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OPTIMAL CONTROL OF STATIC CONTACT IN FINITE STRAIN ELASTICITY

ANTON SCHIELA, MATTHIAS STOECKLEIN

Abstract. We consider the optimal control of elastic contact problems in the regime of finite deformations. We derive a result on existence of optimal solutions and propose a regularization of the contact constraints by a penalty formulation. Subsequential convergence of sequences of solutions of the regularized problem to original solutions is studied. Based on these results, a numerical path-following scheme is constructed and its performance is tested.

1. Introduction

Due to their relevance in mechanics, elastic contact problems have been the subject of intensive research in the past decades. If two elastic bodies come into contact, they may interact by contact forces that are supported by the contact boundary. Since this contact boundary depends on the deformation, already the simple case of linear elasticity, the Signorini problem [Sig33, Coc84, KO88], is a non-linear, non-smooth problem, a variational inequality induced by a convex optimization problem on a Sobolev space. In a general geometric setting already the simulation of linearly elastic contact is challenging [KO88].

In nonlinearly elastic contact, in the context of hyperelastic materials with polyconvex energy function, additional difficulties arise: Solutions of hyperelastic problems can be modeled as energy minimizers. These energy minimizers do not have to be unique due to the non-convexity of the respective energy functional. Also, local minimizers do not have to satisfy the weak form of the equilibrium equation in general. Only modified equilibrium equations can be derived [Bal02]. Classical equilibrium conditions can only be shown under additional structural assumptions on the energy minimizer, and even then, local stability of solutions under perturbation of forces can only be achieved in very regular settings. All these factors have significant consequences for the theoretical and numerical analysis of this class of problems.

In many cases, not only simulation of elastic bodies is of interest, but also optimization problems in the context of elasticity may be considered. In [Lub15, LSW14], the authors studied the design of implants which can be modeled by an optimal control problem of a hyperelastic body using a tracking type objective functional. In these works, a rigorous proof for the existence of optimal solutions to such kinds of problems was elaborated for the first time. Also, a specially suited composite step method was developed to efficiently solve optimal control problems in nonlinear elasticity. In [GH16], an optimal control problem using a non-tracking type objective functional was analyzed to describe biological models. The resulting problems were solved by a quasi-Newton approach.

In this work, we extend the results from [Lub15] to optimal control of static contact problems in non-linear hyperelasticity. Our aim is to establish basic results, concerning the existence of optimal solutions and to analyze a regularization scheme for their numerical computation.

Our paper is structured as follows: In the following section, we introduce the setting for a hyperelastic contact problem which is already a challenging problem by itself. The existence of solutions to hyperelastic problems was shown by John Ball in the context of polyconvexity [Bal77] and was extended to the case of contact in [CN85]. Since the techniques developed there are crucial for the analysis of optimal control problems, we are going to give a short recapitulation of this topic. Additionally, we introduce the so-called normal compliance approach [OM85, MO87] as a regularization method for the contact constraints. From this, we obtain a regularized problem with relaxed constraints. Existence results for this problem will be discussed as well. Also, we examine the convergence of solutions of the regularized problem to solutions of the original problem.

Key words and phrases. nonlinear elasticity, optimal control, contact problem.

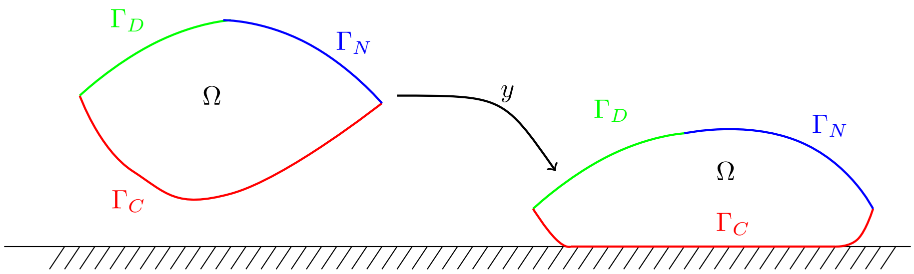


FIGURE 1. Contact problem

In Section 3, we work out the necessary structural assumptions to derive convergence rates for our regularization approach. For the derivation of explicit convergence rates, we will utilize ideas and techniques from [Bal02] and [HSW14].

In Section 4, we study the optimal control of contact problems in the setting of nonlinear elasticity. Optimal control of linear contact problems has been considered in [Bet15, MS17, Weh07], but the non-linear case has not been treated so far, to the best knowledge of the authors. In our setting we aim to minimize an objective functional while the state has to be an energy minimizer of a nonlinear elastic energy functional with contact constraints. By applying a regularization method to make this problem tractable, we additionally obtain a regularized optimal control problem with relaxed constraints. The central point of this study will be to work out a convergence result which states that solutions of the regularized problem converge to solutions of the original one. Due to the non-uniqueness of energy minimizers, this study is very delicate and cannot be done without structural assumptions.

Thereafter, we combine a path-following method with an affine covariant composite step method as the inner solver for the numerical solution. This method was developed in [LSW17, Lub15] and has been proven to be well suited for large-scale problems involving nonlinear elasticity. Finally, we will present some numerical examples to assess the viability of our approach.

2. Contact Problems in Hyperelasticity

In this section, we derive a suitable model for hyperelastic contact problems and summarize the most important theoretical aspects which will prove essential for the further study. We consider the deformations of a three-dimensional body governed by a hyperelastic isotropic material law. The deformation is caused by an external boundary force density and is constrained by an obstacle. We will give a short introduction into the theory of nonlinear elastic problems. In particular, we address the issue of existence of solutions to such problems as far as it will be required for the later examination. A detailed summary of the analysis of nonlinear elastic problems can be found in [Cia94].

2.1. **Nonlinear elasticity.** First, we introduce the required notation and assumptions. Our setting is illustrated in Figure 1. By $\Omega \subset \mathbb{R}^3$, we denote a bounded Lipschitz domain (in the sense of [Neč12]) representing the three-dimensional nonlinear elastic body. Its boundary Γ consists of three disjoint relatively open subsets such that

$$\Gamma = \overline{\Gamma_D \cup \Gamma_N \cup \Gamma_C},$$

whereby each segment has a non-zero boundary measure. Here, Γ_D denotes the part of the boundary where Dirichlet boundary conditions are enforced. Further, Γ_N denotes the Neumann boundary where the external pressure load acts and Γ_C denotes the contact boundary where the nonpenetration conditions are imposed. For the sake of brevity, we will suppress the notation of all trace operators. The deformation of the body is denoted by

$$y : \overline{\Omega} \to \mathbb{R}^3,$$

and is an element of the vector valued Sobolev space $W^{1,p}(\Omega; \mathbb{R}^3)$ for $p \geq 2$. If there is no risk of an ambiguity, we use the shorter notation $W^{1,p}(\Omega)$ and skip the image space in general for all vector valued spaces. We denote the deformation gradient by ∇y, using the notation from [Cia94]. Concerning boundary conditions, we require that y is the identity mapping on Γ_D. On Γ_N, we consider a boundary force density $u \in L^q(\Gamma_N, \mathbb{R}^3)$ which causes the deformation of the body. Later, u will be used as the control of our optimization problem, where state and control space will be denoted by $Y = W^{1,p}(\Omega)$ and $U = L^q(\Gamma_N)$, respectively. The specific choice of the index q will be discussed later. Similarly, volume forces could be included in our problem and treated in an analogous way.

Next, we derive the problem description with the respective hyperelastic model. In the context of hyperelasticity, finding the deformation of a body corresponds to minimizing the total energy functional $I : Y \times U \to \mathbb{R}$, defined by

$$I(y,u) := \int_\Omega \hat{W}(x, \nabla y(x))\, dx - \int_{\Gamma_N} yu \; ds.$$

If $u \in U$ is fixed, we call minimizers of the functional $y \to I(y,u)$ solutions of the elastic problem. Denoting by $\mathbb{M}^3_+$ the set of 3×3 matrices with positive determinant, $\hat{W} : \Omega \times \mathbb{M}^3_+ \to \mathbb{R}$ is called the stored energy function. It is used to model the properties of the specific material which is described. The choice of $\hat{W}$ will be discussed in detail, below.

We introduce the following splitting

$$I(y,u) = I_{\text{strain}}(y) - I_{\text{out}}(y,u)$$

with

$$I_{\text{strain}}(y) = \int_\Omega \hat{W}(x, \nabla y(x))\, dx \quad \text{ and } \quad I_{\text{out}}(y,u) = \int_{\Gamma_N} yu \; ds.$$

In this paper, we will concentrate on polyconvex stored energy functions. This is a class of functionals that, although non-convex, are still weakly lower semicontinuous, and thus allows an existence theory on energy minimizers.

We summarize the necessary assumptions. Let $id : \overline{\Omega} \to \overline{\Omega}$ be the identity mapping, $\|M\| := \sqrt{\operatorname{tr} M^T M}$ the norm on the space of 3×3 matrices $\mathbb{M}^3$ and let $\operatorname{Cof} M := \det(M) M^{-T}$ denote the cofactor matrix for $M \in \mathbb{M}^3_+$.

Assumption 2.1. *Let $\hat{W} : \Omega \times \mathbb{M}^3_+ \to \mathbb{R}$ be the stored energy function. We assume that the following properties hold.*

(1) *Polyconvexity: For almost all $x \in \Omega$, there exists a convex function $\mathbb{W}(x,\cdot,\cdot,\cdot) : \mathbb{M}^3 \times \mathbb{M}^3 \times]0,+\infty[\to \mathbb{R}$ such that*

$$\hat{W}(x,M) = \mathbb{W}(x, M, \operatorname{Cof} M, \det M), \quad \textit{for all } M \in \mathbb{M}^3_+,$$

whereby the function

$$\mathbb{W}(\cdot, M, \operatorname{Cof} M, \det M) : \Omega \to \mathbb{R}$$

is measurable for all $(M, \operatorname{Cof} M, \det M) \in \mathbb{M}^3_+ \times \mathbb{M}^3_+ \times]0,+\infty[$.

(2) *For almost all $x \in \Omega$, the implication*

$$\det M \to 0^+ \Rightarrow \hat{W}(x,M) \to \infty$$

holds.

(3) *The sets of admissible deformations are defined by*

$$\begin{aligned}\mathcal{A}_c := \{&y \in W^{1,p}(\Omega),\ \operatorname{Cof} \nabla y \in L^s(\Omega),\ \det \nabla y \in L^r(\Omega),\\ &y = id \textit{ a.e. on } \Gamma_D,\ \det \nabla y > 0 \textit{ a.e. in } \Omega,\ y_3 \ge 0 \textit{ a.e. on } \Gamma_c\},\end{aligned}$$

and

$$\begin{aligned}\mathcal{A} := \{&y \in W^{1,p}(\Omega),\ \operatorname{Cof} \nabla y \in L^s(\Omega),\ \det \nabla y \in L^r(\Omega),\\ &y = id \textit{ a.e. on } \Gamma_D,\ \det \nabla y > 0 \textit{ a.e. in } \Omega\},\end{aligned}$$

for $p \ge 2$, $s \ge \frac{p}{p-1}$, $r > 1$.

(4) *Coerciveness: There exist $a \in \mathbb{R}$, and $b > 0$, such that*

$$\hat{W}(x,M) \ge a + b(\|M\|^p + \|\operatorname{Cof} M\|^s + |\det M|^r),$$

for all $M \in \mathbb{M}^3_+$.

(5) *Let the index p' satisfy*

$$\frac{1}{p'} > \frac{3-p}{2p},$$

for $p \leq 3$ and $p' = \infty$ for $p > 3$. Further, q satisfies

$$\frac{1}{q} = 1 - \frac{1}{p'}.$$

(6) *The identity mapping $id : \overline{\Omega} \to \overline{\Omega}$ is a natural state, i.e.*

$$I_{\text{strain}}(id) = 0,$$

and

$$id_3 \geq 0 \text{ a.e. on } \Gamma_C.$$

Since the mappings $M \to \operatorname{Cof} M$ and $M \to \det M$ are nonlinear, polyconvex energy-functionals are non-convex. However, these mappings have special properties, summarized in the following theorem:

Theorem 2.1. *Let $p \geq 2$, and let $r, s > 0$ satisfy*

$$r^{-1} = p^{-1} + s^{-1} \leq 1.$$

Further, let y_n be a sequence in $W^{1,p}(\Omega)$. Then, the following implication holds:

$$\left.\begin{array}{r} y_n \rightharpoonup \hat{y} \ \text{ in } W^{1,p}(\Omega), \\ \operatorname{Cof} \nabla y_n \rightharpoonup N \ \text{ in } L^s(\Omega), \\ \det \nabla y_n \rightharpoonup d \ \text{ in } L^r(\Omega), \end{array}\right\} \Rightarrow \begin{cases} N = \operatorname{Cof} \nabla \hat{y}, \\ d \ = \det \nabla \hat{y}. \end{cases}$$

Proof. For the proof, we refer to [Bal77, Lemma 6.1 and Theorem 6.2]. □

With its help, the weak lower semicontinuity of the total energy functional can be shown.

