Topology Optimization for Additive Manufacturing Involving High-Cycle Fatigue

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L-shaped beam with non-proportional loads, mass minimization problem subjected to a fatigue constraint.

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Preface

The work presented in this Licentiate thesis has been performed at the division of Solid Mechanics at Linköping University. The work was performed within the Centre for Additive Manufacturing-Metal (CAM²) financed by Sweden's Innovation Agency under grant agreement No 2016-05175.

Firstly, I would like to express my sincere gratitude to my main supervisor Professor Anders Klarbring and my co-supervisors Dr. Stefan Lindström, Dr. Carl-Johan Thore, and Dr. Bo Torstenfelt who have supported and guided me throughout the project with their patience, motivation and immense knowledge. Their continuous suggestions and encouragement helped me in all the time of research and writing of this thesis. I would also like to thank my colleagues at Linköping University for their support and having interesting work-related, as well as off-topic related, discussions.

Finally, I am deeply grateful to my family and my lovely wife Priya, for all their unconditional support and sacrifices they have made for my life in general.

Thank you!

Shyam Suresh

Linköping, May 2020

Abstract

Additive Manufacturing (AM) is gaining popularity in aerospace and automotive industries. This is a versatile manufacturing process, where highly complex structures are fabricated and together with topology optimization, a powerful design tool, it shares the property of providing a very large freedom in geometrical form. The main focus of this work is to introduce new developments of Topology Optimization (TO) for metal AM.

The thesis consists of two parts. The first part introduces background and theory, where TO and adjoint sensitivity analysis are described. Furthermore, methodology used to identify surface layer and high-cycle fatigue are introduced. In the second part, three papers are appended, where the first paper presents the treatment of surface layer effects, while the second and third papers provide high-cycle fatigue constraint formulations.

In Paper I, a TO method is introduced to account for surface layer effects, where different material properties are assigned to bulk and surface regions. In metal AM, the fabricated components in as-built surface conditions significantly affect mechanical properties, particularly fatigue properties. Furthermore, the components are generally in-homogeneous and have different microstructures in bulk regions compared to surface regions. We implement two density filters to account for surface effects, where the width of the surface layer is controlled by the second filter radius. 2-D and 3-D numerical examples are treated, where the structural stiffness is maximized for a limited mass.

For Papers II and III, a high-cycle fatigue constraint is implemented in TO. A continuous-time approach is used to predict fatigue-damage. The model uses a moving endurance surface and the development of damage occurs only if the stress state lies outside the endurance surface. The model is applicable not only for isotropic materials (Paper II) but also for transversely isotropic material properties (Paper III). It is capable of handling arbitrary load histories, including non-proportional loads. The anisotropic model is applicable for additive manufacturing processes, where transverse isotropic properties are manifested not only in constitutive elastic response but also in fatigue properties. Two optimization problems are solved: In the first problem the structural mass is minimized subject to a fatigue constraint while the second problem deals with stiffness maximization subjected to a fatigue constraint and mass constraint. Several numerical examples are tested with arbitrary load histories.

List of papers

In this thesis, the following papers have been included:

- I. S. Suresh, C.-J. Thore, B.Torstenfelt, A. Klarbring (2020). Topology optimization accounting for surface layer effects, *Submitted and revised*.
- II. S. Suresh, S. B. Lindström, C.-J. Thore, B.Torstenfelt, A. Klarbring (2019). Topology optimization using a continuous-time high-cycle fatigue model, *Published in Structural and Multidisciplinary Optimization* **61**, 1011-1025 (2020). <https://doi.org/10.1007/s00158-019-02400-w>
- III. S. Suresh, S. B. Lindström, C.-J. Thore, A. Klarbring (2020). Topology optimization for transversely isotropic materials with high-cycle fatigue as a constraint, *Submitted*.

The author's contribution

Anders Klarbring and Carl-Johan Thore have been responsible for writing and modelling with the author performing the optimizations in Paper I. The research, as well as the writing expressed in Papers II and III, has been performed primarily by the author.

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Part I

Background and Theory

Introduction

This thesis deals with developments of Topology Optimization (TO) methods for application to metal Additive Manufacturing (AM). AM offers the capability of manufacturing very complex component geometries, which can be the outcome from TO. This makes TO a good design tool for AM.

Figure 1 shows the holistic process for component fabrication using TO for AM. Starting with the initial part design with appropriate boundary conditions and loads, a lightweight design can be obtained through TO. During optimization, we should preferably consider AM-specific properties such as amount of support structures used, residual stresses, fatigue properties and anisotropic material properties. The optimized design is then converted into some computer aided design (CAD) format, and then possibly subjected to manual modifications. The final CAD part is then fabricated by an AM process.

Figure 1: Holistic process for fabrication of components based on topology optimization for additive manufacturing.

1.1 Topology optimization (TO)

TO is a type of structural optimization (Bendsoe and Sigmund, 2004) that offers conceptual design for lighter structures. This is a mathematical method that deals with optimal distribution of materials within a given design domain and ultimately strives for so-called black-and-white designs, in which structural members are identified as black regions and void regions as white regions. The goal of TO is to maximize the system performance for a given set of loads, boundary conditions and constraints.

In density-based TO, the design domain is discretized by the finite element (FE) method and each design variable is associated to a single FE. The design variable indicates whether the corresponding element contains the structural material or a hole, and during optimization the optimal positions of holes are determined. For a given set of loads and boundary condition, Figure 2 shows a typical black-and-white

design for the FE discretized space in which the structural stiffness is maximized for a limited volume.

Figure 2: A typical black-and-white (material and void) design

A traditional gradient-based TO workflow, shown in Figure 3, is used to obtain such optimized designs. The first step is to define a design domain, discretized by the FE method. A TO problem is formulated with an appropriate objective function and constraints for a given load and boundary conditions. The structural design is iterated in a loop until the convergence of objective function and satisfactory constraints are obtained. The FE analysis is done to compute the displacements, stresses etc. Sensitivity analysis forms the core of any gradient-based structural optimization. It involves finding the derivatives of the objective function and constraints to guide the updating of the design. The optimized design is obtained after fulfilling the convergence criteria.

Figure 3: A typical gradient-based optimization workflow

1.2 Additive manufacturing (AM)

AM is a fabrication process that uses a CAD three-dimensional model generated by TO to fabricate a structural component by adding material layer-by-layer. Compared to conventional manufacturing processes, AM can produce highly complex and lighter structures, and this form of manufacturing is gaining popularity in aerospace and automotive industries.

A very good introduction to AM and its techniques can be found in Gibson et al. (2015). One of the most commonly used AM techniques is Powder Bed Fusion

(PBF). Metal AM is treated in this work and commonly used materials are stainless steel 316L, titanium Ti6Al4V (or TA6V) alloy, Nickel-based super-alloys: Inconel 718, Inconel 625, and Hastelloy X.

Figure 4: AM generic process

The generic AM process is shown in Figure 4. This 8-step process starts with the drawing of a three-dimensional model by CAD. For AM machine readability, the CAD model is converted into a STL format. Using build techniques like PBF, the part is fabricated layer-wise and after fabrication the support structures are removed using conventional techniques. AM parts in as-built surface conditions have bad surface properties, hence post-surface treatments are required before they can be used.

In AM, several key properties such as support material, anisotropic material properties, fatigue properties must be considered. Support material in AM will increase the print time, the material cost and the resources to remove the support structures. The anisotropic properties in AM-fabricated components are introduced due to layer-wise generation which also affects the fatigue behaviour.

1.3 High-cycle fatigue (HCF)

In this work, we are concerned with high-cycle fatigue (HCF) due to periodic loads, multiaxial loads and non-proportional loads. HCF implies that the fatigue process predominantly happens due to elastic deformations with more than 10^4 cycles to failure.

Most HCF models are based on stress approaches. The classical multiaxial approaches like in Sines (1955), Cristofori et al. (2008) use stress invariants to predict fatigue-damage. However, the applicability of these models is limited in non-proportional loads especially for rotary stress states. Another stress approach is based on the critical plane criterion (Findley, 1959; Dang Van et al., 1982), where it is assumed that the maximal loaded material plane is decisive for fatigue development. Other HCF models use cycle-counting algorithms, like rainflow counting (Amzallag et al., 1994), and the fatigue-damage accumulation is based on the Palmgren-Miner rule. An alternative to these methods, is to integrate fatigue-damage for some whole

load history using some evolution equations constituting to what is here referred as continuous-time fatigue model. Such a fatigue model can be found in Ottosen et al. (2008).

