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Optimal reliability for components under thermomechanical cyclic loading*

by

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Abstract: We consider the existence of optimal shapes in a context of the thermo-mechanical system of partial differential equations (PDE) using the recent approach based on elliptic regularity theory (Gottschalk and Schmitz, 2015; Agmon, Douglis and Nirenberg, 1959,1964; Gilbarg and Trudinger, 1977). We give an extended and improved definition of the set of admissible shapes based on a class of sufficiently differentiable deformation maps applied to a baseline shape. The obtained set of admissible shapes again allows to prove a uniform Schauder estimate for the elasticity PDE. In order to deal with thermal stress, a related uniform Schauder estimate will be derived for the heat equation. Special emphasis is put on Robin boundary conditions, which are motivated by the convective heat transfer processes. It is shown that these thermal Schauder estimates can serve as an input to the Schauder estimates for the elasticity equation (Gottschalk and Schmitz, 2015). This is needed to prove the compactness of the (suitably extended) solutions of the entire PDE system in some state space that carries a C^2-Hölder topology for the temperature field and a C^3-Hölder topology for the displacement. From this, one obtains the property of graph compactness, which is the essential tool to prove the existence of optimal shapes. Due to the topologies employed, the method works for objective functionals that depend on the displacement and its derivatives up to third order, as well as on the temperature field and its derivatives up to second order. This general result in shape optimization is then applied to the problem of optimal reliability, i.e. the problem of finding shapes that have minimal failure probability under cyclic thermomechanical loading.

Keywords: shape optimization, probabilistic failure times, optimal reliability

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1. Introduction

Objective functionals that are motivated by failure probabilities of mechanical components subject to cyclic mechanical loading have been introduced in Bolten, Gottschalk and Schmitz (2015), Gottschalk and Schmitz (2015) and Schmitz (2014) to the field of shape optimization (Delfour and Zolesio, 2011; Haslinger and Mäkinen, 2003; Sokolowski and Zolesio, 1992). Here, failure times are modelled by the spatio-temporal Poisson Point Processes (PPP) and their first occurrence times. In this paper, we take enhanced material damage into account that occurs at elevated temperature. This is due to thermal stresses and also due to reduced durability of materials at higher temperatures. The assumed design objective is to choose the shape of a component from a set of admissible shapes such that the failure probability after a given number of load cycles is minimal.

The reliability assessment of the cooled components, e.g. in gas turbines or vessels, leads to a set of multi-physical partial differential equations that is known as the the thermo-mechanical equation, see Hetnarski and Eslami (2009). In this paper, we investigate the shape optimization problems with the thermo-mechanical system of PDEs as state equation. We consider a rather uncommon set of objective functionals, depending on differentiable functions and boundary integrals. These functionals are motivated by the probability of failure under cyclic thermo–mechanical loading - as it is the case for low cycle fatigue (LCF) - and generalize the objective functionals, appearing in Gottschalk and Schmitz (2015), and Schmitz et al. (2013a,b) by temperature dependence. Appropriate regularity assumptions on the admissible shapes and the boundary conditions finally allow us to show the existence of shapes with minimal failure probability.

The boundary conditions to the thermal equation that we study in this paper are of Robin type. This corresponds to convective heat transfer at the component's boundary, which is most frequently used in engineering applications. To insert the temperature distribution into to the mechanical equation, we follow a partially coupled approach, see, e.g., Hetnarski and Eslami (2009). When writing the coupled system in its strong form, the gradient of the temperature field becomes a part of the volume force density in the elasticity equation. Moreover, the temperature difference between the current temperature and a baseline temperature will be integrated in the new surface load density. This re-defines the right hand side of the elasticity problem.

In this situation, uniform regularity estimates for the temperature field serve the following purpose: regarding shape optimization with PDE constraints, the temperature field itself is a part of the solution of the state equation. So, following Haslinger and Mäkinen (2003), we will need some kind of compactness properties on the state space. Furthermore, regularity assumptions, on the now temperature influenced volume forces and surface loads, are a crucial input for the regularity estimates applied to the solution of the elasticity equation. Here, uniform bounds on C^1-Hölder norms for the volume force densities and C^2-Hölder for the surface load densities are required to obtain uniform

Schauder estimates via Agmon, Douglis and Nirenberg (1959, 1964), Gilbarg and Fradinger (1977), Gottschalk and Schmitz (2015). In this paper, we prove that these estimates remain valid if the pure mechanical problem is extended by thermal influences. Having established the suitable uniform Schauder estimates on both parts of the state space - the mechnical and the thermal one - we can proceed to prove graph compactness using precompact embeddings in Hölder spaces (Alt, 2006, Section 8). This implies the existence of optimal shapes in the class of admissible shapes for all objective functionals that are continuous with respect to the state space topology.

Proofs for the existence of optimal shapes are not new in shape optimization, see, e.g., Bolton, Gottschalk and Schmitz (2015), Bucur and Buttazzo (2005), Chenais (1975), Delfour and Zolesio (2011), and Haslinger and Mäkinen (2003). However, the class of objective functionals that arises from component reliability is only defined for differentiable functions, which, in turn, are only specified locally, i.e. on bounded sets. Therefore, this special class of functionals can not be treated in the framework of weak solutions, as done in the references cited. Like in Gottschalk and Schmitz (2015) and Schmitz (2014), we need to adapt the general strategy of shape optimization and include strong solution theory in order to be able to deal with these irregular objective functionals that arise from component reliability.

The objective of this paper is to give a mathematical existence proof for a shape optimization problem in a context, which is as close to a real design problem as possible – taking high temperature design in gas turbine engineering as a model. Although this intention can not be completely realized, we show that the machinery of elliptic regularity theory and the general theory of shape optimization, see Haslinger and Mäkinen (2003), is powerful enough to deal with certain non oversimplified problems in a mathematically rigorous way.

The paper is organized as follows: in Section 2 we review the crack initiation processes and their relation to shape optimization following, essentially, Gottschalk and Schmitz (2015). However, more and different notions of optimal reliability are introduced and compared. It is shown that in the case of Weibull models, all these different notions coincide, which allows to prove the existence of shapes with optimal reliability in a stronger sense than given in Gottschalk and Schmitz (2015). It is shown in which way the problem of optimal reliability is related to shape optimization problems. We also extend the crack initiation model for LCF to the case of non constant temperature fields using an approach based on Arrhenius' law.

In Section 3 we review the thermo-mechanical PDE as the state equation to our problem. Section 4 gives some background from the abstract theory of shape optimization following Haslinger and Mäkinen (2003). In Section 5 we present a new and enlarged set of admissible domains based on $C^{k,\alpha}$ deformations of a baseline shape. Compactness results on the set of admissible shapes are given.

Section 6 discusses the uniform Schauder estimates for the mechanical, the thermal, and the thermo-mechanical state equations. Here, special emphasis is laid on realistic convective (Robin) boundary conditions for the heat equation.

The exposition is based on Gilbarg and Trudinger (1977) and proves the uniformity of the regularity estimates in this reference with respect to our set of admissible shapes.

In the following Section 7, the uniform Schauder estimates are used to prove graph compactness of a large class of locally defined and rather irregular shape optimization problems, including those derived from optimal reliability.

Finally, we give a summary and outlook in Section 8. An appendix collects some technical results from the literature for the convenience of the reader.

2. Failure probabilities and objective functionals in shape optimization

In this section, we derive failure probabilities of mechanical components under thermo-mechanical loading and give some specific models that are motivated, in a wide sense, by the gas turbine or vessel design.

2.1. Stochastic failure time models and point processes

For describing a mechanical device filled with some material, we choose a bounded domain $\Omega \subseteq \mathbb{R}^3$ with boundary $\partial\Omega$ - the component's surface. By $\overline{\Omega}$ we denote the closure of Ω in $\mathbb{R}^3$. Initially, the component has a given reference temperature T_0 and there are no loads acting on it, whereas under operation there are several loads causing deformation. These deformations are characterized by the displacement field $u = u(\Omega) : \bar{\Omega} \to \mathbb{R}^3$. The mentioned loads can be splitted into two types: on the one hand, there are volume loads $f_M(\Omega) : \Omega \to \mathbb{R}^3$ (e.g. gravity or centrifugal loads) and on the other hand, surface loads $g_M(\Omega) : \partial\Omega \to \mathbb{R}^3$ (e.g. gas pressure) have to be taken into account. Furthermore, the device is clamped at a part of its surface. There exists a part $\partial\Omega_D \subset \partial\Omega$ of the boundary such that $u = 0$ on $\partial\Omega_D$. $\partial\Omega_D$ is assumed to have a surface volume larger than zero.

If we consider, for example, a gas turbine's blade, then heating and cooling takes place during the single load cycle and causes thermal expansion and shrinkage of the material. This results in the dependence of $u(\Omega)$ on the temperature distribution $T(\Omega) : \bar{\Omega} \to \mathbb{R}$ in the component. The temperature distribution inside Ω, in turn, is influenced by the external temperature field $T_e(\Omega) : \partial\Omega \to \mathbb{R}$ and the thermal conductivity $k \in \mathbb{R}$ of the material*.

During the device's lifetime, the thermal and mechanical loads lead to a deterioration of the material, which is also known as fatigue. This degeneration will result in the formation of cracks that finally destroy the component. A deterministic prediction of the number of load cycles (or time) that will be passed safely before crack formation takes place is problematic, due to significant

*In technical applications that involve cooling, $T_e(\Omega)$ is significantly different on internal and external portions of the boundary, e.g. $\sim 400°$C vs $\sim 1350°$C in contemporary design of front stage turbine blades.

scatter in life times. Hence, it is more functional to set up a probabilistic models for crack formation.

Let $\mathcal{C} = \mathbb{R}_+ \times \bar{\Omega}$ be the configuration space for crack initiation. I.e. each crack initiation on the originally crack free component is identified with time $t \in \mathbb{R}_+$ and location $x \in \bar{\Omega}$.

Let $\mathcal{R}(\mathcal{C})$ be the space of Radon measures on $\mathcal{C}$ and $\mathcal{R}_c(\mathcal{C})$ the space of Radon counting measures. This kind of measures maps measurable sets in the Borel σ-Algebra $\mathcal{B}(\mathcal{C})$ to $\mathbb{N}_0 \cup \{\infty\}$. For any continuous function h on $\mathcal{C}$ with compact support, $h \in C_c(\mathcal{C})$, and $\gamma \in \mathcal{R}(\mathcal{C})$ the integral $\int_{\mathcal{C}} h d\gamma$ is well defined and the mappings $\mathcal{R}(\mathcal{C})\,(\mathcal{R}_c(\mathcal{C})) \ni \gamma \to \int_{\mathcal{C}} h d\gamma$, $h \in C_c(\mathcal{C})$ induce the weak-*-topology on the space of the Radon (counting) measures. The associated Borel σ-algebra is denoted by $\mathcal{B}(\mathcal{R})$ $(\mathcal{B}(\mathcal{R}_c))$.

A Radon counting measure γ is called simple if for every bounded set $A \in \mathcal{B}(\mathcal{C})$ there exists $n < \infty$ and $c_j \in A$, $j = 1, \dots, n$, all distinct, such that $\gamma\restriction_A = \sum_{j=1}^{n} \delta_{c_j}$.

Definition 1 (Crack Initiation Process) *Let $(\Xi, \mathcal{A}, P)$ be a probability space and $\gamma : (\Xi, \mathcal{A}, P) \to (\mathcal{R}(\mathcal{C}), \mathcal{B}(\mathcal{R}_c))$ be measurable. Then γ is called a point process.*

(i) If a point process γ is almost surely simple and non-atomic, i.e. $\gamma(\{c\}) = 0$ holds P a.s. $\forall c \in \mathcal{C}$, then we call γ a crack initiation process on $\overline{\Omega}$.

(ii) For a crack initiation process γ we define the time of first failure associated with γ by $\tau = \tau(\gamma) = \inf\{t \geq 0 : \gamma([t, \infty) \times \overline{\Omega}) > 0\}$. Note that $\tau : (\Xi, \mathcal{A}, P) \to ([0, \infty], \mathcal{B})$ is a random variable, where $\mathcal{B}$ is the Borel σ-Algebra on $[0, \infty)$ extened to $t = \infty$.

The notion of a crack initiation process reflects the stochastic nature of crack formation that has been widely studied in the materials science literature, see, e.g., Bäker, Harder and Rösler (2008). The process is chosen to be simple since two cracks cannot be initiated at the same location and the same time (in that case they would form one crack). Non atomicity is motivated by the fact that in non deterministic crack formation processes there should be no point on the component where the probability that a crack originates exactly there is larger than zero.

We now investigate the situation, when cracks have not yet grown to a size where they can influence the macroscopic stress field. Therefore, and due to the fact that we are interested in first failure times, we assume that the various crack initiations are independent of each other.

Definition 2 (Independent Increments and Poisson Point Process) *Let $\gamma : (\Xi, \mathcal{A}, P) \to (\mathcal{R}(\mathcal{C}), \mathcal{B}(\mathcal{R}_c))$ be a point process on $\mathcal{C} = [0, \infty) \times \bar{\Omega}$.*

(i) The point process γ has independent increments, if for $C_1, \dots, C_n \in \mathcal{B}(\mathcal{C})$ mutually disjoint we have that $\gamma(C_1), \dots, \gamma(C_n)$ are independent random variables.

(ii) The point process γ is a Poisson Point Process (PPP) if $\exists \rho \in \mathcal{R}(\mathcal{C})$ such that $\forall C \in \mathcal{B}(\mathcal{C})$, $\gamma(C)$ is Poisson distributed with intensity $\rho(C)$, i.e. $P(\gamma(C) = n) = e^{-\rho(C)}\, {\rho(C)^n}/{n!}$.

For a crack initiation process the property of having independent increments is equivalent to being a PPP, see Watanabe (1964) and Kallenberg (1983). Thus, we only have to model the intensity measure ρ as a function of the stress and the temperature state on $\overline{\Omega}$ if we accept the assumption of independent increments.

Let $\Omega \subseteq \mathbb{R}^3$ model the component with associated temperature field $T = T(\Omega)$ and displacement field $u = u(\Omega)$. It is then natural to model the local crack initiation intensity as a function of time and local values of the temperature and the displacement along with their derivatives. Here we restrict ourselves to derivatives up to third order in u and up to second order in T:

$$\rho(\Omega, C) = \int_{C\cap(\mathbb{R}_+\times\Omega)} \varrho_{vol}(t, x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dt\, dx + \int_{C\cap(\mathbb{R}_+\times\partial\Omega)} \varrho_{sur}(t, x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dt\, dA,\ C \in \mathcal{B}(\mathcal{C}). \tag{1}$$

Here dA stands for the surface measure on $\partial\Omega$ and $\varrho_{vol/sur}$ are some non negative functions that depend on the physics of the crack formation that will be specified in detail in Subsection 2.3 below. The function ϱ_{vol} represents the volume driven failure mechanisms, like, e.g., creep, whereas ϱ_{sur} models surface driven crack formation, like e.g. low cycle fatigue (LCF). Here we derive some immediate consequences on the probability distribution of the first failure time:

Lemma 1 *Let $\gamma = \gamma(\Omega)$ be the PPP associated with (2.1) and $\tau = \tau(\gamma)$ the associated first failure time. Let $C_t = [0, t] \times \overline{\Omega}$ and $H(\Omega, t) = \rho(\Omega, C_t)$. Then, $H(\Omega, t)$ is the cumulative hazard rate of the random variable τ, i.e. we have for the cumulative distribution function $F_\tau(t)$*

$$F_\tau(t) = P(\tau \leq t) = 1 - e^{-H(\Omega,t)}, \quad t \in \mathbb{R}. \tag{2}$$

Proof Note that $P(\tau > t) = P(\gamma(C_t) = 0) = e^{-\rho(\Omega,C_t)}$ and go over to the complementary probabilities. □

2.2. Optimal reliability problems

The problem of optimal reliability of a technical device can be formulated on several levels. Every choice of a component shape Ω in the design process induces a probability distribution (2). Hence, it is not obvious how to compare the distribution of $\tau = \tau(\Omega)$ with that of $\tau' = \tau(\Omega')$. The following definition gives a number of alternatives:

Definition 3 (Different Notions of Reliability) *Let τ and τ' be two first failure times associated to the design alternatives $\Omega, \Omega' \subseteq \mathbb{R}^3$ via Definition 2 and (2.1).*

(i) The design Ω is more or equally reliable than Ω' at fixed time $t \in \mathbb{R}_+$, if the probability of failure is less for Ω than for Ω', hence $F_\tau(t) \leq F_{\tau'}(t)$.