Lemma 2.1. *Let Assumption 2.1 hold. Then, the outer energy functional $I_{out} : Y \times U \to \mathbb{R}$ is weakly continuous. Additionally, the total energy functional is weakly lower semicontinuous w.r.t. sequences that leave the strain energy I_{strain} bounded.*

Proof. First, we show the weak continuity of the outer energy function I_{out}. Let $(y_n, u_n) \subset Y \times U$ be a weakly converging sequence with the limit $(\overline{y}, \overline{u}) \in Y \times U$. We know from [Neč12, Theorem 6.2] and Assumption 2.1(5) that there exists a continuous and compact trace operator $\tau : Y \to L^{p'}(\Gamma)$. Hence, $\tau(y_n) \to \tau(\overline{y})$. Additionally, we obtain by Hölder's inequality and by continuity of the trace operator that

$$|I_{\text{out}}(y, u)| \leq \int_{\Gamma_N} |\tau(y)u| \, ds \leq \|\tau(y)\|_{L^{p'}(\Gamma_N)} \|u\|_U \leq C \|y\|_Y \|u\|_U,$$

for some constant $C > 0$. As a result, the outer energy I_{out} is bilinear and bounded and thus continuous. Next, we can rewrite

$$I_{\text{out}}(y_n, u_n) - I_{\text{out}}(\overline{y}, \overline{u}) = I_{\text{out}}(y_n - \overline{y}, u_n) + I_{\text{out}}(\overline{y}, u_n) - I_{\text{out}}(\overline{y}, \overline{u}).$$

By combining the boundedness of u_n, the continuity of I_{out} and the existence of a compact trace operator τ, it can be conclude that the term $I_{\text{out}}(y_n - \overline{y}, u_n)$ approaches zero. The second term $I_{\text{out}}(\overline{y}, u_n) - I_{\text{out}}(\overline{y}, \overline{u})$ converges to zero due to the definition of weak convergence. This concludes the first part of the proof. The arguments applied here are analogous to the ones in [Cia94, Proof of Theorem 7.1-5].

The second statement follows from [Cia94, Proof of Theorem 7.7-1]. □

In the next lemma, which is a slightly modified version of the results in [Cia94, Proof of Theorem 7.3-2], we obtain a lower bound of the total energy functional.

Lemma 2.2. *Let $u_n \subset U$ be a bounded sequence. Then, there exist uniform constants $a > 0$ and $b \in \mathbb{R}$ such that the total energy functional satisfies the estimate*

$$I(v, u_n) \geq a\|v\|_Y^p + b, \quad \text{for all } v \in \mathcal{A} \text{ and for all } n \in \mathbb{N}.$$

Proof. Assumption 2.1(4) implies that there exist constants $c > 0$ and $d \in \mathbb{R}$ such that the strain energy satisfies

$$I_{\text{strain}}(v) \geq c\|v\|_Y^p + d, \quad \text{for all } v \in \mathcal{A}.$$

See [Cia94, Proof of Theorem 7.3-2]. Following the argumentation above, the existence of a trace operator $\tau : Y \to L^{p'}(\Gamma)$ and Hölder's inequality yield the estimate

$$|I_{\text{out}}(v, u_n)| \leq \int_{\Gamma_N} |\tau(v)u_n| \, ds \leq \|\tau(v)\|_{L^{p'}(\Gamma_N)}\|u_n\|_U \leq C\|v\|_Y,$$

for some $C > 0$. Since $p > 1$,

$$I(v, u_n) \geq I_{\text{strain}}(v, u_n) - |I_{\text{out}}(v, u_n)| \geq a\|v\|_Y^p + b$$

holds for some $a > 0$ and $b \in \mathbb{R}$ which concludes the proof. □

From this lemma, we also obtain the coercivity of the total energy functional I w.r.t. to the first argument if the sequence u_n is bounded.

The established Assumption 2.1(2) corresponds to the physical interpretation that in order to compress a given volume to zero, an infinite amount of energy is necessary. This conditions already rules out convexity of the stored energy function [Cia94] and thus leads to potential non-uniqueness of possible minimizers. It also has consequences for the numerical analysis, where non-convex solution algorithms have to be applied. Besides non-convexity, the second requirement yields possible singularities of the total energy functional which have to be taken into account as well.

The other important restriction to the deformation of a body is that it has to be injective in the interior of the domain Ω to be physically reasonable. In the Sobolev sense, this can at least locally be enforced by requiring that $\det \nabla y > 0$ a.e. in Ω is satisfied.

2.2. **Contact constraints.** Next, we are going to incorporate the contact constraints into our model. For simplicity, we restrict ourselves to simple constraints of the form

$$y_3 \geq 0 \text{ a.e. on } \Gamma_C,$$

for some a-priori chosen contact boundary Γ_C, meaning that the third component y_3 of y should be non-negative. This restriction corresponds to a setting in which the body has to stay above the plane that is spanned by the first two canonical basis vectors.

The techniques developed in [Bal77, Theorem 4.8-1] were first extended to contact problems in [CN85], in a more general setting.

In order to analyze the resulting contact problem in elasticity, we need the following result:

Lemma 2.3. *The set*

$$\mathcal{C} = \{v \in W^{1,p}(\Omega) \mid v_3 \geq 0 \textit{ a.e. on } \Gamma_C\}$$

is weakly closed in Y.

Proof. The following argumentation is analogous to the one in [CN85, Proof of Theorem 4.1].

Let $v_n \rightharpoonup \overline{v}$ be a weakly converging sequence in Y. Given the existence of a compact trace operator $\tau : Y \to L^{p'}(\Gamma)$, see [Neč12], we can extract a subsequence that converges pointwise ds-almost everywhere on Γ. Since the set

$$\mathcal{K} = \{z \in \mathbb{R}^3 \mid z_3 \leq 0\}$$

is closed, it follows that $\overline{v}_3 \geq 0$ a.e. on Γ_C. Thus, $\mathcal{C}$ is weakly closed. □

For a detailed introduction into elasticity, we refer here to the analysis in [Bal77]. From there, we obtain the admissible set for deformations $\mathcal{A}_c$ as defined in Assumption 2.1(3). With this at hand, finding the resulting deformation caused by some boundary pressure load u corresponds to solving the minimization problem

$$y \in \operatorname*{argmin}_{v \in \mathcal{A}_c} I(v, u). \tag{1}$$

One of the essential parts of proving the existence of solutions is to verify the weak closedness of the sets $\mathcal{A}_c$ and $\mathcal{A}$ w.r.t. infimizing sequences.

Lemma 2.4. *Let $y_n \rightharpoonup \overline{y}$ be a weakly converging sequence in $\mathcal{A}$ that leaves the strain energy $I_{strain}(y_n)$ bounded. Then, $\overline{y} \in \mathcal{A}$.*

Proof. See [Cia94, Proof of Theorem 7.7-1]. □

We note that this result can be transferred to the set $\mathcal{A}_c$ since the set $\mathcal{C}$ is weakly closed.

Next, we can derive the following existence result which was first established in [CN85, Theorem 4.2] in a more general setting.

Theorem 2.2. *Let $u \in U$ be some fixed boundary force and let Assumption 2.1 hold. Further, we assume that the admissible set $\mathcal{A}_c$ is not empty and that $\inf_{v\in\mathcal{A}_c} I(v,u) < \infty$. Then, the total energy functional $I(\cdot,u)$ has at least one minimizer in $\mathcal{A}_c$.*

Proof. Let $y_n \subset \mathcal{A}_c$ be an infinimizing sequence. By applying Lemma 2.2 we obtain the boundedness of $I(y_n,u)$ and y_n. Due to reflexivity of Y, there exists a weakly converging subsequence, also denoted by y_n. The weak limit is denoted by $\overline{y}$. Since $I(y_n,u)$ and y_n are bounded, we obtain the boundedness of the strain energy $I_{\text{strain}}(y_n)$ as well. As previously established, Lemma 2.4 and the weak closedness of the set $\mathcal{C}$ yield $\overline{y} \in \mathcal{A}_c$.

Accordingly, Lemma 2.1 yields that the total energy functional I is weakly lower semicontinuous w.r.t. the sequence y_n. Then, the fact that $\overline{y}$ is again a minimizer results from

$$\inf_{y\in\mathcal{A}_c} I(y,u) \le I(\overline{y},u) \le \liminf_{n\to\infty} I(y_n,u) = \inf_{y\in\mathcal{A}_c} I(y,u).$$

□

2.3. **Regularization of contact constraints.** Solving nonlinear elasticity problems numerically is already highly challenging due to the non-convexity and the singularities of the total energy functional. Additionally, contact constraints add a non-smoothness to the problem. As a result, regularization approaches for those kinds of problems are very popular.

In our analysis, we conduct the so-called normal compliance approach which has been studied in [OM85, MO87]. In this context, we drop the contact constraints by adding a penalty functional $P : Y \to \mathbb{R}_0^+$ of the form

$$P(v) := \frac{1}{k}\int_{\Gamma_C} [-v_3]_+^k \, ds, \quad k \in \mathbb{N},\ k > 1, \quad v \in Y$$

to the total energy functional I. Here, the functional P locally penalizes the violation of the constraint. We multiply the penalty functional with a positive parameter γ. The idea behind this approach is that by minimizing the penalized function, the resulting solutions approach solutions of the original contact constraint problem for increasing parameter γ. The resulting penalized total energy functional reads as follows:

$$I_\gamma(y,u) := I(y,u) + \gamma P(y).$$

For sufficiently large p, there exists a trace operator $\tau : Y \to L^k(\Gamma)$, see [Neč12]. Thus, in this case, the penalty function is well defined, convex and weakly lower semicontinuous.

With the regularized total energy functional at hand, we can drop the contact constraint and obtain the relaxed admissible set $\mathcal{A}$ as defined in Assumption 2.1(3). Consequently, for some fixed penalty parameter $\gamma > 0$, this leads to the relaxed minimization problem

$$y \in \operatorname*{argmin}_{v\in\mathcal{A}} I_\gamma(v,u). \tag{2}$$

In order to analyze whether the normal compliance approach is a reasonable regularization, two properties have to be proven. First, we have to verify if the regularized problem (2) admits at least one optimal solution. Secondly, solutions of the regularized problem (2) have to approach solutions of the original one (1) as the penalty parameter γ approaches infinity. The first condition is addressed in the following theorem.

Theorem 2.3. *Let $\gamma > 0$ be a fixed penalty parameter and $u \in U$ be some fixed boundary force. We assume that the admissible set $\mathcal{A}$ is not empty and that $\inf_{v\in\mathcal{A}} I_\gamma(v,u) < \infty$. Then, under Assumption 2.1, the regularized total energy functional $I_\gamma(\cdot,u)$ has at least one minimizer in $\mathcal{A}$.*

Proof. Since the penalty function P is weakly lower semicontinuous, we can apply the arguments from the constrained case, and the proof follows analogously. □

Before we can address the second condition, we need to establish the following theoretical result that in hyperelasticity, bounded boundary forces leave the resulting total energy bounded.

Lemma 2.5. *Let Assumption 2.1 hold. Further, let $\gamma_n \to \infty$ be a positive sequence of penalty parameters and let $u_n \subset U$ be a bounded sequence. Additionally, let $y_n \subset \mathcal{A}$ be a sequence of corresponding energy minimizers which satisfy*

$$y_n \in \operatorname*{argmin}_{v \in \mathcal{A}} I_{\gamma_n}(v, u_n).$$

Then, $I_{\gamma_n}(y_n, u_n)$ and $I(y_n, u_n)$ are bounded, and y_n is bounded in Y.

Proof. The boundedness from below results from Lemma 2.2. For the boundedness from above, we derive from Theorem 2.2 the existence of a state $\tilde{y} \in \mathcal{A}_c$ satisfying $I_{\text{strain}}(\tilde{y}) < \infty$. Then, there exists a constant $C > 0$ such that

$$I_{\gamma_n}(y_n, u_n) \leq I_{\gamma_n}(\tilde{y}, u_n) = I(\tilde{y}, u_n) \leq I_{\text{strain}}(\tilde{y}) + |I_{\text{out}}(\tilde{y}, u_n)| < C.$$

The last estimate follows from Hölder's inequality as applied in the proof of Lemma 2.2. The boundedness from above of $I(y_n, u_n)$ simply follows from the previous estimate and the fact that $\gamma_n P(y_n) > 0$. Again, Lemma 2.2, which also holds for $I_{\gamma_n} \geq I$, implies the boundedness of y_n. This concludes the proof. □

With this at hand, we prove a continuity result that allows us to pass to the limit later:

Lemma 2.6. *Let $\gamma_n \to \infty$ be a monotonically increasing sequence of penalty parameters. Consider a weakly convergent sequence $(y_n, u_n) \rightharpoonup (\overline{y}, \overline{u})$ such that*

$$y_n \in \operatorname*{argmin}_{v \in \mathcal{A}} I_{\gamma_n}(v, u_n).$$

Then, $(\overline{y}, \overline{u}) \in \mathcal{A}_c \times U$ and

$$\overline{y} \in \operatorname*{argmin}_{v \in \mathcal{A}_c} I(v, \overline{u}).$$

Additionally,

$$\lim_{n \to \infty} I_{\gamma_n}(y_n, u_n) = I(\overline{y}, \overline{u}).$$

Proof. The weak convergence of (y_n, u_n) implies its boundedness in $Y \times U$. Thus, we also obtain the boundedness of the outer energy $I_{\text{out}}(y_n, u_n)$ just as in the proof of Lemma 2.2. Consequently, $I_{\text{strain}}(y_n)$ is bounded as well. Hence, Lemma 2.4 applies and $\overline{y} \in \mathcal{A}$.

