Optimal Control Governed by a Regularized Fracture Propagation Model: Optimality Conditions and Numerical Methods

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Abstract

This thesis addresses the analysis of an optimal control problem in the context of fracture or damage propagation. The problem formulation is given by a tracking type optimal control problem which is governed by a state equation being a (system of) internally coupled regularized quasilinear elliptic partial differential equation(s), which is derived from a variational phase-field fracture propagation model. Due to the coupled structure and the involved need for improved regularity results for the state equation, well-posedness, uniqueness, as well as differentiability and Lipschitz continuity results of the associated solution operator are both interesting and challenging. As a consequence of the state equation being nonlinear, the objective functional of the overall optimal control problem is further nonconvex. In this thesis, we prove second-order conditions and conduct a convergence analysis of the SQP method for such a phase-field fracture propagation optimal control problem. These results extend the already in the literature available existence and first-order necessary optimality results. In the context of the involved penalization, which regularizes inequality constraints incorporated to model the nonhealing presumption of the fracture evolution, we further extend available convergence results for the penalization.

After a brief introduction and a general overview of the fracture propagation model problem in Chapter 1, we recapitulate the derivation and motivation of the model optimal control problem from several key publications of the literature in Chapter 2. The main results of this thesis are contributions towards the topic of optimal control theory, i.p. optimal control problems subject to partial differential equations: In Chapter 4, we study necessary and sufficient optimality conditions of second-order, which do not involve a two-norm discrepancy, and have a minimal gap. Here, we extend recent publications concerning solution and first-order condition results, which cannot deliver sufficient conditions for the optimal control problem due to the objective functional being nonconvex. We also use second-order sufficient conditions in a similar form as a foundation for the convergence analysis of the sequential quadratic programming (SQP) method in the later chapters. To establish our main second-order optimality results, we show the prerequisites of an available framework for second-order optimality conditions. To do this, we rely on a thorough investigation of second-order (local) Lipschitz continuity results of the associated solution operator, which is made beforehand in Chapter 3. The latter results in turn are nontrivial due to the

structure of the involved coupled quasilinear PDE.

In Chapter 5, in the context of first-order necessary conditions and for a setting restricted to one time step, we prove convergence of the dual variables in the penalization (w.r.t. the fracture irreversibility) limit. Here, we rely on already available results which ensure the penalization limit of the primal variables, and norm bounds of the optimal solution which are independent of the penalization parameter in appropriate spaces. We further utilize a similar norm bound of the adjoint state, which we establish again in Chapter 3. We can then ensure that the limits of both the primal and dual variables suffice to a stationarity condition that is associated to the related unpenalized optimal control problem. Note that since we recover the to the nonhealing presumption associated inequality constraints in the limit, the obtained stationarity condition is the optimality condition of a mathematical program with complementarity constraints (MPCC), i.e. our work is also related to this field.

The final main contribution of this thesis is the study of local quadratic convergence of the sequential quadratic programming method for the fracture propagation optimal control problem in Chapter 6. Here, we assume rather weak (σ- strongly active) second-order sufficient conditions, which are close to the minimal-gap second-order conditions, both studied in previous chapters. However, this means that for the theoretical proofs we have to confine the involved SQP subproblem to certain local neighborhoods. We prove local quadratic convergence of the SQP method both for subproblems localized in L^∞ and L^2. Finally, the theoretical convergence result are substantiated by numerical simulations of the SQP method for a simplified phase-field optimal control problem.

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Contents

1. Introduction

The main topic of this thesis is optimal control governed by fracture propagation. In particular, we investigate an optimal control problem which can be used to model the control process of the propagation of a fracture or damage in a brittle material, like e.g. concrete or glass. As an entry point for the model problem, think of the following setting: On the surface of an object of a brittle material, a force is applied. This force shall be used to steer the propagation of an existing or arising crack in the object in a way to achieve a desired fracture pattern. Alternatively, in hope of preserving essential properties of the object, the aim could also be the prevention of the propagation of the fracture in the sense of not having it spread to specific parts of the object. We present a model formulation which can address such a problem setting, recapitulate available solution results, and then dedicate the major parts of this work on how such solutions can be described and how they finally can be (approximately) calculated. Questions like these are of ongoing interest in many real world applications like the construction industry or in mechanical engineering.

