Optimizing Fracture Propagation Using a Phase-Field Approach

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Abstract. We consider an optimal control problem of tracking type governed by a time-discrete phase-field fracture or damage, respectively, propagation model. Pointwise inequality constraints on the phase-field, that model an irreversibility condition for the fracture growth are first regularized by a smooth regularization term, removing the inequality constraints from the lower level problem and resulting in an Euler-Lagrange equation as optimality condition for the lower level problem. We take the regularization limit in the first order optimality conditions and prove convergence of first order necessary points of the regularized control problem to certain limits satisfying an optimality system of a limit problem governed by a variational inequality. Moreover, SQP methods for the regularized problem and its limit are analyzed with respect to solvability of the subproblems. In the case of convergence, it is proven that the limit is a first order necessary point of the respective problem. Finally, the finite element discretization and its convergence for the linear-quadratic SQP subproblems are discussed.

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1. Introduction

In this survey, we consider the problem investigated in [18, 19], i.e., an optimal control problem of tracking type for fracture or damage propagation, which is governed by the Euler-Lagrange equations of a regularized fracture propagation problem modeled by a phase-field approach, which has first been proposed in [3, 4, 7].

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This approach, which we will explain in more detail in Section 2, allows to treat almost arbitrary fracture paths, as opposed to the first results on the control of fractures with prescribed path [14], or fixed length [12]. In a first step, to circumvent the difficulties posed by a pointwise irreversibility condition, this inequality constraint was regularized by a smooth penalization term. In [18], existence of global solutions as well as first order KKT-like necessary optimality conditions under a regularity assumption were proven for the regularized problem. Constraint violation estimates as well as convergence of solutions with respect to taking this penalization parameter to its limit were then shown in [19] for a problem formulation with viscous regularization corresponding to a time-step restriction in the spatially continuous but time-discrete model problem, cf. [13].

In Section 2, we will give a precise description of the model problem under consideration. Then, building on the results from [19], we will prove convergence of the optimality systems with respect to taking the limit in the penalty parameter in Section 3. To elaborate, let us point out that the (uncontrolled) fracture propagation problem is itself an energy minimization problem, the so-called lower level problem. Adding an outer optimal control problem leads to a bilevel optimization problem, where the lower level problem is usually replaced by its first order necessary conditions. In case of the regularized problem, this is a system of Euler-Lagrange equations, so that the control problem resembles a PDE-constrained optimization problem without inequality constraints but a quasilinear PDE constraint. We formulate the optimality conditions for this problem, and then derive a system satisfied by certain limit points when the penalization parameter tends to infinity. In addition to the convergence results for the primal variables, i.e., control, displacement, and phase-field towards a solution of the unregularized problem, we now obtain a limit optimality system, which exhibits the presence of a variational inequality as constraint of the outer optimal control problem.

In Section 4, we formulate the method of sequential quadratic programming (SQP) for the regularized problem formulation and show that the limit point of convergent sequences produced by the SQP method actually satisfies the first order optimality system for the regularized problem. The results are combined with convergence results for the finite element discretization of a linearized fracture control problem, such as the SQP subproblems, from [17]. A key ingredient for obtaining a priori error estimates is an improved regularity of the solutions giving a gap between the norm in which the error is calculated and the regularity of the approximated function. Such estimates have been shown only recently in [10].

Eventually, in Section 5, an SQP method for the unregularized problem is formulated and convergence of the finite element method for the quadratic subproblems is derived.

2. Problem Setting

We consider the problem investigated in [18, 19], i.e., an optimal control problem of tracking type for fracture propagation, which is governed by the Euler-Lagrange equations of a regularized fracture propagation problem modeled by a phase-field approach.

Before presenting the precise control problem, let us elaborate on the fracture propagation problem, which we want to control. The model goes back to Griffith's model of brittle fracture, [8], or more precisely, a variational formulation by Francfort and Marigo in [7]. Within this model, fracture propagation occurs when the elastic energy restitution rate reaches a critical value $G_{\mathcal{C}}$, leading to a minimization problem where the total energy

$$E(u,\mathcal{C}) = \frac{1}{2}\left(\mathbb{C}e(u), e(u)\right)_{\Omega\setminus\mathcal{C}} - (\tau, u)_{\partial_N\Omega} + G_{\mathcal{C}}\mathcal{H}^{d-1}(\mathcal{C})$$

is to be minimized. Here, u denotes a vector-valued displacement field, $\mathcal{C}$ denotes the crack, assumed to be compactly contained in the domain Ω without reaching the boundary, τ is a force applied to the part $\partial_N\Omega$ of the boundary, which will later be our optimization variable in the optimal control problem, and $\mathcal{H}^{d-1}$ is the $d-1$ dimensional Hausdorff measure, when $d \in \{2, 3\}$ denotes the dimension of Ω. By means of $\mathbb{C}$ and $e(u)$, a linear elasticity model is described.

This energy functional is to be minimized with respect to all kinematically admissible displacements u, and any fracture set satisfying a fracture growth condition, making sure that once a fracture has appeared it does not close again. To avoid the difficulty introduced by the Hausdorff measure, we use a regularization proposed by Bourdin et. al., [4, 3]. Precisely, we introduce a time-dependent phase-field variable φ, defined on $\Omega \times (0, T)$, where $\varphi = 1$ describes non-fractured regions, and $\varphi = 0$ fractured regions, with a smooth transition. Using such an Ambrosio-Tortorelli regularization, cf. [1, 2], of the fracture function leads to a regularized energy functional to be minimized:

$$\begin{aligned} E_\varepsilon(u,\varphi) = \frac{1}{2}\big(((1-\kappa)\varphi^2 + \kappa)\mathbb{C}e(u), e(u)\big) - (\tau, u)_{\partial_N\Omega} \\ + G_{\mathcal{C}}\left(\frac{1}{2\varepsilon}\|1-\varphi\|^2 + \frac{\varepsilon}{2}\|\nabla\varphi\|^2\right), \end{aligned} \tag{2.1}$$

where ε is a positive parameter, which, when sent to zero leads to the Hausdorff measure in the sense of a Γ-limit, and $\kappa = o(\varepsilon)$ is a positive parameter used to avoid degeneracy of the energy function when $\varphi = 0$.

The critical issue here is that the energy functional is not convex in both solution variables simultaneously, but only in each single variable when the other one is fixed. While the forward model problem is relatively well-studied, the control of fractures remains to pose a lot of challenges. Controlling this energy functional would lead to a bilevel minimization problem in function spaces, where the lower level problem is nonconvex and subject to additional inequality constraints

$$\varphi(t_2) \le \varphi(t_1) \quad \forall\, t_1 \le t_2, \tag{2.2}$$

describing the irreversibility condition. Fixing the spatial dimension $d = 2$, we obtain for a control space Q, to be specified later, the following problem formulation:

$$\begin{aligned} \min_{q,\mathbf{u}} J(q,\mathbf{u}) &:= \frac{1}{2}\|u-u_d\|^2_{L^2(\Omega;\mathbb{R}^2)} + \frac{\alpha}{2}\|q\|^2_Q \\ &\text{subject to } \mathbf{u} \text{ solves (2.1) given } \tau = q \\ &\text{as well as (2.2).} \end{aligned} \tag{2.3}$$

We tackle the difficulties by the following adaptations to the model problem:

- We will consider a time-discrete, but spatially continuous problem formulation.
- We regularize the inequality constraints in the lower level problem by a penalty approach introduced by Meyer, Rademacher, and Wollner, [15], i.e., adding a term $\frac{\gamma}{4}\|\max(0,\varphi_i-\varphi_{i-1})\|^4_{L^4}$ when φ_i denotes the value of the phase field at time t_i. One of our main goals is then to analyze the problem with respect to considering the limit $\gamma \to \infty$.
- We will follow standard procedure and replace the lower level problem by its Euler-Lagrange equations, leading to a PDE-constrained optimization problem with quasilinear PDE.
- For some of our results, it proved helpful to introduce a further viscous regularization of the energy functional with a regularization parameter $\eta \geq 0$, see below.