Next, the relation

$$P(y_n) = \frac{I_{\gamma_n}(y_n, u_n) - I(y_n, u_n)}{\gamma_n}$$

yields $\lim_{n \to \infty} P(y_n) \to 0$ since the numerator is bounded as previously established. By combining this with the weak lower semicontinuity of P, we obtain

$$0 \leq P(\overline{y}) \leq \liminf_{n \to \infty} P(y_n) = 0.$$

This yields $\overline{y} \in \mathcal{A}_c$.

Finally, we show that $\overline{y}$ is again a solution to the original contact problem (1). From Theorem 2.2, we derive the existence of a state $\tilde{y} \in \mathcal{A}_c$ which satisfies

$$\tilde{y} \in \operatorname*{argmin}_{v \in \mathcal{A}_c} I(v, \overline{u}).$$

Furthermore, the weak lower semicontinuity of the total energy I w.r.t. (y_n, u_n) follows from the boundedness of $I_{\text{strain}}(y_n)$ and Lemma 2.1. Next, we obtain

$$\begin{aligned}\limsup_{n \to \infty} I_{\gamma_n}(y_n, u_n) &\leq \limsup_{n \to \infty} I_{\gamma_n}(\overline{y}, u_n) = \limsup_{n \to \infty} I(\overline{y}, u_n) = \lim_{n \to \infty} I(\overline{y}, u_n) \\ &= I(\overline{y}, \overline{u}) \leq \liminf_{n \to \infty} I(y_n, u_n) \leq \liminf_{n \to \infty} I_{\gamma_n}(y_n, u_n).\end{aligned}$$

Hence,

$$\lim_{n \to \infty} I_{\gamma_n}(y_n, u_n) = I(\overline{y}, \overline{u}).$$

A similar argumentation was applied in [LSW14, Proof of Lemma 3.3].

From the above results, we derive

$$I(\tilde{y}, \overline{u}) \leq I(\overline{y}, \overline{u}) = \lim_{n \to \infty} I_{\gamma_n}(y_n, u_n) \leq \lim_{n \to \infty} I_{\gamma_n}(\tilde{y}, u_n) = I(\tilde{y}, \overline{u})$$

which shows that $\overline{y}$ is again a minimizer of the total energy functional.

□

Finally, we prove that limit points of regularized solutions exist and satisfy the original contact problem:

Proposition 2.1. *Let $u \in U$, $\gamma_n \to \infty$ be a monotonically increasing sequence of penalty parameters and $y_n \in \operatorname{argmin}_{v\in\mathcal{A}} I_{\gamma_n}(v,u)$. Then, y_n has a weakly converging subsequence. The limit point y of any such sequence satisfies $y \in \operatorname{argmin}_{v\in\mathcal{A}_c} I(v,u)$.*

Proof. Boundedness of y_n follows from Lemma 2.5 so that we can extract a weakly converging subsequence. Application of Lemma 2.6 to each of these subsequences yields the desired result. □

3. Asymptotic rates of the energy

By using refined arguments and an assumption on the geometric setting, it is possible to derive a-priori estimates on the rate of convergence of the energy if $\gamma \to \infty$. We are thus interested in estimates of the form:

$$\min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_\gamma(v,u) \le c\gamma^{-\rho},$$

for some positive constants ρ and c.

To this end, we will use ideas from [HSW14] and [Bal02]. We consider the case $p > 3$ so that $W^{1,p}(\Omega)$ is continuously embedded into the space $C^\beta(\Omega)$ of Hölder continuous functions for some suitable $\beta \in]0,1[$. Further, we make the following assumption on the geometry of the boundary conditions:

Assumption 3.1. *Assume that there is a constant $K > 0$ such that for each $\varepsilon > 0$ there exists an invertible mapping $\psi_\varepsilon \in W^{1,\infty}(\mathbb{R}^3)$, such that*

$$\|\psi_\varepsilon - id\|_{W^{1,\infty}} \le K\varepsilon,$$

$\psi_\varepsilon = id$ on Γ_D and

$$\forall x \in \mathbb{R}^3 : x_3 \ge -\varepsilon \quad \Rightarrow \quad \psi_\varepsilon(x)_3 \ge 0.$$

Denoting

$$\mathcal{C}_\varepsilon := \{y \in \mathcal{A} : y_3(x) \ge -\varepsilon, \forall x \in \Gamma_C\},$$

we see that $y \in \mathcal{C}_\varepsilon$ implies $\psi_\varepsilon \circ y \in \mathcal{C}$.

Next, we utilize the growth assumption (C1) from [Bal02].

Assumption 3.2. *We assume that $\hat{W}$ describes the stored energy function of some homogeneous material. Further, we assume that there exists a constant $K > 0$ such that $\hat{W}$ satisfies the following growth condition*

$$|\hat{W}'(M)M^T| \le K(\hat{W}(M) + 1), \quad \text{for all } M \in \mathbb{M}^3_+. \tag{3}$$

From there, we can show the following estimate:

Lemma 3.1. *Let $u \in U$ be a fixed boundary force. If Assumption 3.1 and 3.2 hold and if $\varepsilon > 0$ is sufficiently small, then there is a constant $C > 0$, such that*

$$|I(\psi_\varepsilon \circ y, u) - I(y,u)| \le C(I(y,u) + 1)\varepsilon,$$

for all $y \in \mathcal{C}_\varepsilon$.

Proof. Let $M \in \mathbb{M}^3_+$, satisfying $\|M - Id\| < \varepsilon$. Here, Id denotes the identity matrix. Further, we define $M(t) := tM + (1-t)Id$, with $t \in [0,1]$. From $\|M - Id\| < \varepsilon$ and $\|Id\| = \sqrt{3} < 2$, we derive $\|M(t)^{-1}\| \le 2$.

Following the arguments in the proof of Lemma 2.5 in [Bal02], we obtain

$$\hat{W}(MA) + 1 \le \frac{3}{2}(\hat{W}(A) + 1), \quad \text{for all } A \in \mathbb{M}^3_+. \tag{4}$$

Next, we define

$$\Theta(A) := \sup_{\|M-Id\|<\varepsilon} \hat{W}(MA)$$

and we denote by $K > 0$ the constant from the growth condition (3). Then, applying again the arguments of the proof of Lemma 2.5 in [Bal02] yields the estimate:

$$
\begin{aligned}
\hat{W}(MA) - \hat{W}(A) &= \int_0^1 (\hat{W}'(M(t)A)) \cdot ((M - Id)A)\, dt \\
&\overset{(3)}{\leq} K \int_0^1 (\hat{W}(M(t)A) + 1)\|M - Id\|\|M(t)^{-1}\|\, dt \\
&\leq 2K\varepsilon \int_0^1 (\hat{W}(M(t)A) + 1)\, dt \\
&\leq 2K\varepsilon(\Theta(A) + 1) \overset{(4)}{\leq} 3K\varepsilon(\hat{W}(A) + 1).
\end{aligned}
$$

Integrating over the domain Ω yields the desired result. □

This implies the following result:

Corollary 3.1. *Under the above assumptions we have:*

$$\min_{v \in \mathcal{A}_c} I(v, u) \leq \min_{y \in \mathcal{A} \cap \mathcal{C}_\varepsilon} I(v, u) + C\varepsilon.$$

3.1. **An estimate for the constraint violation in L^∞.** It remains to show that for sufficiently large γ, energy minimizers of I_γ are contained in $\mathcal{C}_\varepsilon$, where $\varepsilon = O(\gamma^{-\rho})$ at a certain rate. For this, we use that the corresponding sequence of minimizers y_γ is bounded in C^β in the setting $p > 3$.

Our analysis here is based on the techniques applied in Proposition 2.4 in [HSW14]. First, we derive an upper bound for the supremum norm in a general setting.

At this point, we require additional assumptions on the boundary segment Γ_C in order to simplify the computations. In the setting here, we assume that Γ_C is a flat two-dimensional sub-manifold of $\mathbb{R}^3$. Nevertheless, under suitable assumptions, the following results still hold if Γ_C is curved. However, this is fairly technical and does not yield further insight. Thus, we restrict ourselves to the simple case.

Additionally, we require the following assumption on the boundary segment Γ_C.

Assumption 3.3. *Assume that Γ_C satisfies a uniform interior cone condition in the following sense: For each point $x \in \Gamma_C$, we can construct a two-dimensional circular sector*

$$S_{R',\theta}(x) \subset \Gamma_C \tag{5}$$

with center at x, radius $R' > 0$ and center angle $\theta > 0$. We assume that R' and θ can be chosen independently of x.

Here, each circular sector $S_{R',\theta}(x) \subset \Gamma_C$ is interpreted as a two-dimensional sub-manifold in $\mathbb{R}^3$. Due to the flatness assumption on Γ_C, this is a meaningful definition. With some abuse of notation, we denote by $(y)_+^k$ the function $\max(0, -y_3)^k$ on Γ_C. From here, we can derive the following estimate:

Proposition 3.1. *Let $\beta \in]0, 1[$ and $s \geq 1$. Further, let $f \in C^\beta(\Gamma_C) \cap L^s(\Gamma_C)$ be a positive function. Additionally, let Assumption 3.3 hold and let $\|f\|_{C^\beta(\Gamma_C)} \leq M$ and $\|f\|_{L^s(\Gamma_C)} \leq 1$. Without loss of generality, we assume that $0 \in \Gamma_C$ and $f(0) = \|f\|_{L^\infty(\Gamma_C)}$. Due to Assumption 3.3, we can deduce the existence of a circular sector $S_{R',\theta}(0) \subset \Gamma_C$ with $R' \leq 1$.*

Then, we obtain the following estimate:

$$\|f\|_{L^\infty(\Gamma_C)} \leq c(s, \beta, R', \theta, M)\|f\|_{L^s(\Gamma_C)}^{\frac{\beta s}{\beta s + 2}},$$

where the positive constant $c(s, \beta, R', \theta, M)$ only depends on the exponents β and s, the angle θ, the radius R' and the upper bound M.

Proof. First, we define

$$R = \left(\frac{f(0)}{\|f\|_{C^\beta(\Gamma_C)}}\right)^{\frac{1}{\beta}} = \left(\frac{\|f\|_{L^\infty(\Gamma_C)}}{\|f\|_{C^\beta(\Gamma_C)}}\right)^{\frac{1}{\beta}}. \tag{6}$$

Next, we choose the maximum positive $\alpha \leq 1$ such that for $\tilde{R} := \alpha R$, the inequalities

$$\left(\tfrac{\tilde{R}}{R}\right)^\beta s \leq 1 \Leftrightarrow \alpha^\beta s \leq 1 \tag{7}$$

and $\tilde{R} \le R'$ hold. As a result, we obtain the inclusion

$$S_{\tilde{R},\theta}(0) \subset S_{R',\theta}(0). \tag{8}$$

In addition, we recall Bernoulli's inequality

$$(1+x)^n \ge 1 + nx, \tag{9}$$

for real numbers $x \ge -1$ and $n \ge 1$.

Next, the Hölder continuity of f yields the estimate

$$f(x) \ge f(0) - \|f\|_{C^\beta(\Gamma_c)} \|x - 0\|^\beta, \quad \text{for all } x \in S_{R',\theta}(0). \tag{10}$$

From there, we obtain the following estimate:

$$\begin{aligned}
\|f\|^s_{L^s(\Gamma_C)} &= \int_{\Gamma_C} |f(x)|^s \, dx \ge \int_{S_{R',\theta}(0)} |f(x)|^s \, dx \\
&\overset{(8)(10)}{\ge} \int_{S_{\tilde{R},\theta}(0)} |f(0) - \|f\|_{C^\beta(\Gamma_C)} \|x - 0\|^\beta|^s \, dx \\
&\overset{(6)}{=} \|f\|^s_{C^\beta(\Gamma_C)} \int_{S_{\tilde{R},\theta}(0)} |R^\beta - \|x - 0\|^\beta|^s \, dx \\
&= 2|S_{1,\theta}(0)| \|f\|^s_{C^\beta(\Gamma_C)} \int_0^{\tilde{R}} |R^\beta - r^\beta|^s r \, dr \\
&\overset{(7)(9)}{\ge} 2|S_{1,\theta}(0)| \|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \int_0^{\tilde{R}} \left(1 - s\tfrac{r^\beta}{R^\beta}\right) r \, dr.
\end{aligned}$$

At this point, we have to distinguish between two cases. The first case is $\alpha^\beta s = 1$ which implies $\tilde{R} \le R'$. In this case, we obtain

$$\begin{aligned}
&2|S_{1,\theta}(0)| \|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \int_0^{\tilde{R}} \left(1 - s\tfrac{r^\beta}{R^\beta}\right) r \, dr \\
&= 2|S_{1,\theta}(0)| \|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \left[\tfrac{1}{2} r^2 - \tfrac{s r^{\beta+2}}{(\beta+2) R^\beta}\right]_0^{\alpha R} \\
&= 2|S_{1,\theta}(0)| \|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s + 2} \tfrac{\alpha^2}{\beta+2} \left(\tfrac{1}{2}(\beta+2) - s\alpha^\beta\right).
\end{aligned}$$

Due to the condition $\alpha^\beta s = 1$, we know that the constant

$$c_0(s, \beta, R', \theta) := 2|S_{1,\theta}(0)| \tfrac{\alpha^2}{\beta+2} \left(\tfrac{1}{2}(\beta+2) - s\alpha^\beta\right) \overset{(7)}{>} 0$$

does not approach zero even if $R \to 0$. Thus, we can insert the definition of R and obtain the estimate

$$\|f\|^s_{L^s(\Gamma_C)} \ge c_0(s, \beta, R', \theta) \|f\|^s_{C^\beta(\Gamma_C)} \left(\frac{\|f\|_{L^\infty(\Gamma_C)}}{\|f\|_{C^\beta(\Gamma_C)}}\right)^{\frac{\beta s + 2}{\beta}}.$$

Now, solving for $\|f\|_{L^\infty(\Gamma_C)}$ yields

$$\begin{aligned}
\|f\|_{L^\infty(\Gamma_C)} &\le c_0(s, \beta, R', \theta)^{-\frac{\beta}{\beta s+2}} \|f\|^{\frac{2}{\beta s+2}}_{C^\beta(\Gamma_C)} \|f\|^{\frac{\beta s}{\beta s+2}}_{L^s(\Gamma_C)} \\
&\le c(s, \beta, R', \theta, M) \|f\|^{\frac{\beta s}{\beta s+2}}_{L^s(\Gamma_C)}
\end{aligned}$$

which shows the desired result.