(ii) *The design Ω is more or equally reliable than Ω' in first stochastic order, if it is more or equally reliable if (i) holds at any time $t \in \mathbb{R}_+$.*

(iii) *Suppose that τ and τ' are continuously distributed. Then Ω is more reliable than Ω' in terms of instantaneous hazard, if $h_\tau(t) \leq h_{\tau'}(t)$ holds for any $t \geq 0$. Here $h_\tau(t) = f_\tau(t)/(1 - F_\tau(t))$ is the hazard rate and f_τ the density function of τ.*

Clearly, each of these notions gives rise to an optimal reliability problem:

Definition 4 (Optimal Reliability Problem) *Let $\mathcal{O}$ be some set of admissible domains (shapes) $\Omega \subseteq \mathbb{R}^3$. Then, $\Omega^* \in \mathcal{O}$ solves the problem of optimal reliability on $\mathcal{O}$ according to Definition 3 (i), (ii) or (iii) if it is more or equally reliable than any other design $\Omega \in \mathcal{O}$ regarding (i), (ii) or (iii), respectively.*

Solutions of the optimal reliability problem, according to Definition 4 w.r.t. first order stochastic dominance are interesting, because a product with optimal design Ω^* serves the customer most reliably during any time span $[0, t]$ of its life cycle – design to life is excluded. The concept of higher reliability in terms of instantaneous hazard enhances this notion: One design is most reliable at each instance in time. Since $F_\tau(t) = 1 - e^{-\int_0^t h_\tau(s)ds}$ (see Escobar and Meeker, 1998), the estimate $h_\tau(t) \leq h_{\tau'}(t)$ $\forall t \in \mathbb{R}_+$ implies $F_\tau(t) \leq F_{\tau'}(t)$ $\forall t \in \mathbb{R}_+$ and thus the concept of higher reliability in instantaneous hazard is more restrictive than the concept of higher reliability in first stochastic order.

Let $\mathcal{F}_{vol/sur}(t, \cdot) = \int_0^t \varrho_{vol/sur}(s, \cdot)\, ds$ and

$$\mathcal{J}_t(\Omega, u, T) = \mathcal{J}_{vol,t}(\Omega, u, T) + \mathcal{J}_{sur,t}(\Omega, u, T) \tag{3}$$

with

$$\begin{array}{rcl} \mathcal{J}_{vol,t}(\Omega, u, T) &=& \int_\Omega \mathcal{F}_{vol}(t, x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dx \\ \mathcal{J}_{sur,t}(\Omega, u, T) &=& \int_{\partial\Omega} \mathcal{F}_{sur}(t, x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dA \end{array} . \tag{4}$$

Here and further on we use the following conventions on derivatives: ∇u (∇T) are the Jacobi matrix (gradient) of the $\mathbb{R}^3$ (scalar) valued real function u (T). By $\nabla_i u$ we denote a partial derivative in the direction of the i-th coordinate vector. $\nabla^r u$ is the $r+1$-level tensor of r-th partial derivatives of u. Finally, for a multi index α, $\nabla^\alpha u$ stands for the repeated partial derivative of u as specified by α. Related conventions hold for T and for $\mathbb{R}^n$-valued functions u on domains in $\mathbb{R}^n$.

Then, the optimal reliability problems from Definition 4 can be translated to the following shape optimization problems:

Lemma 2 *Let the crack initiation process $\gamma = \gamma(\Omega)$ for some $\Omega \in \mathcal{O}$ be a PPP with intensity measure (2.1).*

(i) A shape $\Omega^* \in \mathcal{O}$ solves the optimal reliability problem (i) at fixed time $t \in \mathbb{R}_+$ if and only if

$$\mathcal{J}_t(\Omega^*, u, T) \leq \mathcal{J}_t(\Omega, u, T) \quad \forall \, \Omega \in \mathcal{O}. \tag{5}$$

(ii) Furthermore, a shape Ω^* solves the optimal reliability problem from Definition 4 in terms of first order stochastic dominance from Definition 3 (ii) if and only if Ω^* solves (5) for all $t \in \mathbb{R}_+$.

(iii) Finally, a shape Ω^* also solves the optimal reliability problem in terms of instantaneous hazard, if an only if

$$\frac{d\mathcal{J}_t(\Omega^*, u, T)}{dt} \leq \frac{d\mathcal{J}_t(\Omega, u, T)}{dt} \quad \forall t \in \mathbb{R}_+, \; \Omega \in \mathcal{O}. \tag{6}$$

Proof This follows from $P(\tau \leq t) = 1 - e^{-\mathcal{J}_{vol,t}(\Omega,u,T)}$, see Lemma 1 and equations (2.1) and (3–4). Thus, $h_\tau(t) = \frac{d\mathcal{J}_t(\Omega^*,u,T)}{dt}$. □

Remark 1 *Another perspective on the problem of optimal reliability is given by the notion of acceptability functionals:*

Let $\mathcal{A}(\tau)$ be an acceptability functional according to Pflug and Römisch (2007). Common choices include the life expectation $\mathcal{A}(\tau) = \mathbb{E}[\tau]$ or risk adjusted versions of it, e.g. $\mathcal{A}(\tau) = \mathbb{E}[\tau] - \delta \mathrm{Var}[\tau]$ for some $\delta > 0$. For $\iota : \mathbb{R} \to \mathbb{R}$ measurable and provided that $\iota(\tau)$ is in $L^1(\Xi, P)$ also $\mathcal{A}_\iota(\tau) = \mathbb{E}[\iota(\tau)]$ defines an acceptability functional. Then, the design Ω is more or equally reliable than Ω' with respect to $\mathcal{A}$, if $\mathcal{A}_\iota(\tau) \geq \mathcal{A}_\iota(\tau')$.

Hence, a shape Ω^* solves the optimal reliability problem in the sense of acceptability for all $\mathcal{A}_\iota$ with increasing ι, if and only if it solves (5) $\forall t \in \mathbb{R}_+$, see the equivalent formulations of first order stochastic dominance in Pflug and Römisch (2007, Theorem 1.13 (i)).

Obviously, the ranking of failure or survival probabilities at a given warranty time or service interval according to Definition 3 (i) is a special case of the general notion of acceptability with $\iota = 1_{\{\tau > t\}}$.

Interestingly, there exists a special situation, when the solution of the optimal reliability problem in terms of instantaneous hazard can be obtained by finding at least one solution to the related problem at a fixed time t.

Definition 5 (Local Weibull Model) *Let $m > 0$ be a Weibull shape parameter and*

$$\varrho_{vol/sur}(t, \cdot) = \frac{m}{N_{vol/sur}(\cdot)} \left(\frac{t}{N_{vol/sur}(\cdot)} \right)^{m-1} \tag{7}$$

for some functions $N_{vol/sur}(\cdot) = N_{vol/sur}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)$ with values in $[0, \infty]$. The associated crack initiation processes are called local Weibull models.

Note that the convention $\frac{1}{\infty} = 0$ is used here and one of $N_{vol/sur}(\cdot)$ could be identically infinite.

Since $N_{vol/sur}$ can be interpreted as the number of load cycles passed until crack formation, $N_{vol} = 0$ (or $N_{sur} = 0$) means that the rupture originates in the volume (at the surface) of the mechanical device. An example for the systematic derivation of such a functional N_{sur} will be presented in the next section.

We recall that a random variable $\tau \sim \text{Wei}(N, m)$ is Weibull distributed with scale parameter $N > 0$ and shape parameter $m > 0$ iff $F_\tau(t) = 1 - e^{-\left(\frac{t}{N}\right)^m}$.

Lemma 3 *Let $\gamma = \gamma(\Omega)$ be the PPP from a local Weibull model. Then, the first failure time $\tau = \tau(\gamma)$ is Weibull distributed with parameters $N = N(\Omega) > 0$ and $m > 0$ given by*

$$N = \left(\int_\Omega \left(\frac{1}{N_{vol}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)}\right)^m dx + \int_{\partial\Omega} \left(\frac{1}{N_{sur}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)}\right)^m dA\right)^{-\frac{1}{m}}. \tag{8}$$

Proof Insert (7) into (2.1) and (2). The integral in time now up to some maximal time t can be easily solved as it factors out. We obtain $F_\tau(t) = 1 - e^{-t^m N^{-m}}$ with N given by (3).

In the context of a local Weibull model, the problem of optimal reliability in first order stochastic dominance can be reduced to a simple shape optimization problem, as the following proposition shows:

Proposition 1 *Let $\gamma = \gamma(\Omega)$ be the crack initiation process associated with a local Weibull model where $m \geq 1$ and let $\mathcal{O}$ be the set of admissible shapes. Then,*

(i) $\Omega^* \in \mathcal{O}$ is a solution to the optimal reliability problem from Definition 4 (iii) if and only if it solves the optimal reliability problem from Definition 4 (i) at a given time t.

(ii) $\Omega^* \in \mathcal{O}$ is a solution to the optimal reliability problem from Definition 4 (i) if and only if

$$\mathcal{J}(\Omega^*, u, T) \leq \mathcal{J}(\Omega, u, T) \quad \forall \Omega \in \mathcal{O}. \tag{9}$$

for

$$\mathcal{J}(\Omega^*, u, T) = \int_\Omega \left(\frac{1}{N_{vol}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)}\right)^m dx + \int_{\partial\Omega} \left(\frac{1}{N_{sur}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)}\right)^m dA. \tag{10}$$

Proof (i) Let $t \in \mathbb{R}_+$ be fixed. If Ω^* solves the optimal reliability problem from Definition 4 (iii) with respect to that time, we have $F_{\tau(\Omega^*)}(t) \leq F_{\tau(\Omega)}(t)$ $\forall\, \Omega \in \mathcal{O}$ and thus

$$1 - e^{-t^m N(\Omega^*)^{-m}} \leq 1 - e^{-t^m N(\Omega)^{-m}} \;\Leftrightarrow\; N(\Omega^*) \geq N(\Omega) \quad \forall \Omega \in \mathcal{O}.$$

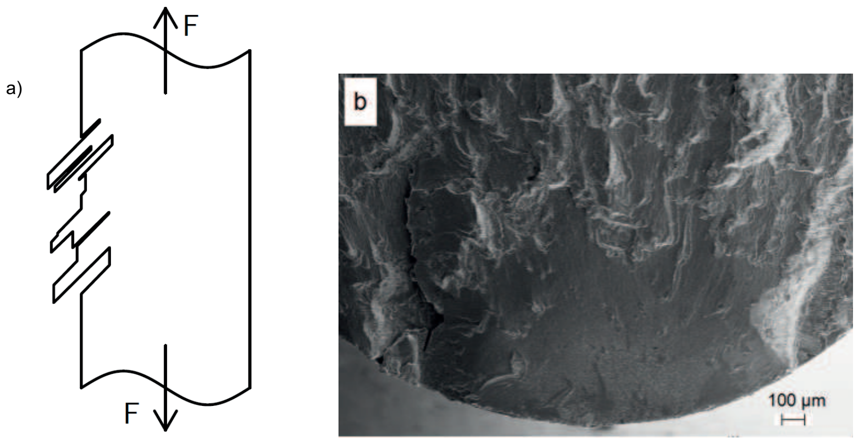

Figure 1: (a) Intrusions and extrusions at the surface forming under cyclic application of the force F. (b) Crack initation at the lower boundary of a specimen cracked during a cyclic life test for the Ni-based superalloy RENE80.

But then, the hazard rates fulfill for $m \geq 1$

$$h_{\tau(\Omega^*)}(t) = \frac{m}{N(\Omega^*)}\left(\frac{t}{N(\Omega^*)}\right)^{m-1} \leq \frac{m}{N(\Omega)}\left(\frac{t}{N(\Omega)}\right)^{m-1} = h_{\tau(\Omega)}(t)\ ,\ \ \forall t \in \mathbb{R}_+ . \tag{11}$$

(ii) Combine (i) for $t = 1$, Lemma 3, Definition 5 and Lemma 2 (i). □

2.3. The example of low cycle fatigue

In this subsection, we extend the local Weibull model for Low Cycle Fatigue (LCF) for the purely mechanical load case, discussed in Gottschalk and Schmitz (2015), to the case of thermo-mechanical loading. It is well known, see Bäker, Harders and Rösler (2008), that repeated loading of a mechanical component ultimately leads to failure, even if the single loads are well below the ultimate tensile strength of the material. This degradation of strength is known as fatigue. LCF is a damage mechanism that is best understood for polycrystalline metal: shear stress acting on atomic layers with the densest packing leads to the intragranular displacement of one dimensional lattice defects. When these defects reach the surface of the component, then intrusions and extrusions form, see Fig. 1 (a). This leads to stress concentration at the tip of the intrusion, from which a crack originates. Percolation over grain boundaries then causes macroscopic cracks to start from the initial intragranular crack, see Bäker, Harders and Rösler (2008). This is why LCF is a stress and surface driven failure mechanism, see Fig. 1 (b).

Let $\sigma = \sigma(\nabla u, T) : \Omega \to \mathbb{R}^{3\times 3}$ be the stress field associated with the displacement field u (the first derivatives thereof, in particular) and the temperature field T via a material equation. Here we suppress the Ω dependence for notational simplicity. For the example of linear thermo-elasticity, we refer to the following Section 3 Eq. (18).

If I stands for the identity matrix on $\mathbb{R}^3$, then $\sigma' = \sigma - \frac{1}{3}\mathrm{tr}(\sigma)I$ denotes the trace free part of the stress field. We shortly recall the steps that lead to the calculation of the approximate number of load cycles to crack initiation N_{sur} for the case of cyclic, purely mechanical loading.