Fatigue is the most common source behind failures of mechanical structures. It is therefore important to consider fatigue phenomena while designing the mechanical components and we use TO to implement HCF as a constraint. The problem is solved using the workflow shown in Figure 5.

Figure 5: Fatigue optimization workflow

1.4 Developments in TO for AM

Current and future developments in TO for AM have been thoroughly reviewed in Liu et al. (2018).

With overhang constraint in TO, the goal is to achieve self-supporting structures without additional support material. Leary et al. (2014) proposed a direct method where the topology of optimized designs is modified to account for AM. The methods by Langelaar (2016a,b) and Gaynor and Guest (2016) introduce density-filter and projection schemes to control the support material presence in the optimal structure.

Another important feature in AM is material anisotropy. AM-fabricated components have material anisotropy that generally cannot be totally avoided and thus, should be carefully addressed when designing AM parts. Anisotropy is introduced in two ways: The first way is through constitutive elastic properties and the second way is through directional strengths (stress criteria or fatigue strength). Anisotropy in constitutive response depends on the build direction. Ulu et al. (2015), Umetani and Schmidt (2013) and Alm Grundström (2017) studied the effects of build direction on structural performance in optimization. The second way in which anisotropy is introduced through directional strengths has not been studied in TO. In this work, we introduce directional strengths in the fatigue criterion in a TO problem.

1.5 Developments in TO accounting for HCF constraint

There are developments in TO which account for HCF as a constraint. Holmberg et al. (2014) introduces fatigue constraints in TO that are based on the highest

tensile principal stresses. Other examples of TO formulations with fatigue constraints are found in Jeong et al. (2018), who use cycle-counting techniques, in Collet et al. (2017), and in Oest and Lund (2017), where the fatigue prediction is done for a simplified damage model. However, the mentioned methods are restricted to proportional loads. The contribution from Zhang et al. (2019), gives a rare TO formulation with a fatigue constraint that handles non-proportional loads. It uses all classical techniques, including rainflow-counting, mean stress correction and the Palmgren-Miner rule.

1.6 Aims of the work

The mechanical properties of metal AM structures frequently show a pronounced member size dependency, which originate from surface or boundary effects. These effects are so far not modelled and incorporated in TO methods. In AM-fabricated components, another important design criterion that is not sufficiently considered is high-cycle fatigue (HCF) behaviour. The fatigue behaviour is heavily influenced by surface effects. Hence, in this thesis we develop the following:

1. **Paper I:** A TO method is developed that accounts for surface layer effects, where we assign different material properties to bulk and surface regions.
2. **Paper II:** We propose a new TO method that considers HCF as a constraint which can handle arbitrary load histories. The method is developed for isotropic materials (Suresh et al., 2020).
3. **Paper III:** An extension is made to Paper II, to account for anisotropic (in particular transversely isotropic) material properties in the HCF model.

Optimization formulation

We use a standard density-based TO method (Bendsoe and Sigmund, 2004; Christensen and Klarbring, 2009) in this work and this chapter provides a brief introduction to various concepts related to TO.

The elastic continuum problem defined on a design domain Ω , shown in Figure 6, is spatially discretized by the Finite Element (FE) Method (Hughes, 2000). A single design variable x_e is associated to a single FE and these variables are collected in a vector $\mathbf{x} = [x_1, x_2, \dots, x_{n_e}]^T$, with n_e as the total number of elements. As an integer representation, these ideally should take either one of the values 0 (void) or 1 (material).

Figure 6: Design domain Ω with load and boundary conditions.

2.1 Problem formulation

A typical TO problem reads:

$$(\mathbb{TO}_1) \begin{cases} \min_{\mathbf{x}} f_0(\mathbf{x}) \\ \text{s.t.} \begin{cases} f_c(\mathbf{x}) \leq \bar{f}_c, & c = 1, 2, \dots, n_c, \\ 0 \leq x_e \leq 1, & e = 1, 2, \dots, n_e, \end{cases} \end{cases}$$

where $f_0(\mathbf{x})$ is the objective function, while $f_c(\mathbf{x})$, with $c = 1, 2, \dots, n_c$, are constraint functions whose values are bounded by the constraint limits $\bar{f}_c$.

The displacement vector $\mathbf{u}$ is uniquely defined by the design variables $\mathbf{x}$, i.e. $\mathbf{u} = \mathbf{u}(\mathbf{x})$ and is calculated by standard FE analysis. This is called a nested approach, and is used in this work. Another possibility is the simultaneous approach, where

both displacements and design variables are treated as optimization variables and the equilibrium condition is added as an explicit constraint (Christensen and Klarbring, 2009).

We consider a steady-state response and for the given external load $\mathbf{F}$, the equilibrium equation is

$$\mathbf{K}(\mathbf{x})\mathbf{u} = \mathbf{F}, \quad (1)$$

where $\mathbf{K}(\mathbf{x})$ is the global stiffness matrix. The displacement vector $\mathbf{u}$ is then calculated from (1) as

$$\mathbf{u} = \mathbf{u}(\mathbf{x}) = \mathbf{K}^{-1}(\mathbf{x})\mathbf{F}.$$

When $x_e = 0$, the stiffness matrix $\mathbf{K}$ in (1) may become singular and to avoid such instances, we introduce a lower bound $\varepsilon > 0$ to the design variables, i.e., $x_e \geq \varepsilon$.

A very popular TO problem is to maximize stiffness for a limited mass or volume. The stiffness is quantified inversely in the form of compliance, i.e. $\mathbf{F}^T \mathbf{u}(\mathbf{x})$. Using the compliance measure and introducing the lower bound ε , the TO problem is written as

$$(\text{TO}_2) \quad \begin{cases} \min_{\mathbf{x}} \mathbf{F}^T \mathbf{u}(\mathbf{x}) \\ \text{s.t.} \quad \begin{cases} \sum_{e=1}^{n_e} v_e \rho_e(\mathbf{x}) \leq \bar{V}, \\ \varepsilon \leq x_e \leq 1, \end{cases} \end{cases} \quad e = 1, 2, \dots, n_e,$$

where v_e is the volume of element e and $\bar{V}$ is the upper bound on the total volume.

2.2 Design variable filter

Common numerical problems that appear in TO are checkerboards and mesh dependence (Sigmund and Petersson, 1998). Checkerboards refer to regions with alternate solid and void elements that are ordered in a checkerboard pattern, shown in Figure 8(a). Mesh dependence means that we obtain different optimal solutions with mesh refinement. We need filtering techniques to avoid mesh dependence and remove checkerboards, particularly for lower-order elements. Commonly used filtering technique is the density-based filter or design variable filter.

In this work, we use a linear design variable filter by Bruns and Tortorelli (2001), Bourdin (2001). We start with the continuous linear filter operator which takes the design variable x , defined in the design domain Ω , and returns the field ρ by the convolution

$$\rho(\tilde{\mathbf{x}}) = \int_{\Omega} x(\tilde{\mathbf{y}}) \psi(\tilde{\mathbf{x}}, \tilde{\mathbf{y}}) d\tilde{\mathbf{y}}, \quad (2)$$

where the integral kernel ψ is defined as

$$\psi(\tilde{\mathbf{x}}, \tilde{\mathbf{y}}) = \frac{\max(0, R - |\tilde{\mathbf{x}} - \tilde{\mathbf{y}}|)}{\int_{\Omega} \max(0, R - |\tilde{\mathbf{x}} - \tilde{\mathbf{z}}|) d\tilde{\mathbf{z}}}.$$

In the above expression, R is the filter radius, $\tilde{\mathbf{x}}$, $\tilde{\mathbf{y}}$ and $\tilde{\mathbf{z}}$ indicate positions in the design domain Ω , and $|\cdot|$ is the Euclidean norm. In Paper I, we use the continuous design filter as a starting point to calculate the gradients of a field ρ .

Figure 7: Filter for the design variable x_e , with R as the filter radius and $R_k = |\tilde{\mathbf{x}}_k^C - \tilde{\mathbf{x}}_e^C|$ is the Euclidean distance between centroids of elements e and k .