For the second case, we have $\alpha^\beta s < 1$ which implies $\tilde{R} = R'$. Here, we get the estimate

$$\begin{aligned}
&2|S_{1,\theta}(0)|\|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \int_0^{\tilde{R}} \left(1 - s\tfrac{r^\beta}{R^\beta}\right) r\,dr \\
&= 2|S_{1,\theta}(0)|\|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \left[\tfrac{1}{2}r^2 - \tfrac{sr^{\beta+2}}{(\beta+2)R^\beta}\right]_0^{\tilde{R}} \\
&= 2|S_{1,\theta}(0)|\|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \left(\tfrac{1}{2}\tilde{R}^2 - \tfrac{s\tilde{R}^{\beta+2}}{(\beta+2)R^\beta}\right) \\
&\overset{(7)}{\geq} 2|S_{1,\theta}(0)|\|f\|^s_{C^\beta(\Gamma_C)} R^{\beta s} \tilde{R}^2 \left(\tfrac{1}{2} - \tfrac{1}{(\beta+2)}\right).
\end{aligned}$$

By applying $\tilde{R} = R'$, we can define the constant

$$c_0(s, \beta, R', \theta) := 2|S_{1,\theta}(0)|(R')^2 \left(\tfrac{1}{2} - \tfrac{1}{(\beta+2)}\right) > 0$$

which does not depend on R. Analogously to the computations above, we insert the definition of R and obtain

$$\|f\|^s_{L^s(\Gamma_C)} \geq c_0(s, \beta, R', \theta)\|f\|^s_{C^\beta(\Gamma_C)} \left(\frac{\|f\|_{L^\infty(\Gamma_C)}}{\|f\|_{C^\beta(\Gamma_C)}}\right)^{\frac{\beta s}{\beta}}.$$

Solving for $\|f\|_{L^\infty(\Gamma_C)}$ and using $\|f\|_{L^s(\Gamma_C)} \leq 1$ yields

$$\|f\|_{L^\infty(\Gamma_C)} \leq c_0(s, \beta, R', \theta)^{-\frac{1}{s}} \|f\|_{L^s(\Gamma_C)} \leq c(s, \beta, R', \theta)\|f\|^{\frac{\beta s}{\beta s+2}}_{L^s(\Gamma_C)}.$$

Taking both estimates together, we obtain the desired result. □

In the following, we assume that Assumption 3.3 holds throughout the whole section.

We extend the previous result to sequences that leave the term $\gamma P(\cdot)$ bounded.

Corollary 3.2. *Let $\gamma_n \to \infty$ and let $y_n \subset Y$ be a bounded sequence with $\gamma_n P(y_n)$ being bounded as well. Then, there exists a constant $C > 0$ such that we obtain the following estimate:*

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq C\gamma_n^{-\frac{\beta}{k\beta+2}}.$$

Proof. From the boundedness of $P(y_n)\gamma_n$, we deduce the existence of a constant $c > 0$ such that

$$P(y_n) \leq c\gamma_n^{-1}.$$

Next, the continuous embedding of $W^{1,p}(\Omega)$ into the space $C^\beta(\Omega)$ yields the boundedness of $(y_n)_+$ in the space $C^\beta(\Gamma_C)$. By definition, $P(y_n) = \|(y_n)_+\|^k_{L^k(\Gamma_C)}$. Thus, Corollary 3.1 applies, and we obtain the stated estimate. □

From this, we can directly deduce a convergence rate for the regularized total energy.

Corollary 3.3. *Let $u \in U$ be some fixed boundary force. Additionally, let $\gamma_n \to \infty$ be an arbitrary sequence of penalty parameters and y_n a sequence of minimizers to the corresponding regularized contact problems* (2)*. Further, we assume $W^{1,p}(\Omega)$ is continuously embedded into the space $C^\beta(\Omega)$ and that Assumption 3.1 and 3.2 hold. Then, there exists a constant $C > 0$ such that we obtain the following convergence rate*

$$\min_{v\in\mathcal{A}_c} I(v, u) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v, u) \leq C\gamma_n^{-\frac{\beta}{k\beta+2}}.$$

Proof. Let $y_n \subset \mathcal{A}$ denote a sequence of minimizers to problem (2) corresponding to the sequence γ_n. From Lemma 2.5, we deduce that $I_{\gamma_n}(y_n, u)$ and $I(y_n, u)$ are bounded. Consequently, $\gamma_n P(y_n)$ is bounded as well. Therefore, Corollary 3.2 applies and we obtain

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c\gamma^{-\frac{\beta}{k\beta+2}},$$

for some constant $c > 0$.

Utilizing Lemma 3.1, we obtain the transformation functions ψ_{ϵ_n}, where ϵ_n denotes the respective maximum constraint violation $\|(y_n)_+\|_{L^\infty(\Gamma_C)}$.

In addition, for sufficiently large γ_n, Lemma 3.1 yields the estimate

$$0 \leq \min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v,u) \leq |I(\psi_{\varepsilon_n}\circ y_n,u) - I(y_n,u)| \leq c_0(I(y_n,u)+1)\varepsilon_n,$$

for a constant $c_0 > 0$. Inserting the estimate for ε_n and utilizing the boundedness of $I(y_n,u)$ yield

$$\min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v,u) \leq c_1 c\gamma^{-\frac{\beta}{k\beta+2}},$$

for some $c_1 > 0$. This shows the desired result. We note here that the same convergence rate holds for the sequence $I(y_n,u)$. In addition, due to the relation

$$0 \leq \min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v,u),$$

we obtain

$$0 \leq \gamma_n P(y_n) \leq \min_{v\in\mathcal{A}_c} I(v,u) - I(y_n,u) \leq c_1 c\gamma^{-\frac{\beta}{k\beta+2}}.$$

This estimate can be used to derive sharper convergence rates. □

3.2. **A bootstrapping argument.** The previous results can be refined by applying a bootstrapping argument, similar to the one in [HSW14, Theorem 2.12].

Corollary 3.4. *Let $u \in U$ be some fixed boundary force and let $\gamma_n \to \infty$ be an arbitrary sequence of penalty parameters. Further, we denote by $y_n \subset \mathcal{A}$ a sequence of minimizers to the corresponding regularized contact problems* (2). *We assume $W^{1,p}(\Omega)$ is continuously embedded into the space $C^\beta(\Omega)$ and that Assumption 3.1 and 3.2 hold. Then, there exists a constant $c > 0$ such that we obtain the following convergence rate:*

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c\gamma_n^{-\frac{\beta}{(k-1)\beta+2}}.$$

Proof. From the Corollaries 3.3 and 3.2, we deduce that there exist positive constants c_0, c_1 and c_2 such that the following estimates hold:

$$P(y_n) \leq c_0\gamma^{-1}.$$

From there, we derive the convergence rate for the maximum constraint violation

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c_1 c_0^{\frac{\beta}{k\beta+2}} \gamma_n^{-\frac{\beta}{k\beta+2}}.$$

Subsequently, we obtain the rates for the regularized total energy

$$\min_{v\in\mathcal{A}_c} I(v,u) - I_{\gamma_n}(y_n,u) \leq c_2 c_1 c_0^{\frac{\beta}{k\beta+2}} \gamma_n^{-\frac{\beta}{k\beta+2}}$$

and

$$\min_{v\in\mathcal{A}_c} I(v,u) - I(y_n,u) \leq c_2 c_1 c_0^{\frac{\beta}{k\beta+2}} \gamma_n^{-\frac{\beta}{k\beta+2}}.$$

As discussed in the proof of Corollary 3.3, it can be concluded that

$$\gamma_n P(y_n) \leq c_2 c_1 c_0^{\frac{\beta}{k\beta+2}} \gamma_n^{-\frac{\beta}{k\beta+2}}.$$

In comparison to the analysis above, this allows the refined estimate

$$P(y_n) \leq c_2 c_1 c_0^{\frac{\beta}{k\beta+2}} \gamma_n^{-1-\frac{\beta}{k\beta+2}}.$$

By writing $\overline{c} := c_2 c_1 c_0^{\frac{\beta}{k\beta+2}}$ and inserting it into the estimate of Corollary 3.2, we can further improve the estimate for the convergence rate of the maximum constraint violation to

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c_1 \overline{c}^{\frac{\beta}{k\beta+2}} \gamma_n^{(-1-\frac{\beta}{k\beta+2})\frac{\beta}{k\beta+2}}.$$

This estimate carries over to the convergence rate of the total energy. Applying this technique recursively yields the formula

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c_1 C_i^{\frac{\beta}{k\beta+2}} \gamma_n^{(-1-\delta_i)\frac{\beta}{k\beta+2}},$$

with $\delta_{i+1} = (1+\delta_i)\frac{\beta}{k\beta+2}$ and $C_{i+1} = c_2 c_1 (C_i)^{\frac{\beta}{k\beta+2}}$. The initial values are $\delta_0 = 0$ and $C_0 = c_0$, respectively.

Next, for $i \geq 1$, we derive the equivalent formulas

$$\delta_i = \sum_{m=1}^{i} \left(\tfrac{\beta}{k\beta+2}\right)^m, \quad C_i = (c_2 c_1)^{\sum_{j=0}^{i-1} (\frac{\beta}{k\beta+2})^j} C_0^{(\frac{\beta}{k\beta+2})^i}.$$

As $i \to \infty$, we can compute the limit δ_∞ by

$$\delta_\infty = \sum_{m=1}^{\infty} \left(\tfrac{\beta}{k\beta+2}\right)^m = \frac{1}{1-\frac{\beta}{k\beta+2}} - 1 = \frac{\beta}{(k-1)\beta+2}.$$

Analogously, the limit C_∞ can be computed by

$$C_\infty = \lim_{i\to\infty} ((c_2 c_1)^{\sum_{j=0}^{i-1} (\frac{\beta}{k\beta+2})^j} C_0^{(\frac{\beta}{k\beta+2})^i}) = (c_2 c_1)^{\frac{k\beta+2}{(k-1)\beta+2}}.$$

Finally, we obtain

$$\|(y_n)_+\|_{L^\infty(\Gamma_C)} \leq c_1 C_\infty^{\frac{\beta}{k\beta+2}} \gamma_n^{(-1-\delta_\infty)\frac{\beta}{k\beta+2}} = c_1 C_\infty^{\frac{\beta}{k\beta+2}} \gamma_n^{-\frac{\beta}{(k-1)\beta+2}}.$$

This concludes the proof. □

This result carries over to a refined version of Corollary 3.3.

Corollary 3.5. *Let $u \in U$ be some fixed boundary force. Additionally, let $\gamma_n \to \infty$ be an arbitrary sequence of penalty parameters and y_n a sequence of minimizers to the corresponding regularized contact problems* (2)*. Further, we assume $W^{1,p}(\Omega)$ is continuously embedded into the space $C^\beta(\Omega)$ and that Assumption 3.1 and 3.2 hold. Then, there exists a constant $C > 0$ such that we obtain the following convergence rate:*

$$\min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v,u) \leq C\gamma_n^{-\frac{\beta}{(k-1)\beta+2}}.$$

Proof. The proof simply follows by combining the results from Corollary 3.4 and the techniques applied in the proof of Corollary 3.3. □

From a theoretical point of view, the convergence of the energy hinges on an a-priori bound on the Hölder continuity of the solutions for some $\beta > 0$. In practical computations, as presented below, β can be quite large, e.g., $\beta = 1$. Nevertheless, we will see in our numerical results (below) that the rate of convergence of the energy is faster than predicted by theory.

4. Optimal Control of Nonlinear Elastic Contact Problems

In the optimal control setting, we want to minimize an objective functional

$$J : Y \times U \to \mathbb{R}.$$

As a constraint for the optimal control problem, we require that the optimal state y_* is a minimizer of the total energy functional i.e.

$$y_* \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,u_*),$$

where u_* is the corresponding optimal control.