2.1. Model Problem, Notation and Assumptions

Following the before-mentioned steps, we arrive at the following short description of the model problem. Note that while the original problem formulation is spatially continuous, but time-discrete, for simplicity of notation we consider only one time-step of the fracture evolution, giving us the regularized optimization problem for finding $q_\gamma \in Q$ and $\mathbf{u}_\gamma = (u_\gamma, \varphi_\gamma) \in V$ solving

$$\begin{aligned} \min_{q_\gamma,\mathbf{u}_\gamma} J(q_\gamma,\mathbf{u}_\gamma) &:= \frac{1}{2}\|u_\gamma-u_d\|^2_{L^2(\Omega;\mathbb{R}^2)} + \frac{\alpha}{2}\|q_\gamma\|^2_Q \\ &\text{subject to } A(\mathbf{u}_\gamma) + R(\gamma;\varphi) = B(q_\gamma). \end{aligned} \tag{NLP$^\gamma$}$$

Here, for spaces to be defined below, $A\colon W^{1,p}(\Omega;\mathbb{R}^2) \times W^{1,p}(\Omega) \subset V \to V^*$ denotes a nonlinear phase-field operator, $R\colon V_\varphi \to V_\varphi^*$ is a regularization operator penalizing deviation from an irreversibility condition for the fracture growth, and $B\colon Q \to V^*$ is the control-action operator. They are defined by

$$\begin{aligned} \langle A(\mathbf{u}),\mathbf{v})\rangle &:= \Big(g(\varphi)\mathbb{C}e(u), e(v^u)\Big) + \varepsilon(\nabla\varphi,\nabla v^\varphi) - \frac{1}{\varepsilon}(1-\varphi, v^\varphi) \\ &\quad + \eta(\varphi-\varphi^-, v^\varphi) + (1-\kappa)(\varphi\mathbb{C}e(u):e(u), v^\varphi), \\ \langle R(\gamma;\varphi), v^\varphi\rangle &:= \gamma([(\varphi-\varphi^-)^+]^3, v^\varphi), \\ \langle Bq,(v^u,v^\varphi)\rangle &:= (q, v^u)_Q \end{aligned}$$

for any $\mathbf{v} = (v^u, v^\varphi) \in V$. Here g is given as

$$g(x) := (1-\kappa)x^2 + \kappa,$$

$\kappa, \varepsilon, \gamma > 0$ are given parameters as explained above, and $\eta \geq 0$ is an additional parameter which can be regarded as a viscous regularization, cf. [13]. Choosing η sufficiently large serves two purposes: On the one-hand, it makes the lower-level energy function strictly convex and hence uniquely solvable. On the other hand, this helps to include damage problems in addition to pure fracture. It also corresponds to choosing a sufficiently small time-step in the temporal discretization of the problem. φ^- is the given initial phase-field, and $\mathbb{C}$ is the rank-4 elasticity tensor with the usual properties. The problem is defined on a polygonal domain $\Omega \subset \mathbb{R}^2$ with boundary $\partial\Omega = \Gamma \dot{\cup} \Gamma_D$, such that the union $\Omega \cup \Gamma$ is Gröger regular [9].

Note that the term $\eta(\varphi - \varphi^-, v^\varphi)$ corresponds to a viscous regularization of the problem for $\eta > 0$ that can also be interpreted as a restriction on the time-step in the temporal discretization of the problem, cf. [13]. In [18], a setting with $\eta = 0$ was considered, requiring additional assumptions due to a lack of convexity.

We define

$$\begin{aligned}
V_u &= H^1_D(\Omega;\mathbb{R}^2) := \{v \in H^1(\Omega;\mathbb{R}^2) \,|\, v = 0 \text{ on } \Gamma_D\},\\
V_\varphi &= H^1(\Omega),\\
V &= V_u \times V_\varphi,\\
Q &= L^2(\Gamma),
\end{aligned}$$

and denote the respective dual spaces with a superscript *, e.g., V^*. For spaces such as $W^{s,p}$ and $H^s = W^{s,2}$, we understand that they are defined on the domain Ω unless otherwise stated. We will further use the following notation for the scalar product/norm: $(\cdot,\cdot)$ denotes the usual L^2 scalar product with corresponding norm $\|\cdot\|$, and $(\cdot,\cdot)_Q$ corresponds to the scalar product of Q. In addition, $\langle\cdot,\cdot\rangle$ stands for a duality pairing where the spaces are omitted if obvious from the context. In what follows, we also define

$$W = W_u \times W_\varphi = W^{1,p}_D \cap H^{1+s} \times W^{2,q}$$

and the corresponding space for the right-hand side of the equation

$$W^\times = W^{-1,p} \cap H^{-1+s} \times L^q,$$

where $W^{-1,p} = (W^{1,p'})^*$, and $H^{-1+s} = (H^{1-s})^*$ are the respective dual spaces. As common, for any $p \in [1,\infty]$ we denote the dual exponent by p', i.e., $\frac{1}{p} + \frac{1}{p'} = 1$. Finally, we will implicitly rely on the following standing assumptions: For the parameters p, q, and s, we require

$$p > 2, \quad q = p/2 > 1, \quad \text{and} \quad s \in (0, 1/2).$$

Further, we assume, that p and s are chosen such that $H^{1+s} \subset W^{1,p}$.

With this notation, we point out that taking the limit $\gamma \to \infty$ in (NLP$^\gamma$) yields the MPCC

$$\min_{q,\mathbf{u}} J(q,\mathbf{u})$$
$$\text{subject to} \begin{cases} A(\mathbf{u}) + \lambda = B(q) & \text{in } V^*, \\ \lambda \geq 0 & \text{in } V_\varphi^*, \\ \varphi \leq \varphi^- & \text{a.e. in } \Omega, \\ \langle \lambda, \varphi - \varphi^- \rangle = 0, \end{cases} \tag{NLP$^{\text{VI}}$}$$

where $\lambda \in V_\varphi^*$ and we implicitly use the natural embedding $V_\varphi^* \ni \lambda \mapsto (0,\lambda) \in V^*$.

We remark, that if $\varphi^- \in W_\varphi$ and $q_\gamma, q \in Q$, by [10, Section 7], the solutions $\mathbf{u}_\gamma$ for the equality constraint in (NLP$^\gamma$) and $\mathbf{u}$ for the constraints in (NLP$^{\text{VI}}$) satisfy $\mathbf{u}_\gamma, \mathbf{u} \in W$ for some $p > 2$.

2.2. The Phase-Field Equation

This section provides a short analysis of the linearized operators $A'(\mathbf{u})\colon V \to V^*$ and $R'(\gamma,\varphi)\colon V_\varphi \to V_\varphi^*$, which for $\mathbf{u} \in V \cap W$, are defined via

$$\begin{aligned} \langle A'(\mathbf{u})\mathbf{d^u}, \mathbf{v}\rangle := {} & \Big(g(\varphi)\mathbb{C}e(d^u), e(v^u)\Big) + 2(1-\kappa)(\varphi\mathbb{C}e(u) : e(d^u), v^\varphi) \\ & + \varepsilon(\nabla d^\varphi, \nabla v^\varphi) + \frac{1}{\varepsilon}(d^\varphi, v^\varphi) + \eta(d^\varphi, v^\varphi) \\ & + (1-\kappa)(d^\varphi \mathbb{C}e(u) : e(u), v^\varphi) + 2(1-\kappa)(\varphi\mathbb{C}e(u)d^\varphi, e(v^u)), \\ \langle R'(\gamma;\varphi)d^\varphi, v^\varphi\rangle := {} & 3\gamma([(\varphi-\varphi^-)^+]^2 d^\varphi, v^\varphi), \end{aligned} \tag{2.4}$$

for any $\mathbf{v} = (v^u, v^\varphi)$, introducing the notation $\mathbf{d^u} := (d^u, d^\varphi)$.

A quick calculation shows two properties of importance for the following calculations. Firstly, coercivity of A', i.e., for $\eta \geq 0$ sufficiently large there exists a $\beta_\eta > 0$ such that

$$\langle (A'(\mathbf{u}))\mathbf{v}, \mathbf{v}\rangle \geq \beta_\eta \|\mathbf{v}\|_V^2 \quad \forall\, \mathbf{v} \in V, \tag{2.5}$$

and, secondly, the following non-negativity statement for R' for all $v^\varphi \in V_\varphi$:

$$\langle R'(\gamma;\varphi)v^\varphi, v^\varphi\rangle \;= 3\gamma([(\varphi-\varphi^-)^+]^2 v^\varphi, v^\varphi) \geq 0. \tag{2.6}$$

Following the results of [10], $A'(\mathbf{u})\colon V \mapsto V^*$ is well-defined and an isomorphism if $\eta \geq 0$ is sufficiently large. In particular, for $\mathbf{u} \in V \cap W$, the operator

$$\mathbf{d^u} \mapsto A'(\mathbf{u})\mathbf{d^u} + R'(\gamma,\varphi)d^\varphi \colon V \to V^* \tag{2.7}$$

is invertible. In a similar way to [18, Lemma 5.2], we can establish the following improved regularity result for data in $W^\times \hookrightarrow V^*$.