1. Define the amplitude comparison stress as the von Mises stress associated with σ, i.e. $\sigma_v = \sqrt{\frac{3}{2}\sigma' : \sigma'}$ and define the amplitude stress as $\varepsilon_a = \sigma_v/2$.
2. If σ is obtained from a linear thermo-elasticity, convert the amplitude stress σ_a to elastic-plastic amplitude stress, e.g. via the Neuber relation

$$\frac{\sigma_a^2}{E} = \frac{(\sigma_a^{el-pl})^2}{E} + \sigma_a^{el-pl}\left(\frac{\sigma_a^{el-pl}}{K}\right)^{1/n'}. \tag{12}$$

   Otherwise, i.e. if σ is obtained from an thermo-elastoplastic problem, set $\sigma_a^{el-pl} = \sigma_a$. In equation (12) E stands for Young's modulus, K for the hardening constant and n' for the hardening exponent.
3. Convert the elastic-plastic comparison stress amplitude to the elastic-plastic strain amplitude ε_a^{el-pl} via the Ramberg-Osgood relation:

$$\varepsilon_a^{el-pl} = \frac{\sigma_a^{el-pl}}{E} + \left(\frac{\sigma_a^{el-pl}}{K}\right)^{1/n'}. \tag{13}$$

4. Solve the Coffin-Manson-Basquin equation for $\mathcal{N}_{sur}$,

$$\varepsilon_a^{el-pl} = \frac{\sigma_f'}{E}(2\mathcal{N}_{sur})^b + \varepsilon_f'(2\mathcal{N}_{sur})^c. \tag{14}$$

   Here $\sigma_f', \varepsilon_f' > 0$ and $b, c < 0$ are material constants.

Let us now turn to the case when, additionally, a temperature change from the baseline temperature T_0 to the temperature field T takes place. Then, it is usually assumed that the durability changes with temperature. Dissemination of displacements through the crystal is facilitated by the thermal excitation of the atomic oscillations in the lattice. Therefore, LCF life to crack initiation usually decreases with temperature. Here, we take a simplistic Arrhenius law (Bäker, Harders and Rösler, 2008) for the temperature dependence of LCF life. This is an 'import' from creep damage modelling and not necessarily the most adequate temperature model. Alternatively, one could consider temperature dependent CMB parameters $\sigma_f'(T), \varepsilon_f(T), b(T)$ and $c(T)$, modelled by continuous functions. The field of temperature models in fatigue, however, is vast and lies beyond the scope of this article. We thus choose

$$N_{sur}(\cdot) = e^{-Q(T-T_0)}\mathcal{N}_{sur}(\cdot). \tag{15}$$

Here Q plays the rôle of an activation energy. Using (14) it is easily shown that this corresponds to constant $b(T) = b$ and $c(T) = c$, as well as $\frac{\sigma'_f(T)}{E} = e^{-Qb(T-T_0)}\frac{\sigma'_f}{E}$ and $\varepsilon'_f(T) = e^{-Qc(T-T_0)}\varepsilon'_f$. Wrapping up these modeling steps we obtain the following:

Lemma 4 *Let $N_{sur} = N_{sur}(\nabla u, T)$ be defined as above. Then, $\left(\frac{1}{N_{sur}}\right)^m$ depends continuously on ∇u and T.*

Note that models which include notch support factors (Bäker, Harders and Rösler, 2008; Mäde et al., 2017) also require derivatives $\nabla^2 u$. Therefore, second order derivatives will enter into the definition of N_{sur}.

We have thus shown that in realistic models, the functions $\mathcal{F}_{vol/sur}$ from (4) can be assumed to be continuous, as long as the temperature does not exceed a certain limit close to the melting temperature.

3. The thermomechanic formulation of linear elasticity

Up till now, we have seen that volume forces, surface forces, and changes in temperatures acting on a device have an impact on its durability. In linear thermo-elasticity both aspects are taken into account, see Hetnarski amd Eslami (2009).

As proposed in Gottschalk and Schmitz (2015) and for reasons of simplification, we restrict ourselves to the case, in which the load vector fields f_M and g_M and the temperature distribution field T are independent of time. This means that time t only counts the number of load cycles passed. Then, according to Ciarlet (1988), and Ern and Guermond (2004), the disjoint displacement-traction problem of linear isotropic elasticity is defined by

$$\begin{array}{ll} \mathrm{div}(\sigma(u)) + f_M = 0 & \text{in } \Omega \\ \sigma(u) = \lambda \mathrm{div}(u) I + \mu(\nabla u + (\nabla u)^\top) & \text{in } \Omega \\ u = 0 & \text{auf } \partial\Omega_D \\ \sigma(u)\cdot\nu = g_M & \text{auf } \partial\Omega_N \end{array} \tag{16}$$

on $\Omega \subset \mathbb{R}^3$. Here, $\partial\Omega_N \dot\cup \partial\Omega_D$ is a partition of the domain's boundary, where on $\partial\Omega_N$ a force surface density g_M is imposed on $\partial\Omega_N$ and $\partial\Omega_D$ is clamped. Let ν be the outward normal on $\partial\Omega$. The load vector field $f_M : \Omega \to \mathbb{R}^3$ corresponds to a force imposed on the volume of Ω and every solution $u : \overline{\Omega} \to \mathbb{R}^3$ is called displacement field on Ω. In addition, we assume that the Lamé coefficients $\lambda, \mu > 0$ are constants. For the computation of approximative numerical solutions a finite element approach can be used, see Ern and Guermond (2004), and Hetnarski and Eslami (2009).

Temperature gradients, as for example occurring in materials that are heated and cooled at the same time, encourage fatigue as already explained in the preceding section. Therefore, they have to be taken into account when dealing with durability of devices that are run under changing temperatures. For implementation, we use a combination of the PDE (16) and heat equation. But, since simulation of heat transfer from the exterior to the interior of the component is necessary, we propose Robin boundary conditions instead of the most common Dirichlet or Neumann conditions.

Let $T : \overline{\Omega} \to \mathbb{R}$ be a two times continuously differentiable temperature field solving

$$\begin{aligned} &\Delta T = 0 && \text{in } \Omega \\ &\kappa \frac{\partial T}{\partial \nu} = \eta(T_e - T) && \text{on } \partial\Omega, \end{aligned} \tag{17}$$

where $T_e : \Omega^{ext} \to \mathbb{R}$, $\Omega^{ext} \supset \Omega$ denotes the component's ambient temperature, $\eta : \partial\Omega \to \mathbb{R}$ the heat transfer coefficient and $\kappa > 0$ the thermal conductivity. Taking into account a non constant temperature field $T : \overline{\Omega} \to \mathbb{R}$ in (16) leads to a new stress formulation, Hetnarski and Eslami (2009),

$$\tilde{\sigma}(u) = \lambda \mathrm{div}(u) I + \mu(\nabla u + (\nabla u)^\top) - \rho(3\lambda + 2\mu)(T - T_0)I, \tag{18}$$

where $T_0 \in \mathbb{R}$ is a reference temperature and ρ the coefficient of linear thermal expansion. If we insert the thermo-mechanical stress tensor field into (16) and rewrite it as an expression of its mechanical component, the resulting combined equation reads

$$\begin{aligned} &\Delta T = 0 && \text{in } \Omega \\ &\kappa \frac{\partial T}{\partial \nu} = \eta(T_e - T) && \text{on } \partial\Omega, \\ &\mathrm{div}(\sigma(u)) + f_M - \rho(3\lambda + 2\mu)\nabla T = 0 && \text{in } \Omega \\ &\sigma(u) = \lambda(\mathrm{div}(u))I + \mu(\nabla u + (\nabla u)^\top) && \text{in } \Omega \\ &u = 0 && \text{on } \partial\Omega_D \\ &\sigma(u) \cdot \nu = g_M + \rho(3\lambda + 2\mu)(T - T_0) \cdot \nu && \text{on } \partial\Omega_N. \end{aligned} \tag{19}$$

4. Basic notations and abstract setting for shape design problems

In the following, we analyse the generalized shape optimization problems

$$\begin{aligned} &\min \mathcal{J}(\Omega) \\ &s.t \;\; \Omega \text{ satisfies a given condition } P(\Omega), \\ &\qquad \Omega \in \mathcal{O}. \end{aligned} \tag{$\mathbb{P}$}$$

We adopt the concepts that are presented, e.g., in Chenais (1975) and Haslinger and Mäkinen (2003), and apply the suggested solution strategy to the problem of LCF. Further introductions to shape optimization can be found in Sokolowski and Zolesio (1992), Bucur and Butazzo (2005), and Delfour and Zolesio (2011).

A solution of $\mathbb{P}$ is sought as a set Ω in some family of admissible domains $\mathcal{O}$. First, we collect the assumptions, which have to be made on the cost functional $\mathcal{J}$, the restrictions $P(\Omega)$ and the family $\mathcal{O}$.

Let $\mathcal{O}$ be the set of admissible domains, contained in a larger system $\tilde{\mathcal{O}}$, on which we assume some kind of convergence, that has to be adjusted according to the respective problem. This convergence will be denoted by $\Omega_n \xrightarrow{\tilde{\mathcal{O}}} \Omega$ as $n \to \infty$ for a sequence $(\Omega_n)_{n\in\mathbb{N}}$ in $\tilde{\mathcal{O}}$ and its limit $\Omega \in \tilde{\mathcal{O}}$. Further, we define a state space $V(\Omega)$ of real functions on Ω for every $\Omega \in \tilde{\mathcal{O}}$ that contains possible solutions of $P(\Omega)$.

Since functions $y_n \in V(\Omega_n)$, $\Omega_n \in \tilde{\mathcal{O}}$ are defined on changing sets, a suitable specification of convergence is necessary and has to be defined properly for each problem[†]. Generally, we write $y_n \rightsquigarrow y$ as $n \to \infty$. Moreover, we require that any subsequence of a convergent sequence tends to the same limit as the original one.

In every $\Omega \in \tilde{\mathcal{O}}$ a state problem $P(\Omega)$ has to be solved. This can be a PDE, ODE or variational inequality. Assuming that there is a unique solution $u(\Omega)$ for every state problem $P(\Omega)$ and every $\Omega \in \tilde{\mathcal{O}}$, we are able to define the map $u : \Omega \to u(\Omega) \in V(\Omega)$. The resulting set $\mathcal{G} = \{(\Omega, u(\Omega)) \,|\, \Omega \in \mathcal{O}\}$ is called the graph of u restricted to a chosen subfamily $\mathcal{O}$ of $\tilde{\mathcal{O}}$. In this context, we say that the graph $\mathcal{G}$ is compact iff every sequence $((\Omega_n, u(\Omega_n)))_{n\in\mathbb{N}} \subset \mathcal{G}$ has a subsequence $(\Omega_{n_k}, u(\Omega_{n_k}))_{k\in\mathbb{N}}$ satisfying the condition

$$\begin{array}{ccc} \Omega_{n_k} & \xrightarrow{\tilde{\mathcal{O}}} & \Omega \\ u(\Omega_{n_k}) & \rightsquigarrow & u(\Omega) \end{array} \tag{20}$$

as $k \to \infty$ for some $(\Omega, u(\Omega)) \in \mathcal{G}$.

A cost functional $\mathcal{J}$ on $\tilde{\mathcal{O}}$ maps a pair (Ω, y), $\Omega \in \tilde{\mathcal{O}}$, $y \in V(\Omega)$ onto $\mathcal{J}(\Omega, y)$, e.g. the functional introduced in Definition 4. Here, lower semi-continuity is defined as follows:

Let the sequences $(\Omega_n)_{n\in\mathbb{N}}$ in $\tilde{\mathcal{O}}$ and $(y_n)_{n\in\mathbb{N}}$, $y_n \in V(\Omega_n)$ be convergent to $\Omega \in \mathcal{O}$ and $y \in V(\Omega)$, respectively. Then

$$\left.\begin{array}{ccc} \Omega_n & \xrightarrow[n\to\infty]{\tilde{\mathcal{O}}} & \Omega \\ y_n & \underset{n\to\infty}{\rightsquigarrow} & y \end{array}\right\} \Rightarrow \liminf_{n\to\infty} \mathcal{J}(\Omega_n, y_n) \geq \mathcal{J}(\mathcal{O}, y). \tag{21}$$

Now, let $\mathcal{O}$ be a subfamily of $\tilde{\mathcal{O}}$ and let $u(\Omega)$ be the unique solution of a given state problem $P(\Omega)$ for every $\Omega \in \mathcal{O}$. An optimal shape design problem can be defined by

$$\text{Find } \Omega^* \in \mathcal{O} \text{ such that } \mathbb{P} \text{ is solved.} \tag{22}$$

The following theorem that can be found in Haslinger and Mäkinen (2003, Ch. 2) provides conditions for the existence of optimal shapes. It is based on the

[†]See for example Definition 13 further on for the convergence applied in this work.

general fact, that lower semicontinuous functions always possess a minimum on a compact set.

THEOREM 1 *Let $\tilde{\mathcal{O}}$ be a family of shapes with an admissible subfamily $\mathcal{O}$. It is assumed that every $\Omega \in \mathcal{O}$ has an associated state problem $P(\Omega)$ with state space $V(\Omega)$, which is uniquely solved by $u(\Omega) \in V(\Omega)$. Finally, require*

(i) compactness of $\mathcal{G}$,

(ii) lower semi-continuity of $\mathcal{J}$.

Then there is at least one solution of the optimal shape design problem.

5. $C^{k,\alpha}$-admissible domains via deformation maps

In this section, we adjust the terms and results introduced in the last section to our present problem. Among others, we have to define the family of domains $\tilde{\mathcal{O}}$ and the admissible subfamily $\mathcal{O}$. We consider $C^{k,\alpha}$-admissible domains‡, on which we later impose the boundary value problems of linear elasticity and heat equation that were introduced in Section 3. We will see that $C^{k,\alpha}$-domains are very useful in relation to compactness properties.

DEFINITION 6 (**$C^{k,\alpha}$-Diffeomorphisms**)

(i) A $C^{k,\alpha}$-diffeomorphism on a bounded domain $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$ is a one to one mapping $\Phi : \Omega \to \Omega'$, $\Omega' \subset \mathbb{R}^n$ such that $\Phi \in [C^{k,\alpha}(\Omega)]^n$ and $\Phi^{-1} \in [C^{k,\alpha}(\Omega')]^n$.

(ii) The set of $C^{k,\alpha}$-diffeomorphisms on $\Omega \subset \mathbb{R}^n$ will be denoted by $\mathcal{D}^{k,\alpha}(\Omega, \Omega')$ or $\mathcal{D}^{k,\alpha}(\Omega)$ if $\Phi : \Omega \to \Omega$ §.

DEFINITION 7 (**$C^{k,\alpha}$-Admissible Domains**) *Let $K > 0$ be a positive constant and $\Omega^0 \Subset \Omega^{ext} \subset \mathbb{R}^3$ be $C^{k,\alpha}$-domains.*

The elements of

$$U^{ad}_{k,\alpha}(\Omega^{ext}) := \left\{ \Phi \in \mathcal{D}^{k,\alpha}(\overline{\Omega^{ext}}) \,\middle|\, \|\Phi\|_{[C^{k,\alpha}(\Omega^{ext})]^3} \leq K,\ \|\Phi^{-1}\|_{[C^{k,\alpha}(\Omega^{ext})]^3} \leq K \right\}$$

are called design-variables. In a natural way, this induces the set of admissible shapes

$$\mathcal{O}_{k,\alpha}(\Omega^0, \Omega^{ext}) := \left\{ \Phi(\Omega^0) \,|\, \Phi \in U^{ad}_{k,\alpha}(\Omega^{ext}) \right\}$$

assigned to Ω^0.

In this context it is obvious to define convergence of sets in $\mathcal{O}$ through $\left[C^{k,\alpha'}\right]^3$-convergence of admissible functions.

‡For explanations see Section 7 of Agmon, Douglis and Nirenberg (1964) or Sections 4 and 6 of Gilbarg and Trudinger (1977)

§Note that $\Phi \in [C^{k,\alpha}(\overline{\Omega})]^n$ if $\Phi \in [C^{k,\alpha}(\Omega)]^n$ has a k, α-regular extension to $\overline{\Omega}$.