In our analysis we choose a tracking type functional defined by

$$J(y,u) := \frac{1}{2}\|y-y_{\mathrm{d}}\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Gamma_N)},$$

where $y_{\mathrm{d}} \in L^2(\Omega)$ denotes the desired state and $\alpha > 0$. This standard tracking type functional is obviously weakly lower semicontinuous and coercive w.r.t. its second argument. Here, we require $q \geq 2$ for the space $U = L^q(\Gamma_N)$. Next, we state the optimal control problem and analyze the existence of optimal solutions.

4.1. **Optimal control of elastic contact problems.** With the objective functional at hand, the optimal control problem reads as follows:

$$\begin{aligned} &\min_{(y,u)\in Y\times U} J(y,u) \\ &s.t.\ y \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,u). \end{aligned} \tag{11}$$

In proving the existence of optimal solutions to this problem, we encounter several difficulties. First, we are dealing with a bi-level optimization problem where it is not possible to derive first-order optimality conditions without strong additional assumptions [Bal77]. Additionally, the total energy functional I is non-convex and therefore, its minimizers do not have to be unique. In [LSW14], the existence of solutions to an optimal control problem in hyperelasticity without contact constraints has been proven. We can directly transfer the results from [LSW14] to our analysis.

Before we address the existence of solutions, we introduce the following definition.

Definition 4.1 (Solution set)**.** The solution set $\mathcal{S}$ is defined as

$$\mathcal{S} := \{(y,u)\in Y\times U \mid y\in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,u)\}.$$

Next, we can state an existence result in the following theorem.

Theorem 4.1. *We assume that Assumption 2.1 holds. Then, the optimal control problem* (11) *hast at least one optimal solution in* $\mathcal{S}$*.*

Proof. The proof follows the lines of [LSW14, Proof of Theorem 3.1]. Let $(y_n,u_n)\subset\mathcal{S}$ be an infimizing sequence whereby $J(y_n,u_n)$ is bounded. We know that such a sequence exists due to Assumption 2.1 and due to the definition of the tracking functional J. The coerciveness of J w.r.t. the second variable yields the boundedness of u_n.

The boundedness of $I(y_n,u_n)$ follows from the same arguments as applied in the proof of Lemma 2.5. Accordingly, Lemma 2.2 implies the boundedness of y_n. From there, we can deduce the boundedness of the strain energy $I_{strain}(y_n)$.

Now, reflexivity of $Y\times U$ yields the existence of a weakly converging subsequence which we also denote by (y_n,u_n). Its weak limit is denoted by $(\overline{y},\overline{u})\in Y\times U$. Here, Lemma 2.4 and the weak closedness of $\mathcal{C}$ ensure that $\overline{y}\in\mathcal{A}_c$.

Next, we have to verify that $(\overline{y},\overline{u})$ satisfies again the constraints of the optimal control problem (11) i.e.

$$\overline{y}\in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,\overline{u}).$$

Theorem 2.2 guarantees the existence of a state $\tilde{y}\in\mathcal{A}_c$ satisfying

$$\tilde{y}\in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,\overline{u}).$$

As a result, Lemma 2.1 yields the weak lower semicontinuity of I w.r.t. the sequence (y_n,u_n) and the weak continuity of the outer energy I_{out}.

Then,

$$\limsup_{n\to\infty} I(y_n,u_n) \le \limsup_{n\to\infty} I(\overline{y},u_n) = I(\overline{y},\overline{u}) \le \liminf_{n\to\infty} I(y_n,u_n),$$

and consequently,

$$\lim_{n\to\infty} I(y_n,u_n) = I(\overline{y},\overline{u}).$$

From there, we obtain

$$I(\tilde{y},\overline{u}) \le I(\overline{y},\overline{u}) = \lim_{n\to\infty} I(y_n,u_n) \le \lim_{n\to\infty} I(\tilde{y},u_n) = I(\tilde{y},\overline{u}).$$

Thus, $(\overline{y},\overline{u})$ satisfies the constraints of the optimal control problem (11).

Finally, the estimate

$$\inf_{(y,u)\in\mathcal{S}} J(y,u) \le J(\overline{y},\overline{u}) \le \liminf_{n\to\infty} J(y_n,u_n) = \inf_{(y,u)\in\mathcal{S}} J(y,u)$$

concludes the proof. $\square$

4.2. **Regularized optimal control problem.** Although it is possible to show the existence of optimal solutions, the numerical computation of such solutions poses significant challenges due to the contact constraints and the resulting non-smoothness. In order to apply the specialized algorithm developed in [LSW17], we deploy the normal compliance approach to relax the constraints. Consequently, we obtain the regularized problem:

$$\begin{aligned} &\min_{(y,u)\in Y\times U} J(y,u) \\ &s.t.\ y \in \operatorname*{argmin}_{v\in\mathcal{A}} I_\gamma(v,u), \end{aligned} \tag{12}$$

for some fixed parameter $\gamma > 0$.

Next, we can state the following existence result.

Theorem 4.2. *We assume that Assumption 2.1 holds. Furthermore, let $\gamma > 0$ be some fixed penalty parameter. Then, the optimal control problem* (12) *has at least one optimal solution.*

Proof. The regularization does not alter the two crucial properties of the total energy functional which are coerciveness and weak lower semicontinuity w.r.t. infimizing sequences. Thus, the existence of optimal solutions can be proven analogously to the constrained case. □

5. Convergence of Solutions of the Regularized Problem

In this section, we analyze how the regularized optimal control problem (12) relates to the original one (11). The crucial part of every regularization scheme is to verify that as the regularization parameter approaches its limit, solutions of the regularized problem approach solutions of the original problem.

However, in optimal control of nonlinear elasticity, we encounter several difficulties. First of all, we have a bi-level optimization problem with no solution operator for the second level problem due to the non-uniqueness of energy minimizers in hyperelasticity. Secondly, the lack of first-order optimality conditions also rules out usual techniques to show convergence. Thus, in order to obtain a satisfactory convergence result, we will need some additional structure or information on the problem. In this section, we discuss two alternative approaches to show the desired convergence result. In the first approach, we utilize a structural assumption, namely that optimal solutions can be approximated by regularized solutions. In the second approach, we modify the regularized energy-functional by adding a small fraction of the cost functional. This allows us to drop the reachability assumption.

5.1. **Convergence under a reachability assumption.** In our setting so far, one critical case cannot be excluded. If no optimal solution pair of the original problem (11) can be approximated by a sequence of solutions of the regularized contact problem (2), we have no chance of proving any convergence result at all. In the general setting of hyperelastic contact problems, this case cannot be ruled out. Therefore, we have to require additional structure in order to get an analytical relation between solutions of the regularized contact problem (2) and solutions of the original problem (1).

In this context, we introduce a property which ensures that solutions of the original contact problem (1) can be approximated by solutions of the regularized contact problem (2).

Definition 5.1 (Reachable)**.** A feasible solution $(y,u) \in \mathcal{S}$ is called reachable, if for each sequence $\gamma_n \to \infty$ there exists a subsequence γ_{n_k} and a corresponding sequence $(\tilde{y}_{n_k}, \tilde{u}_{n_k}) \subset \mathcal{A}\times U$, satisfying $\tilde{y}_{n_k} \rightharpoonup y$, $\tilde{u}_{n_k} \to u$ and

$$\tilde{y}_{n_k} \in \operatorname*{argmin}_{v\in\mathcal{A}} I_{\gamma_{n_k}}(v, \tilde{u}_{n_k}).$$

We denote the set of all reachable pairs by $\mathcal{R} \subset \mathcal{S}$.

Since $\mathcal{R} \subset \mathcal{S}$, we obtain $\min_{\mathcal{S}} J \le \inf_{\mathcal{R}} J$. However, it is not clear, whether both values coincide.

Assumption 5.1. *We assume that*

$$\min_{\mathcal{S}} J = \inf_{\mathcal{R}} J$$

Next, we address the convergence result.

Theorem 5.1. *Let Assumption 2.1 and Assumption 5.1 hold. Further, let $\gamma_n \to \infty$ be a positive and monotonically increasing sequence of penalty parameters. In addition, let $(y_n, u_n) \subset \mathcal{A} \times U$ be a sequence of optimal solutions to the corresponding regularized problems* (12)*. Then,*

$$\lim_{n\to\infty} J(y_n, u_n) = \min_{\mathcal{S}} J.$$

Furthermore, there exists a subsequence (y_{n_k}, u_{n_k}) and a pair $(\overline{y}, \overline{u}) \in \mathcal{A}_c \times U$ such that we obtain the weak convergence $y_{n_k} \rightharpoonup \overline{y}$ in Y and the strong convergence $u_{n_k} \to \overline{u}$ in $L^2(\Gamma_N)$. Additionally, $(\overline{y}, \overline{u})$ solves the original optimal control problem

$$\min_{(y,u)\in Y\times U} J(y, u)$$
$$s.t.\ y \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v, u).$$

Proof. We start by proving the boundedness of $J(y_n, u_n)$. Recalling the identity mapping id, we know that $J(id, 0) < \infty$. Due to Assumption 2.1(6), the pair $(id, 0) \in Y \times U$ satisfies the regularized constraint for every parameter γ_n. This is due to the fact that the identity mapping id is a natural state and that $id \in \mathcal{C}$. Therefore, the boundedness of $J(y_n, u_n)$ can be concluded so that $\limsup_{n\to\infty} J(y_n, u_n) < \infty$.

Let (y, u) be any reachable pair. Then, we can choose a subsequence γ_{n_k}, such that

$$\limsup_{n\to\infty} J(y_n, u_n) = \lim_{k\to\infty} J(y_{n_k}, u_{n_k}).$$

Simultaneously, there exists a sequence $(\tilde{y}_{n_k}, \tilde{u}_{n_k}) \subset \mathcal{A} \times U$ corresponding to γ_{n_k} with $\tilde{y}_{n_k} \rightharpoonup y$ in Y and $\tilde{u}_{n_k} \to u$ in U satisfying

$$\tilde{y}_{n_k} \in \operatorname*{argmin}_{v\in\mathcal{A}} I_{\gamma_{n_k}}(v, \tilde{u}_{n_k}).$$

The compact embedding $W^{1,p}(\Omega) \hookrightarrow L^p(\Omega)$, (see [Ada75]), implies $\tilde{y}_{n_k} \to y$ in $L^p(\Omega)$. Consequently, we conclude by optimality of (y_{n_k}, u_{n_k}) and strong continuity of J:

$$\limsup_{n\to\infty} J(y_n, u_n) = \lim_{k\to\infty} J(y_{n_k}, u_{n_k}) \le \lim_{k\to\infty} J(\tilde{y}_{n_k}, \tilde{u}_{n_k}) = J(y, u), \quad \forall (y, u) \in \mathcal{R}.$$

Hence,

$$\limsup_{n\to\infty} J(y_n, u_n) \le \inf_{\mathcal{R}} J.$$

The coercivity of the objective functional J w.r.t. the second variable yields the boundedness of u_n and thus, by Lemma 2.5, the boundedness of y_n. Hence, by reflexivity, there exists a subsequence of (y_{n_k}, u_{n_k}), such that simultaneously

$$\lim_{k\to\infty} J(y_{n_k}, u_{n_k}) = \liminf_{n\to\infty} J(y_n, u_n) \quad \text{and} \quad (y_{n_k}, u_{n_k}) \rightharpoonup (\overline{y}, \overline{u}).$$

By Lemma 2.6, we conclude that $(\overline{y}, \overline{u})$ satisfies the original constraint

$$\overline{y} \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v, \overline{u}).$$

By weak lower semicontinuity of J, we obtain

$$\min_{\mathcal{S}} J \le J(\overline{y}, \overline{u}) \le \lim_{k\to\infty} J(y_{n_k}, u_{n_k}) = \liminf_{n\to\infty} J(y_n, u_n) \le \limsup_{n\to\infty} J(y_n, u_n) \le \inf_{\mathcal{R}} J.$$

Invoking Assumption 5.1, namely $\min_{\mathcal{S}} J = \inf_{\mathcal{R}} J$, we obtain

$$\min_{\mathcal{S}} J = J(\overline{y}, \overline{u}) = \lim_{n\to\infty} J(y_n, u_n).$$

Thus, $(\overline{y}, \overline{u})$ is an optimal solution.

Finally, we show strong convergence of the sequence u_{n_k}. By the Sobolev embedding theorem, y_{n_k} converges strongly in $L^2(\Omega)$ and thus,

$$\frac{1}{2}\|y_{n_k} - y_{\mathrm{d}}\|_{L^2}^2 \to \frac{1}{2}\|\overline{y} - y_{\mathrm{d}}\|_{L^2}^2.$$

By incorporating the convergence $J(y_{n_k}, u_{n_k}) \to J(\overline{y}, \overline{u})$, we can deduce that

$$\frac{\alpha}{2}\|u_{n_k}\|_{L^2(\Gamma_N)}^2 \to \frac{\alpha}{2}\|\overline{u}\|_{L^2(\Gamma_N)}^2.$$

Since u_{n_k} is weakly converging in U, this implies the strong convergence in $L^2(\Gamma_N)$. □

5.2. **A modified regularization.** Although we have been able to show a convergence result, this was only possible under the assumption of reachability. However, in applications, it is usually not possible to verify whether this assumption holds.