Proposition 2.1. *Let $\mathbf{u} \in V \cap W$, $\varphi^- \in W_\varphi$ and $b \in W^\times \hookrightarrow V^*$, recalling $p > 2$. Then the solution $\mathbf{d^u} = (d^u, d^\varphi) \in V$ of*

$$A'(\mathbf{u})\mathbf{d^u} + R'(\gamma,\varphi)d^\varphi = b$$

has improved regularity $\mathbf{d^u} \in V \cap W$.

Further, for regular $\mathbf{u} \in W$, we can define the second derivative operators $A''(\mathbf{u})\colon V \times V \to (V \cap W^{1,p})^*$ and $R''(\gamma,\varphi)\colon V_\varphi \times V_\varphi \to V_\varphi^*$ by

$$\begin{aligned}
\langle A''(\mathbf{u})[\mathbf{d}_1^{\mathbf{u}}, \mathbf{d}_2^{\mathbf{u}}], \mathbf{v}\rangle &= 2(1-\kappa)(d_2^\varphi \mathbb{C}e(u) d_1^\varphi, e(v^u)) \\
&\quad + 2(1-\kappa)(d_2^\varphi \mathbb{C}e(d_1^u)\varphi, e(v^u)) \\
&\quad + 2(1-\kappa)(d_2^\varphi \mathbb{C}e(u) : e(d_1^u), v^\varphi) \\
&\quad + 2(1-\kappa)(\varphi \mathbb{C}e(d_2^u) d_1^\varphi, e(v^u)) \\
&\quad + 2(1-\kappa)(d_1^\varphi \mathbb{C}e(d_2^u) : e(u), v^\varphi) \\
&\quad + 2(1-\kappa)(\varphi \mathbb{C}e(d_2^u) : e(d_1^u), v^\varphi), \\
\langle R''(\gamma;\varphi)[d_1^\varphi, d_2^\varphi], v^\varphi\rangle &= 6\gamma([(\varphi - \varphi^-)^+] d_1^\varphi d_2^\varphi, v^\varphi).
\end{aligned}$$

We note, that for regular data $\mathbf{u}, \mathbf{v}$ the second derivatives are continuous on V in the following sense:

Lemma 2.2. *Let $\mathbf{u}, \mathbf{v} \in V \cap W^{1,p}$ be given. Then there exists a constant c depending on $\|\mathbf{u}\|_{1,p}, \|\mathbf{v}\|_{1,p}$ such that*

$$|\langle A''(\mathbf{u})[\mathbf{d}_1^{\mathbf{u}}, \mathbf{d}_2^{\mathbf{u}}], \mathbf{v}\rangle| \le c \|\mathbf{d}_1^{\mathbf{u}}\|_V \|\mathbf{d}_2^{\mathbf{u}}\|_V.$$

Analogue estimates hold if any two of the four variable $\mathbf{u}, \mathbf{v}, \mathbf{d}_1^{\mathbf{u}}, \mathbf{d}_2^{\mathbf{u}}$ are in $V \cap W^{1,p}$.

Following the regularity results of [10] any solution $\mathbf{u}_\gamma$ to the equation in (NLP$^\gamma$) satisfies the additional regularity $\mathbf{u}_\gamma \in W$ and thus $A'(\mathbf{u})$, and $A''(\mathbf{u})$ are well-defined for all points $\mathbf{u}$ of the same regularity. Further, by (2.5) $A'(\mathbf{u})$ is an isomorphism if η is sufficiently large.

To simplify the following arguments, we assume throughout

Assumption 2.3. Let $\eta \ge 0$ be chosen such that $A'(\mathbf{u})\colon V \mapsto V^*$ is coercive, i.e., (2.5) holds.

3. The Limiting First Order Necessary Conditions

We see that for a local minimizer $(q_\gamma, \mathbf{u}_\gamma)$ of (NLP$^\gamma$) there exists $\mathbf{z}_\gamma \in V$, $\lambda_\gamma, \mu_\gamma \in V_\varphi^*$, $\theta_\gamma \in V_\varphi$ such that the following system is satisfied:

$$\begin{aligned}
A(\mathbf{u}_\gamma) + \lambda_\gamma &= Bq_\gamma && \text{in } V^*, \\
\lambda_\gamma &= R(\gamma;\varphi_\gamma) && \text{in } V_\varphi^*, \\
(A'(\mathbf{u}_\gamma))^* \mathbf{z}_\gamma &= u_\gamma - u_d - \mu_\gamma && \text{in } V^*, \\
B^* \mathbf{z}_\gamma + \alpha q_\gamma &= 0 && \text{in } V^*, \\
z_\gamma^\varphi - \theta_\gamma &= 0 && \text{in } V_\varphi, \\
\mu_\gamma - R'(\gamma;\varphi_\gamma)\theta_\gamma &= 0 && \text{in } V_\varphi^*.
\end{aligned} \tag{FON$^\gamma$}$$

Clearly, the variables λ_γ, μ_γ, and θ_γ can easily be eliminated, but they are useful as separate quantities as they have a meaning as multipliers for the limit, cf. [15]

as well as (FON$^{\mathrm{VI}}$). Moreover, improved regularity for $\mathbf{u}_\gamma \in W$ and $\lambda_\gamma \in L^q(\Omega)$ hold as remarked at the end of Section 2.

We will see, that certain limits $(\bar{q}, \bar{\mathbf{u}}, \bar{\lambda}, \bar{\theta}, \bar{\mu})$ of first order necessary points of (NLP$^\gamma$) satisfy the system (C-stationarity)

$$\begin{aligned}
A(\bar{\mathbf{u}}) + \bar{\lambda} &= B\bar{q} && \text{in } V^*,\\
\bar{\lambda} &\geq 0 && \text{in } V_\varphi^*,\\
\bar{\varphi} &\leq \varphi^- && \text{a.e. in } \Omega,\\
\langle \bar{\lambda}, \bar{\varphi} - \varphi^- \rangle &= 0,\\
(A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}} &= \bar{u} - u_d - \bar{\mu} && \text{in } V^*,\\
B^*\bar{\mathbf{z}} + \alpha\bar{q} &= 0 && \text{in } V^*,\\
\bar{z}^\varphi - \bar{\theta} &= 0 && \text{in } V_\varphi,\\
\langle \bar{\theta}, \bar{\lambda} \rangle &= 0,\\
\langle \bar{\mu}, \bar{\varphi} - \varphi^- \rangle &= 0,\\
\langle \bar{\theta}, \bar{\mu} \rangle &\geq 0.
\end{aligned} \tag{FON$^{\mathrm{VI}}$}$$

Indeed, the following theorem holds:

Theorem 3.1. *Let $q_\gamma \to \bar{q}$ be a convergent sequence of local minimizers of* (NLP$^\gamma$) *for $\gamma \to \infty$. Then, up to selecting a subsequence, the following convergence*

$$\begin{aligned}
\mathbf{u}_\gamma &\to \bar{\mathbf{u}} && \textit{in } V,\\
u_\gamma &\to \bar{u} && \textit{in } W_u,\\
\varphi_\gamma &\rightharpoonup \bar{\varphi} && \textit{in } W_\varphi,\\
\lambda_\gamma &\to \bar{\lambda} && \textit{in } V_\varphi^*,\\
\mathbf{z}_\gamma &\rightharpoonup \bar{\mathbf{z}} && \textit{in } V,\\
\mu_\gamma &\rightharpoonup \bar{\mu} && \textit{in } V_\varphi^*,\\
\theta_\gamma &\rightharpoonup \bar{\theta} && \textit{in } V_\varphi
\end{aligned}$$

holds. Further, any such limit satisfies (FON$^{\mathrm{VI}}$)*.*

Proof. By [19, Corollary 3.10], we obtain the first three convergence claims as well as the satisfaction of the first four lines of (FON$^{\mathrm{VI}}$). Further, from this convergence, the convergence of λ_γ in V_φ^* follows from the first equation.