Definition 8 ($C^{k,\alpha'}$**-Convergence of Sets**) *Let* $0 \leq \alpha' \leq \alpha$ *be fixed and suppose that* $\Omega^0 \subset \Omega$. *Then,* $\Omega_n \xrightarrow{\mathcal{O}} \Omega$, $n \to \infty$ *iff there is a sequence* $(\Phi_n)_{n\in\mathbb{N}} \subset U^{ad}_{k,\alpha}(\Omega^{ext})$, $\Phi \in U^{ad}_{k,\alpha}(\Omega^{ext})$ *such that* $\Phi_n(\Omega^0) = \Omega_n \, \forall n \in \mathbb{N}$, $\Phi(\Omega^0) = \Omega$ *and* $\Phi_n \to \Phi$, $n \to \infty$ *in* $[C^{k,\alpha'}(\overline{\Omega^{ext}})]^3$.

Lemma 5 $U^{ad}_{k,\alpha}(\Omega^{ext})$ *is compact in the Banach space* $\left([C^{k,\alpha'}(\overline{\Omega^{ext}})]^3, \|.\|_{[C^{k,\alpha'}(\Omega^{ext})]^3}\right)$ *for any* $0 \leq \alpha' < \alpha$ *and* $k \in \mathbb{N}$.

Proof The set $S := \left\{\Phi \in [C^{k,\alpha}(\overline{\Omega^{ext}})]^3 \,\middle|\, \|\Phi\|_{[C^{k,\alpha}(\Omega^{ext})]^3} \leq K\right\}$ is precompact in the Banach space $\left([C^{k,\alpha'}(\overline{\Omega^{ext}})]^3, \|.\|_{[C^{k,\alpha'}(\Omega^{ext})]^3}\right)$ as stated in Ramberg and Osgood (1943, 6.36).

Now, let Φ^* be the limit of a convergent sequence $(\Phi_n)_{n\in\mathbb{N}}$ in S regarding $\|.\|_{[C^{k,\alpha'}(\Omega^{ext})]^3}$. We use the abbreviation $\|.\|_{k,\alpha'}$ for the $\left[C^{k,\alpha'}\right]^3$-Norms on Ω^{ext} and define $K_n := \|\Phi_n\|_k$ and $\tilde{K_n} := \sup_{\substack{x,y\in\Omega^{ext} \\ |\beta|=k}} \frac{\left|\nabla^\beta\Phi_n(x)-\nabla^\beta\Phi_n(y)\right|}{|x-y|^\alpha}$. From the inequality

$$\|\Phi_n\|_{k,\alpha} = \|\Phi_n\|_k + \sup_{\substack{x,y\in\Omega^{ext} \\ |\beta|=k}} \frac{\left|\nabla^\beta\Phi_n(x) - \nabla^\beta\Phi_n(y)\right|}{|x-y|^\alpha} \leq K$$

and the $C^{k,\alpha'}$-convergence we conclude that $\tilde{K}_n \leq K - K_n$ for all $n \in \mathbb{N}$, as well as $K_n \xrightarrow{n\to\infty} K^* = \|\Phi^*\|_k \leq K$. What remains to be shown is that $\left|\nabla^\beta\Phi^*(x) - \nabla^\beta\Phi^*(y)\right| \leq (K-K^*)|x-y|^\alpha$ holds for every $|\beta| = k$, $x, y \in \Omega^{ext}$.

We apply triangle inequality to the left hand term and obtain

$$\begin{aligned}\left|\nabla^\beta\Phi^*(x) - \nabla^\beta\Phi^*(y)\right| \leq \left|\nabla^\beta\Phi^*(x) - \nabla^\beta\Phi_n(x)\right| + \left|\nabla^\beta\Phi_n(x) - \nabla^\beta\Phi_n(y)\right| \\ + \left|\nabla^\beta\Phi_n(y) - \nabla^\beta\Phi^*(y)\right|.\end{aligned}$$

Because of the uniform convergence of the k-th order derivatives, the first and the third term on the right hand side become zero as $n \to \infty$. The second one can be estimated by $\left|\nabla^\beta\Phi_n(x) - \nabla^\beta\Phi_n(y)\right| \leq (K-K_n)|x-y|^\alpha$ what leads to $\left|\nabla^\beta\Phi^*(x) - \nabla^\beta\Phi^*(y)\right| \leq (K-K^*)|x-y|^\alpha$ when passing to the limit. Therefore, S is closed. The latter is also true for $S^{-1} := \left\{\Phi^{-1} \,|\, \Phi \in S\right\}$. Since $\Phi_n \circ \Phi_n^{-1} = \Phi_n^{-1} \circ \Phi_n = id$ for all $n \in \mathbb{N}$ and $\Phi_n \in U^{ad}_{k,\alpha}$, it holds that $\lim_{n\to\infty} \Phi_n^{-1} = \Phi^*$ if $\Phi^* = \lim_{n\to\infty} \Phi_n$. Thus, $U^{ad}_{k,\alpha}$ is a closed subset of the compact set S and the statement holds. □

Definition 9 (**Baseline Design and Admissible Shapes**) *Let* $\Omega_0 \subset \mathbb{R}^3$ *be a* $C^{k,\alpha}$*-domain for some* $\alpha \in (0,1]$, $k > 0$. *Further let* $B := B_r(z) \subset \Omega_0$, $z \in int(\Omega_0)$, *be a ball in its interior having positive distance* $D := dist(B_r(z), \partial\Omega_0) > 0$ *from the boundary. Then we define the baseline design by* $\Omega_b := \Omega_0 \setminus B$. *The partition of the boundary requested in* (16) *shall be given by* $\partial\Omega_D := \partial B$ *and* $\partial\Omega_N := \partial\Omega_b \setminus \partial B$.

Let $R > r > 0$ be a radius such that $B_R(z) \Supset \Omega_0$ and choose $\Omega^{ext} = B_R(z)$, $\Omega^0 = \Omega_b$ together with the associated sets of design variables $U^{ad}_{k,\alpha} = U^{ad}_{k,\alpha}(\Omega^{ext})$ and admissible shapes $\mathcal{O}_{k,\alpha} = \mathcal{O}_{k,\alpha}(\Omega_b, \Omega^{ext})$.

With regard to the following sections we state here that, in particular, any $C^{k,\alpha}$-domain with $k + \alpha > 1$ has a $C^{0,1}$-boundary, and therefore satisfies a uniform cone property as explained in Chenais (1975). This is obviously the case for Ω_b. Moreover, for any admissible shape $\Omega = \Phi(\Omega_b) \in \mathcal{O}_{k,\alpha}$, the partition of the boundary is given by $\partial\Omega_D := \partial\Phi(B)$ and $\partial\Omega_N := \partial\Phi(\Omega_b) \setminus \partial\Omega_D$.

Remark 2 (Volume Constraints) *One can easily restrict the set of admissible domains with geometric constraints. Let us take the volume constraint as an example and let $V = \int_{\Omega_b} dx$ be the volume of the considered baseline design Ω_b (or Ω^0 instead). We then consider only those deformation maps $\Phi \in U^{ad}_{k,\alpha}$ that preserve the volume of Ω_b, i.e.*

$$V = \int_{\Omega_b} dx = \int_{\Phi(\Omega_b)} dx = \int_{\Omega_b} |\det(\nabla\Phi)| \, dx. \tag{23}$$

Let $U^{ad}_{k,\alpha,V}$ be the set of all $\Phi \in U^{ad}_{k,\alpha}$ that fulfil (23). From this equation it is clear that $U^{ad}_{k,\alpha,V}$ is closed in $U^{ad}_{k,\alpha}$ (if $k \geq 1$) and therefore compact in the $C^{k,\alpha'}$-topology for $\alpha' < \alpha$.

Taking this into account, we see that all arguments of this article are equally valid for the set of admissible shapes $\mathcal{O}_{k,\alpha,V} = \{\Phi(\Omega_b) : \Phi \in U^{ad}_{k,\alpha,V}\}$ with volume constraint V.

6. Uniform Schauder estimates

Recall the mixed problem (19) from Section 3 and the definitions of design variables and admissible shapes from Section 5.

At the end of this paper we want to apply Theorem 1. In this section, suitable assumptions on $\mathcal{O}$ and on the functions appearing in (16) and (17) will be presented, such that the requirement of unique solubility of (19) is satisfied. This ensures the existence of the graph $\mathcal{G} = \{(\Omega, T(\Omega), u_T(\Omega)) \,|\, \Omega \in \mathcal{O}\}$, as claimed. We will also see that under appropriate assumptions the resulting solutions u_T and T are Hölder functions which ensures a proper definition of convergence of solution sequences $(u(\Omega_n))_{n\in\mathbb{N}}$ and $(T(\Omega_n))_{n\in\mathbb{N}}$. The crucial step, when showing compactness of $\mathcal{G}$ (see Lemma 11) by means of (20), is the application of Schauder estimates to prove the solution's uniform boundedness with respect to $\mathcal{O}$. This gives us the possibility to apply Lemma 13 which leads to the desired conclusion. Throughout Lemma 11 we will finally show lower semi continuity for a very general class of cost functionals, containing especially the one of ours.

6.1. Schauder estimates for linear elasticity equation

We start with a review of regularity results for the disjoint displacement-traction problem of linear elasticity, presented in Gottschalk and Schmitz (2015) and point out the main characteristics of the shape's geometry that lead to the uniformity of certain estimates. Since C^4-regularity is needed in Theorems 6.3-5 and 6.3-6 in Ciarlet (1988), which are used in the proof of Theorem 5.1 et seq. in Gottschalk and Schmitz (2015). Accordingly, we set $U^{ad} := U^{ad}_{4,\alpha}$, $\alpha \in (0,1)$ for the set of feasible design-variables and $\mathcal{O} := \mathcal{O}_{4,\alpha}$ for the set of admissible shapes.

Lemma 6 *Each $\Omega \in \mathcal{O}$ satisfies a hemisphere property where the corresponding hemisphere transformations are of class $C^{4,\alpha'}$, $\alpha' \in [0,\alpha]$ and have a uniform bound $\mathcal{K}$ with respect to $\mathcal{O}$.*

Proof First, we note that Ω_b satisfies a hemisphere condition, see Definition 14. This can be proven analogously to Lemma 5.4 in Gottschalk and Schmitz (2015) because Ω_b is a $C^{4,\alpha}$ domain and thus its compact boundary can be parametrized by a finite family of uniformly bounded $C^{4,\alpha}$-functions in two variables. The resulting hemisphere transformations depend on the point $z_0 \in \Omega_b$, lying at a sufficient small distance $0 < d < \frac{D}{2}$ from the boundary that depends on the curvature of the boundary and on D, which is given in Definition 9.

Since every $\Phi \in U^{ad}$ is a $C^{4,\alpha}$-diffeomorphism, the compositions $\mathcal{T}_{\Phi,z_0} := \Phi \circ \mathcal{T}_{z_0}$ are again hemisphere transformations: the functions $\Phi \in U^{ad}$ are one to one mappings from Ω_b to $\Phi(\Omega_b)$ that are uniformly bounded. Therefore, we have a constant $\mathcal{K} > 0$, depending on Ω_b, but not on the choice of Φ, where

$$\mathcal{K}^{-1}|x-y| \leq |\Phi(x) - \Phi(y)| \leq \mathcal{K}|x-y| \tag{24}$$

for all $x, y \in \Omega_b$, see (6.29) in Gilbarg and Trudinger (1977). As a consequence, we set $d' = K^{-1}d$ (uniformly for all $\Omega \in \mathcal{O}$) and construct the new neighborhood U' as a proper extension of $\Phi(U \cap \Omega_b)$ beyond the boundary. At last, we apply the chain rule and see that the transformations $\mathcal{T}_{\Phi,z_0}$ are even uniformly (with respect to $\mathcal{O}$) bounded in the $C^{4,\alpha'}$-norms, $0 \leq \alpha' \leq \alpha$, because the functions Φ and $\mathcal{T}_{z_0}$ are. This is also true for the inverse functions by analogous arguments.□

Example 1 *Let $O \subset \mathbb{R}^3$ be a C^1-domain where $\psi : B_a(0) \subset \mathbb{R}^2 \to \mathbb{R}$ describes a part of the upper boundary. Then, $\mathcal{T} : \Sigma_a \subset \mathbb{R}^3 \to \tilde{\Sigma} \subset \Omega$, where*

$$\mathcal{T}(z_1, z_2, z_3) := \begin{pmatrix} z_1 \\ z_2 \\ \psi(z_1, z_2) - z_3 \end{pmatrix}, \tag{25}$$

defines a one to one mapping from the half ball Σ_a with radius a at $0 \in \mathbb{R}^3$ to $\tilde{\Sigma}_a$.

Due to its construction, every shape $\Omega \in \mathcal{O}$ has a Lipschitz-boundary and the associated Lipschitz constant can be chosen uniformly, what is proved to be equivalent to a uniform cone property in Chenais (1975). Hence, the following Lemma is applicable:

LEMMA 7 *(Gottschalk and Schmitz, 2015) Suppose that $\mathcal{M}$ is a set of bounded domains in $\mathbb{R}^n$ satisfying a uniform cone property and let $\Omega \in \mathcal{M}$. Then, for every $\varepsilon > 0$ there is a constant $C(\varepsilon) > 0$ that is uniform with respect to $\mathcal{M}$ and that satisfies $\|v\|_{C^0(\Omega)} \leq \varepsilon \|v\|_{C^1(\Omega)} + C(\varepsilon) \int_\Omega |v| dx$ for all $v \in C^1(\Omega)$.*

One of the complications when setting up a realistic shape optimization problem is the definition of the surface force density g. While the volume force densities are easily defined as gravitational or centrifugal loads, the surface load g generally depends on the shape Ω in a non trivial way. Often, $g = g(\Omega)$ will be defined by the static pressure of a fluid surrounding Ω. In this paper we do not intend to give a solution to this problem. The following definition sets a framework that is capable to deal with such effects.

DEFINITION 10 (ADMISSIBLE SURFACE FORCE MODEL) *Let $G(\mathcal{O}, \phi) := \dot{\bigcup}_{\Omega \in \mathcal{O}} [C^{2,\phi}(\partial\Omega)]^3$ be a collection of surface forces in $[C^{2,\phi}(\partial\Omega)]^3$ over $\Omega \in \mathcal{O}$. We define the space of admissible surface force models as continuous mapping¶ $\mathcal{O} \ni \Omega \to g(\Omega) \in [C^{2,\phi}(\partial\Omega)]^3 \subseteq G(\mathcal{O}, \phi)$ with uniform bound.*

Continuity here means that for $\Omega_n \to \Omega$ in $\mathcal{O}$, there exists $\Omega^{ext} \Supset \Omega_n, \Omega$ and norm-preserving extensions of $g(\Omega_n)$ to $[C^{2,\phi}(\Omega^{ext})]^3$ such that $g(\Omega)_n^{ext}\restriction\partial\Omega$ converges in $[C^{2,\phi}(\partial\Omega)]^3$.

We set $G^{ad}(\mathcal{O}, \phi) := \{\bar{g} : \mathcal{O} \to G(\mathcal{O}, \phi)$ continuous s.t. $\bar{g}(\Omega) \in [C^{2,\phi}(\partial\Omega)]^3$ and $\exists\, 0 < k_1 < \infty$ s.t. $\|\bar{g}(\Omega)\|_{[C^{2,\phi}(\partial\Omega)]^3} \leq k_1\ \forall \Omega \in \mathcal{O}\}$.

