depicted in Figure 3. On the left and right side the domain is fixed, and ambient temperature is prescribed, which is also the initial temperature for the whole domain. The top and bottom side are thermally isolated. On the red elements a heat load is applied from t = 0. The objective is to minimize the thermal error from t = 30s to t = 60s. The thermal error is defined as: $|u_{obj} - 1.5 \cdot 10^{-3}|$, which means that a displacement of 1.5mm



Figure 3: Transient TM test case. Red elements are fixed, green elements are design variables. The heat load is applied equally on the red elements.



(a) Final design without penalization. (b) Final design with conventional penalization. (c) Final design with material penalization.

Figure 4: TO results for the transient TM case for different penalization settings.

is desired over the time frame of interest.

The solution without penalization is displayed in Figure 4a. The design shows a mechanism that pushes the area on which the heat load is applied upward, to reach the target displacement. Around the fixed domain there is a ring that provides heat capacity and slightly decreases the objective displacement when it expands. This complex design gives a clue for the engineer in what direction the final design can be made, but it leaves a lot undecided. No design for the suspension of the domain on which the heat load is applied can be deduced because it is suspended in intermediate densities. Adding conventional penalization does not improve the situation, as can be seen in Figure 4b. When material penalization is applied, it becomes much clearer what the final design should look like. This is displayed in Figure 4c. Now there are hardly any intermediate densities left. The remaining intermediate densities are in areas where for example a certain stiffness is required: around hinge points. These are areas to which the engineer should pay special attention, for example, when determining the exact required thickness.

This also shows that a black-and-white design is only achieved when there are competing material properties. On the hinge points, where intermediate densities are present, only the stiffness of the elements is dominant (and desires an intermediate value). When this is the case, material penalization will not be able to result into a black-and-white design.

8. Conclusion

In this research TO is applied to a transient TM problem. A new penalization method, material penalization, is presented for transient TM TO problems. Every element is given its unique set of penalization parameters which are optimized to maximize the objective function, where the overall goal is to minimize the objective function. Material penalization will not always be able to create a black-and-white design, as it needs counteracting material properties. However, when this is the case, it is shown that material penalization, unlike conventional penalization, is able to result in a manufacturable, intermediate density free, design for a complex transient TM problem.

Further investigation into the relative optimization speeds of the density and penalization variables and how this compares to the total number of iterations will be relevant in order to reduce the total number of iterations. Furthermore, when minimizing the penalization parameters instead of maximizing them, this method might be used to investigate which material properties (and thus material) are favourable at different locations of the design.

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10. References

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