In the FE context, the discrete version of the density filter gives a relation between the design variable vector $\mathbf{x}$ and the filtered variables $\boldsymbol{\rho} = \boldsymbol{\rho}(\mathbf{x}) = [\rho_1(\mathbf{x}), \rho_2(\mathbf{x}), \dots, \rho_{n_e}(\mathbf{x})]^T$. Figure 7 shows an FE mesh with the design variable x_e . Here the filtered variable $\rho_e(\mathbf{x})$ is calculated as a weighted average of neighbouring design variables x_k . For the FE e , and $\tilde{\mathbf{x}}_k^C$, the centroid of element k , a neighbourhood is defined as

$$N_e = \{k : |\tilde{\mathbf{x}}_k^C - \tilde{\mathbf{x}}_e^C| \leq R\}.$$

The density filter relation is given as

$$\rho_e(\mathbf{x}) = \frac{\sum_{k \in N_e} w_{k,e} v_k x_k}{\sum_{k \in N_e} w_{k,e} v_k}, \quad (3)$$

where v_k is the volume of the element k and the weight $w_{k,e}$ is given by the linearly decaying (cone-shaped) function:

$$w_{k,e} = R - |\tilde{\mathbf{x}}_k^C - \tilde{\mathbf{x}}_e^C|.$$

Figure 8(b) provides an optimized result with filter, and thus no checkerboard patterns. A drawback with density filter is that there exist a transition region of intermediate design variable values at the boundaries. In other words, there is a grey region in between the black-and-white designs.

The filtered variables $\boldsymbol{\rho}(\mathbf{x})$ are used to define the structural stiffness and mass, hence are often referred as the physical densities.

Figure 8: Optimized model: (a) No filter and thus checkerboards; (b) Filter having filter radius R as 1.5 times element size and thus no checkerboards.

2.3 Penalization of stiffness and stresses

Stiffness penalization

To solve TO problems, we introduce some form of penalty to obtain discrete 0-1 valued solutions, i.e. black-and-white, design. A common penalization technique is Solid Isotropic Material with Penalization or SIMP method. This approach was first introduced by Bendsoe (1989) and later named as SIMP by Rozvany et al. (1992).

Using the SIMP method, the intermediate design variables are penalized for appropriate constraints and objectives (Rietz, 2001). The penalization function $\eta_K(\rho_e(\mathbf{x}))$ is inserted when the global stiffness matrix $\mathbf{K}(\boldsymbol{\rho}(\mathbf{x}))$ is assembled from the elemental stiffness matrices $\mathbf{K}_e$, as

$$\mathbf{K}(\boldsymbol{\rho}(\mathbf{x})) = \sum_{e=1}^{n_e} \eta_K(\rho_e(\mathbf{x})) \mathbf{K}_e. \quad (4)$$

The SIMP penalization is given as

$$\eta_K(\rho_e(\mathbf{x})) = (\rho_e(\mathbf{x}))^q, \quad (5)$$

where $q > 1$ is a penalization parameter, usually taken as $q = 3$.

Other penalization techniques such as the RAMP (Rational Approximation of Material Properties) approach by Stolpe and Svanberg (2001) exist. In this work we use the SIMP approach for stiffness penalization.

Stress penalization

In Papers II and III, we propose a TO method with HCF as a constraint. The fatigue estimation is based on stresses calculated from the FE analysis. Hence, we need to penalize stresses to avoid stress singularity phenomenon.

From the FE analysis and for the given global nodal displacements $\mathbf{u}(\mathbf{x})$, the stress vector $\hat{\boldsymbol{\sigma}}$ at a stress evaluation point is calculated as

$$\hat{\boldsymbol{\sigma}}(\mathbf{x}) = \hat{\boldsymbol{\sigma}}(\mathbf{x}, \mathbf{u}(\mathbf{x})) = \mathbf{E} \mathbf{B} \mathbf{u}(\mathbf{x}), \quad (6)$$

where $\mathbf{E}$ is the constitutive tensor in Voigt form and $\mathbf{B}$ is the strain-displacement matrix.

Following Bruggi (2008) and Holmberg et al. (2013), the penalization function $\eta_S(\rho_e(\mathbf{x}))$ of stresses is

$$\eta_S(\rho_e(\mathbf{x})) = (\rho_e(\mathbf{x}))^r, \quad (7)$$

where $r < q$ is a parameter introduced to avoid the stress singularity phenomenon and r is usually taken as 0.5.

To avoid artificial damage at the lower bound, we modify (7). Hence, in Papers II and III, we use

$$\eta_S(\rho_e(\mathbf{x})) = \left(\frac{\rho_e(\mathbf{x}) - \varepsilon}{1 - \varepsilon} \right)^r. \quad (8)$$

Figure 9 provides a comparison between (7) and (8). We notice that with (7), the penalization factor does not give zero values, when $\rho_e(\mathbf{x}) = \varepsilon$. However, with (8), the penalization factor gives exactly zero values when $\rho_e(\mathbf{x}) = \varepsilon$.

Figure 9: Stress penalization functions with $\eta_S = \rho_e^{0.5}$ ($\circ$ points), $\eta_S = ((\rho_e - \varepsilon)/(1 - \varepsilon))^{0.5}$ (solid line).

The penalized stress at an integration point reads

$$\boldsymbol{\sigma}(\mathbf{x}) = \eta_S(\rho_e(\mathbf{x})) \hat{\boldsymbol{\sigma}}(\mathbf{x}). \quad (9)$$

On substituting (8) in (9), we get exact zero stress values in voids, and as a result there is no artificial damage development. It also gives $\boldsymbol{\sigma} = \hat{\boldsymbol{\sigma}}$ when $\rho_e(\mathbf{x}) = 1$ as desired.

2.4 Domain extension approach

An important concept is the domain extension approach by Clausen and Andreassen (2017) which is shown in Figure 10(a). Here, the external boundaries are treated in

the same way as the internal boundaries. This is crucial for identifying the domain boundary which could be potentially affected by boundary effects. In this method, the design variables $\mathbf{x}$ are prescribed to the lower limit ε in the extended parts, which relate to free boundaries, while we solve the elasticity problem for the whole domain. The width of the grey region is usually taken as at-least one filter radius.

Figure 10: Domain extension approach: (a) The grey region indicate the extended regions where the design variables $\mathbf{x}$ are fixed to the lower bound value ε ; Optimized results: (b) Without domain extension approach, (c) With domain extension approach.

We implement the domain extension approach in Papers I and III. In Paper I, this approach accounts for surface effects at the domain boundary whereas in Paper III, we get a smoother profile at the boundary and avoid artificial structural reinforcement at the domain boundary. Figure 10(b), provides optimized result without using the domain extension approach, while Figure 10(c) provides an optimized design with the domain extension approach. We can notice that at the boundary of the optimized design, the profile obtained from the domain extension approach is smoother than the profile obtained without domain extension approach.

To utilize the domain extension in a TO problem, we can modify the problem (TO_2) as

$$(\mathbb{P}_1) \begin{cases} \min_{\mathbf{x}} \mathbf{F}^T \mathbf{u}(\mathbf{x}) \\ \text{s.t.} \begin{cases} \sum_{e=1}^{n_e} v_e \rho_e(\mathbf{x}) \leq \bar{V}, \\ \varepsilon \leq x_e \leq 1, & e = 1, 2, \dots, n_d, \\ x_e = \varepsilon, & e = n_d + 1, \dots, n_e, \end{cases} \end{cases}$$

where we assume that the last set of elements $n_e - n_d$ represent the region containing extended elements that take the design variable value $x_e = \varepsilon$.

Adjoint sensitivity analysis

Sensitivity analysis deals with finding the derivatives of the objective function and constraints with respect to the design variables. It forms the core of gradient-based TO methods. The calculation of derivatives in this thesis is done using the adjoint method (Haftka and Adelman, 1989; Tortorelli and Michaleris, 1994).

In this chapter, we present the adjoint method for a steady-state response and for a transient response, respectively.