With every $\bar{g} \in G^{ad}$ we can thus associate surface force boundary conditions $\bar{g}(\Omega)$ to any set $\Omega \in \mathcal{O}$ that has a uniform common bound on their $[C^{2,\phi}(\partial\Omega)]^3$ norm. The following example has been used in Gottschalk and Schmitz (2015):

EXAMPLE 2 *Let $g^{ext} \in [C^{2,\phi}(\Omega^{ext})]^3$ be an arbitrary mapping. Then we can define $\bar{g} \in G^{\mathrm{ad}}(\mathcal{O}, \phi)$ by $\bar{g}(\Omega) := g^{ext}\restriction_{\partial\Omega}$ with $k_1 = \|g^{ext}\|_{[C^{2,\phi}(\partial\Omega)]^3}$.*

THEOREM 2 *(Gottschalk and Schmitz, 2015, Theorems 5.6, 5.7) Recall the PDE ($\mathbb{P}$) with $\Omega = \Phi(\Omega_b)$ for some $\Phi \in U^{ad}$.*

(i) Let $f_M \in [C^{1,\phi}(\overline{\Omega^{ext}})]^3$, $g_M \in [C^{2,\phi}(\overline{\Omega^{ext}})]^3$ for some $\phi \in (0,1)$ ‖. Then there exists a unique solution $u \in [C^{3,\phi}(\overline{\Omega})]^3$ that satisfies

$$\|u\|_{[C^{3,\varphi}(\Omega)]^3} \leq C\big(\|f_M\|_{[C^{1,\phi}(\Omega)]^3} + \|g_M\|_{[C^{2,\phi}(\partial\Omega)]^3} + \|u\|_{[C^0(\Omega)]^3}\big) \quad (26)$$

for any $\varphi \in (0, \phi)$ and some positive constant C independent from $\Omega \in \mathcal{O}$.

(ii) Let $f_M \in [C^{2,\phi}(\overline{\Omega^{ext}})]^3$. Moreover, let $g_M = \bar{g}(\Omega)$ be the mapping associated to some $\bar{g} \in G^{ad}(\mathcal{O}, \phi)$. Then, the term $\|u\|_{[C^0(\Omega)]^3}$ can be replaced by $\int_\Omega |u|\, dx$ by means of Lemma 7 and even

$$\|u\|_{[C^{3,\varphi}(\Omega)]^3} \leq C^M \quad (27)$$

¶ g can be seen as a section of the fibre bundle $G(\mathcal{O}, \phi)$.

‖ $C^{k,\alpha}(\overline{\Omega})$ and $C^{k,\alpha}(\Omega)$-functions can be identified and therefore replaced by each other, see Gilbarg and Trudinger (1977) *holds for any* $\varphi \in [0, \phi)$ *and constant* $C^M > 0$ *which can be chosen uniformly w.r.t.* $\mathcal{O}$.

Proof The proof is essentially the same as in Theorem 5.6 in Gottschalk and Schmitz (2015). We only have to show that it also holds for the extended set of geometries $\mathcal{O} = \mathcal{O}_{k,\alpha}$ that is considered in this paper. Two aspects of the geometry definition are relevant for the uniform Schauder estimates: uniform bounds θ of hemisphere transformations that (locally) straighten out the boundary $\partial\Omega$ are build in our definition of admissible shapes $\mathcal{O}$ and enter the minor constant, see Agmon, Douglis and Nirenberg (1964). In fact, let $\Phi_i : U_i \to \Sigma$ be a finite collection of $C^{4,\alpha}$-hemisphere transformations on Ω_b such that U_i cover $\partial\Omega$, see Definition 14. Obviously, the $C^{4,\alpha}$ norms of Φ_i and Φ_i^{-1} are uniformly bounded. However, for $\Omega = \Phi(\Omega)$ with $\Phi \in U^{\mathrm{ad}}_{k,\alpha}$, the same applies to the sets $U_i' = \Phi(U_i)$ with hemisphere transformations $\Phi_i' = \Phi_i \circ \Phi$. Clearly, the $C^{4,\alpha}$-norms of these transformations and their inverses only depend on the related norms of the Φ_i and the constant K, used in the definition of $U^{ad}_{k,\alpha}$.

We also need a uniform lower bound $\delta^* > 0$ of the radii of the balls on which the boundary is straightened by hemisphere transformations. This bound δ^* can be constructed as shown in Lemma 8 further on.

6.2. Schauder estimates for the heat equation

Recall the heat equation (17) presented in Section 3. By application of Theorem 6.31 from Gilbarg and Trudinger (1977) it is easy to see that there is a unique solution $T \in C^{2,\phi}(\overline{\Omega})$ of (17) for every $\Omega \in \mathcal{O}$ and every $\phi \in (0,1)$, supposing that $\eta \in C^{1,\phi}(\overline{\Omega})$, $\eta > 0$ and $T_e \in C^{1,\phi}(\overline{\Omega})$.

Assume that $T \in C^{2,\phi}(\overline{\Omega})$ is a solution of (17) for some $\Omega \in \mathcal{O}$ and suppose that $0 < \varphi < \phi$. Then we can apply inequality (26) to (19), which is equivalent to the problem (16) with load vector fields $\tilde{f}_M = f_M - \rho(3\lambda + 2\mu)\nabla T$ and $\tilde{g}_M = g_M + \rho(3\lambda + 2\mu)(T - T_0) \cdot \nu$. Together with triangle inequality and Lemma 7 we obtain for the unique solutions u of (16) and u_T of (19)

$$\begin{aligned}
&\|u_T\|_{[C^{3,\varphi}(\Omega)]^3}\\
&\le C\left(\|f_M - c\nabla T\|_{[C^{1,\phi}(\Omega)]^3} + \|g_M - c(T - T_0)\cdot\nu\|_{[C^{2,\phi}(\partial\Omega)]^3} + \|u\|_{[C^0(\Omega)]^3}\right)\\
&\le C\big(\|f_M\|_{[C^{1,\phi}(\Omega)]^3} + \|g_M\|_{[C^{2,\phi}(\partial\Omega)]^3} + \varepsilon\|u\|_{[C^1(\Omega)]^3} + C(\varepsilon)\int_\Omega |u|\,dx\big)\\
&+Cc\left(\|\nabla T\|_{[C^{1,\phi}(\Omega)]^3} + \|T - T_0\|_{C^{2,\phi}(\partial\Omega)}\|\nu\|_{[C^{2,\phi}(\partial\Omega)]^3}\right)
\end{aligned}$$

with $c = \rho(3\lambda + 2\mu)$. Thus,

$$\begin{aligned}
&(1 - \varepsilon C)\|u_T\|_{[C^{3,\varphi}(\Omega)]^3} \le C_{f,g} + C\rho(3\lambda + 2\mu)\\
&\left(\|\nabla T\|_{[C^{1,\phi}(\Omega)]^3} + \|T - T_0\|_{C^{2,\phi}(\partial\Omega)}\|\nu\|_{[C^{2,\phi}(\partial\Omega)]^3}\right). \qquad (28)
\end{aligned}$$

As explained in the proof of Theorem 5.7 in Gottschalk and Schmitz (2015) it can be shown by applying two times the Korn's second inequality to the L^1-Norm of u that the constant $C_{f,g}$ can be chosen to be uniform w.r.t $\mathcal{O}$. The latter is also true for $\|\nu\|_{[C^{2,\phi}(\partial\Omega)]^3} \leq \tilde{C}$, see the proof of Lemma 8. Hence, it will be sufficient to show that $\|T\|_{C^{2,\phi}(\Omega)} \leq C^T$ for a constant C^T independent of $\Omega \in \mathcal{O}$ to derive uniform boundedness of the solutions u of (19).

The following result is presented, but not proven in detail in Gilbarg and Trudinger (1977). In order to prove the uniformity of the constant C^T, occurring in the subsequent Lemma, we revisit the results presented in Gilbarg and Trudinger (1977) Lemma 6.5 and Theorem 6.6:

Theorem 3 (***Schauder Estimates for Elliptic PDE with Convective BC***) *Let Ω be a $C^{2,\phi}$ domain in $\mathbb{R}^n$ and let $T \in C^{2,\phi}(\overline{\Omega})$ be a solution of the boundary value problem (BVP)*

$$\begin{aligned} LT &= f_T \text{ on } \Omega, \\ BT &\equiv g_T \text{ on } \partial\Omega. \end{aligned} \tag{29}$$

Define the convective (Robin) boundary condition by

$$BT(x) = \gamma(x)T + \sum_{i=1}^{n} \beta_i(x)\nabla_i T(x),\ x \in \partial\Omega \tag{30}$$

where the normal component $\beta_\nu = \beta \cdot \nu$ of the vector $\beta = (\beta_1, ..., \beta_n)$ is non zero and $|\beta_\nu(x)| \geq \theta > 0$ on $\partial\Omega$ for some constant θ. It is assumed that the operator L, defined by

$$LT(x) = \sum_{i,j=1}^{n} a_{i,j}(x)\nabla_i\nabla_j T(x) + \sum_{i=1}^{n} b_i(x)\nabla_i T(x) + c(x)T(x),\ x \in \Omega \tag{31}$$

is strictly elliptic with ellipticity constant l and that

$$f_T \in C^{\phi}(\overline{\Omega}),\ g_T \in C^{1,\phi}(\overline{\Omega}),\ a_{i,j},\ b_i,\ c \in C^{\phi}(\overline{\Omega})$$

and γ, $\beta_i \in C^{1,\phi}(\overline{\Omega})$ with

$$\|a_{i,j},\ b_i,\ c\|_{C^{0,\phi}(\Omega)},\ \|\gamma,\ \beta_i\|_{C^{1,\phi}(\Omega)} \leq \mathcal{L},\ i,j = 1, \ldots, n. \tag{32}$$

Then

$$\|T\|_{C^{2,\phi}(\Omega)} \leq C\left(\|T\|_{C^0(\Omega)} + \|g_T\|_{C^{1,\phi}(\Omega)} + \|f_T\|_{C^{0,\phi}(\Omega)}\right) \tag{33}$$

where $C = C_{n,\phi,l,\mathcal{L},\theta,\Omega}$.

Proof We choose a $C^{2,\phi}$-diffeomorphism $\tau = \tau(x_0)$ that straightens the boundary in a neighborhood N of a point $x_0 \in \partial\Omega$. Let $B_\delta(x_0) \Subset N$ and set

$$B_0 = B_\delta(x_0) \cap \Omega, \qquad \Gamma_0 = B_\delta(x_0) \cap \partial\Omega \subset \partial B_0. \tag{34}$$

Consider the local problem

$$\begin{aligned} LT &= f_T && \text{in } B_0 \\ \gamma(x)T_e(x) &= \gamma(x)T(x) + \textstyle\sum_{i=1}^n \beta_i(x)\nabla_i T(x) && \text{on } \Gamma_0, \end{aligned}$$

which is transformed to

$$\begin{aligned} \tilde{L}\tilde{T}(y) &= \tilde{f}_T(y) && \text{in } \tilde{B}_0 \\ \tilde{\gamma}(y)\tilde{T}_e &= \tilde{\gamma}(y)\tilde{T}(y) + \textstyle\sum_{i=1}^n \tilde{\beta}_i(x)\nabla_i \tilde{T}(y) && \text{on } \tilde{\Gamma}_0, \end{aligned}$$

by τ. For $y = \tau(x)$, $\tilde{T}(y) = T(x)$, the equation

$$[\tilde{L}\tilde{T}](y) = \sum_{i,j=1}^n \tilde{a}_{i,j}(y)\nabla_i\nabla_j\tilde{T}(y) + \sum_{i=1}^n \tilde{b}_i(y)\nabla_i\tilde{T}(y) + \tilde{c}(y)\tilde{T}(y) = \tilde{f}_T(y)^{**}$$

holds for $y \in \tilde{B}_0 = \tau(B_0)$. This defines again an elliptic PDE: since $\tilde{a}_{i,j}(y) = \sum_{r,s=1}^n (\nabla_r\tau_i(x))(\nabla_s\tau_j(x))a_{r,s}(x)$ we obtain for $x \in B_0$, $\xi \in \mathbb{R}^n$

$$\sum_{i,j=1}^n \tilde{a}_{i,j}\xi_i\xi_j \geq l\|\nabla\tau(x)\xi\|^2_{\mathbb{R}^3} = l\xi^\top\nabla\tau(x)^\top\nabla\tau(x)\xi.$$

Since τ is an $C^{2,\phi}$-diffeomorphism, its determinant is nowhere equal to zero and $\nabla\tau(x)^\top\nabla\tau(x)$ is symmetric, positive definite for any $x \in B_0$. Hence, $\nabla\tau^\top\nabla\tau = (S\mathcal{D}^{1/2})^\top\mathcal{D}^{1/2}S$ on B_0, where S is a suitable orthogonal matrix and $\mathcal{D}$ is a diagonal matrix, whose diagonal elements are the positive eigenvalues λ_i^τ, $i = 1,\ldots,n$ of $\nabla\tau^\top\nabla\tau$. We conclude that

$$\sum_{i,j=1}^3 \tilde{a}_{i,j}(y)\xi_i\xi_j \geq l\|\mathcal{D}^{1/2}(x)S(x)\xi\|^2_{\mathbb{R}^3} \geq l\,\lambda^\tau_{min}(x)\|\xi\|^2_{\mathbb{R}^3} \quad x \in B_0,\ \xi \in \mathbb{R}^n.$$

The eigenvalues depend continuously on x lying in the compact set $\overline{B_0}$, what gives us the possibility to choose a lower bound $l\,\lambda^\tau_{min}(x) \geq \tilde{l} > 0$.

By application of (6.30) from Gilbarg and Trudinger (1977) one sees that

$$\|\tilde{a}_{i,j}\|_{C^{0,\phi}(B_0)},\ \|\tilde{b}_i\|_{C^{0,\phi}(B_0)}, \|\tilde{c}\|_{C^{0,\phi}(B_0)} \leq \tilde{\mathcal{L}} = C_\tau\mathcal{L},$$

because τ is bounded from above in $\|.\|_{C^{2,\phi}(\Omega)}$. The latter is also true for $\|\tilde{\gamma}\|_{C^{1,\phi}(\tilde{B}_0)}$, where $\tilde{\gamma}(y) = \gamma(x)$, and $\|\tilde{\beta}_i\|_{C^{1,\phi}(\tilde{B}_0)}$ with $\tilde{\beta}_i(y) = \sum_{j=1}^n \beta_j(x)\nabla_j\tau_i(x)$ on the hyperplane portion $\tilde{\Gamma}_0 = \tau(\Gamma_0)$. Now we will show that $|\tilde{\beta}_n| \geq \tilde{\theta} > 0$, what is required for the statement in Lemma 6.29†† from Gilbarg and Trudinger (1977).