The following critical case is conceivable: the original contact problem may have several solutions, some of which are in contact and some of which are not. In this case, our regularization scheme is biased towards those that are in contact because violating the contact allows reducing the energy.

To compensate for this bias, we introduce an alternative regularized total energy function $\mathcal{E}_\gamma$ which contains an additional term from the objective functional. Roughly speaking, this introduces a bias of energy-minimizers towards optimality of the objective functional J.

Our modified new regularized energy functional is

$$\mathcal{E}_\gamma(y,u) := I_\gamma(y,u) + \varphi(\gamma)\frac{1}{2}\|y - y_d\|^2_{L^2(\Omega)}, \tag{13}$$

where $\varphi : [0,\infty[\to]0,\infty[$ is a positive function in γ, that is monotonically decreasing, such that

$$\lim_{\gamma\to\infty} \varphi(\gamma) = 0.$$

The latter property ensures that solutions of this new regularized problem can approach solutions of the original contact problem (1).

First of all, we observe existence of regularized solutions:

Theorem 5.2. *Let Assumption 2.1 hold. Further, let $u \in U$ be some fixed boundary force and let $\gamma > 0$ be a fixed penalty parameter. If $\mathcal{A}$ is not empty and if $\inf_{v\in\mathcal{A}} I(v,u) < \infty$, then, the energy minimization problem*

$$y \in \operatorname*{argmin}_{v\in\mathcal{A}} \mathcal{E}_\gamma(v,u)$$

has at least one solution.

Proof. We note that the functional $\mathcal{E}_\gamma$ is weakly continuous w.r.t. the second variable and weakly lower semicontinuous w.r.t. sequences that leave the strain energy I_{strain} bounded. Thus, the proof is completely analogous to the proof of Theorem 2.2. □

Without giving the details of the proof, we remark that the results of Lemma 2.2 and Lemma 2.5 also hold for $\mathcal{E}_\gamma$.

Next, we establish the result that limits of regularized problems solve the original contact problem:

Lemma 5.1. *Let $\gamma_n \to \infty$ be a monotonically increasing sequence of penalty parameters. Consider a weakly convergent sequence $(u_n, y_n) \rightharpoonup (\overline{u}, \overline{y})$ such that*

$$y_n \in \operatorname*{argmin}_{v\in\mathcal{A}} \mathcal{E}_{\gamma_n}(v,u_n).$$

Then, $(\overline{y},\overline{u}) \in \mathcal{A}_c \times U$ with

$$\overline{y} \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,\overline{u})$$

and

$$\lim_{n\to\infty} \mathcal{E}_{\gamma_n}(y_n,u_n) = I(\overline{y},\overline{u}).$$

Proof. Theorem 2.2 guarantees the existence of a state $\hat{y} \in \mathcal{A}_c$ such that $I_{\text{strain}}(\hat{y}) < \infty$. From there, it follows that the sequence $\mathcal{E}_{\gamma_n}(\hat{y},u_n)$ is bounded since u_n is bounded and

$$\gamma_n P(\hat{y}) = 0, \quad \text{for all } n \in \mathbb{N}.$$

Therefore, we deduce that the sequence $\mathcal{E}_{\gamma_n}(y_n,u_n)$ is bounded due to

$$\mathcal{E}_{\gamma_n}(y_n,u_n) \le \mathcal{E}_{\gamma_n}(\hat{y},u_n).$$

We have to show that the pair $(\overline{y},\overline{u})$ satisfies the original constraint (1). First, boundedness of (y_n,u_n) and $\mathcal{E}_{\gamma_n}(y_n,u_n)$ implies the boundedness of $I_{\text{strain}}(y_n)$, and thus Lemma 2.4 implies $\overline{y} \in \mathcal{A}$. By the same argumentation as in the proof of Theorem 2.6, we even obtain $\overline{y} \in \mathcal{A}_c$.

Again, by using the techniques applied in the proof of Theorem 2.6 and by applying $\varphi(\gamma_n) \to 0$, we obtain:

$$\begin{aligned}\limsup_{n\to\infty} \mathcal{E}_{\gamma_n}(y_n,u_n) &\le \limsup_{n\to\infty} \mathcal{E}_{\gamma_n}(\overline{y},u_n) = \limsup_{n\to\infty} I(\overline{y},u_n) + \varphi(\gamma_n)\frac{1}{2}\|\overline{y} - y_d\|^2_{L^2(\Omega)} \\ &= I(\overline{y},\overline{u}) \le \liminf_{n\to\infty} I(y_n,u_n) \le \liminf_{n\to\infty} \mathcal{E}_{\gamma_n}(y_n,u_n).\end{aligned}$$

Thus,

$$\lim_{n\to\infty} \mathcal{E}_{\gamma_n}(y_n, u_n) = I(\overline{y}, \overline{u}).$$

Next, Theorem 2.2 yields the existence of a state $\check{y}$ with

$$\check{y} \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v, \overline{u}).$$

Consequently, it follows that

$$I(\check{y}, \overline{u}) \le I(\overline{y}, \overline{u}) = \lim_{n\to\infty} \mathcal{E}_{\gamma_n}(y_n, u_n) \le \lim_{n\to\infty} \mathcal{E}_{\gamma_n}(\check{y}, u_n) = I(\check{y}, \overline{u}).$$

□

Applying this new approach to the optimal control problem yields:

$$\begin{aligned} &\min_{(y,u)\in Y\times U} J(y,u) \\ &s.t.\ y \in \operatorname*{argmin}_{v\in\mathcal{A}} \mathcal{E}_\gamma(v,u). \end{aligned} \tag{14}$$

Next, we can state the existence result.

Theorem 5.3. *We assume that Assumption 2.1 holds. Further let $\gamma > 0$ be some fixed penalty parameter. Then, the optimal control problem* (14) *has at least one optimal solution.*

Proof. The proof is analogous to the proof of Theorem 4.1. □

So far, no further restrictions of the regularization function φ have been necessary. However, in order to overcome the lack of structure for the convergence proof, we have to ensure that minimizing a part of the objective functional in the constraint is sufficiently weighted as the penalty parameter approaches infinity. Therefore, we need to introduce an additional condition for the function φ.

Recall that for fixed u, the function $\gamma \to \min_{v\in\mathcal{A}} I_\gamma(v,u)$ is monotonically increasing and bounded. Moreover, by Lemma 2.6, we obtain

$$\lim_{\gamma\to\infty} \min_{v\in\mathcal{A}} I_\gamma(v,u) = \min_{v\in\mathcal{A}_c} I(v,u).$$

Assumption 5.2. *Let $u \in U$ be fixed. Assume that*

$$\lim_{\gamma\to\infty} \frac{\min_{v\in\mathcal{A}_c} I(v,u) - \min_{v\in\mathcal{A}} I_\gamma(v,u)}{\varphi(\gamma)} = 0.$$

With this at hand, we can state a convergence result without the structural assumption of reachability.

Theorem 5.4. *Let Assumption 2.1 hold and let $\gamma_n \to \infty$ be a positive and monotonically increasing sequence of penalty parameters. Furthermore, let (y_*, u_*) denote an optimal solution to problem* (11). *In addition, let $(y_n, u_n) \subset \mathcal{A} \times U$ be a sequence of optimal solutions to the corresponding regularized problems* (14), *where the regularization function φ satisfies Assumption 5.2 w.r.t. u_*. Then,*

$$\lim_{n\to\infty} J(y_n, u_n) = J(y_*, u_*).$$

Further, there exists a subsequence (y_{n_k}, u_{n_k}) and a pair $(\overline{y}, \overline{u}) \in \mathcal{A}_c \times U$ such that we obtain the weak convergence $y_{n_k} \rightharpoonup \overline{y}$ in Y and the strong convergence $u_{n_k} \to \overline{u}$ in $L^2(\Gamma_N)$. Additionally, the pair $(\overline{y}, \overline{u})$ solves the original optimal control problem

$$\begin{aligned} &\min_{(y,u)\in Y\times U} J(y,u) \\ &s.t.\ y \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v,u). \end{aligned}$$

Proof. Let us construct a sequence $(\tilde{y}_n, u_*) \subset \mathcal{A} \times U$ that satisfies the regularized constraints for each element in γ_n and that fulfills the condition

$$\limsup_{n\to\infty} J(\tilde{y}_n, u_*) \le J(y_*, u_*).$$

To this end, let $\tilde{y}_n \subset \mathcal{A}$ be a sequence satisfying

$$\tilde{y}_n \in \operatorname*{argmin}_{v\in\mathcal{A}} \mathcal{E}_{\gamma_n}(v, u_*).$$

We know from Theorem 5.2 that such sequences exist. The minimization property of $\tilde{y}_n$ yields

$$\mathcal{E}_{\gamma_n}(\tilde{y}_n, u_*) - \mathcal{E}_{\gamma_n}(y_*, u_*) \leq 0, \quad \text{for all } n \in \mathbb{N}. \tag{15}$$

Then, we can derive the estimate

$$\begin{aligned}\mathcal{E}_{\gamma_n}(\tilde{y}_n, u_*) - \mathcal{E}_{\gamma_n}(y_*, u_*) &= I_{\gamma_n}(\tilde{y}_n, u_*) - I(y_*, u_*) \\ &\quad + \varphi(\gamma_n)\left(\frac{1}{2}\|\tilde{y}_n - y_d\|^2_{L^2(\Omega)} - \frac{1}{2}\|y_* - y_d\|^2_{L^2(\Omega)}\right) \\ &\geq \min_{v\in\mathcal{A}} I_{\gamma_n}(v, u_*) - \min_{v\in\mathcal{A}_c} I(v, u_*) \\ &\quad + \varphi(\gamma_n)(J(\tilde{y}_n, u_*) - J(y_*, u_*)).\end{aligned}$$

In combination with (15), this yields

$$J(\tilde{y}_n, u_*) \leq J(y_*, u_*) + \frac{\min_{v\in\mathcal{A}_c} I(v, u_*) - \min_{v\in\mathcal{A}} I_{\gamma_n}(v, u_*)}{\varphi(\gamma_n)}.$$

Since (y_n, u_n) is optimal and φ satisfies Assumption 5.2, we obtain

$$\limsup_{n\to\infty} J(y_n, u_n) \leq \limsup_{n\to\infty} J(\tilde{y}_n, u_*) \leq J(y_*, u_*).$$

By coercivity of J in the second variable, u_n is bounded. Consequently, y_n is also bounded due to Lemma 2.5. Thus, we can choose a subsequence such that simultaneously

$$\lim_{k\to\infty} J(y_{n_k}, u_{n_k}) = \liminf_{n\to\infty} J(y_n, u_n) \quad \text{and} \quad (y_{n_k}, u_{n_k}) \rightharpoonup (\overline{y}, \overline{u}).$$

By Lemma 5.1, the pair $(\overline{y}, \overline{u})$ satisfies

$$\overline{y} \in \operatorname*{argmin}_{v\in\mathcal{A}_c} I(v, \overline{u}).$$

Due to the weak lower semicontinuity of J, we conclude

$$\begin{aligned}J(y_*, u_*) \leq J(\overline{y}, \overline{u}) &\leq \lim_{k\to\infty} J(y_{n_k}, u_{n_k}) \\ &= \liminf_{n\to\infty} J(y_n, u_n) \leq \limsup_{n\to\infty} J(y_n, u_n) \leq J(y_*, u_*).\end{aligned}$$

This yields

$$\lim_{n\to\infty} J(y_n, u_n) = J(y_*, u_*) = J(\overline{y}, \overline{u}).$$

The strong convergence of u_n follows from the same arguments which have been applied in the proof of Theorem 5.1. □

In short, if $\varphi(\gamma)$ tends to zero *sufficiently slowly*, then we can recover an optimal solution of the original problem. In view of Section 3, we can even quantify a-priori, what *sufficiently slowly* means. Depending on the problem characteristics, Section 3 yields a rate of convergence of the energy that yields a theoretically backed choice of $\varphi(\gamma)$.

6. A Numerical Path-Following Algorithm

Based on our regularization approach, we present a numerical algorithm for the solution of the optimization problems introduced above. We combine an affine covariant path-following method in the spirit of [Deu11, Chap. 5], which sends the regularization parameter γ to infinity, with an affine covariant composite step method, as introduced in [LSW17]. The composite step method is used as a corrector in the path-following scheme. The latter has a globalization mechanism and has been successfully applied for the numerical solution of optimization problems subject to nonlinear elasticity [Lub15]. Such a globalized corrector seems appropriate in our context of non-convex problems, adding additional robustness to our overall method, compared to a plain Newton corrector.

To apply the composite step method in our setting, we to have replace the minimizing problem (2) by its formal first order optimality conditions.

6.1. **Equilibrium conditions of energy minimizers.** In the context of elasticity, it cannot be guaranteed in general that a local minimizer $y_* \in Y$ of the total energy functional I satisfies

$$\partial_y I(y_*, u)v = 0, \quad \text{for all } v \in Y,$$

see [Bal02]. The crucial point here is the assumed singularity of the stored energy function:

$$\det \nabla y \to 0_+ \Rightarrow \hat{W}(x, \nabla y(x)) \to \infty.$$

From a physical point of view, this condition prevents local self-penetration of the body and yields extreme compressions "expensive" in terms of the total energy. As a result, the set

$$Y_\infty := \{v \in Y \mid \int_\Omega \hat{W}(x, \nabla v(x))\, dx = \infty\}$$

is a dense subset of $W^{1,p}(\Omega)$ for $p < \infty$. This already rules out Gâteaux differentiability in $W^{1,p}(\Omega)$.