3.1 Steady-state response

A general system response is defined as

$$J(\mathbf{x}) = J(\mathbf{x}, \mathbf{u}(\mathbf{x})). \quad (10)$$

The derivative of $J(\mathbf{x})$ with respect to a design variable x_k is

$$\frac{\partial J(\mathbf{x})}{\partial x_k} = \frac{\partial J(\mathbf{x})}{\partial x_k} + \frac{\partial J(\mathbf{x})}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x_k}. \quad (11)$$

The structural residual for the equilibrium equation (1) is defined as

$$\mathbf{R}(\mathbf{x}) = \mathbf{R}(\mathbf{x}, \mathbf{u}(\mathbf{x})) = \mathbf{0}. \quad (12)$$

Taking the derivative of (12) with respect to a design variable x_k , we get

$$\frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_k} = \frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_k} + \frac{\partial \mathbf{R}(\mathbf{x})}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x_k}. \quad (13)$$

As any system response should preserve the structural residuum (12), we multiply the equation by a Lagrange multiplier $\boldsymbol{\lambda}$, referred to as adjoint variable, to obtain the following augmented version of (10)

$$\hat{J}(\mathbf{x}) = J(\mathbf{x}) - \boldsymbol{\lambda}^T \mathbf{R}(\mathbf{x}). \quad (14)$$

Since the residuum $\mathbf{R}(\mathbf{x})$ is zero, the augmented function $\hat{J}(\mathbf{x}) = J(\mathbf{x})$. Taking the derivative of (14) and after substituting (11) and (13) we get

$$\frac{\partial \hat{J}(\mathbf{x})}{\partial x_k} = \frac{\partial J(\mathbf{x})}{\partial x_k} + \frac{\partial J(\mathbf{x})}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x_k} - \boldsymbol{\lambda}^T \left(\frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_k} + \frac{\partial \mathbf{R}(\mathbf{x})}{\partial \mathbf{u}} \frac{\partial \mathbf{u}}{\partial x_k} \right).$$

Rearranging the terms we get

$$\frac{\partial J(\mathbf{x})}{\partial x_k} = \frac{\partial J(\mathbf{x})}{\partial x_k} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_k} + \left(\frac{\partial J(\mathbf{x})}{\partial \mathbf{u}}^T - \boldsymbol{\lambda}^T \frac{\partial \mathbf{R}(\mathbf{x})}{\partial \mathbf{u}} \right) \frac{\partial \mathbf{u}}{\partial x_k}.$$

Since the adjoint variable $\boldsymbol{\lambda}$ is arbitrary, computing the derivatives of the state variables can be avoided by choosing $\boldsymbol{\lambda}$ such that the following adjoint system is satisfied:

$$\frac{\partial \mathbf{R}(\mathbf{x})}{\partial \mathbf{u}}^T \boldsymbol{\lambda} = \frac{\partial J(\mathbf{x})}{\partial \mathbf{u}}. \quad (15)$$

The adjoint variable $\boldsymbol{\lambda}$ is obtained from (15), and the final sensitivity expression is

$$\frac{\partial J(\mathbf{x})}{\partial x_k} = \frac{\partial J(\mathbf{x})}{\partial x_k} - \boldsymbol{\lambda}^T \frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_k}.$$

3.2 Transient (Time-dependent) response

For a transient response, we follow the adjoint sensitivity method from Panagiotis et al. (1994). For such a response, we not only discretize in space (by the FE method) but also in time. The time domain $[0, T]$ is divided into a finite number of time steps of equal length Δt , i.e. $t_i = i\Delta t$, with $i = 0, 1, 2, \dots, N$. The fatigue model presented in Chapter 5 has a state variable $\mathbf{v}$. We therefore consider a model with two state variables $\tilde{\mathbf{u}}$ and $\mathbf{v}$ as a function of time t , where $\mathbf{v}$ is governed by a system of discretized ordinary differential equations (ODEs).

For each time step i , the residuals $\mathbf{R}(\mathbf{x})|_i$ and $\mathbf{H}(\mathbf{x})|_i$, with $|_i$ denoting function evaluation at time step i , are expressed as

$$\mathbf{R}(\mathbf{x})|_i = \mathbf{R}(\mathbf{x}, \tilde{\mathbf{u}}_i(\mathbf{x}), \mathbf{v}_i(\mathbf{x})) = \mathbf{0}, \quad (16)$$

$$\mathbf{H}(\mathbf{x})|_i = \mathbf{H}(\mathbf{x}, \tilde{\mathbf{u}}_i(\mathbf{x}), \tilde{\mathbf{u}}_{i-1}(\mathbf{x}), \mathbf{v}_i(\mathbf{x}), \mathbf{v}_{i-1}(\mathbf{x})) = \mathbf{0}. \quad (17)$$

The residual $\mathbf{H}(\mathbf{x})|_i$ in (17) is developed from the discrete version of the ODEs. A general system response, G can be expressed as a function of the design variables $\mathbf{x}$ and the field variables $\tilde{\mathbf{u}}$ and $\mathbf{v}$, i.e.

$$G(\mathbf{x}) = G(\mathbf{x}, \tilde{\mathbf{u}}_1(\mathbf{x}), \tilde{\mathbf{u}}_2(\mathbf{x}), \dots, \tilde{\mathbf{u}}_N(\mathbf{x}), \mathbf{v}_1(\mathbf{x}), \mathbf{v}_2(\mathbf{x}), \dots, \mathbf{v}_N(\mathbf{x})). \quad (18)$$

The sensitivity of $G(\mathbf{x})$ with respect to a design variable x_j is

$$\frac{\partial G(\mathbf{x})}{\partial x_j} = \frac{\partial G}{\partial x_j} + \sum_{i=1}^N \frac{\partial G}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \sum_{i=1}^N \frac{\partial G}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j}. \quad (19)$$

Taking the derivative of $\mathbf{R}(\mathbf{x})|_i$ from (16) with respect to design variable x_j , we get

$$\frac{\partial \mathbf{R}(\mathbf{x})}{\partial x_j}|_i = \frac{\partial \mathbf{R}}{\partial x_j}|_i + \frac{\partial \mathbf{R}}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \frac{\partial \mathbf{R}}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j}. \quad (20)$$

Similarly, the derivative of $\mathbf{H}(\mathbf{x})|_i$ from (17) with respect to design variable x_j is

$$\frac{\partial \mathbf{H}(\mathbf{x})}{\partial x_j}|_i = \frac{\partial \mathbf{H}|_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_{i-1}} \frac{\partial \tilde{\mathbf{u}}_{i-1}}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_{i-1}} \frac{\partial \mathbf{v}_{i-1}}{\partial x_j}. \quad (21)$$

As any system response should preserve structural residuum, (16) and (17), we multiply these equations by the Lagrange multipliers λ_i and γ_i , to obtain the following augmented version of (18):

$$G(\mathbf{x}) = G(\mathbf{x}) - \sum_{i=1}^N \lambda_i^T \mathbf{R}(\mathbf{x})|_i - \sum_{i=1}^N \gamma_i^T \mathbf{H}(\mathbf{x})|_i. \quad (22)$$

Substituting (19), (20) and (21) into the derivative of (22) with respect to design variable x_j , we get

$$\begin{aligned} \frac{\partial G(\mathbf{x})}{\partial x_j} &= \frac{\partial G}{\partial x_j} + \sum_{i=1}^N \frac{\partial G}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \sum_{i=1}^N \frac{\partial G}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j} \\ &\quad - \sum_{i=1}^N \lambda_i^T \left[\frac{\partial \mathbf{R}|_i}{\partial x_j} + \frac{\partial \mathbf{R}|_i}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \frac{\partial \mathbf{R}|_i}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j} \right] \\ &\quad - \sum_{i=1}^N \gamma_i^T \left[\frac{\partial \mathbf{H}|_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_i} \frac{\partial \tilde{\mathbf{u}}_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_{i-1}} \frac{\partial \tilde{\mathbf{u}}_{i-1}}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_i} \frac{\partial \mathbf{v}_i}{\partial x_j} + \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_{i-1}} \frac{\partial \mathbf{v}_{i-1}}{\partial x_j} \right]. \end{aligned}$$

Rearranging the terms, we get

$$\begin{aligned} \frac{\partial G(\mathbf{x})}{\partial x_j} &= \frac{\partial G}{\partial x_j} - \sum_{i=1}^N \lambda_i^T \frac{\partial \mathbf{R}|_i}{\partial x_j} - \sum_{i=1}^N \gamma_i^T \frac{\partial \mathbf{H}|_i}{\partial x_j} - \underbrace{\left[\lambda_N^T \frac{\partial \mathbf{R}|_N}{\partial \tilde{\mathbf{u}}_N} + \gamma_N^T \frac{\partial \mathbf{H}|_N}{\partial \tilde{\mathbf{u}}_N} - \frac{\partial G}{\partial \tilde{\mathbf{u}}_N} \right]}_{=0} \frac{\partial \tilde{\mathbf{u}}_N}{\partial x_j} \\ &\quad - \underbrace{\left[\lambda_N^T \frac{\partial \mathbf{R}|_N}{\partial \mathbf{v}_N} + \gamma_N^T \frac{\partial \mathbf{H}|_N}{\partial \mathbf{v}_N} - \frac{\partial G}{\partial \mathbf{v}_N} \right]}_{=0} \frac{\partial \mathbf{v}_N}{\partial x_j} \\ &\quad - \sum_{i=2}^N \underbrace{\left[\lambda_{i-1}^T \frac{\partial \mathbf{R}|_{i-1}}{\partial \tilde{\mathbf{u}}_{i-1}} + \gamma_{i-1}^T \frac{\partial \mathbf{H}|_{i-1}}{\partial \tilde{\mathbf{u}}_{i-1}} + \gamma_i^T \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_{i-1}} - \frac{\partial G}{\partial \tilde{\mathbf{u}}_{i-1}} \right]}_{=0} \frac{\partial \tilde{\mathbf{u}}_{i-1}}{\partial x_j} \\ &\quad - \sum_{i=2}^N \underbrace{\left[\lambda_{i-1}^T \frac{\partial \mathbf{R}|_{i-1}}{\partial \mathbf{v}_{i-1}} + \gamma_{i-1}^T \frac{\partial \mathbf{H}|_{i-1}}{\partial \mathbf{v}_{i-1}} + \gamma_i^T \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_{i-1}} - \frac{\partial G}{\partial \mathbf{v}_{i-1}} \right]}_{=0} \frac{\partial \mathbf{v}_{i-1}}{\partial x_j} \\ &\quad - \underbrace{\gamma_1^T \frac{\partial \mathbf{H}|_1}{\partial \tilde{\mathbf{u}}_0}}_{=0} \frac{\partial \tilde{\mathbf{u}}_0}{\partial x_j} - \underbrace{\gamma_1^T \frac{\partial \mathbf{H}|_1}{\partial \mathbf{v}_0}}_{=0} \frac{\partial \mathbf{v}_0}{\partial x_j}, \end{aligned}$$