It remains to show the convergence of the dual variables and the limits in the adjoint equation, the gradient equation, as well as the complementary slackness conditions. We start with the weak convergence of $\mathbf{z}_\gamma$ in V. To this end, we replace μ_γ and θ_γ in the equation for $\mathbf{z}_\gamma = (z_\gamma^u, z_\gamma^\varphi)$ in (FON$^\gamma$) and obtain

$$(A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma + R'(\gamma, \varphi_\gamma)z_\gamma^\varphi = u_\gamma - u_d.$$

Testing with $\mathbf{z}_\gamma$, we arrive at

$$\langle (A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma, \mathbf{z}_\gamma \rangle + \langle R'(\gamma; \varphi_\gamma)z_\gamma^\varphi, z_\gamma^\varphi \rangle = \langle u_\gamma - u_d, z_\gamma^u \rangle, \tag{3.1}$$

and using (2.5) and (2.6), from (3.1) we receive

$$\|\mathbf{z}_\gamma\|_V \leq \frac{1}{\beta_\eta}\|u_\gamma - u_d\|_{H^{-1}}. \tag{3.2}$$

Since u_γ is bounded independently of γ in $W_u \hookrightarrow V_u \hookrightarrow H^{-1}$ as proven in [19, Lemma 3.1], $\mathbf{z}_\gamma$ is bounded in V and we deduce the existence of a subsequence that converges weakly to some $\bar{\mathbf{z}}$ in V.

Next, we want to take the limit in the adjoint equation, so we have to establish weak convergence of $(A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma$ in V^* first. Using the already shown convergence $u_\gamma \to \bar{u}$ in W_u and $\varphi_\gamma \rightharpoonup \bar{\varphi}$ in W_φ we obtain $A'(\mathbf{u}_\gamma) - A'(\mathbf{u}) \to 0$ in $L(V, V^*)$ showing

$$(A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma \rightharpoonup (A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}} \text{ in } V^*.$$

Since u_γ converges strongly in $W_u \hookrightarrow V_\varphi^*$, the convergence of μ_γ and the limit in the adjoint equation $(A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}} = \bar{u} - u_d - \bar{\mu}$ in (FON$^{\text{VI}}$) follow by

$$\mu_\gamma = u_\gamma - u_d - (A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma \rightharpoonup \bar{u} - u_d - (A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}} =: \bar{\mu} \text{ in } V_\varphi^*.$$

Since $\theta_\gamma = z_\gamma^\varphi$, the weak convergence of θ_γ to $\bar{\theta} = \bar{z}^\varphi$ is an immediate consequence.

Next, we can pass to the limit in the gradient equation $B^*\mathbf{z}_\gamma + \alpha q_\gamma = 0$ in (FON$^\gamma$), to obtain

$$B^*\bar{\mathbf{z}} + \alpha\bar{q} = 0.$$

We have shown the convergence results for all functions as stated in the theorem, and established the limits in the first seven lines of (FON$^{\text{VI}}$). We can now verify the complementary slackness conditions given by the last three lines of (FON$^{\text{VI}}$). By definition of $\lambda_\gamma := R(\gamma, \varphi_\gamma) = \gamma[(\varphi_\gamma - \varphi^-)^+]^3$ and introducing the set $\mathcal{A} := \{x \in \Omega \,|\, \varphi_\gamma > \varphi^-\}$, we find that

$$|\langle\lambda_\gamma, \theta_\gamma\rangle| = \left|\int_{\mathcal{A}} \gamma[(\varphi_\gamma - \varphi^-)^+]^3\theta_\gamma \, dx\right| \leq \|\lambda_\gamma\|_{L^q(\mathcal{A})}\|\theta_\gamma\|_{L^{q'}(\mathcal{A})} \tag{3.3}$$

is true. By [19, Lemma 3.8], we know that $\|\lambda_\gamma\|_q \leq C$ holds independently of γ, which implies a uniform bound for $\|\lambda_\gamma\|_{L^q(\mathcal{A})}$. For the second term of (3.3), exploiting (3.2), we receive a uniform bound on the subsequence θ_γ in $H^1 \hookrightarrow L^{q'}$ noting that $q' \in (1, \infty)$. By the convergence result for the primal variables, it has already been proven that $\varphi_\gamma \to \bar{\varphi}$ in V_φ as well as $\bar{\varphi} \leq \varphi^-$, hence for $\gamma \to \infty$ it holds $|\mathcal{A}| \to 0$ and thus

$$\|\theta_\gamma\|_{L^{q'}(\mathcal{A})} \to 0 \text{ for } \gamma \to 0.$$

So overall, from (3.3) we obtain:

$$|\langle\lambda_\gamma, \theta_\gamma\rangle| \leq C\|\theta_\gamma\|_{L^{q'}(\mathcal{A})} \to 0 \text{ for } \gamma \to \infty. \tag{3.4}$$

We already know that λ_γ converges strongly in V_φ^*. In combination with the weak convergence of θ_γ in V_φ, (3.4) yields

$$\langle\bar{\lambda}, \bar{\theta}\rangle = \lim_{\gamma\to\infty}\langle\lambda_\gamma, \theta_\gamma\rangle = 0,$$

which is the third-to-last line of ($\mathrm{FON}^{\mathrm{VI}}$).

Next, by definition of $\mu_\gamma := R'(\gamma;\varphi_\gamma)\theta_\gamma = 3\gamma[(\varphi_\gamma - \varphi^-)^+]^2\theta_\gamma$, using (3.4), it holds

$$\begin{aligned}\langle \mu_\gamma, \varphi_\gamma - \varphi^-\rangle &= 3\int_\Omega \gamma[(\varphi_\gamma - \varphi^-)^+]^2\theta_\gamma(\varphi_\gamma - \varphi^-)\,dx\\ &= 3\gamma\int_\Omega [(\varphi_\gamma - \varphi^-)^+]^3\theta_\gamma\,dx\\ &= 3\langle \lambda_\gamma, \theta_\gamma\rangle \to 0.\end{aligned}$$

Since $\mu_\gamma \rightharpoonup \bar\mu$ in V_φ^* and $\varphi_\gamma \to \bar\varphi$ in V_φ, this proves $\langle \bar\mu, \bar\varphi - \varphi^-\rangle = 0$.

Finally, it remains to show the last line in ($\mathrm{FON}^{\mathrm{VI}}$), $\langle \bar\theta, \bar\mu\rangle \geq 0$. We test both $(A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma + \mu_\gamma = u_\gamma - u_d$ and $(A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}} + \bar\mu = \bar u - u_d$ with $\mathbf{z}_\gamma - \bar{\mathbf{z}}$ and subtract the equations to arrive at

$$\begin{aligned}\langle \mu_\gamma - \bar\mu, \theta_\gamma - \bar\theta\rangle &= \langle \mu_\gamma - \bar\mu, z_\gamma^\varphi - \bar z^\varphi\rangle\\ &= \langle u_\gamma - \bar u, z_\gamma^u - \bar z^u\rangle - \langle (A'(\mathbf{u}_\gamma))^*\mathbf{z}_\gamma - (A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}}, \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle\\ &= \langle u_\gamma - \bar u, z_\gamma^u - \bar z^u\rangle - \langle (A'(\mathbf{u}_\gamma))^*(\mathbf{z}_\gamma - \bar{\mathbf{z}}), \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle\\ &\quad - \langle (A'(\mathbf{u}_\gamma) - A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}}, \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle\\ &\leq \langle u_\gamma - \bar u, z_\gamma^u - \bar z^u\rangle - \langle (A'(\mathbf{u}_\gamma) - A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}}, \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle,\end{aligned} \tag{3.5}$$

where the last inequality follows from coercivity of A', i.e., Assumption 2.3. As before, convergence of $\mathbf{u}_\gamma$ provides

$$\langle (A'(\mathbf{u}_\gamma) - A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}}, \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle \to 0 \text{ for } \gamma \to \infty. \tag{3.6}$$

By definition of μ_γ we also find that

$$\langle \mu_\gamma, \theta_\gamma\rangle = 3\int_\Omega \gamma[(\varphi_\gamma - \varphi^-)^+]^2\theta_\gamma^2\,dx \geq 0. \tag{3.7}$$

We thus arrive at

$$\begin{aligned}\langle \bar\mu, \bar\theta\rangle &= \langle \bar\mu, \theta_\gamma\rangle + \langle \mu_\gamma, \bar\theta\rangle - \langle \mu_\gamma, \theta_\gamma\rangle + \langle \mu_\gamma - \bar\mu, \theta_\gamma - \bar\theta\rangle\\ &\leq \langle \bar\mu, \theta_\gamma\rangle + \langle \mu_\gamma, \bar\theta\rangle + \langle u_\gamma - \bar u, z_\gamma^u - \bar z^u\rangle - \langle (A'(\mathbf{u}_\gamma))^*\bar{\mathbf{z}} - (A'(\bar{\mathbf{u}}))^*\bar{\mathbf{z}}, \mathbf{z}_\gamma - \bar{\mathbf{z}}\rangle,\end{aligned}$$

where we used the non-negativity of $\langle \mu_\gamma, \theta_\gamma\rangle$ from (3.7) in the second line as well as (3.5). Because $u_\gamma \to \bar u$ in V_u, $\theta_\gamma \rightharpoonup \bar\theta$ in V_φ and $\mu_\gamma \rightharpoonup \bar\mu$ in V_φ^*, the first two terms of the right-hand side converge to $2\langle \bar\mu, \bar\theta\rangle$ and the third term converges to zero. By (3.6), also the last term converges to zero, and the desired sign condition in the last line of ($\mathrm{FON}^{\mathrm{VI}}$) follows.