By an additional assumption on y_*, the situation can be improved slightly:

Assumption 6.1. *Let $y \in \mathcal{A}$ be a deformation. We call y non-degenerate if $y \in W^{1,\infty}(\Omega)$ and if for an $\epsilon > 0$*

$$\det \nabla y(x) \geq \epsilon, \quad \text{for a.e. } x \in \Omega,$$

is satisfied.

In [LSW14, Theorem 4.6], it was proven that for a compressible Mooney-Rivlin model these assumptions guarantee that an energy minimizer satisfies the stationarity optimality condition

$$\partial_y I(y, u) = 0.$$

However, it cannot be shown a-priori that an energy minimizer y satisfies Assumption 6.1.

6.2. **Formal KKT conditions for the optimal control problem.** These considerations show that, at best, a useful framework for differentiability of I_{strain} is $W^{1,\infty}(\Omega)$. To proceed towards KKT-conditions of our optimal control problem, a local sensitivity of energy minimizers with respect to perturbations in the control would be necessary, e.g., by the application of an implicit function theorem. Such sensitivity studies have been conducted (cf. e.g. [Cia94, Section 6]), however, within a $W^{2,p}(\Omega)$ framework, with $p > 3$, so that $W^{2,p}(\Omega) \hookrightarrow W^{1,\infty}(\Omega)$. Unfortunately, this theory requires very strong regularity assumptions on the problem data, because application of the implicit function theorem requires $W^{2,p}$-regularity of the solution of the linearized elastic problems. Such assumptions are unlikely to be satisfied for many problems of interest. In particular, the important case of mixed boundary conditions is ruled out, in general. Therefore, we will only derive KKT-conditions in a formal way.

Let us introduce the notation $x = (y, u)$ and

$$c_\gamma(x)v = \partial_y I(y, u)v - \gamma \int_{\Gamma_C} [-y_3]_+^{k-1}\, v_3\, ds, \quad v \in Y.$$

Then, formally, the KKT-conditions at a minimizer x_* state the existence of an adjoint state p such that:

$$\begin{aligned} J'(x_*) + c_\gamma'(x_*)^* p &= 0 \\ c_\gamma(x_*) &= 0. \end{aligned}$$

6.3. **Composite step method.** We start by sketching our correction algorithm. More details on this method can be found in [LSW17]. For a fixed penalty parameter γ, we have to solve the respective regularized optimal control problem (12). In order to algorithmically approach this problem, we formally replace the energy minimizing constraint by its first order optimality condition. Then, the reformulated problem reads as follows:

$$\begin{aligned} &\min_{(y,u) \in Y \times U} J(y, u) \\ &s.t.\ c_\gamma(y, u) = 0. \end{aligned} \tag{16}$$

In the following, we abbreviate $x := (y, u)$ and $X = Y \times U$ and obtain the problem:

$$\begin{aligned} &\min_{x \in X} J(x) \\ &s.t.\ c_\gamma(x) = 0. \end{aligned} \tag{17}$$

Then, the formal KKT conditions are

$$
\begin{aligned}
J'(x) + c_\gamma'(x)^* p &= 0 \quad \text{in } X^* \\
c_\gamma(x) &= 0 \quad \text{in } Y^*.
\end{aligned} \tag{18}
$$

This system can be solved (under appropriate assumptions) by a Lagrange Newton method. The defining idea of composite step methods is to split the Lagrange Newton step δx into a normal step $\delta n \in \ker c_\gamma'(x)^\perp$ and into a tangential step $\delta t \in \ker c_\gamma'(x)$. The normal step approaches feasibility, whereas the tangential step approaches optimality. This class of methods is popular in equality constrained optimization and optimal control [Var85, Omo89, Rid06, HR14, ZU11].

The algorithm, proposed in [LSW17] adds a simplified normal step, which we denote by δs, at the end of each iteration. This allows for an affine covariant globalization scheme and also acts as a second order correction to avoid the well known Maratos effect. The resulting composition of the step δx is illustrated in Figure 2.

The special feature of this algorithm, affine covariance, means that norms are only evaluated in the domain space X, but not in the image space of c_γ. In particular, in the context of PDE-constraints, meaningful norms in the image space (which usually is some dual space) are hard to define, whereas problem suited norms in the domain space can be constructed much more easily.

Roughly speaking, our globalization mechanism combines affine covariant Newton techniques for underdetermined problems, due to [Deu11, Chap. 4.4] for feasibility, with a cubic regularization approach [Gri81, WDE07, CGT11], applied to the tangent step for optimality.

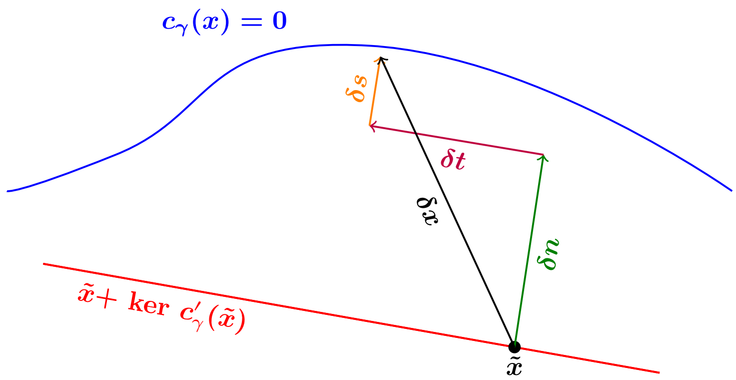


FIGURE 2. Composite Step

In the case of nonlinear elastic problems, some additional modifications have to be made to address the local injectivity constraint $\det y > 0$. Due to Assumption 2.1(2), we can assume that this constraint is inactive at an energy minimizer, but computed trial iterates may violate this condition. If this is the case, say for a trial iterate $x + \delta x$, we reduce the length of δx until $x + \delta x$ is feasible with respect to this constraint by a simple back-tracking procedure. Only afterwards, the globalization scheme of [LSW17] is applied for possibly further reduction of the step size.

In the context of function space problems, the choice of an appropriate norm is important. For our experiments, we took the simple choice:

$$\|\delta x\|^2 = \|(\delta y, \delta u)\|^2 := \|\delta y\|_{M_y}^2 + \alpha \|\delta u\|_{M_u}^2.$$

Here, $\|\cdot\|_{M_y}$ and $\|\cdot\|_{M_u}$ denote the norms induced by the H^1-scalar product on Ω and by the L^2-scalar product on Γ_N, respectively.

6.4. **A simple path-following algorithm.** It is to be expected that the difficulty of (17) depends on the regularization parameter γ, which should be driven to ∞ in order to approximate the original problem. Thus, we augment our optimization algorithm by a path-following method, which is equipped with a simple adaptive step-size strategy.

Introducing the notation $Z := X \times Y$ and $z = (x, p)$, the KKT-system (18) system can be interpreted as an parameter dependent nonlinear system

$$F(z, \gamma) = 0.$$

Path-following methods are widely applied to solve highly nonlinear or non-smooth systems. In convex problems, the existence of a homotopy-path $\gamma \to z(\gamma)$ of zeros of $F(\cdot, \gamma)$ can often be shown, and even sensitivity and a-priori length estimates can be derived. In our non-convex setting, such results can only be observed a-posteriori by a numerical algorithm, and it may happen, that several paths exist that may converge to local solutions or end prematurely. The possible occurrence of such situations is another reason to employ a robust correction method, as described above.

The idea of a path-following method is to successively compute solutions on the homotopy path for a increasing sequence of parameters γ_k. We assume (z_k, γ_k) to be an initial solution close to the path. For the next solution, we increase γ_k by some factor $s > 1$:

$$\gamma_{k+1} = s\gamma_k.$$

Typically, due to the robustness of the corrector, a simple, constant choice of $s = 10$ is appropriate. However, an adaptive choice of the update parameter, depending on the progress of the corrector is advisable.

Next, we apply the composite step method to compute the corresponding solution pair (z_{k+1}, γ_{k+1}) close to the path, whereby z_k is used as starting point. This resembles a classical continuation method for parameter dependent systems. This process is repeated until a solution close to the path with the desired parameter $\gamma_{\max}$ is found. Here, we restrict ourselves to the simple approach, where s is some fixed update parameter. In case the parameter γ is increased too rapidly, we expect that the globalization mechanism of the composite step method will steer the iterate back to the path. This basic approach is illustrated in the following algorithm.

Algorithm 1 Basic Path-following

initial guess: (z_0, γ_0)
fixed update factor: s

function PATH-FOLLOWING(z_0, γ_0)
    $(z_0, \mathit{converged}) \leftarrow \mathit{compositeStepMethod}(z_0, \gamma_0)$
    if not *converged* **then**
        return; (No initial solution on the path found)
    end if
    do
        $z_{k+1} \leftarrow z_k$
        $\gamma_{k+1} \leftarrow s\gamma_k$
        $\gamma_{k+1} \leftarrow \min(\gamma_{k+1}, \gamma_{\max})$
        $(z_{k+1}, \mathit{converged}) \leftarrow \mathit{compositeStepMethod}(z_{k+1}, \gamma_{k+1})$
        if not *converged* **then**
            return; (Algorithm did not converge)
        else
            $k \leftarrow k + 1$
        end if
    while $\gamma_k < \gamma_{\max}$
    return z_{k+1}; (Algorithm converged)
end function

7. Examples

In the numerical examples, we test our combined composite step path-following approach at the following model problem. As mentioned above, we choose to minimize a tracking type functional defined by

$$J(y, u) := \frac{1}{2}\|y - y_{\mathrm{d}}\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Gamma_N)},$$

whereby we aim at approximating a reference deformation $y_{\mathrm{d}} \in L^2(\Omega)$. As regularization parameter we choose $\alpha = 0.25$. It is obvious that the tracking type functional satisfies all the required properties stated above. In the context of nonlinear elasticity, we choose a compressible Mooney-Rivlin model for the stored energy function:

$$\hat{W}(\nabla y) = a\|\nabla y\|^2 + b\|\mathrm{Cof}\ \nabla y\|^2 + c(\det \nabla y)^2 - d \log \det \nabla y.$$

The material is determined by its parameters which are chosen as follows:

$$a = 0.08625, \quad b = 0.08625, \quad c = 0.68875, \quad d = 1.895.$$

This corresponds to a model for soft tissue [Lub15]. In addition, we choose $k = 3$ as exponent in the penalty function P. Further, we apply homogeneous Dirichlet boundary conditions on Γ_D.

The domain is described by a discretized cuboid $\overline{\Omega} = [0, 2] \times [0, 2] \times [0, 0.2]$ which is displayed in Figure 3. Here, the respective grid is uniform. For the discretization of the variables, linear finite elements are used. The degrees of freedom for the state and the control are 44415 and 5043, respectively. Additionally, for the implementation, the finite element library KASKADE7 [GWS12] was applied. This library has been developed at the Zuse Institute Berlin and is based on the DUNE library [BBE+06].

The software package UMFPACK [DD97] was used to directly solve the sparse linear systems that arise during the computations. This limits, of course, the size of tractable problems, but keeps the implementation simple. For larger problems, problem suited iterative solvers, based on a block-decomposition of the linearized KKT-matrix, are currently under investigation.

The optimization and path-following algorithms were implemented in Spacy [1] which is a C++ library designed for optimization algorithms in a general setting. Also, the library FunG [Lub17] for automatic differentiation was applied to compute the required derivatives of the total energy functional.

As reference deformation, we choose a precomputed deformation displayed in Figure 3. The contact constraint $y_3 \geq 0$ a.e. on Γ_C corresponds to a plane which the body cannot penetrate. This plane, in relation to the reference deformation, is also illustrated in Figure 3. For the convenience of the reader, the figures have been rotated.

In order to solve this problem, we apply our previously introduced approach which combines the composite step method with a path-following algorithm. Here, each subproblem is described by the regularized optimal control problem (12) for a corresponding parameter γ. The resulting optimal solutions are displayed in Figure 4 for some chosen parameters. There, we observe that the optimal solutions approach the contact constrained solution as the penalty parameter γ increases.

In order to numerically examine our theoretical results, we also combine the path-following approach with the extended regularized optimal control problem (14) and compare the two approaches. As regularization function we choose $\varphi(\gamma) = \gamma^{-\frac{1}{4}}$. In the following figures, we will distinguish solutions corresponding to this problem by adding the letter φ in the subscript. The respective numerical quantities of the two approaches are displayed in the Figures 5 to 9. The simple geometric situation suggests that energy minimizers are unique in this problem instance so that the reachability assumption is satisfied. This coincides with our observation that the additional regularization is not necessary for convergence in this particular problem setting.