Since the adjoint variables are arbitrary, the derivatives of the state variables with respect to design variables can be eliminated if the following discrete terminal value problems are satisfied:

$$\begin{bmatrix} \frac{\partial \mathbf{R}|_N}{\partial \tilde{\mathbf{u}}_N}^T & \frac{\partial \mathbf{H}|_N}{\partial \tilde{\mathbf{u}}_N}^T \\ \frac{\partial \mathbf{R}|_N}{\partial \mathbf{v}_N}^T & \frac{\partial \mathbf{H}|_N}{\partial \mathbf{v}_N}^T \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_N \\ \boldsymbol{\gamma}_N \end{bmatrix} = \begin{bmatrix} \frac{\partial G}{\partial \tilde{\mathbf{u}}_N} \\ \frac{\partial G}{\partial \mathbf{v}_N} \end{bmatrix}, \quad (23)$$

$$\begin{bmatrix} \frac{\partial \mathbf{R}|_{i-1}}{\partial \tilde{\mathbf{u}}_{i-1}}^T & \frac{\partial \mathbf{H}|_{i-1}}{\partial \tilde{\mathbf{u}}_{i-1}}^T \\ \frac{\partial \mathbf{R}|_{i-1}}{\partial \mathbf{v}_{i-1}}^T & \frac{\partial \mathbf{H}|_{i-1}}{\partial \mathbf{v}_{i-1}}^T \end{bmatrix} \begin{bmatrix} \boldsymbol{\lambda}_{i-1} \\ \boldsymbol{\gamma}_{i-1} \end{bmatrix} = - \begin{bmatrix} \frac{\partial \mathbf{H}|_i}{\partial \tilde{\mathbf{u}}_{i-1}}^T \\ \frac{\partial \mathbf{H}|_i}{\partial \mathbf{v}_{i-1}}^T \end{bmatrix} \boldsymbol{\gamma}_i + \begin{bmatrix} \frac{\partial G}{\partial \tilde{\mathbf{u}}_{i-1}} \\ \frac{\partial G}{\partial \mathbf{v}_{i-1}} \end{bmatrix}, \quad (24)$$

where $i = N, N-1, \dots, 2$. The final sensitivity expression is

$$\frac{\partial G(\mathbf{x})}{\partial x_j} = \frac{\partial G}{\partial x_j} - \sum_{i=1}^N \boldsymbol{\lambda}_i^T \frac{\partial \mathbf{R}|_i}{\partial x_j} - \sum_{i=1}^N \boldsymbol{\gamma}_i^T \frac{\partial \mathbf{H}|_i}{\partial x_j}. \quad (25)$$

Surface layer effects

AM metallic parts are commonly fabricated via PBF process. The PBF process includes the following printing techniques: Direct metal laser sintering (DMLS), Electron beam melting (EBM), Selective heat sintering (SHS), Selective laser melting (SLM) and Selective laser sintering (SLS). It uses either a laser or an electron-beam to melt and fuse the powder into a part.

Several process parameters, such as laser power, scanning speed and layer thickness, could influence the material microstructure and thus the mechanical behaviour. Therefore, in this chapter, a brief review of important factors that affect the mechanical properties of AM-fabricated components, are presented. One of the major factors that is considered is surface roughness. Hence, in this chapter, we incorporate surface effects in a TO method where different material properties are assigned to bulk and surface regions.

4.1 Factors to consider in metal AM design

Mechanical properties such as strength, structural performance, and fatigue behaviour must be considered while designing AM-fabricated parts (Molaei and Fatemi, 2018). There are several factors, including build direction, surface roughness, residual stresses, multiaxial stress states and fabrication process parameters that significantly influence the mechanical properties.

The build direction of AM metallic parts can have a significant influence on the material anisotropy. The layer-wise generation in metal AM parts, induces strong directional dependencies. Kumara et al. (2018) modelled anisotropic elastic properties in AM alloy 718 made by EBM. It is found that the Young's modulus is lowest in the build direction and the plane perpendicular to it has isotropic properties. It is thus concluded that the material properties closely resemble transversely isotropic properties.

Several studies confirmed that fatigue properties are influenced by build orientation. For example, Yadollahi et al. (2017) showed that for the AM built 17-4 PH stainless steel specimens built by the SLM process have higher fatigue strength when the specimen is horizontally built compared to a vertically built specimen. However, another example by Qiu et al. (2013), shows a higher fatigue strength for the vertically AM built Ti6Al4V specimens as compared to the horizontally built specimens.

Surface effects in metal AM parts also influences mechanical behaviour. The

mechanical properties, in particular fatigue properties, of Ti6Al4V AM specimens built by EBM and SLM processes are studied by Molaei and Fatemi (2018) and Kahlin et al. (2017). AM components used in as-built surface condition (without any post surface treatments) will have significantly worse fatigue-life compared to a post-treated surface finished AM part. With good surface finish, the fatigue-life in these components is greatly improved.

Another major concern in AM parts is the variation in the microstructure and the produced defects, which arise due to the fabrication process. Balachandramurthi et al. (2019) studied the microstructural influence on fatigue properties of AM alloy 718 fabricated components. It is found that the bulk region has strong directional properties, resulting in anisotropic behaviour, while at the surface region, the material properties are close to isotropic.

4.2 Material interpolation using density filter

Paper I introduces a methodology for accounting of surface effects in TO problem with help of linear density filters. Here, three density-like field variables are introduced, namely

- The optimization variable (design variable) x .
- The physical density ρ , obtained from x by standard linear filtering with filter radius R , shown in Chapter 2.
- The surface layer identifier ρ_S , also obtained from x by standard linear filtering, but with a larger filter radius $R_S \geq R$.

Schematic illustrations of the density-like field variables are shown in Figure 11. From the optimized design shown in Figure 11, the optimization variable x takes value one (black representing structural members) for the length AB and the value zero (white representing void) outside this length. Both the physical density variable ρ and the surface layer identifier ρ_S are obtained from x by linear filtering. Since, a larger filter radius ($R_S \geq R$) is taken for ρ_S , when compared to ρ , there would be lot of intermediate density values closer to the boundary (A and B). Taking the Euclidean norm of the gradient of ρ_S would lead to non-zero positive values around domain boundary, while the value of gradient takes zero values when moved away from the boundary. Using the Heaviside function H , these non-zero gradient values become one around the boundary and this function plays a key role in interpolating the material properties.

In Paper I, we study two cases: In the first case, we use isotropic material properties for both bulk and surface regions, but different Young's moduli in the bulk E_B and in the surface layer E_S are considered. The interpolation of Young's modulus, using SIMP for the shape density, is then

$$E = \rho^q (H(|\nabla \rho_S(x)|^2) E_S + (1 - H(|\nabla \rho_S(x)|^2)) E_B), \quad (26)$$

where ∇ is the gradient operator. The Heaviside function H takes the value zero in the bulk of the structure and the value one close to the boundary.

Figure 11: Two linear filter operations, with different filter radii R and R_S , $R \leq R_S$, are applied to a zero-one-valued optimization variable x , producing ρ and ρ_S .