□

4. An SQP-Method for (NLP$^\gamma$)

In this section, we introduce the sequential quadratic programming method for the regularized problem (NLP$^\gamma$). Towards a complete convergence analysis of this algorithm, we are interested in the following tasks: After introducing the algorithm, we discuss solvability of the SQP-subproblem (QP$^\gamma$) in the spaces provided by the regularity of the prior iterates, relying on a typical coercivity condition on the second derivative of the Lagrangian which is expected to be used when deriving second order sufficient optimality conditions. Typically, conditions like that allow to prove local convergence of the algorithm. For the purpose of this chapter, we assume the existence of a convergent sequence and show that the limit satisfies (FON$^\gamma$), i.e., in case of convergence the limit is in fact a critical point of the problem under consideration. Last, we are interested in the convergence behavior of finite element discretizations of the SQP subproblems.

4.1. The SQP Algorithm

Let us start by defining the Lagrangian $\mathcal{L}$ corresponding to (NLP$^\gamma$) via

$$\mathcal{L}(q, \mathbf{u}, \mathbf{z}) := J(q, \mathbf{u}) - \langle A(\mathbf{u}) + R(\gamma, \varphi) - B(q), \mathbf{z}\rangle.$$

Let $(q^k, \mathbf{u}^k) = (q^k, u^k, \varphi^k) \in Q \times V \cap W$ with associated $z^k \in V \cap W$ denote a given iterate of the solution algorithm, and define the notation

$$\mathbf{d} := (d^q, \mathbf{d}^\mathbf{u}) := (d^q, d^u, d^\varphi) = (q - q^k, \mathbf{u} - \mathbf{u}^k) = (q - q^k, u - u^k, \varphi - \varphi^k)$$

for the update directions. We note first that the second derivative of the Lagrangian, twice with respect to (q, u) for directions $[\mathbf{d}, \mathbf{d}]$ at the current iterate as linearization point, is given and denoted by

$$\begin{aligned}\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \mathbf{z}^k)[\mathbf{d}, \mathbf{d}] = \|d^u\|^2 + \alpha\|d^q\|_Q^2 - \langle A''(\mathbf{u}^k)[\mathbf{d}^\mathbf{u}, \mathbf{d}^\mathbf{u}], \mathbf{z}^k\rangle \\ - \langle R''(\gamma, \varphi^k)[d^\varphi, d^\varphi], z^{\varphi,k}\rangle.\end{aligned}$$

Together with the first order derivative of the objective function J with respect to (q, u) at point $(q^k, \mathbf{u}^k)$ in direction $\mathbf{d}$, denoted by

$$J'_{(q,\mathbf{u})}(q^k, \mathbf{u}^k)\mathbf{d},$$

we formulate for given $\varphi^- \in W_\varphi$ the linear-quadratic subproblem (QP$^\gamma$) as follows:

Find the solution $\mathbf{d} = (d^q, \mathbf{d}^\mathbf{u}) \in Q \times V \cap W$ of

$$\min_{\mathbf{d}} J'_{(q,\mathbf{u})}(q^k, \mathbf{u}^k)\mathbf{d} + \frac{1}{2}\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \mathbf{z}^k)[\mathbf{d}, \mathbf{d}] \tag{QP$^\gamma$}$$

$$\text{s. t. } A'(\mathbf{u}^k)\mathbf{d}^\mathbf{u} + R'(\gamma; \varphi^k)d^\varphi = B(d^q) + B(q^k) - A(\mathbf{u}^k) - R(\gamma; \varphi^k). \tag{4.1}$$

The local SQP algorithm for solving (NLP$^\gamma$) then reads as:

Algorithm 4.1. Sequential quadratic programming method for (NLP$^\gamma$):

0. Choose $(q^0, \mathbf{u}^0, \mathbf{z}^0) \in Q \times V \cap W \times V \cap W$, sufficiently close to the optimal triple $(\bar{q}, \bar{\mathbf{u}}, \bar{\mathbf{z}})$ and set $k = 0$.
1. STOP, if $(q^k, \mathbf{u}^k, \mathbf{z}^k)$ is a KKT point of (NLP$^\gamma$), i.e., satisfies (FON$^\gamma$).

2. Solve (QP$^\gamma$) to receive $\mathbf{d}$ with associated adjoint $\mathbf{z}$.
3. Set $(q^{k+1}, \mathbf{u}^{k+1}) := (q^k, \mathbf{u}^k) + \mathbf{d}$, $\mathbf{z}^{k+1} = \mathbf{z}$, $k := k+1$ and go to step 1.

Solvability of (QP$^\gamma$) will be shown in Proposition 4.3 and the optimality conditions to be satisfied in the second step of Algorithm 4.1 are stated in (4.3). To derive these results, we need the solvability of (4.1), which follows from Proposition 2.1 and the properties of $A'(\mathbf{u})$ in Section 2.2.

Corollary 4.2. *Assuming $(q^k, \mathbf{u}^k, \mathbf{z}^k) \in Q \times W \times W$, the linearized partial differential equation given in* (4.1) *has a solution $\mathbf{d}^\mathbf{u} \in V \cap W$ for data $d^q \in Q$.*

Proof. By the regularity assumptions on $(q^k, \mathbf{u}^k) \in Q \times W$, one can see that all terms of $A(\mathbf{u}^k) - R(\gamma, \varphi^k)$ are at least in $W^\times$. Also, by assumption on the data it holds $d^q, q^k \in Q \hookrightarrow W^\times$. Thus the right-hand side of (4.1) is an element of $W^\times$, and the desired result follows by Proposition 2.1. □

Next, we discuss solvability of the quadratic subproblem (QP$^\gamma$):

Proposition 4.3. *Let $(\bar{q}, \bar{\mathbf{u}})$ be a locally optimal solution to* (NLP$^\gamma$) *and let the linearization triple $(q^k, \mathbf{u}^k, \mathbf{z}^k) \in Q \times V \cap W \times V \cap W$ be given. Assume there exists an $\alpha'' > 0$ such that*

$$\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \mathbf{z}^k)[(d^q, \mathbf{d}^\mathbf{u}), (d^q, \mathbf{d}^\mathbf{u})] \geq \alpha'' \|(d^q, \mathbf{d}^\mathbf{u})\|^2_{Q \times L^2(\Omega;\mathbb{R}^3)} \tag{4.2}$$

holds for all $(d^q, \mathbf{d}^\mathbf{u}) \in Q \times V \cap W$ that satisfy

$$A'(\mathbf{u}^k)\mathbf{d}^\mathbf{u} + R'(\gamma, \varphi^k) d^\varphi = B(d^q).$$

Then, there exists a unique global solution $(d^q, \mathbf{d}^\mathbf{u}) \in Q \times V \cap W$ to (QP$^\gamma$).