** For a detailed description see the proof of Lemma 6.5 in Gilbarg and Trudinger (1977).

†† Lemma 6.29 is analogous to Lemma 6.4, which is used in the proof of Lemma 6.5

Since $\tau : \Omega \subset \mathbb{R}^n \to \Sigma_R \subset \mathbb{R}^n$, we can consider $\nabla\tau(x)$ as a mapping between the tangential spaces at x and y, respectively, where $T_x \cong \mathbb{R}^n$ and $\mathbb{R}^n \cong T_y$. We choose an orthonormal basis (ONB) of vectorfields $(e'_1(x), \ldots, e'_{n-1}(x))$ of the tangential space assigned to the $n-1$ dimensional submanifold $\partial\Omega$ at $x \in \Gamma_0$ and extend it to an ONB $E'(x)$ of $\mathbb{R}^n$ by $e'_n(x) = \nu(x)$. Furthermore, we define $E = (e_1, \ldots, e_n)$ to be the standard ONB of $\mathbb{R}^n$. Then, it holds that

$$\begin{aligned}|\tilde{\beta}_n(y)| =& |e_n^\top \nabla\tau(x)\beta(x)| = |e_n^\top \nabla\tau(x) \left(\|\beta_\nu(x)\|_{\mathbb{R}^n} \nu(x) + \beta_T \right)| \\ =& |\beta_\nu(x)| \left| e_n^\top \nabla\nu(x) \right| \geq \theta \left| e_n^\top \nabla\tau(x) e'_n(x) \right| .\end{aligned}$$

We contemplate the matrix $B_{i,j} = e_i^\top \nabla\tau e'_j$, $i,j = 1, \ldots, n$ for $x \in \Gamma_0$. Because both, E and $E'(x)$, are ONB of the $\mathbb{R}^n$, there exists an orthogonal matrix $O(x)$, $x \in \Gamma_0$ where $e'_i(x) = O(x)e_i$, $\forall\, x \in \{1, \ldots, n\}$. Thereby we deduce

$$B_{i,j} = \sum_{k=1}^{n} e_i \nabla\tau e_k O_{k,j} = (\nabla\tau O^\top)_{i,j},\ i,j = 1, \ldots, n$$

and

$$|\det(B(x))| = \left| \det\left(\nabla\tau(x) O(x)^\top \right) \right| = |\det\left(\nabla\tau(x)\right)| \geq C_1 > 0.$$

On the other hand, $B_{n,j} = e_n^\top \nabla\tau e'_j = e_n e_j = 0$ for every $j \neq n$ and $B_{n,n} = e_n^\top \nabla\tau e'_n$. Thus, the matrix B has the structure

$$B = \left(\begin{array}{c|c} \left(\nabla\tau(x)O(x)^\top\right)_{i,j=1,\ldots,n-1} & \vec{b} \\ \hline \vec{0}^\top & e_n^\top \nabla\tau e'_n \end{array} \right), \quad \vec{b}, \vec{0} \in \mathbb{R}^{n-1},$$

and its determinant can be calculated by

$$|\det(B(x))| = \left| \det\left(\nabla\tau(x)O(x)^\top\right)_{i,j=1,\ldots,n-1} \right| \left| e_n^\top \nabla\tau(x) e'_n(x) \right| \leq C_2 \left| e_n^\top \nabla\tau_x e'_n(x) \right| .$$

In consequence,

$$C_2 \left| e_n^\top \nabla\tau_x e'_n(x) \right| \geq C_1 > 0 \ \Leftrightarrow\ \left| e_n^\top \nabla\tau_x e'_n(x) \right| \geq \frac{C_1}{C_2} := C > 0$$

and finally

$$|\tilde{\beta}_n(y)| \geq \theta C := \tilde{\theta} > 0.$$

All conditions requested in the mentioned Lemma 6.29 from Gilbarg and Trudinger (1977) are fulfilled, what yields

$$\|\tilde{T}\|^*_{C^{2,\phi}(\tilde{B}_0 \cup \tilde{\Gamma}_0)} \leq \tilde{C} \left(\|\tilde{T}\|_{C^0(\tilde{B}_0)} + \|\tilde{g}_T\|_{C^{1,\phi}(\tilde{\Gamma}_0)} + \|\tilde{f}_T\|_{C^{0,\phi}(\tilde{B}_0)} \right),$$

with a constant $\tilde{C}$ that depends on n, ϕ, $\tilde{l}$, $\tilde{\mathcal{L}}$, $\tilde{\theta}$, $\mathrm{diam}(\tilde{B}_0)$. Now we use exactly the same arguments which are applied in Gilbarg and Trudinger (1977) and obtain for $B_0' = B_{\delta/2}(x_0)$

$$\|T\|_{C^{2,\phi}(B_0')} \leq C\left(\|T\|_{C^0(B_0)} + \|g_T\|_{C^{1,\phi}(\Gamma_0)} + \|f_T\|_{C^{0,\phi}(B_0)}\right) \tag{35}$$

where $C = C_{n,\phi,l,\mathcal{L},\theta,\mathrm{diam}(B_0),\tau}$ due to the construction of the coefficients $\tilde{l}$, $\tilde{\mathcal{L}}$, $\tilde{\theta}$, and the structure of the set $\tilde{B}_0$.

Since the boundary of Ω is compact, one needs only a fixed number m of points x_i and radii δ_i to cover the whole boundary. We choose $\delta^* = \min \delta_i/4$, $B = B_{\delta^*}(x_0)$ and assert that

$$\|T\|_{C^{2,\phi}(B\cap\Omega)} \leq C\left(\|T\|_{C^0(\Omega)} + \|g_T\|_{C^{1,\phi}(\partial\Omega)} + \|f_T\|_{C^{0,\phi}(\Omega)}\right) \tag{36}$$

for the maximum $C = C_i$ that is assigned to x_i, $i = 1, \ldots, m$, appearing in (35). Therefore, $C = C_{n,\phi,l,\mathcal{L},\theta,\Omega}$, where the dependence on Ω is through the radius δ^*, the transformations τ and $\mathrm{diam}(\Omega)$.

The remainder of the proof is essentially the same as for Theorem 6.6 in Gilbarg and Trudinger (1977), but with (36) instead of (6.32). Using the same distinction of cases as in the just mentioned theorem we end up with

$$\|T\|_{C^{2,\phi}(\Omega)} \leq C\left(\|T\|_{C^0(\Omega)} + \|g_T\|_{C^{1,\phi}(\Omega)} + \|f_T\|_{C^{0,\phi}(\Omega)}\right) \tag{37}$$

where $C = C_{n,\phi,l,\mathcal{L},\theta,\Omega}$ and the dependence of Ω is subject to δ^*, τ and $\mathrm{diam}(\Omega)$. □

In practical applications, the shape dependence of the external temperature and heat transfer coefficient, as coded by $T_e = T_e(\Omega)$ and $\eta = \eta(\Omega)$, requires the solution of further (fluid dynamical and thermal) PDEs in a computational domain external to Ω, see e.g. Incropera and DeWitt (1998), and Kays, Crawford and Weigand (2004). As we do not intend to investigate these processes here, we encode this dependence‡‡ in the following definitions.

Definition 11 (Admissible Heat Transfer Boundary Conditions) *We consider an assignment of heat transfer coefficients $\eta = \eta(\Omega)$ and external temperatures $T_e = T_e(\Omega)$ in a related way as we did for the admissible surface force model, see Definition 10. In particular, the continuity of such assignments is defined in an analogous way with $C^{2,\phi}$ replaced by $C^{1,\phi}$.*

We set $\mathcal{E}^{ad}(\mathcal{O},\phi) := \{\bar{\eta} : \mathcal{O} \to \mathcal{E}(\mathcal{O},\phi)$ continuous s.t. $\bar{\eta}(\Omega) \in C^{1,\phi}(\partial\Omega)$, $\bar{\eta}(\Omega) > 0$ and $\exists 0 < k_2 < \infty$ s.t. $\|\bar{\eta}(\Omega)\|_{C^{1,\phi}(\partial\Omega)} \leq k_2\ \forall \Omega \in \mathcal{O}\}$ where $\mathcal{E}(\mathcal{O},\phi) = \dot{\bigcup}_{\Omega\in\mathcal{O}} C^{1,\phi}(\partial\Omega)$.

Furthermore, $\mathcal{T}^{ad}(\mathcal{O},\phi) = \{\tilde{T}_e : \mathcal{O} \to \mathcal{E}(\mathcal{O},\phi)$ continuous s.t. $\tilde{T}_e(\Omega) \in C^{1,\phi}(\partial\Omega)$ and $\exists 0 < k_3 < \infty$ s.t.$\|\bar{\eta}(\Omega)\|_{C^{1,\phi}(\partial\Omega)} < k_3\}$.

‡‡On physical grounds, we expect such conditions to hold for stationary, laminar subsonic external flow fields, but not necessarily for fields that show shocks during the transition from sub- to supersonic fluid speed. Related problems with shocks are also expected for surface force models.

Lemma 8 *Let the heat equation* (17) *be given on a domain* $\Omega = \Phi(\Omega_b) \in \mathcal{O}$. *Suppose that* $\eta \in \mathcal{E}^{ad}(\mathcal{O}, \phi)$ *and* $T_e \in \mathcal{T}^{ad}(\mathcal{O}, \phi)$ *are admissible heat transfer boundary conditions in the sense of Definition 11. Then, there is a constant* $C > 0$ *such that*

$$\|T\|_{C^{2,\phi}(\Omega)} \leq C \left(\|T\|_{C^0(\Omega)} + \|\eta T_e\|_{C^{1,\phi}(\Omega)} \right) \tag{38}$$

holds for the unique solution $T \in C^{2,\phi}(\overline{\Omega})$ *of* (17). *Moreover, the constant* C *can be chosen uniformly with respect to* $\mathcal{O}$.

Proof We apply Theorem 3 and Theorem 6.31 from Gilbarg and Trudinger (1977) to

$$\begin{aligned} \Delta T &= 0 && \text{in } \Omega \\ \left(\tfrac{\eta}{\kappa}\right) T_e &= \left(\tfrac{\eta}{\kappa}\right) T + \textstyle\sum_{i=1}^{3} \nu_i \nabla_i T && \text{on } \partial\Omega, \end{aligned}$$

for $\Omega \in \mathcal{O}$.

Hence, the existence of a unique solution is ensured and we essentially have to comprehend the proof of the last mentioned theorem in detail in order to obtain precise information regarding the appearing constants:

We first notice that any $l \leq 1$ can be chosen for the ellipticity parameter and so we set $l = 1$. The outward normal ν is a $[C^{3,\alpha}(\partial\Omega)]^3$-function (the boundary is of class $C^{4,\alpha}$) and a parametrization of the boundary can be constructed using the uniformly bounded hemisphere transformations, what implies that $\|\nu\|_{[C^{1,\phi}(\overline{\Omega})]^3} \leq \|\nu\|_{[C^{2,\phi}(\overline{\Omega})]^3} \leq \mathcal{L}_1$ independent of Ω. The $C^{0,\phi}$-norms of $a_{i,j}(x) \in \{0, 1\}$, $b_i(x) = c(x) = 0$ surely cannot be greater than $\mathcal{L}_2 = 1$ and $\|\eta\|_{C^{1,\phi}(\overline{\Omega})} \leq \mathcal{L}_3(= k_2)$ holds by choice of η. Therefore, we choose $\mathcal{L}$ in (32) as their maximum. Finally, let $\theta < 1 = \|\nu\|_{\mathbb{R}^3}$. Then we derive from inequality (38) that

$$\|T\|_{C^{2,\phi}(\Omega)} \leq C \left(\|T\|_{C^0(\Omega)} + \|\eta T_e\|_{C^{1,\phi}(\Omega)} \right)$$

applies with $C = C_\Omega$ and that the dependence of Ω is subject to the choice of δ, τ and $\mathrm{diam}(\Omega)$ appearing in the proof of Theorem 6.7 in Gilbarg and Trudinger (1977).

Because every $\Omega \in \mathcal{O}$ satisfies the uniform hemisphere condition with uniform $d' > 0$ and transformations $\tau_i = \tau(z_i), z_i \in \Omega, i = 1, \ldots, n$ *s.t.* $\mathrm{dist}(z_i, \partial\Omega) < d'$ (constructed as in Lemma 6) we can choose $\delta = {d'}/{2}$ in (34) and as a consequence $\delta^* = {d'}/{8}$ in (36). Furthermore, for any $\tau \in \{\tau_i\}$ the minimal eigenvalue function $\lambda^\tau_{\underline{min}}(x) > 0$ depends continuously on τ and on $x \in \Omega$. However, we know that $\overline{\Omega}$ is compact, and the set of transformations is as well, regarding the $C^{k,\alpha'}$-norms, where $k + \alpha' < 4 + \alpha$. We conclude that there has to be a lower bound $\lambda^* \leq \lambda^\tau_{min}(x)$ for all $x \in \Omega$ and hemisphere transformations $\tau \in \{\tau_i\}$. Consequently, it is uniform w.r.t. $\mathcal{O}$. The global boundedness of $\|\tau\|_{[C^1(\Omega)]^3} \leq \|\tau\|_{[C^{4,\alpha}(\Omega)]^3}$ implies that $\tilde{\mathcal{L}} = \mathcal{L}C_\tau \leq \mathcal{L}^*$ is as well, and for essentially the same reasons the assertion $\tilde{\theta} = \theta\frac{C_1}{C_2} > \theta^*$ holds, too. For $\mathrm{diam}(\Omega)$ we notice that

$$\operatorname{diam}(\Omega) = \sup_{x,y\in\Omega} \|x-y\|_{\mathbb{R}^3} \leq \mathcal{K} \sup_{x',y'\in\Omega_b} \|x'-y'\|_{\mathbb{R}^3} \leq \mathcal{K}\operatorname{diam}(\Omega_b),$$

where $\mathcal{K}$ is a constant depending again only on the transformation τ and Ω_b, compare (24). □

The norms of η and T_e are naturally bounded by the choice of these functions. What is left to be shown, is that the latter is also true for $\|T\|_{C^0(\Omega)}$:

Lemma 9 *Let the setting of the previous Lemma be given and suppose that $T \in C^{2,\phi}(\overline{\Omega})$ is the unique solution of (17). For the constants $T_- = \min\{T_e(x) \,|\, x \in \overline{\Omega^{ext}}\}$ and $T_+ = \max\{T_e(x) \,|\, x \in \overline{\Omega^{ext}}\}$ it holds that*

$$T_- \leq \min_{x\in\overline{\Omega}} T(x) \leq \max_{x\in\overline{\Omega}} T(x) \leq T_+. \tag{39}$$

Proof We prove the statement for T_+ only, because the proof for T_- proceeds analogously.

The solution $T \in C^{2,\phi}(\overline{\Omega})$ satisfies $\Delta T = 0$ on Ω and therefore it is harmonic as well as subharmonic. By application of the maximum and minimum principle, see Evans (2010) and Gilbarg and Trudinger (1977), we conclude that $\min_{x\in\overline{\Omega}} T(x) = \min_{x\in\partial\Omega} T(x)$ and $\max_{x\in\overline{\Omega}} T(x) = \max_{x\in\partial\Omega} T(x)$.