In the second case we interpolate between transversely isotropic material in the bulk, represented by a matrix $\mathbf{E}_B$ and isotropic material in the surface layer, represented by a matrix $\mathbf{E}_S$. Expression (26) is then replaced by

$$\mathbf{E} = \rho^q (H(|\nabla \rho_S(x)|^2) \mathbf{E}_S + (1 - H(|\nabla \rho_S(x)|^2)) \mathbf{E}_B). \quad (27)$$

The precise form of the material matrix $\mathbf{E}$ for both isotropic and transversely isotropic material is given in Paper I. In Chapter 2, the continuous form of the density filter is given in (2). With this as a starting point, a detailed derivation of the gradient $\nabla \rho_S$ is given in Paper I.

4.3 Formulation of optimization problem accounting for surface effects

There are previously developed TO methods for coated structures, where the coating material is assigned higher stiffness in the surface region than the bulk material. For example, the density-based methods in Clausen et al. (2015), Yoon and Yi (2019) and a level-set method in Wang and Kang (2018) identify boundary regions and assign coating material properties. However, for AM components in as-built surface conditions, the material in surface regions will have lower stiffness (converse of the coated material) than the bulk material.

Using the material interpolation schemes from the previous section, we formulate the stiffness matrix accordingly. Firstly, for the pure isotropic case, the stiffness matrix is written as

$$\mathbf{K}(\mathbf{x}) = \sum_{e=1}^{n_e} \mathbf{K}_e(\mathbf{x}) = \sum_{e=1}^{n_e} E_e(\mathbf{x}) \mathbf{K}_e^I, \quad (28)$$

where $\mathbf{K}_e^I$ is elemental stiffness matrix for unit Young's modulus and E_e is defined in (26). Similarly, for the second case, the stiffness matrix is written as

$$\mathbf{K}(\mathbf{x}) = \sum_{e=1}^{n_e} \rho_e^q \left(H_e(|\nabla \rho_S(x)|^2) \mathbf{K}_{S,e} + (1 - H_e(|\nabla \rho_S(x)|^2)) \mathbf{K}_{B,e} \right), \quad (29)$$

where $\mathbf{K}_{S,e}$ and $\mathbf{K}_{B,e}$ are the elemental stiffness matrices at the surface and bulk material, respectively that are formulated from material matrices $\mathbf{E}_S$ and $\mathbf{E}_B$. The TO problem ($\mathbb{P}_1$) is solved in Paper I, where the stiffness is maximized for a limited volume. The domain extension approach from Chapter 2 is used in the problem ($\mathbb{P}_1$) as this is important for identification of boundary regions in the boundaries of the design domain.

The problem ($\mathbb{P}_1$) is solved for two cases using the Method of Moving Asymptotes (MMA) (Svanberg, 1987). The sensitivity of the objective function measured in terms of compliance is calculated by the adjoint method by following the procedure from Chapter 3.

4.4 Results and discussion

The proposed method is implemented in the in-house finite element program TRINITAS (Torstenfelt B., 2012). Several numerical results (for both cases) are tested, which include 2D and 3D examples, and are shown in Paper I.

A cantilever beam, shown in Figure 12, with $L = 200$ mm is studied for the isotropic case. The model is discretized by 200×120 bi-linear quadrilateral plane stress elements with thickness of 1mm. The beam is clamped at the left end and a static load $F = 150$ N is applied at the other end. The grey regions indicate elements that are part of domain extension.

Figure 12: Geometry of the 2D cantilever beam

The problem ($\mathbb{P}_1$) is solved with the maximum bound on the volume set as $\bar{V} = 0.4V_0$, taking V_0 as the original volume. The filter radius for the shape density is taken as $R = 1.2$ mm, while the second filter radius for identifying the surface layer thickness is taken as $R_S = 3.2$ mm.

Figure 13 provides optimization results. The first row provides the topology of the optimized design while the second row shows the material distribution within

Figure 13: Optimization result for the cantilever beam with isotropic material properties in both bulk and surface layer. The first row provides the topology of the optimized design and the second row shows the material distribution within the structure, with E_B (red) and E_S (green) being the Young's modulus in the respective regions.

the structure, with $E_B = 210$ GPa in red colour and $E_S = 105$ GPa in green colour. For comparison, the standard optimized problem with no surface layer is shown in the upper left corner. In Paper I, the effect of varying the filter radius R_S , implying different surface layer thickness, is studied. It is evident that for a thicker surface layer, the topology of the optimized model is simpler.

Continuous-time fatigue model

As seen in Chapter 4, the mechanical properties in metal AM, particularly fatigue properties are influenced by build directions, material anisotropy and surface effects. Thus, it is important to consider these influences when designing AM-fabricated components.

We are concerned with HCF due to periodic loads, multiaxial loads and non-proportional loads. We incorporate the continuous-time HCF model by Ottosen et al. (2008), Holopainen et al. (2016) in a TO problem. This evolution-based model integrates the fatigue-damage for the whole load history without use of any cycle-counting algorithm. The model is capable of handling arbitrary load histories, including non-proportional loads. The method is developed for isotropic materials (Paper II) and also extended for transversely isotropic materials (Paper III).

The flexibility of the model has led to further developments. For example, Brighenti et al. (2012) studied the assessment of fatigue for complex multiaxial load histories. Another example can be found in Ottosen et al. (2018), where the multiaxial fatigue criterion considers stress gradient effects in critical regions like holes and notches. Furthermore, the validity range and the computational acceleration of the model are investigated in Lindström et al. (2020).

5.1 Theory

We are concerned with HCF, which means that the fatigue-damage neither influences the geometry nor the material properties. For each design, the stress evolution $\boldsymbol{\sigma}(t)$, with t belonging to the time interval $[0, T]$, is considered as given in the fatigue analysis.

The HCF model is based on the concept of an endurance surface $\{\boldsymbol{\sigma} | \beta(\boldsymbol{\sigma}, \boldsymbol{\alpha}) = 0\}$, with $\boldsymbol{\alpha}$ as the back-stress tensor and β as the endurance function. It is assumed that the development of fatigue-damage only occurs if the stress-state lies outside the endurance surface, i.e. $\beta > 0$, and the endurance function is increasing, i.e. $\dot{\beta} > 0$, where a superposed dot indicates the time derivative of the function.

The rate-of-change of the back-stress tensor $\boldsymbol{\alpha}$ and the fatigue-damage D are given as

$$\dot{\boldsymbol{\alpha}} = C(\mathbf{s} - \boldsymbol{\alpha})H(\beta)H(\dot{\beta})\dot{\beta}, \quad \boldsymbol{\alpha}(0) = \mathbf{0}, \quad (30)$$

$$\dot{D} = K \exp(L\beta)H(\beta)H(\dot{\beta})\dot{\beta}, \quad D(0) = 0, \quad (31)$$

where $C > 0$, $K > 0$ and $L > 0$ are material parameters, $\mathbf{s} = \boldsymbol{\sigma} - \frac{1}{3}\text{tr}(\boldsymbol{\sigma})\mathbf{I}$ is the deviatoric stress, with $\text{tr}(\cdot)$ being the trace of the tensor and $\mathbf{I}$ being the second-order identity tensor. The formulations of the endurance function and its rate are given for transversely isotropic material properties in the next section. However, it is possible to specialize the model for isotropic materials.

5.2 Transversely-isotropic HCF model

The fatigue model in Holopainen et al. (2016) considers transversely isotropic material properties and the overview of the model is given in Paper III. A unit vector $\mathbf{m}$ in the longitudinal (build) direction is defined and we write the structural tensor as $\mathbf{M} = \mathbf{m} \otimes \mathbf{m}$.

The idea of the transversely-isotropic HCF model is to split the stress tensor into longitudinal $\boldsymbol{\sigma}_{\parallel}$ and transverse $\boldsymbol{\sigma}_{\perp}$ stress tensors, i.e. $\boldsymbol{\sigma} = \boldsymbol{\sigma}_{\parallel} + \boldsymbol{\sigma}_{\perp}$. The transverse component $\boldsymbol{\sigma}_{\perp}$ is obtained using the projection tensor $\mathbf{P} = \mathbf{I} - \mathbf{M}$, as $\boldsymbol{\sigma}_{\perp} = \mathbf{P}\boldsymbol{\sigma}\mathbf{P}$.