Proof. For every $d^q \in Q$, the linearized partial differential equation (4.1) in (QP$^\gamma$) has a unique solution $\mathbf{d}^\mathbf{u} \in V \cap W$ by Corollary 4.2. Let M_{feas} denote the feasible set, i.e.,

$$M_{\text{feas}} := \{(d^q, \mathbf{d}^\mathbf{u}) \in \ Q \times V \cap W \text{ satisfying (4.1)}\}.$$

It is immediate that M_{feas} is nonempty, closed, and convex. Due to (4.2), the cost functional of (QP$^\gamma$) is strictly convex and continuous, hence weakly lower semicontinuous, as well as radially unbounded, so (QP$^\gamma$) is uniquely solvable in $Q \times V$. Due to Corollary 4.2, $\mathbf{d}^\mathbf{u}$ is an element of W. □

4.2. First Order Optimality Conditions for (QP$^\gamma$) and its Limit

In order to prove that any limit point of sequences generated by Algorithm 4.1 is in fact a first order necessary point for (NLP$^\gamma$) let us point out that for $(q^k, \mathbf{u}^k, \mathbf{z}^k)$ be given as in Algorithm 4.1, in the $(k+1)^{\text{st}}$-step, the functions

$$\mathbf{d}^\mathbf{u} = (d^u, d^\varphi) = (u^{k+1} - u^k, \varphi^{k+1} - \varphi^k)$$

with associated adjoint $\mathbf{z}^{k+1}$, satisfy the first-order optimality conditions of (QP$^\gamma$), which are given by:

$$\begin{aligned} A'(\mathbf{u}^k)\mathbf{d}^\mathbf{u} + R'(\gamma;\varphi^k)d^\varphi &= B(d^q) + B(q^k) - A(\mathbf{u}^k) - R(\gamma;\varphi^k), && \text{(4.3a)}\\ (A'(\mathbf{u}^k))^*\mathbf{z}^{k+1} + R'(\gamma,\varphi^k)z^{\varphi,k+1} &= -A''(\mathbf{u}^k)[\mathbf{d}^\mathbf{u},\cdot]^*\mathbf{z}^k - R''(\gamma,\varphi^k)[d^\varphi,\cdot]z^{\varphi,k}\\ &\quad + \mathbf{d}^\mathbf{u} + u^k - u_d, && \text{(4.3b)}\\ B^*\mathbf{z}^{k+1} + \alpha(d^q+q^k) &= 0. && \text{(4.3c)} \end{aligned}$$

These optimality conditions are necessary and sufficient, since (QP$^\gamma$) is a convex linear-quadratic problem due to (4.2). These properties allow to prove our desired convergence result.

Theorem 4.4. *Assume that Algorithm* 4.1 *generates an infinite sequence* $(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k, \theta^k, \mu^k)$ *with a limit point* $(\hat{q}, \hat{\mathbf{u}}, \hat{\lambda}, \hat{\mathbf{z}}, \hat{\theta}, \hat{\mu})$ *in the sense that*

$$\begin{aligned} q^k &\to \hat{q} && \text{in } Q, & \mathbf{u}^k &\to \hat{\mathbf{u}} && \text{in } V,\\ u^k &\to \hat{u} && \text{in } W_u, & \varphi^k &\rightharpoonup \hat{\varphi} && \text{in } W_\varphi,\\ \lambda^k &\to \hat{\lambda} && \text{in } V_\varphi^*, & \mathbf{z}^k &\rightharpoonup \hat{\mathbf{z}} && \text{in } V,\\ \mu^k &\rightharpoonup \hat{\mu} && \text{in } V_\varphi^*, & \theta^k &\rightharpoonup \hat{\theta} && \text{in } V_\varphi. \end{aligned}$$

Then, the limit satisfies (FON$^\gamma$).

Proof. We examine the limit for $k \to \infty$ in the equations (4.3a), (4.3b), and (4.3c) separately, starting with (4.3a):

By definition, we have $\mathbf{d}^\mathbf{u} = \mathbf{u}^{k+1} - \mathbf{u}^k = (u^{k+1} - u^k, \varphi^{k+1} - \varphi^k)$. Thus, by the given convergence and regularity assumptions, there exists a limit point $\hat{\mathbf{d}}^\mathbf{u} = (\hat{d}^u, \hat{d}^\varphi) = 0$ in V and $\hat{d}^q = 0$ in Q.

Analogous to the proof of Theorem 3.1, convergence of $\mathbf{u}^k$ in (4.3a) shows that this limit solves

$$0 = A'(\hat{\mathbf{u}})\hat{\mathbf{d}}^\mathbf{u} + R'(\gamma;\hat{\varphi})\hat{d}^\varphi - B(\hat{d}^q) = B(\hat{q}) - A(\hat{\mathbf{u}}) - R(\gamma;\hat{\varphi}).$$

Defining $\hat{\lambda} = R(\gamma;\hat{\varphi})$ gives the first two lines of (FON$^\gamma$).

Taking the limit in (4.3b), and defining $\hat{\theta} = \hat{z}^\varphi$ and $\hat{\mu} = R'(\gamma;\hat{\varphi})\hat{\theta}$, shows the the third, fifth, and sixth line of (FON$^\gamma$).

Finally, convergence in (4.3c) gives the fourth line of (FON$^\gamma$). □

4.3. Approximation of (QP$^\gamma$) by Finite Elements

For a practical implementation of Algorithm 4.1, the QP-step cannot be performed exactly. Instead, an approximate solution of (QP$^\gamma$) is needed, where the PDE (4.1) is discretized by finite elements. To this end, let $\mathcal{T}_h$ be a sequence of shape regular and quasi uniform meshes with element diameter $h_T \le h \to 0$ for all $T \in \mathcal{T}_h$. We assume, for simplicity, that the elements T are open triangles, pairwise disjoint, and provide a decomposition of the domain Ω, i.e., $\overline{\Omega} = \bigcup_{T\in\mathcal{T}_h} \overline{T}$. Further, we assume that the elements match the splitting of the boundary into Γ and Γ_D.

Now, we define the finite element space of piecewise linear finite elements

$$V_h = \{v \in V \mid v\big|_T \in P_1(T), \quad \forall T \in \mathcal{T}_h\}.$$

Then, for $\mathbf{u}^k \in V \cap H^{1+s}$ and $q^k \in Q$, we can define the discretized QP-subproblem

$$\begin{aligned} \min_{\mathbf{d} \in Q \times V_h} \; & J'_{(q,\mathbf{u})}(q^k, \mathbf{u}^k)\mathbf{d} + \frac{1}{2}\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \mathbf{z}^k)[\mathbf{d}, \mathbf{d}] \\ \text{s. t. } & \langle A'(\mathbf{u}^k)\mathbf{d}^{\mathbf{u}}, \mathbf{v}_h\rangle + \langle R'(\gamma; \varphi^k)d^\varphi, v_h^\varphi\rangle \\ & = \langle B(d^q) + B(q^k) - A(\mathbf{u}^k), \mathbf{v}_h\rangle \\ & \quad - \langle R(\gamma; \varphi^k), v_h^\varphi\rangle \quad \forall \mathbf{v}_h \in V_h. \end{aligned} \tag{QP_h^γ}$$

Note that, although no discretization is enforced for d^q, the optimality conditions immediately induce a natural discretization, see, e.g., [11].

Under the growth condition (4.2), the analysis of [17, Theorem 3.3, Corollary 3.8] can be transferred to this situation and yields the following

Proposition 4.5. *Given $(q^k, \mathbf{u}^k, \mathbf{z}^k)$ satisfying (4.2) and let η be such that Assumption 2.3 holds. Then there exists $h_0 > 0$, depending on $\|q^k\|_Q$, $\|\mathbf{u}^k\|_{1+s}$ only, such that for any $h \le h_0$ problem (QP_h^γ) has a unique solution $(d_h^q, \mathbf{d}_h^u)$ and for the solution $(d^q, \mathbf{d}^u)$ of (QP^γ) it holds the error estimate*

$$\alpha''\Big(\|d^q - d_h^q\|_Q^2 + \|\mathbf{d}^u - \mathbf{d}_h^u\|^2\Big) + \|\mathbf{d}^u - \mathbf{d}_h^u\|_V^2 + \|\mathbf{z} - \mathbf{z}_h\|_V^2 \le ch^{2s}.$$

The constant c depends on $\|\mathbf{u}^k\|_{1+s}$ and $R'(\gamma; \varphi^k)$.

Combining these estimates with the convergence in Theorem 4.4, we see that convergence can be asserted as long as $h \to 0$ sufficiently fast for $k \to \infty$. Of course, to assert global convergence of the sequence, suitable globalization strategies are needed. In these, additional requirements on the accuracy of the iterates need to be required to reliably evaluate sufficient descent conditions, cf. [21, 20].