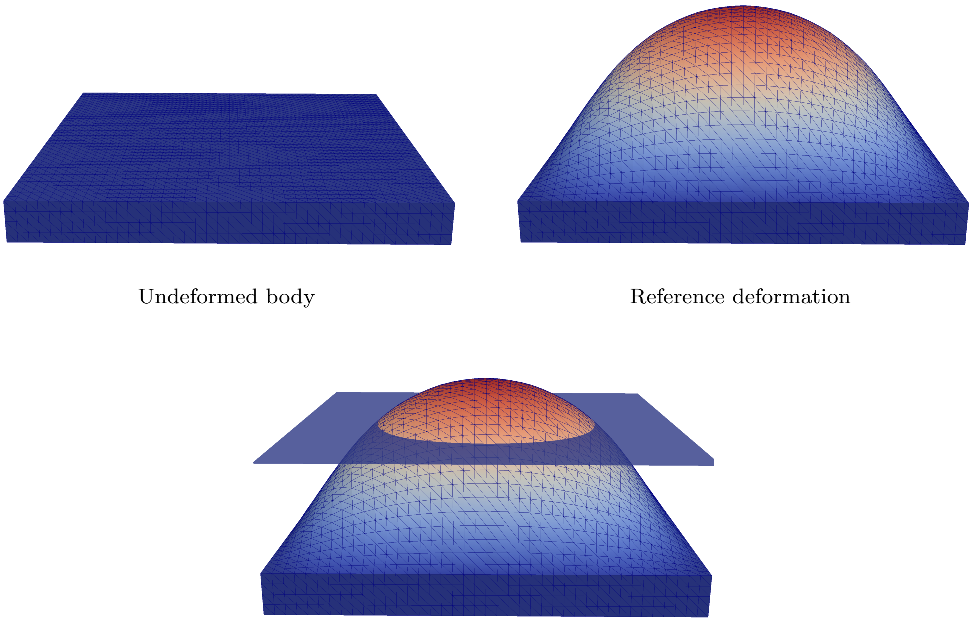
Regarding the number of corrector steps required by the composite step method, Figure 5 shows moderate numbers of corrector steps and quite robust behaviour. This indicates that a path-following method is a reasonable approach for this kind of problem. For very large values of γ, the number of corrector steps becomes smaller. This suggests that γ could be increased more aggressively in this region.

Considering the objective functional values, we observe in Figure 6 that for both approaches, the difference between two consecutive function values approaches zero. These observations coincide with our convergence result elaborated in Theorem 5.1. However, we observe a slower convergence rate for problem (14).

The convergence of the path-following approach is also reflected in behavior of the norm of the updates δx. In this context, Figure 7 shows that the respective updates approach zero at similar rates for both approaches.

Next, we consider the convergence rates of the maximum constraint violation $\|y_+\|_{L^\infty(\Gamma_C)}$ and of the penalty term $\gamma P(y)$. Since we know that both terms approach zero, we can compute local estimates for the convergence rates at each iterate γ_n. Here, y_n denotes the optimal deformation

[1] https://spacy-dev.github.io/Spacy/



Undeformed body

Reference deformation

Reference deformation and obstacle

FIGURE 3. Top left: Undeformed body Ω. Top right: Desired deformation. Bottom: Desired deformation with obstacle (transparent).

of the corresponding optimal control problem. Analogously to the examples in [HSW14], we define these estimates by

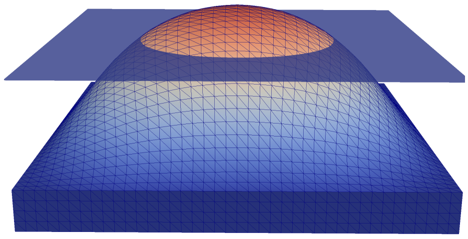
$$\rho_n^y := \frac{\ln(\|(y_n)_+\|_{L^\infty(\Gamma_C)}) - \ln(\|(y_{n+1})_+\|_{L^\infty(\Gamma_C)})}{\ln(\gamma_{n+1}) - \ln(\gamma_n)}$$

and

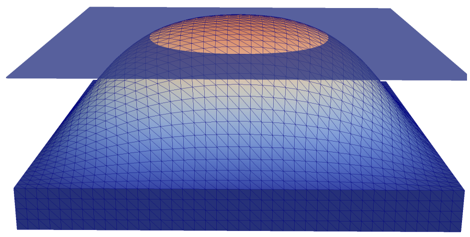
$$\rho_n^P := \frac{\ln(\gamma_n P(y_n)) - \ln(\gamma_{n+1} P(y_{n+1}))}{\ln(\gamma_{n+1}) - \ln(\gamma_n)},$$

respectively.

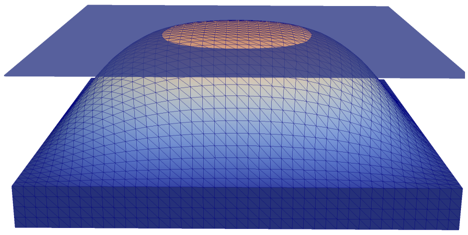
From Corollary 3.4 and 3.5, we expect the same asymptotic convergence rate of $\rho = \frac{\beta}{2\beta+2}$ for both terms. Inserting the reasonable value $\beta = 1$ for the Hölder exponent yields the minimal convergence rate $\rho = \frac{1}{4}$. We note here that in the path-following setting, the boundary force u is not fixed. Therefore, the comparison between the theoretical convergence rates and the observed ones is only a heuristical analysis. Numerically, we observe in Figure 8 and 9 the estimated asymptotic convergence rate $\rho \approx \frac{1}{2}$ for both approaches. This is significantly better than the predicted value, suggesting that further theoretical progress may be possible.



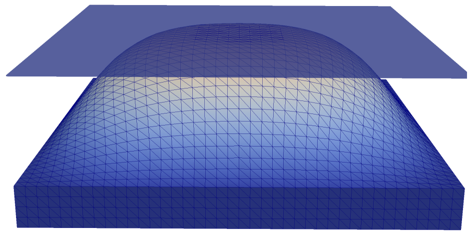
Optimal deformation for $\gamma = 1$



Optimal deformation for $\gamma = 10$



Optimal deformation for $\gamma = 10^2$



Optimal deformation for $\gamma = 10^{10}$

FIGURE 4. Optimal deformations for the respective penalty parameter γ

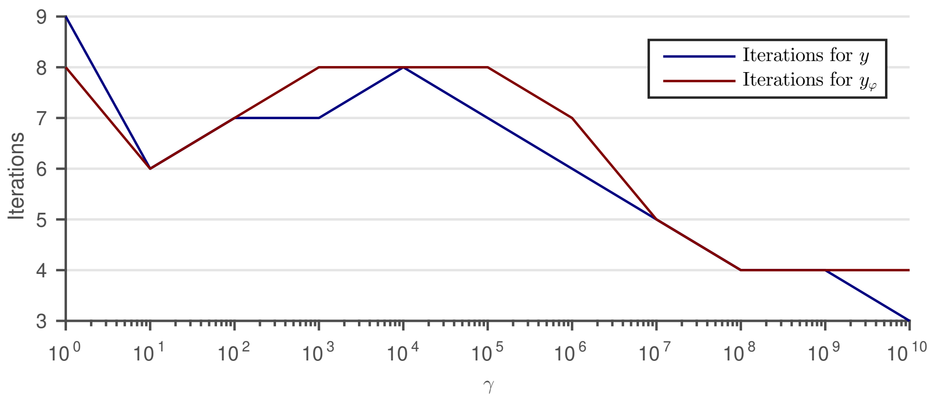


FIGURE 5. Number of composite step iterations in each path step

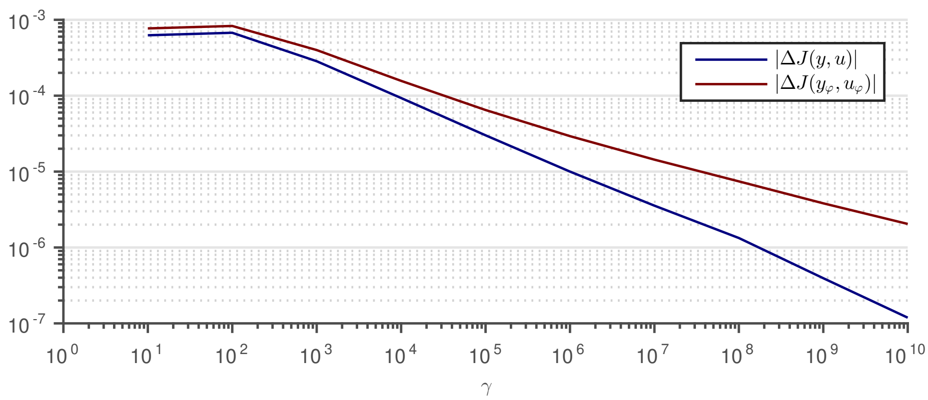


FIGURE 6. Difference of the objective function value compared to the previous iterate

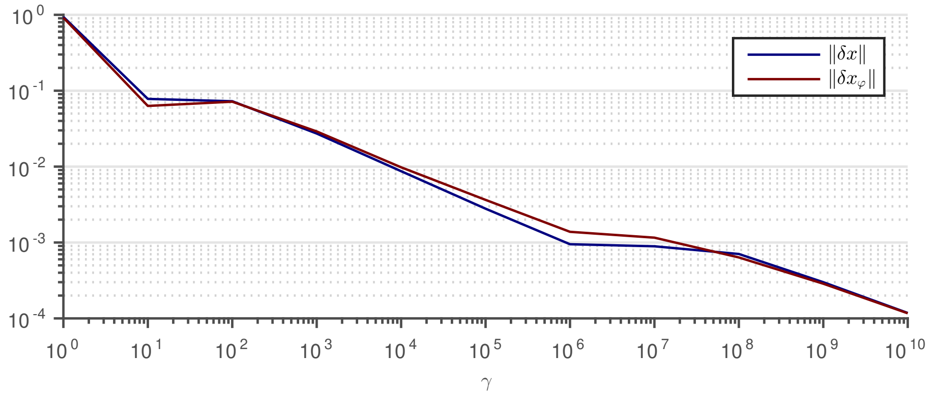


FIGURE 7. Norm of the updates $\|\delta x\|$ of the path-following method

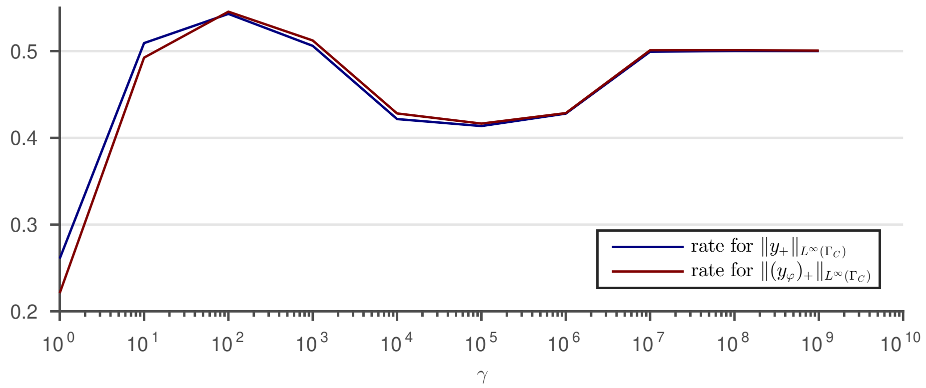


FIGURE 8. Estimates for the convergence rate ρ of $\|y_+\|_{L^\infty(\Gamma_C)}$

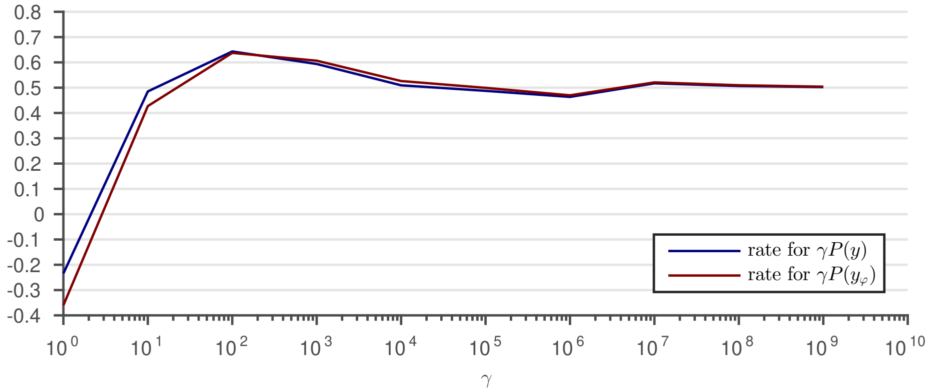


FIGURE 9. Estimates for the convergence rate ρ of $\gamma P(y)$

8. Conclusion and Outlook

In summary, we can conclude that the combined approach of path-following and composite step method converges robustly and efficiently for both regularization variants and thus can be seen as a viable approach for optimal control of contact problems.

While analytic and algorithmic groundwork is laid, some algorithmic extensions are conceivable. First of all, this current implementation is limited by the use of direct sparse solvers for the step computation. To be able to use finer discretizations, iterative solvers have to be employed instead. For works in this direction, we refer to [SSS18]. Second, although our corrector is rather robust due to the underlying composite step method, an adaptive increase of γ is certainly a useful algorithmic extension of the current concept. In particular, for very large values of γ, we expect more aggressive updates, yielding faster local convergence. Finally, our approach should be extended to more complicated geometries, which is, however, a topic of future research.

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