To formulate the endurance function, we introduce four invariants: $I_1 = \text{tr}(\boldsymbol{\sigma})$, $I_2 = \frac{1}{2}\text{tr}(\boldsymbol{\sigma}^2)$, $I_4 = \text{tr}(\boldsymbol{\sigma}\mathbf{M})$ and $I_5 = \text{tr}(\boldsymbol{\sigma}^2\mathbf{M})$. The endurance function is then written as

$$\beta(\boldsymbol{\sigma}, \boldsymbol{\alpha}) = \frac{1}{S_{\perp}} [\bar{\sigma} + A_{\parallel}\text{tr}(\boldsymbol{\sigma}_{\parallel}) + A_{\perp}\text{tr}(\boldsymbol{\sigma}_{\perp}) - ((1 - \xi(\boldsymbol{\sigma}))S_{\perp} + \xi(\boldsymbol{\sigma})S_{\parallel})], \quad (32)$$

where $S_{\parallel} > 0$ and $S_{\perp} > 0$ are the endurance stresses, and $A_{\parallel} > 0$ and $A_{\perp} > 0$ are material parameters in the corresponding directions. It can be shown that $\text{tr}(\boldsymbol{\sigma}_{\parallel}) = I_4$ and $\text{tr}(\boldsymbol{\sigma}_{\perp}) = I_1 - I_4$. The effective stress $\bar{\sigma}$ is obtained by

$$\bar{\sigma} = \sqrt{\frac{3}{2}(\mathbf{s} - \boldsymbol{\alpha}) : (\mathbf{s} - \boldsymbol{\alpha})}.$$

The scalar ξ in (32) is the stress ratio, given as

$$\xi(\boldsymbol{\sigma}) = \frac{\boldsymbol{\sigma}_{\parallel} : \boldsymbol{\sigma}_{\parallel}}{\boldsymbol{\sigma} : \boldsymbol{\sigma}} = \frac{2I_5 - I_4^2}{2I_2}. \quad (33)$$

Using (33) and (30), the rate-of-change of (32) is

$$\begin{aligned} \dot{\beta}(\boldsymbol{\sigma}, \dot{\boldsymbol{\sigma}}, \boldsymbol{\alpha}) = & \frac{1}{S_{\perp} + H(\beta)C\bar{\sigma}} \left[\frac{3}{2} \frac{(\mathbf{s} - \boldsymbol{\alpha})}{\bar{\sigma}} + (A_{\parallel} - A_{\perp})\mathbf{M} + A_{\perp}\mathbf{I} \right. \\ & \left. - \frac{(S_{\parallel} - S_{\perp})}{2I_2^2} (I_2(4\boldsymbol{\sigma} - 2I_4\mathbf{I})\mathbf{M} - (2I_5 - I_4^2)\boldsymbol{\sigma}) \right] : \dot{\boldsymbol{\sigma}}. \end{aligned} \quad (34)$$

The isotropic HCF model due to Ottosen et al. (2008) emerges as a special case when $A_{\perp} = A_{\parallel} = A > 0$ and $S_{\perp} = S_{\parallel} = S_0 > 0$. Then the endurance function (32) and its rate (34) simplify to

$$\begin{aligned} \beta(\boldsymbol{\sigma}, \boldsymbol{\alpha}) &= \frac{1}{S_0} [\bar{\sigma} + A\text{tr}(\boldsymbol{\sigma}) - S_0], \\ \dot{\beta}(\boldsymbol{\sigma}, \boldsymbol{\alpha}, \dot{\boldsymbol{\sigma}}) &= \frac{1}{S_0 + H(\beta)C\bar{\sigma}} \left[\frac{3}{2} \frac{(\mathbf{s} - \boldsymbol{\alpha})}{\bar{\sigma}} + A\mathbf{I} \right] : \dot{\boldsymbol{\sigma}}. \end{aligned}$$

Figure 14: Endurance surface from Holopainen et al. (2016) in the deviatoric plane: Dotted line shows isotropic case ($S_{\parallel} = S_{\perp}$), Dashed and solid lines represent transversely isotropic case, where $S_{\parallel} = 1.5S_{\perp}$ and $S_{\parallel} = 2S_{\perp}$, respectively

In Figure 14, we can see a comparison of the endurance surface shapes. In the isotropic case, the endurance stress limits have same values, hence we have a circular shape. In the transversely-isotropic case, the shape of the surface starts deviating from circle (isotropic case) to an elliptical shape depending upon the endurance stress limits ($S_{\parallel}/S_{\perp} > 1$). Furthermore, the shape of the endurance surface might lead to non-convexity for higher values of $S_{\parallel}/S_{\perp}$ (shown in Figure 14 for $S_{\parallel}/S_{\perp} = 2$).

For materials, where $S_{\parallel}/S_{\perp} > 1$, the fatigue strength in the longitudinal direction is greater than the transverse direction. In AM, the fatigue strength depends upon the build (longitudinal) direction and load direction. If the build and load directions are in the same direction, the fatigue strength is the greatest, while the fatigue strength is the weakest when these directions are perpendicular to each other.

Having the endurance function and its rate defined in (32) and (34), the fatigue-damage is integrated numerically using (30) and (31). The discretization procedure is shown in Papers II and III.

5.3 Formulation of the fatigue constraints

In Papers II and III, we introduce the required loading conditions to formulate the fatigue constraint in TO problems. Using the terminologies from Chapter 2, we formulate two optimization problems: The first problem is mass minimization subjected to a fatigue constraint. The second problem is compliance minimization subjected to a fatigue constraint and a mass constraint.

In all the problems, we define a global fatigue constraint using a smooth aggregation function (Kennedy and Hicken, 2015). It is approximated using the

p-norm as

$$D^{PN}(\mathbf{x}) = \left[\sum_{e=1}^{n_e} (D_{N,e}(\mathbf{x}))^P \right]^{\frac{1}{P}} \quad (35)$$

with $P > 1$ and D^{PN} as the approximated maximum damage. It holds that $D^{PN}(\mathbf{x}) \rightarrow \max D_{N,e}(\mathbf{x})$ when $P \rightarrow \infty$, but very large values of P can cause numerical difficulties.

Using (35), the TO problems are now formulated. The mass minimization problem is

$$(\mathbb{P}_2) \begin{cases} \min_{\mathbf{x}} \sum_{e=1}^{n_e} m_e \rho_e(\mathbf{x}) \\ \text{s.t.} \begin{cases} \mathbf{F}^T \mathbf{u}(\mathbf{x}) \leq \bar{C}, \\ D^{PN}(\mathbf{x}) \leq \bar{D}, \\ \varepsilon \leq x_e \leq 1, & e = 1, 2, \dots, n_d, \\ x_e = \varepsilon, & e = n_d + 1, \dots, n_e, \end{cases} \end{cases}$$

where m_e is the elemental mass and $\bar{C}$ is the upper bound on the compliance. A compliance constraint is added to prevent all void solutions, further details are found in Paper II. We assume that the last set of elements $n_e - n_d$ represents the region containing extended elements. This is done to get a smoother profile at the domain boundary and also remove artificial reinforcement at the boundary. Note that, when $n_d = n_e$, the domain extension is not used.

The second problem is compliance minimization and it reads

$$(\mathbb{P}_3) \begin{cases} \min_{\mathbf{x}} \mathbf{F}^T \mathbf{u}(\mathbf{x}) \\ \text{s.t.} \begin{cases} \sum_{e=1}^{n_e} m_e \rho_e(\mathbf{x}) \leq \bar{M}, \\ D^{PN}(\mathbf{x}) \leq \bar{D}, \\ \varepsilon \leq x_e \leq 1, & e = 1, 2, \dots, n_d, \\ x_e = \varepsilon, & e = n_d + 1, \dots, n_e, \end{cases} \end{cases}$$

where $\bar{M}$ is maximum allowable mass.

Fatigue sensitivities

The fatigue sensitivities are calculated by the adjoint method. Since we use an evolution-based HCF model, the procedure for deriving the fatigue sensitivities follows that from Chapter 3 (for a transient response).

The state variable $\mathbf{v}_i$ comprises of back-stress $\boldsymbol{\alpha}$ and fatigue damage D , is introduced at each time step, i.e.

$$\mathbf{v}_i = [\mathbf{v}_{i,1}, \mathbf{v}_{i,2}, \dots, \mathbf{v}_{i,n_e}]^T, \quad i = 1, 2, \dots, N, \quad \text{with } \mathbf{v}_{i,e} = [\boldsymbol{\alpha}_{i,e}, D_{i,e}]^T.$$

We are interested in fatigue damage that is evaluated at the final time step $t_N = N\Delta T$ and thus the system response in (18) is specialized to the final time step. Now the general system response in (18) is modified to

$$G(\mathbf{x}) = G(\mathbf{x}, \tilde{\mathbf{u}}_N(\mathbf{x}), \mathbf{v}_N(\mathbf{x})).$$

When we use a HCF model in the TO problem, neither geometry nor material properties are affected, which implies that the stiffness matrix remains constant. This means that the structural residual in (16) does not depend on the internal state variable $\mathbf{v}$, i.e. $\mathbf{R}(\mathbf{x})|_i = \mathbf{R}(\mathbf{x}, \tilde{\mathbf{u}}_i(\mathbf{x}), \mathbf{v}_i(\mathbf{x})) = \mathbf{R}(\mathbf{x}, \tilde{\mathbf{u}}_i(\mathbf{x})) = \mathbf{0}$. The residual $\mathbf{H}(\mathbf{x})|_i$ in (17) is developed from the discrete version of the evolution equations (30) and (31) that are defined for the back-stress $\boldsymbol{\alpha}$ and fatigue damage D , respectively. The detailed derivation of fatigue sensitivities is shown in Paper II.