However, our results [19] only show that it is reasonable to assert bounds on $R(\gamma; \varphi^k)$ but not on $R'(\gamma; \varphi^k)$. Hence it is not clear, whether a uniform bound on the constant in Proposition 4.5 can be proven throughout a globalized SQP-type method. Thus we will also discuss an alternative SQP-like algorithm in which the regularization is not used when building subproblems. However a detailed analysis of this alternative is beyond the scope of this paper.

5. An SQP-Method for $(\mathrm{NLP}^{\mathrm{VI}})$

Along the lines of the last section, we would now like to consider an SQP algorithm for the problem $(\mathrm{NLP}^{\mathrm{VI}})$ and briefly discuss solvability of the SQP subproblems. Instead of investigating the convergence analysis, we place special emphasis on the finite element discretization of the quadratic problem governed by complementarity conditions.

It should be noted that in this setting, the quadratic subproblems contain the linearized operator, while the feasible set is not linearized, similar to the way Newton's method is utilized for generalized equations, e.g., in [6]. This means, our resulting QP still is an MPEC in function space. However, in contrast to Proposition 4.5 we will be able to provide uniform discretization error estimates for the resulting QP problems. Note, again, that in Proposition 4.5 uniform finite element estimates are only true under the assumption that $R'(\gamma;\varphi^k)$ remains bounded, a property which up to now is not even proven for the central path where φ_γ solves (NLP$^\gamma$).

5.1. SQP Algorithm for (NLP$^{\mathrm{VI}}$)

Similar as before, we consider the Lagrangian

$$\mathcal{L}(q,\mathbf{u},\lambda,\mathbf{z}) := J(q,\mathbf{u}) - \langle A(\mathbf{u}) + \lambda - B(q), \mathbf{z}\rangle$$

and point out that we have

$$\mathcal{L}''_{(q,\mathbf{u})(q,\mathbf{u})}(q,\mathbf{u},\lambda,\mathbf{z})[\mathbf{d},\mathbf{d}] = \|d^u\|^2 + \alpha\|d^q\|_Q^2 - \langle A''(\mathbf{u})[\mathbf{d^u},\mathbf{d^u}];\mathbf{z}\rangle.$$

Based on this, we can define the QP-approximation to (NLP$^{\mathrm{VI}}$) in a given point $(q^k,\mathbf{u}^k,\lambda^k,\mathbf{z}^k)$ for $\mathbf{d} = (d^q,\mathbf{d^u}) \in Q\times V$ as

$$\min_{\mathbf{d}\in Q\times V} J'_{(q,\mathbf{u})}(q^k,\mathbf{u}^k)(d^q,\mathbf{d^u}) + \frac{1}{2}\mathcal{L}''_{(q,\mathbf{u})(q,\mathbf{u})}(q^k,\mathbf{u}^k,\lambda^k,\mathbf{z}^k)[\mathbf{d},\mathbf{d}]$$
$$\text{s. t.} \begin{cases} A(\mathbf{u}^k) + A'(\mathbf{u}^k)\mathbf{d^u} + \lambda^{k+1} - B(q^k) - B(d^q) = 0, \\ \lambda^{k+1} \geq 0, \\ \varphi^- - \varphi^k - d^\varphi \geq 0, \\ \langle \lambda^{k+1}, \varphi^k - \varphi^- + d^\varphi\rangle = 0. \end{cases} \tag{QP$^{\mathrm{VI}}$}$$

Indeed, this problem corresponds to the linearization of the PDE operator in (NLP$^{\mathrm{VI}}$) while keeping the inequality constraint. Thus the step d^φ needs to be found in

$$K^k := \{\mathbf{v} = (v^u, v^\varphi) \in V \mid v^\varphi \leq \varphi^- - \varphi^k \text{ a.e. in } \Omega\}$$

to assert $\varphi^{k+1} = \varphi^k + d^\varphi \leq \varphi^-$. Thus, the constraint in (QP$^{\mathrm{VI}}$) can equivalently be written as

$$\langle A(\mathbf{u}^k) + A'(\mathbf{u}^k)\,\mathbf{d^u}, \mathbf{v} - \mathbf{d^u}\rangle \geq \langle B(q^k + d^q), v^u - d^u\rangle, \quad \forall \mathbf{v} \in K^k \tag{5.1}$$

and λ^{k+1} is the corresponding Lagrange-multiplier.

With this, we obtain the following local SQP-type iteration:

Algorithm 5.1. Sequential Quadratic Programming method for (NLP$^{\mathrm{VI}}$):

0. Choose $(q^0,\mathbf{u}^0,\lambda^0,\mathbf{z}^k) \in Q\times V\times V_\varphi^*\times V$, and set $k = 0$.
1. If $(q^k,\mathbf{u}^k,\lambda^k,\mathbf{z}^k)$ is a KKT point of (NLP$^{\mathrm{VI}}$), STOP.
2. Derive a KKT point $(\mathbf{d},\lambda^{k+1},\mathbf{z}^{k+1})$ of the problem (QP$^{\mathrm{VI}}$).
3. Set $(q^{k+1},\mathbf{u}^{k+1}) = (q^k,\mathbf{u}^k) + \mathbf{d}$, $k := k+1$, and go to step 1.

Similar as in the previous section, we need to assume a growth condition to have well-posedness of the QP-subproblem, the analogue to (4.2) is now:

Assumption 5.2. Let us assume, that for given $(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k)$ there exists α'' such that for all $\mathbf{d} = (d^q, \mathbf{d}^\mathbf{u}) \in Q \times V \cap W$ satisfying (5.1) it holds

$$\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k)[\mathbf{d}, \mathbf{d}] \geq \alpha'' \|\mathbf{d}\|^2_{Q \times L^2(\Omega;\mathbb{R}^3)}.$$

Once this assumption holds it follows by standard arguments, that (QP$^{\mathrm{VI}}$) has a global solution, noting that coercivity of $A'(\mathbf{u})$ implies that the variational inequality (5.1) is the necessary and sufficient optimality condition for a strictly convex energy minimization.

5.2. Convergence of FE approximation to (QP$^{\mathrm{VI}}$)

In fact, the subproblem (QP$^{\mathrm{VI}}$) is a quadratic minimization problem with inequality constraints. To analyze its approximation by finite elements, we can proceed similarly as in [16], with the slight complication that the linear second order operator in the obstacle problem (5.1) is not H^2-regular.

We abbreviate the objective function of the QP problem by

$$J^k(\mathbf{d}) := J'_{(q,\mathbf{u})}(q^k, \mathbf{u}^k)(d^q, \mathbf{d}^\mathbf{u}) + \frac{1}{2}\mathcal{L}''_{(q,\mathbf{u})(q,\mathbf{u})}(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k)[\mathbf{d}, \mathbf{d}].$$

By Assumption 5.2 for any $d^q \in Q$ there exists a unique solution $\mathbf{d}^\mathbf{u} \in K^k$ of the constraint (5.1). Therefore, we can define the solution operator $S : Q \to K^k$ which maps d^q to $\mathbf{d}^\mathbf{u}$, and thus we can define the reduced objective function

$$\begin{aligned} j^k &: Q \to \mathbb{R} \\ j^k(d^q) &:= J^k(d^q, S(d^q)) \end{aligned}$$

with which we can equivalently write (QP$^{\mathrm{VI}}$) as

$$\min_{d^q \in Q} j^k(d^q). \tag{5.2}$$

Moreover, if $\varphi^- \in W_\varphi$ and $\mathbf{u}^k \in W$, then (5.1) implies the additional regularity $\mathbf{d}^\mathbf{u} = S(d^q) \in W$, cf., [10, Remark 7]. As a consequence, the corresponding multiplier λ^{k+1} satisfies $\lambda^{k+1} \in H^{-1+s}$.

For the discretization, we proceed as in Section 4.3; except now solutions need to be found in the set

$$K_h^k := \{\mathbf{v}_h \in V_h : v_h^\varphi \leq I_h(\varphi^- - \varphi^k) \,\text{in}\, \Omega\}.$$

Where $I_h : C(\overline{\Omega}) \mapsto V_h$ is the nodal interpolation operator satisfying

$$\|w - I_h w\|_V \leq C_I h^s \|w\|_{1+s}, \quad \|w - I_h w\|_{1-s} \leq C h^{2s} \|w\|_{1+s}, \tag{5.3}$$

for any $w \in H^{1+s}$.