Now suppose that there is some $x_0 \in \partial\Omega$ where $T(x_0) > T_+$. Then,

$$\frac{\partial T}{\partial\nu}(x_0) = \left(\frac{\eta(x_0)}{\kappa}\right)(T_e(x_0) - T(x_0)) \leq \left(\frac{\eta(x_0)}{\kappa}\right)(T_+ - T(x_0)) < 0,$$

because $\frac{\eta}{\kappa} > 0$ on $\overline{\Omega}$ and $T_e(x) \leq T_+$ for all $x \in \overline{\Omega^{ext}}$. Let $\varepsilon > 0$. Consistently, $x_0 - \varepsilon\nu(x_0)$ is contained in $\mathring{\Omega}$ and we obtain, by the first order Taylor series

$$T(x_0 - \varepsilon\nu(x_0)) = T(x_0) - \varepsilon\left[\nu(x_0)^\top \nabla T(x_0) - \frac{1}{\varepsilon}(r(x_0 - \varepsilon\nu(x_0))\right],$$

where

$$\frac{|r(x_0 - \varepsilon\nu(x_0))|}{\|\varepsilon\nu(x_0)\|_{\mathbb{R}^3}} = \frac{|r(x_0 - \varepsilon\nu(x_0))|}{\varepsilon} \to 0 \text{ for } \varepsilon \to 0.$$

On the other hand, it holds that

$$\nu(x_0)^\top \nabla T(x_0) = \frac{\partial T}{\partial\nu}(x_0) < 0.$$

If we choose $\varepsilon > 0$ small enough, the term $\nu(x_0)^\top \nabla T(x_0) - \frac{1}{\varepsilon}(r(x_0 - \varepsilon\nu(x_0))$ will be negative, as well, and thus $T(x_0 - \varepsilon\nu(x_0)) > T(x_0)$, what contradicts the maximum principle. □

Theorem 4 *Let the setting of Lemma 8 be given on a domain $\Omega = \Phi(\Omega_b) \in \mathcal{O}$ and let $T \in C^{2,\phi}(\Omega)$ be the unique solution of* (17)*. Then, $T \in C^{2,\phi}(\overline{\Omega})$ and there is a positive constant $C^T > 0$ such that*

$$\|T\|_{C^{2,\phi}(\Omega)} \leq C^T, \tag{40}$$

where C^T can be chosen uniformly with respect to $\mathcal{O}$.

Proof The statement follows directly from Lemmata 8 and 9 and the assumptions from Definition 11. □

6.3. Schauder estimates for the heat dependent elasticity equation

In the last two sections we established the existence of unique and uniformly bounded solutions for elasticity equation and heat equations separately. In order to derive results for the combined problem we tie up to inequality (6.2): there, we assumed $T \in C^{2,\phi}(\overline{\Omega^{ext}})$, but in fact we only have $T \in C^{2,\phi}(\overline{\Omega})$.

Moreover, extensions of functions will be needed to define convergence of solution sequences in terms of Section 4 and to prove the compactness of the appropriate graph, see Section 7.

Definition 12 (**State Problem and State Space for Thermo–Elasticity)**

(i) Let $\Omega := \Phi(\Omega_b)$ be a $C^{4,\alpha}$-admissible shape for some $\alpha \in (0,1)$. Moreover, decompose the boundary into the interior boundary $\partial\Omega_D := \partial\Phi(B)$ and the complete exterior boundary $\partial\Omega_N = \partial\Omega \setminus \partial\Omega_D$. Then, the corresponding state problem for thermo elasticity $\mathcal{P}(\Omega)$ is given by equation (19).

(ii) Let $0 < \varphi < \phi < 1$. Moreover, assume that $\kappa > 0$ and that the Lamé coefficients λ, $\mu > 0$ are constants, as well as ρ. Additionally, choose $\eta \in \mathcal{E}(\mathcal{O}, \phi)$, and $T_e \in \mathcal{T}(\mathcal{O}, \phi)$ $f_M \in [C^{1,\phi}(\overline{\Omega^{ext}})]^3$, $g_M \in G(\mathcal{O}, \varphi)$, and $0 < \varphi' < \varphi$, $0 < \phi' < \phi$. Then, the state space for thermo elasticity is given by $V_P(\Omega) = C^{2,\phi'}(\overline{\Omega}) \oplus [C^{3,\varphi'}(\overline{\Omega})]^3$.

Note that the chosen decomposition of the boundary depends continuously on the choice of $\Phi \in U^{ad}$. Moreover, the two–dimensional Lebesgue measures of $\partial\Omega_N$ and $\partial\Omega_D$ are always bounded away from zero.

Theorem 5 *Let the state Problem $\mathcal{P}(\Omega)$ be defined as in Definition 12. Then, for every $\varphi \in (0, \phi)$ there exists a unique solution $(T, u_T) \in V_P(\Omega)$ of (19), where*

$$\begin{aligned} \|T\|_{C^{2,\phi}(\Omega)} &\leq C^T \\ \|u_T\|_{[C^{3,\varphi}(\Omega)]^3} &\leq C^{T/M} \end{aligned} \tag{41}$$

holds for the constant $C^T > 0$ of Theorem 4 and some constant $C^{T/M} > 0$ that also can be chosen independently of Ω. Remark that the tuple (T, u_T) is actually an element of $C^{2,\phi}(\overline{\Omega}) \oplus [C^{3,\varphi}(\overline{\Omega})]^3$.

Proof The existence of the unique solutions $T \in C^{2,\phi}(\overline{\Omega})$ and $u \in [C^{3,\varphi}(\overline{\Omega})]^3$ follows directly from Theorem 6.31 in Gilbarg and Trudinger (1977) and Theorem 2, confer Theorems 5.6 and 5.7 in Gottschalk and Schmitz (2015), too. Because $0 < \varphi < \phi$, the estimate (6.2) holds and we can conclude that for $\varepsilon > 0$ small enough, namely $\varepsilon C < 1$,

$$\|u_T\|_{[C^{3,\phi}(\Omega)]^3} \leq$$
$$\tfrac{C_{f,g}}{1-\varepsilon C} + \tfrac{C\rho(3\lambda+2\mu)}{1-\varepsilon C} \left(\|\nabla T\|_{[C^{1,\phi}(\Omega)]^3} + (|T_0| + \|T\|_{C^{2,\phi}(\partial\Omega)})\tilde{C} \right) \leq C^*,$$

since C was chosen uniformly, see Lemma 8. The constant $C_{f,g}$ can be chosen to be the same for any $\Omega \in \mathcal{O}$, due to the choice of f_M and g_M. The latter is also true for $\tilde{C}$ as already mentioned in the beginning of Section 6.2. Additionally, $\|\nabla T\|_{[C^{1,\phi}(\Omega)]^3} \leq c\|(\nabla T)_i\|_{C^{1,\phi}(\Omega)} \leq \|T\|_{C^{2,\phi}(\Omega)} \leq C^T$ uniformly in Ω. The starting temperature T_0 is constant. Therefore, C^* can be chosen to be uniform w.r.t. $\mathcal{O}$.

7. Existence of optimal shapes

In this section, we prove existence of optimal solutions to shape optimization problems where the constraints are given by thermal elasticity, see Section 3. The cost functionals considered are of a quite singular class and include surface integrals which lead to a loss of regularity according to the appearing derivatives of u and T and the trace theorem (see, for instance, Evans, 2010, 5.5). Therefore, they cannot be defined for weak solutions and, in consequence, we have to resort to regularity theory and strong solutions.

Our objective is to find an optimal shape $\Omega = \Phi(\Omega_b)$ within the set of $C^{4,\alpha}$-admissible shapes $\mathcal{O}$, from Definition 7, which minimizes a local cost functional $\mathcal{J}(\Omega, u, T) = \mathcal{J}_{vol}(\Omega, u, T) + \mathcal{J}_{sur}(\Omega, u, T)$, given by

$$\begin{aligned} \mathcal{J}_{vol}(\Omega, u, T) &= \int_\Omega \mathcal{F}_{vol}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)dx \\ \mathcal{J}_{sur}(\Omega, u, T) &= \int_{\partial\Omega} \mathcal{F}_{sur}(x, T, \nabla T, \nabla^2 T, u, \nabla u, \nabla^2 u, \nabla^3 u)dA. \end{aligned} \tag{42}$$

Here, the tuple (T, u) solves the state Problem $\mathcal{P}(\Omega)$.

In Sections 5 and 6 we prepared the application of Theorem 1 in the present constellation. Now, we are able to prove that the graph $\mathcal{G} = \{(\Omega, T, u) \,|\, \Omega \in \mathcal{O}\}$ is compact in the sense of (20). In the following definition we therefore choose $q = 2$, $\beta = \phi'$, respectively $q = 3$, $\beta = \varphi'$.

Definition 13 ($C^{q,\beta}$ Convergence of functions on Variable Domains) *Recall the sets $\mathcal{O}$ and Ω^{ext} from Section 5. Let $m, q \in \mathbb{N}$, $\beta \in (0,1)$ be fixed.*

i) Let $p_\Omega^{m,q,\beta} : \left[C^{q,\beta}(\overline{\Omega})\right]^m \to \left[C_0^{q,\beta}(\Omega^{ext})\right]^m$ be the extension operator that exists by Lemma 15. If $v \in \left[C^{q,\beta}(\overline{\Omega})\right]^m$ set $v^{ext} = p_\Omega^{m,q,\beta} v$.

ii) Let $(\Phi_n)_{n\in\mathbb{N}} \subset U^{ad}$, $\Phi \in U^{ad}$ and $\Omega_n := \Phi_n(\Omega_b) \in \mathcal{O}$, $\Omega = \Phi(\Omega_b) \in \mathcal{O}$. For $(u_n)_{n\in\mathbb{N}}$ with $u_n \in \left[C^{q,\beta}(\overline{\Omega_n})\right]^m$, $n \in \mathbb{N}$ and $u \in \left[C^{q,\beta}(\overline{\Omega})\right]^m$ we define the expression $u_n \rightsquigarrow u$ as $n \to \infty$ by $u_n^{ext} \to u^{ext}$ in $\left[C_0^{q,\beta}(\Omega^{ext})\right]^m$.

Lemma 10 *Let $\Omega \in \mathcal{O}$ be a $C^{4,\alpha}$-admissible shape for some $\alpha \in (0,1)$ and suppose $v \in C^{q,\beta}(\overline{\Omega})$, where $1 \leq q + \beta \leq 4 + \alpha$. Then, there exists a function $w \in C_0^{q,\beta}(\Omega^{ext})$ and a constant $C_q > 0$ such that $w = v$ in Ω^{ext} and*

$$\|w\|_{C^{q,\beta}(\Omega^{ext})} \leq C\|v\|_{C^{q,\beta}(\Omega)}$$

where $C = C_q$ is independent of Ω and Ω^{ext}.

Proof Confer the proof of Lemma 14 (see Gilbarg and Trudinger (1977)) and substitute Ω' by Ω^{ext} and Ω by Ω_b. Furthermore, we replace the $C^{k,\varphi}$ diffeomorphism ψ by the hemisphere transformations $\mathcal{T}_{x_0} : B_d(x_0) \to \Sigma_R$, $x_0 \in \partial\Omega_b$ introduced in Lemma 6, (25). Then, $G^+ = \Sigma_R$ and $G = B_R(0) \supset \Sigma_R$ is a ball with radius R at the origin of the coordinates. For $u \in C^{q,\beta}(\overline{\Omega_b})$, $q + \beta \leq 4 + \alpha$ one sets $\tilde{u}(y) = u \circ \mathcal{T}_{x_0}(y)$, where $y = (y', y_3)$, $y' = (y_1, y_2)$. We follow Gilbarg and Trudinger (1977) and define an extension into $y_3 < 0$ by

$$\tilde{u}(y', y_3) = \sum_{i=1}^{q} c_i \tilde{u}(y', -y_3/i), \ , y_3 < 0, \quad \sum_{i=1}^{q} c_i \left(-1/i\right)^m, \quad m = 0, \ldots, q+1.$$

Furthermore, one obtains that $w = \tilde{u} \circ \mathcal{T}_{x_0}^{-1}$ provides a $C^{4,\alpha}$-extension of u onto $\Omega_b \cup B(x_0)$ for some balls $B(x_0)$ and the related hemisphere transformation. A finite covering argument of $\partial\Omega_b$ and an associated partition of unity leads to the sought extension $w \in C_0^{q,\beta}\Omega^{ext}$. The fact that the constant C appearing in the inequality

$$\|w\|_{C^{q,\beta}(\Omega')} \leq C\|u\|_{C^{q,\beta}(\Omega)} \tag{43}$$

only depends on q, Ω', Ω is due to inequalities (6.29) and (6.30) in Gilbarg and Trudinger (1977), see the proof of Lemma 6.37 there. So, in our case, it depends mainly on Ω^{ext} and Ω_b, which are both fixed sets.

Given a function $v \in C^{q,\beta,}(\Omega)$, $1 \leq q + \beta \leq 4 + \alpha$ on $\Omega = \Phi(\Omega_b)$ for some $\Phi \in U^{ad}$, the mapping $u = v \circ \Phi$ defines a $C^{q,\beta}$ function on Ω_b. Then, an extension $w \in C^{q,\beta}(\Omega^{ext})$ can be defined as described above. Hence, $w = v \circ \Phi$ on Ω_b and $w \circ \Phi^{-1} = v$ on Ω is an extension of v, since Φ is a $C^{4,\alpha}$ diffeomorphism on Ω^{ext}. By application of (6.30) from Gilbarg and Trudinger (1977) and (43) we derive

$$\|w \circ \Phi^{-1}\|_{C^{q,\beta}(\Omega^{ext})} \leq \mathcal{C}\|w\|_{C^{q,\beta}(\Omega^{ext})} \leq \mathcal{C}C\|v \circ \Phi\|_{C^{q,\beta}(\Omega_b)} \leq \mathcal{C}^2 C\|v\|_{C^{q,\beta}(\Omega)},$$

for a suitable positive constant $\mathcal{C}$ that can be chosen uniformly w.r.t U^{ad} due to its construction. □

Lemma 11 (***Compactness of the Graph***) *Let $(\Omega_n)_{n\in\mathbb{N}} = (\Phi_n(\Omega_b))_{n\in\mathbb{N}} \subset \mathcal{O}$ be an arbitrary sequence where on any Ω_n the setting of Theorem 5 is given. By $(T_n, u_n) \in V_P(\Omega_n)$ we denote the corresponding solutions to the state problems $\mathcal{P}(\Omega_n)$. Then, the sequence $(\Omega_n, T_n, u_n)_{n\in\mathbb{N}}$ has a subsequence $(\Omega_{n_k}, T_{n_k}, u_{n_k})_{k\in\mathbb{N}}$ such that $\Omega_{n_k} \underset{k\to\infty}{\overset{\mathcal{O}}{\longrightarrow}} \Omega = \Phi(\Omega_b)$ as well as $T_{n_k} \underset{k\to\infty}{\rightsquigarrow} T$ and $u_{n_k} \underset{k\to\infty}{\rightsquigarrow} u$ such that (T, u) solves $\mathcal{P}(\Omega)$ and $(T, u) \in V_P(\Omega)$.*

Proof In terms of Lemma 5 there is a convergent subsequence $(\Phi_{n_l})_{l\in\mathbb{N}}$, tending to some $\Phi \in C^{4,\alpha}(\overline{\Omega^{ext}})$ as $l \to \infty$ concerning $\|\cdot\|_{[C^{k,\alpha'}(\Omega^{ext})]^3}$, $0 \leq \alpha' < \alpha$. Hence, $\Omega_n \overset{\mathcal{O}}{\longrightarrow} \Omega := \Phi(\Omega_b)$ when it passes to the limit. According to Theorem 4 $T_{n_l} \in C^{2,\phi}(\overline{\Omega_{n_l}})$ for every $n_l \in \mathbb{N}$. Moreover, this theorem leads to

$\|T_{n_l}\|_{C^{2,\phi}(\overline{\Omega_{n_l}})} \leq C^T$ for every n_l. Let $p_{\Omega_{n_l}} := p^{1,2,\phi}_{\Omega_{n_l}}$ be the extension operator from Definition 13 and set $T^{ext}_{n_l} := p_{\Omega_{n_l}} T_{n_l}$. Because of Lemma 14 there is a constant C^{ext} such that $\|T^{ext}_{n_l}\|_{C^{2,\phi}(\Omega^{ext})} \leq C^{ext}\|T_{n_l}\|_{C^{2,\phi}(\Omega_{n_l})} \leq C^{ext}C^T$. The constant C^{ext} can again be chosen uniformly with regard to $\mathcal{O}$, what was shown in the previous lemma. This results in a uniform bound for all $\|T^{ext}_{n_l}\|_{C^{2,\phi}(\Omega^{ext})}$. In view of Lemma 13 there is again a convergent subsequence $T^{ext}_{n_j} \to T^{ext,*}$ as $j \to \infty$ concerning $\|.\|_{C^{2,\phi'}(\Omega^{ext})}$. The limit $T^{ext,*} \in C^{2,\phi'}(\overline{\Omega^{ext}})$ is even an element of $C^{2,\phi}(\overline{\Omega})$, see the proof of Lemma 5. Thus,

$$\Omega_{n_j} \xrightarrow{\mathcal{O}} \Omega,\ T^{ext}_{n_j} \xrightarrow{C^{2,\phi'}} T^{ext,*} \quad \text{for some } T^{ext,*} \in C^{2,\phi}(\overline{\Omega}).$$

Because all derivatives of $T^{ext}_{n_j}$ up to order two converge particularly to those of $T^{ext,*}$ as $j \to \infty$, the function $T^{ext,*}\restriction_\Omega$ solves (17). Here we also apply the continuity of η and T_e in the shapes $\Omega \in \mathcal{O}$. Since Theorem 4 holds, (17) has a unique solution T and $T^{ext,*}$ has to be an extension of T to $\overline{\Omega^{ext}}$.