5.4 Results and discussion

Two materials are considered, namely AISI-SAE 4340 alloy steel and 34CrMo6 forged steel. The fitted fatigue parameters for these materials are shown in Table 1. The AISI-SAE 4340 steel has isotropic fatigue properties ($S_{\parallel} = S_{\perp}$), while the 34CrMo6 forged steel has strong directional fatigue properties, i.e. the longitudinal fatigue strength is greater than the transverse fatigue strength ($S_{\parallel} > S_{\perp}$). We take the values of the penalization parameters as $q = 3$ and $r = 0.5$. The problems are solved with the exponent of the p-norm as $P = 8$.

Table 1: Fitted fatigue material parameters

	$S_{\parallel}$ (MPa)	$S_{\perp}$ (MPa)	$A_{\parallel}$	$A_{\perp}$	C	K	L
AISI-SAE 4340	490	490	0.225	0.225	1.25	2.65E-5	14.4
34CrMo6	447	360	0.225	0.300	7.8	3.39E-5	4.7

The L-shaped beam shown in Figure 15, with $L = 100$ mm is treated. The model is discretized by 6400 bi-linear quadrilateral elements. The top edge of the beam is clamped. Two load cases are created, where the first load case is a static load $F = 1000$ N for compliance evaluation, while the second load case takes the non-periodic load history, $\tilde{F}(t) = FS_f(t)$, shown in Figure 16, with $t = 0, 0.05, \dots, 50$, for fatigue estimation. The grey regions in Figure 15 indicate elements that utilize the domain extension approach, i.e. $x_e = \varepsilon$.

The problem $(\mathbb{P}_2)$ is solved for AISI-SAE 4340 alloy steel and 34CrMo6 forged steel. We take isotropic elastic response for AISI-SAE 4340 alloy steel, where the value of Young's modulus is taken as 210 GPa and Poisson's ratio is 0.3. For 34CrMo6 steel, the five material parameters in the anisotropic material response are $E_1 = 200$ GPa, $E_3 = 150$ GPa, $G_{13} = 78$ GPa, $\nu_{12} = 0.3$ and $\nu_{13} = 0.23$, with direction 3 being the build direction. The maximum bounds on the fatigue limit is $\bar{D} = 0.2\text{E-}5$ and the compliance limit is $\bar{C} = 1.4$ Nmm.

Figure 17 gives the optimization results of the L-shaped beam. Figure 17(a) provides the optimized design when fatigue constraint is not included in $(\mathbb{P}_2)$. We

Figure 15: Geometry of the L-shaped beam **Figure 16:** Non-periodic load history

Figure 17: Optimization results of the L-shaped beam: (a) Without fatigue constraint; (b) With fatigue constraint for AISI-SAE 4340 steel, and (c) for 34CrMo6 forged steel, where x_1 and x_3 are material coordinates that take the Young's modulus E_1 and E_3 , respectively.

notice that the profile obtained in the optimized design still has material at the re-entrant corner and thus the topology will still have high stress concentrations, and thereby not improving fatigue-life. Whereas in Figure 17(b), with fatigue constraint, the profile of the optimized model has a smooth radius at the re-entrant corner, thereby reducing high stress concentrations and thus prolonging life.

Furthermore, we compare results between isotropic and anisotropic material properties. Figure 17(b) provides the optimized design for AISI-SAE 4340 alloy steel (isotropic material), while Figure 17(c) gives the optimized design for 34CrMo6 forged steel. Here we consider a pure anisotropic case (when anisotropic elastic response and fatigue anisotropic material are used). Both profiles have smooth radius at the re-entrant corner.

Conclusion

This work provides developments of TO methods for application to metal AM by considering surface layer effects and HCF behaviour. In Paper I, a TO method is developed to account for surface layer effects, and in Papers II and III, a HCF constraint is implemented in TO.

The surface layer in the optimized structures is identified by linear filtering and by calculation of a filter gradient. Unique material properties are assigned to the bulk region compared to the surface regions. At the surface regions, due to surface roughness, low stiffness material is used. Several examples, which include 2-D and 3-D examples, are tested. It is noted that, with a larger surface layer, the profiles of the optimized structures become less complicated. The computational cost is minutely larger than a standard TO problem.

The fatigue model using the continuous-time approach is capable of handling arbitrary load histories. The HCF model is extended to account for transversely isotropic material properties. The TO formulations with HCF constraint are tested on several numerical examples. The topologies obtained from optimized designs have reduced stress concentrations and thus prolong the life of the components. In addition, a comparison between isotropic and transversely isotropic material properties are given. Furthermore, different build orientations are tested in the case of transversely isotropic materials. Due to high computational costs arising from sensitivity analysis, current TO developments with HCF are restricted to 2-D examples.

Outlook

7.1 Acceleration techniques to treat 3-D problems for fatigue constrained TO problem

The fatigue sensitivities are derived by using the adjoint method. Since the predicted fatigue damage by the continuous-time approach has history dependence, the adjoint variables are obtained by solving a discrete terminal value problem. Due to this, the computational cost spent on sensitivity analysis is quite high. Therefore at the present stage, only 2-D problems are treated. As a result, an important extension is to develop acceleration techniques to improve the overall performance and shorten the computational time.

7.2 Overhang and fatigue constraint

The support material in AM increases the print time and the material cost. Implementing overhang constraint along with a fatigue constraint in a TO problem would enable lightweight designs, which would not only have support structure with minimized support materials but also have improved fatigue-life.

7.3 Fatigue constraint formulation only on the boundary regions

AM-fabricated components with as-built surface conditions, i.e. with no surface treatment, have significantly worse mechanical properties, particularly fatigue behaviour. It may thus be sufficient to evaluate the fatigue at the boundaries rather than computing fatigue for the whole structure.

Review of Appended Papers

Paper I

Topology optimization accounting for surface layer effects

In Paper I, surface layer effects are introduced into topology optimization problems, where the structural stiffness is maximized for a limited volume. For metal AM-fabricated components in as-built surface conditions with no post-surface treatments, the mechanical properties are affected. In addition, the components are generally in-homogeneous and have different microstructure in the bulk region compared to surface region. To account for these effects, two linear density filters are introduced. The first filter defines the topology of the optimized design while the second filter is used to identify the surface regions, where the thickness is controlled by second filter radius. Several numerical examples are tested, which include 2D and 3D models.

Paper II

Topology optimization using a continuous-time high-cycle fatigue model

A high-cycle fatigue constraint is developed in a topology optimization method for isotropic materials. The fatigue model is based on a continuous-time approach, which employs a concept of endurance surface. It follows that the development of damage only occurs if the stress state lies outside the endurance surface. The fatigue-damage is integrated for the whole load history, and thus the model avoids the use of cycle-counting algorithm. The fatigue sensitivities are determined by the adjoint method as we employ a gradient-based optimization. Two optimization problems are solved: The first problem is to minimize mass subject to a high-cycle fatigue constraint and the second problem is to maximize the structural stiffness subject to a high-cycle fatigue constraint and a limited mass. Several numerical examples with both proportional and non-proportional loads are tested.

Paper III

Topology optimization for transversely isotropic materials with high-cycle fatigue as a constraint

We extend the Paper II, to account for transversely isotropic materials. The fatigue constraint is based on a continuous-time model, where the so-called endurance surface is modified to account for stresses in longitudinal and transverse directions. The method is applicable for AM processes, where transverse isotropic properties are often manifested in the form of constitutive elastic response and fatigue properties. We solve a mass minimization problem subject to a high-cycle fatigue constraint, where several numerical examples are tested with arbitrary load histories. Two alloy steels, AISI-SAE 4340 steel and 34CrMo6 steels, are treated, where the comparison between two materials and also the combined impact of transversely isotropic elastic and fatigue properties are studied.

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Part II

Appended Papers

Papers

The papers associated with this thesis have been removed for copyright reasons. For more details about these see:

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