From the discrete analog of (5.1), we get the linearized solution operator $S_h : Q \to K_h^k \subset V_h$, $d^q \mapsto \mathbf{d}_h^{\mathbf{u}}$ and the discretized reduced objective

$$\begin{aligned} &j_h^k : Q \to \mathbb{R} \\ &j_h^k(d^q) := J^k(d^q, S_h(d^q)) \end{aligned}$$

and the discretized problem

$$\min_{d_h^q \in Q} j_h^k(d_h^q). \tag{5.4}$$

Lemma 5.3. *Let Assumption* 2.3 *be satisfied. Let* $(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k) \in Q \times W \times V_\varphi^* \times W$ *and* $d^q \in Q$ *be given.*

Then there exists $c > 0$ *such that* $\mathbf{d}^{\mathbf{u}} = S(d^q)$ *and* $\mathbf{d}_h^{\mathbf{u}} = S_h(d^q)$ *satisfy*

$$\|\mathbf{d}^{\mathbf{u}} - \mathbf{d}_h^{\mathbf{u}}\|_V \leq ch^s(\|d^q\|_Q + 1)$$

where $c = c(\|\lambda^{k+1}\|_{-1+s})$ *depends on the* H^{-1+s}*-norm of the multiplier for the variational inequality* (5.1)*.*

Proof. We follow [5] and derive the best-approximation result

$$\begin{aligned} \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{d}_h^u\rangle \leq{}& \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{v}_h\rangle \\ &- \langle \lambda^{k+1}, \mathbf{v}_h - \mathbf{d}_h^u\rangle \quad \forall \mathbf{v}_h \in K_h^k. \end{aligned} \tag{5.5}$$

Indeed, the result shows the claim using continuity and coercivity of $A'(\mathbf{u}^k)$ as well as the following simple calculation using the complementarity and sign relations of (QP$^{\mathrm{VI}}$):

$$\begin{aligned} -\langle \lambda^{k+1}, \mathbf{v}_h - \mathbf{d}_h^u\rangle ={}& - \langle \lambda^{k+1}, \mathbf{v}_h - I_h(\varphi^- - \varphi^k) - \mathbf{d}^u + \varphi^- - \varphi^+\rangle \\ &- \langle \lambda^{k+1}, \mathbf{d}^u - \varphi^- + \varphi^k\rangle \\ &- \langle \lambda^{k+1}, I_h(\varphi^- - \varphi^k) - \mathbf{d}_h^u\rangle \\ \leq{}& - \langle \lambda^{k+1}, I_h(\mathbf{v}_h - \varphi^- + \varphi^k) - (\mathbf{d}^u - \varphi^- + \varphi^+)\rangle \\ \leq{}& \|\lambda^{k+1}\|_{-1+s}\|I_h(\mathbf{v}_h - \varphi^- + \varphi^k) - (\mathbf{d}^u - \varphi^- + \varphi^+)\|_{1-s}. \end{aligned}$$

Taking $\mathbf{v}_h = I_h\mathbf{d}^u$ in (5.5) thus yields

$$\begin{aligned} \beta_\eta\|\mathbf{d}^u - \mathbf{d}_h^u\|_V^2 \leq{}& C\|\mathbf{d}^u - \mathbf{d}_h^u\|_V\|\mathbf{d}^u - I_h\mathbf{d}^u\|_V \\ &+ \|\lambda^{k+1}\|_{-1+s}\|I_h(\mathbf{d}_h^u - \varphi^- + \varphi^k) - (\mathbf{d}^u - \varphi^- + \varphi^+)\|_{1-s} \end{aligned}$$

and the interpolation error estimate (5.3) yields the assertion.

To show (5.5), we calculate for arbitrary $\mathbf{v}_h \in K_h^k$

$$\begin{aligned}\langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{d}_h^u\rangle &= \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{v}_h\rangle \\ &\quad + \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{v}_h - \mathbf{d}_h^u\rangle \\ &= \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{v}_h\rangle \\ &\quad - \langle \lambda^{k+1} + A(\mathbf{u}^k) - B(q^k + d^q), \mathbf{v}_h - \mathbf{d}_h^u\rangle \\ &\quad - \langle A'(\mathbf{u}^k)\mathbf{d}_h^u, \mathbf{v}_h - \mathbf{d}_h^u\rangle \\ &\le \langle A'(\mathbf{u}^k)(\mathbf{d}^u - \mathbf{d}_h^u), \mathbf{d}^u - \mathbf{v}_h\rangle - \langle \lambda^{k+1}, \mathbf{v}_h - \mathbf{d}_h^u\rangle\end{aligned}$$

where we utilized the Lagrange-multiplier λ^{k+1} for the variational inequality (5.1) for the second equation, and the discretized variational inequality for (5.1) in the last step; showing (5.5). □

With this we obtain a discretization error estimate for the reduced cost functional.

Lemma 5.4. *Let $(q^k, \mathbf{u}^k, \lambda^k, \mathbf{z}^k) \in Q \times W \times V_\varphi^* \times V$ be given. Then it holds for any $d^q \in Q$*

$$|j^k(d^q) - j_h^k(d^q)| \le ch^s \|d^q\|_Q.$$

Proof. By definition, it holds

$$\begin{aligned}j^k(d^q) - j_h^k(d^q) &= J'(q^k, \mathbf{u}^k)(0, (S - S_h)d^q) \\ &\quad + \frac{1}{2}\Big(\mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \lambda^k, z^k)[(d^q, Sd^q), (d^q, Sd^q)] \\ &\qquad - \mathcal{L}''_{(q,\mathbf{u}),(q,\mathbf{u})}(q^k, \mathbf{u}^k, \lambda^k, z^k)[(d^q, S_h d^q), (d^q, S_h d^q)]\Big) \\ &= J'(q^k, \mathbf{u}^k)(0, (S - S_h)d^q) + \frac{1}{2}\Big(\|Sd^q\|^2 - \|S_h d^q\|^2 \\ &\quad - \langle A''(\mathbf{u}^k)[Sd^q, Sd^q], \mathbf{z}^k\rangle + \langle A''(\mathbf{u}^k)[S_h d^q, S_h d^q], \mathbf{z}^k\rangle\Big) \\ &= J'(q^k, \mathbf{u}^k)(0, (S - S_h)d^q) + \frac{1}{2}\Big(\|Sd^q\|^2 - \|S_h d^q\|^2 \\ &\quad + \langle A''(\mathbf{u}^k)[(S + S_h)d^q, (S - S_h)d^q], \mathbf{z}^k\rangle\Big).\end{aligned}$$

Using, that $(S + S_h)d^q \in W^{1,p}$ we get from Lemma 2.2

$$|j^k(d^q) - j_h^k(d^q)| \le c\|(S - S_h)d^q\|_V$$

and Lemma 5.3 shows the assertion. □

In order to derive error estimates for the optimal arguments, we need to rely on the following quadratic growth condition. Let $\bar{d}^q \in Q$ be a local solution to (5.2). We assume the following:

Assumption 5.5. (Quadratic growth condition). There exists $\delta > 0$ such that

$$j^k(\bar{d}^q) \le j^k(d^q) - \delta\|d^q - \bar{d}^q\|_Q^2, \quad \forall\, d^q \in Q. \tag{5.6}$$

In many cases, it can be shown that such a condition is a direct consequence of Assumption 5.2. Whether this holds in the given situation is currently being investigated.

From the quadratic growth condition a standard argument gives the following convergence estimate

Theorem 5.6. *Let $\bar{d}^q$ and $\bar{d}^q_h$ be the optimal solutions to the problems* (5.2) *and* (5.4)*, respectively. Then there exists a constant $c > 0$, independent of the mesh size h, such that the following holds*

$$\|\bar{d}^q - \bar{d}^q_h\|_Q^2 \leq ch^s.$$

Proof. From Assumption 5.5 we get, using the optimality of $\bar{d}^q_h$

$$\begin{aligned}\delta \|\bar{d}^q_h - \bar{d}^q\|_Q^2 &\leq j^k(\bar{d}^q_h) - j^k(\bar{d}^q)\\ &= j^k(\bar{d}^q_h) - j^k_h(\bar{d}^q_h) + j^k_h(\bar{d}^q) - j^k(\bar{d}^q) + j^k_h(\bar{d}^q_h) - j^k_h(\bar{d}^q)\\ &\leq |j^k(\bar{d}^q_h) - j^k_h(\bar{d}^q_h)| + |j^k(\bar{d}^q) - j^k_h(\bar{d}^q)|\\ &\leq ch^s(\|\bar{d}^q\|_Q + \|\bar{d}^q_h\|_Q)\end{aligned}$$

where the last inequality follows from Lemma 5.4. □

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