We apply the same arguments to the solutions $u_{n_j} \in [C^{3,\varphi}(\Omega_{n_j})]^3$ that are allocated to Φ_{n_j} and $T^{ext}_{n_j}$. In this way, we finally obtain a further subsequence $(\Omega_{n_k}, T^{ext}_{n_k}, u^{ext}_{n_k})_{k\in\mathbb{N}}$ where $u^{ext}_{n_k} = p^{3,3,\varphi}_{\Omega_{n_k}} u_{n_k}$ and

$$\Omega_{n_k} \xrightarrow{\mathcal{O}} \Omega,\ \ T^{ext}_{n_k} \xrightarrow{C^{2,\phi'}} T^{ext,*},\ \ u^{ext}_{n_k} \xrightarrow{C^{3,\varphi'}} u^{ext,*} \quad \text{for some } u^{ext,*} \in C^{3,\varphi}(\overline{\Omega}).$$

Actually, $(T^{ext,*}, u^{ext,*})\restriction_\Omega$ solves (19), because $T^{ext,*}\restriction_\Omega$ solves (17) and $u^{ext}_{u_l} \xrightarrow{C^3} u^{ext,*}$, where $(T^{ext,*}, u^{ext,*})$ is an extension of the unique solution (T,u) of (19). Here also the shape continuity of the g_M enters. □

Lemma 12 (***Continuity of Local Cost Functionals)*** *Let* $\mathcal{F}_{vol}$, $\mathcal{F}_{sur} \in C^0(\mathbb{R}^d)$ *with* $d = 3 + \sum_{j=0}^{s} 3^j + \sum_{j=0}^{r} 3^{j+1}$, $s = 2, r = 3$ *and let the set* $\mathcal{O}$ *only consist of* C^0*-admissible shapes. For* $\Omega \in \mathcal{O}$, $T \in C^2(\overline{\Omega})$, *and* $u \in C^3(\overline{\Omega})$ *consider the volume integral* $\mathcal{J}_{vol}(\Omega, T, u)$ *and the surface integral* $\mathcal{J}_{sur}(\Omega, T, u)$ *of* (42).

Let $(\Omega_n)_{n\in\mathbb{N}} \in \mathcal{O}$ *with* $\Omega_n \xrightarrow{\mathcal{O}} \Omega$ *as* $n \to \infty$, $(u_n)_{n\in\mathbb{N}} \in [C^3(\overline{\Omega_n})]^3$ *be a sequence with* $u_n \rightsquigarrow u$ $(q = 3,\ \beta = 0)$ *and* $(T_n)_{n\in\mathbb{N}} \in C^2(\overline{\Omega_n})$ *be a sequence with* $T_n \rightsquigarrow T$ $(q = 2,\ \beta = 0)$. *Then,*

(i) $\mathcal{J}_{vol}(\Omega_n, T_n, u_n) \to \mathcal{J}_{vol}(\Omega, T, u)$ *as* $n \to \infty$.

(ii) If the family $\mathcal{O}$ *consists only of* C^1*-admissible shapes, then* $\mathcal{J}_{sur}(\Omega_n, T_n, u_n) \to \mathcal{J}_{sur}(\Omega, T, u)$ *as* $n \to \infty$.

Proof (i) Statement (i) can be proved in the same way as Lemma 6.3 in Gottschalk and Schmitz (2015).

(ii) Because of its definition, every $\Omega \in \mathcal{O}$ has a boundary that can be considered as a differentiable two-dimensional submanifold in $\mathbb{R}^3$: let $x_0 = \Phi(z_0)$, $z_0 \in \partial\Omega_b$ be some point on the boundary. The mapping $\mathcal{T}_{x_0} : B_d(x_0) \cap \partial\Omega \to F_R \subset \mathbb{R}^2 \times$

$\{0\}$ defines a chart for x_0 if $\mathcal{T}_{x_0}$, d and F_R are defined analogously to Lemma 6. Now we can choose $x_i, i = 1\ldots, l \in \mathbb{N} \in \partial\Omega$, such that $\partial\Omega \subset \bigcup_{i=1}^{l} B_d(x_i) \cap \partial\Omega$. By restriction of these mappings to carefully chosen sets $\mathcal{A}^i \subset B_d(x_0) \cap \partial\Omega$, we can define an atlas $(\mathcal{A}^i)_{i=1,\ldots,l}$ for $\partial\Omega$, where $\mathcal{A}^i \cap \mathcal{A}^j = \emptyset$. In this way, we can write the surface integral as a sum:

$$\begin{aligned}\mathcal{J}_{sur}(\Omega_n, T_n, u_n) &= \int_{\partial\Omega_n} \mathcal{F}_{sur}(x, T_n, \nabla T_n, \nabla^2 T_n, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dA \\ &= \sum_{i=1}^{l} \int_{\mathcal{A}_i^n} \mathcal{F}_{sur}(x, T_n, \nabla T_n, \nabla^2 T_n, u, \nabla u, \nabla^2 u, \nabla^3 u)\, dA.\end{aligned}$$

If we denote the chart-mappings by $h_n^i : \mathcal{A}_n^i \to \tilde{\mathcal{A}}_n^i$ and the correspinding Gram determinants by $g^{h_n^i}$ we can write the integrals in the form

$$\int_{\mathcal{A}_i^n} \mathcal{F}_{sur}\big(h_n^i(s), T_n(h_n^i(s)), \nabla T_n(h_n^i(s)), \nabla^2 T_n(h_n^i(s)), u(h_n^i(s)), \ldots, \\ \ldots, \nabla^3 u(h_n^i(s))\big) \sqrt{g^{h_n^i}(s)}\, ds.$$

Especially, the h_n^i corresponds to the inverse hemisphere transformations on Ω_n. Since $\Phi \in C^1(\overline{\Omega^{ext}}) \leq K$ by some constant K, which is the same for all $\Omega \in \mathcal{O}$ and the hemisphere transformations on Ω_b are uniformly bounded and the Gram determinant is bounded as well. Because of $\mathcal{F}_{sur} \in C^0(\mathbb{R}^d)$, $T_n \rightsquigarrow T$ as $n \to \infty$ and $u_n \rightsquigarrow u$ as $n \to \infty$, there are constants C_i such that

$$\Big|\mathcal{F}_{sur}\big(h_n^i(s), T_n(h_n^i(s)), \nabla T_n(h_n^i(s)), \nabla^2 T_n(h_n^i(s)), u(h_n^i(s)), \\ \ldots, \nabla^3 u(h_n^i(s))\big) \sqrt{g^{h_n^i}(s)}\Big| \leq C_i$$

holds for all $n \in \mathbb{N}$, $i = 1, \ldots, l$. In consequence, Lebesgue's theorem of dominated convergence can be applied (with $C = \max C_i : i = 1, \ldots, l$) and we conclude $\mathcal{J}_{sur}(\Omega_n, T_n, u_n) \to \mathcal{J}_{sur}(\Omega, T, u)$ when passing to the limit. □

Theorem 6 (***Solution to the SO Problem***) *Let the set of admissible shapes be given as in Definition 7 with $k = 4$. Then, the shape optimization problem* (16) *with the objective functionals* (42) *and the thermomechanical state equation* (19) *has at least one solution $\Omega^* \in \mathcal{O}$.*

Proof As demonstrated in the above Lemmata 11 and 12, the conditions of Theorem 1 are fulfilled and the assertion follows. □

The application of this result in shape optimization to the optimal reliability problem now is straightforward:

Corollary 1 (***Solution to the Optimal Reliability Problem***) *For all optimal reliability problems from Definitions 3 and 4 there exists at least one solution in the set of admissible shapes $\mathcal{O}$ for the local, probabilistic failure time model for LCF.*

Proof Combine the results of Lemmata 2 and 4 with the above Theorem 6.□

8. Summary and outlook

In the present paper, we have shown the existence of optimal solutions to a class of shape optimization problems with the thermo-mechanic PDE as the state equation. The objective functionals can be of a rather singular type, as they contain higher derivatives of the solution of the PDE and boundary integrals. This forces us to use elliptic regularity theory and domains defined by smooth deformation of a baseline domain. We have also shown how this relates to the notion of optimal reliability of mechanical design. This generalizes prior work, Gottschalk and Schmitz (2015) and Schmitz (2014), in several respects: a more general setting for optimal reliability problems, a temperature dependent crack initiation process, more flexible admissible shapes and a multi-physical state equation.

A number of new questions naturally arise at this point: The first concerns the construction of boundary value problems that associate surface forces to shapes Ω. This point has been left open in this article and was not even mentioned in previous work by Gottschalk and Schmitz (2015) and Schmitz (2014). From an applied prospective, such models should come from other physical processes, such as static gas pressure $g = P\nu$ on $\partial\Omega$, that will again depend on geometry. Taking a potential flow v in a region exterior to Ω as a simple model, it should be possible to verify the assumptions of Definition 10 for $P = P(v)$ using elliptic regularity theory once again. A quick check, however, reveals that the second order Shauder estimates for the Poisson equation that are proven in this work are one order too low to meet the $C^{2,\phi}$ continuity requirements for g in the mechanical Schauder estimate. One thus has to use the more general framework of Agmon, Douglis and Nirenberg (1964) in order to treat even the simplest physical boundary condition model in the framework of elliptic regularity theory. An even more multi-physical approach, starting with simple flow models in the exterior of Ω and proceeding to more complicated ones, seems to be an interesting research direction for the future.

It would also be desirable to study the continuous shape derivative of failure probabilities in the given context, see Sokolowski and Zolesio (1992) for the general theory and Bolten, Gottschalk and Schmitz (2015) and Schmitz (2014) for some first steps in that direction. The mathematically rigorous treatment of shape derivatives for rather singular objective functionals is not an easy task. Material and shape derivatives should have a similar $C^{k,\phi}$ regularity class as the solutions, but also depend on the solutions, Sokolowski and Zolesio (1992), and so a careful treatment is desirable, in particular if one would like to consider higher derivatives. Furthermore, a formal inspection of the right hand side of the adjoint equation, for the class of objective functionals given by the optimal reliability application, reveals that the adjoint state can not be a Sobolev function, since the formal expressions for $\frac{\partial \mathcal{J}_{sur}(\Omega,T,u)}{\partial u}$ do not define a functional in $H^{-1}(\Omega)$. This raises several interesting questions on the nature and numerical approximation of the adjoint state that are beyond the scope of the present article.

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A. Appendix

LEMMA 13 *(Gilbarg and Trudinger, 1977, Lemma 6.36) Let* Ω *be a* $C^{k,\phi}$*-domain in* $\mathbb{R}^n$ *(with* $k \geq 1$*) and let* S *be a bounded set in* $C^{k,\phi}(\overline{\Omega})$*. Then,* S *is precompact in* $C^{j,\beta}(\overline{\Omega})$ *if* $j + \beta < k + \phi$*.*

DEFINITION 14 (**HEMISPHERE PROPERTY**) *(Agmon, Douglis and Nirenberg, 1959, p. 667)*
Let $\Omega \subset \mathbb{R}^n$ *be a domain with a* $C^{k,\phi}$ *boundary portion* Γ *and* $A \subseteq \Omega$ *be a subdomain such that* $\partial A \cap \partial\Omega \subseteq \mathring{\Gamma}$ *in the* $(n-1)$*-dimensional sense.*
A is said to satisfy a $C^{k,\phi}$*-hemisphere property on* Γ*, if there exists constant* $d > 0$ *such that every* $x \in A$ *with* $dist(x, \Gamma) \leq d$ *possesses a neighborhood* $U_x \subset \mathbb{R}^n$ *where*
(i) $\overline{U}_x \cap \partial\Omega \subseteq \Gamma$*,*
(ii) $B_{d/2}(x) \subseteq U_x$ *and*
(iii) (a) $\overline{U}_x \cap \overline{\Omega} = \mathcal{T}(\Sigma_{R(x)})$*,* *(b)*$\overline{U}_x \cap \partial\Omega = \mathcal{T}(F_{R(x)})$*,* $0 < R(x) \leq 1$
for some hemisphere $\Sigma_{R(x)}$ *and its flat boundary* $F_{R(x)}$*. The transformations* $\mathcal{T}, \mathcal{T}^{-1} \in C^{k,\varphi}$ *are dependent on the point* $x \in A$*.*

LEMMA 14 *(Lemma 6.37, Gilbarg and Trudinger, 1977)*
Let Ω *be a* $C^{k,\phi}$ *domain in* $\mathbb{R}^n$ *(with* $k \geq 1$*) and let* Ω' *be an open set containing* $\overline{\Omega}$*. Suppose* $u \in C^{k,\phi}(\overline{\Omega})$*. Then, there exists a function* $w \in C_0^{k,\phi}(\Omega')$ *such that* $w = u$ *in* Ω' *and*

$$\|w\|_{C^{k,\phi}(\Omega')} \leq C\|u\|_{C^{k,\phi}(\Omega)}, \quad C = C_{k,\Omega,\Omega'}.$$

LEMMA 15 *(Lemma 6.38, Gilbarg and Trudinger, 1977)*
Let Ω *be a* $C^{k,\phi}$ *domain in* $\mathbb{R}^n$ *(with* $k \geq 1$*) and let* Ω' *be an open set containing* $\overline{\Omega}$*. Suppose* $\psi \in C^{k,\phi}(\partial\Omega)$ *or* $\psi \in C^{k,\phi}(\overline{\Omega})$ *(See the explanations concerning* $C^{k,\phi}$ *domains at the beginning of Chapter 6.2 in Gilberg and Trudinger, 1977). Then, there exists a function* $\Psi \in C_0^{k,\phi}(\Omega')$ *such that* $\Psi = \psi$ *on* $\partial\Omega$*,* $\overline{\Omega}$ *respectively.*

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