Let us begin with a quick introduction of the investigated setting, starting with the underlying fracture modelling process: It is given by a regularized variational phase-field fracture model, which is also already used in [132, 133]. We revisit its derivation and motivation in detail in Section 2.1, founded on ideas of [31, 32, 64, 107, 119]. For now, let us only give an informal, nonrigorous explanation. The aim is to model a (two-dimensional) object of a brittle material. The object contains an evolving fracture and is subject to forces applied on the boundary, i.e. by dragging or pulling on the boundary of the object. As a result, an existing crack propagates or new cracks emerge. At this point, the behavior of the material is given by a displacement variable in combination with the occurring fracture set, which together minimize a corresponding energy functional. This is motivated by the common postulate that in many physical contexts, the system desires to be in an energetic favorable state. The involvement of the fracture set inevitably leads to "jumps" in the material and therefore to discontinuities. To handle this, the fracture set is regularized utilizing a phase-field formulation. In short, this means that the fracture set is eliminated from the formulation by introducing an additional phase-field variable, which indicates the condition of the material, with a value of *one* at all points where the material is completely sound, and *zero* where the material is fully broken, and a buffer zone that ensures a smooth transition in between. Subsequently, the state of the material is described by a pair consisting of the displacement and the phase-field variable. Moreover, as the fracture evolves, an irreversibility condition is inevitable, which models the "nonhealing" of a once fractured material. Recalling that lower values of the phase-field variable mean less integrity, in the notion of phase-fields the irreversibility can be modelled by an inequality constraint between the phase-field variables of successive instants of time. At this point, the fracture energy minimization is therefore an obstacle like problem, i.e. a problem where the state variable is subject to pointwise constraints, before a penalization approach is used to incorporate the inequality constraints into the corresponding energy functional. Eventually, the optimality conditions of such an energy minimization problem can then be formulated in the form of a partial differential equation (PDE) with the following properties: It is spatially continuous and time discrete, elliptic, quasilinear, involves boundary forces as (given) data and is coupled in the phase-field and displacement variable. We want to point out that the coupled quasilinear structure makes the analysis of this PDE as well as its associated solution operator nontrivial. Further, although the progression of a fracture is modelled, the resulting PDE is not parabolic. Instead, a time discrete formulation is used and an elliptic PDE is solved for every time step, where the previous time step is involved as given data. Let us further recall that quasilinear means that while the highest-order derivatives are linear, its coefficients are allowed to involve also lower-order derivatives of the unknown function. Quasilinear elliptic equations are studied e.g. in [69]. They are more complicated than linear, or semilinear PDEs, where nonlinearities are only allowed in the lower-order terms, but less challenging than fully nonlinear PDEs, where nonlinearities are also allowed in the highest-order derivatives. For an overview of all four types of partial differential equations, see e.g. [160, Definition 20] or [59, 76]. Finally, before moving on to the optimal control problems, the reader is referred to Section 2.1 for a rigorous derivation and the full formulation of the fracture propagation problem, as well as a summary of current research concerning (variational) phase-field methods.

To obtain a fracture propagation optimal control problem, the PDE given by the fracture propagation model is used as state equation to govern an optimal control problem. To the best of knowledge of the author, this is first done in [132, 133]. The boundary forces of the fracture problem are now given as the control, denoted by $q_{\mathbb{I}}$, of the optimal control problem. The state is denoted by $\mathbf{u}_{\mathbb{I}}$, and due to the phase-field fracture approach, the state variable $\mathbf{u}_{\mathbb{I}} = (u_{\mathbb{I}}, \varphi_{\mathbb{I}})$ is a pair of vectors of displacement $u_{\mathbb{I}}$ and phase-field $\varphi_{\mathbb{I}}$ variables. In this context, the subscript $\mathbb{I}$ indicates the set $\{1, ..., M\}$ of time steps from the discrete time step formulation. The optimal control problem then reads:

$$\left.\begin{array}{ll} \min\limits_{q_{\mathbb{I}},\mathbf{u}_{\mathbb{I}}} & J_{\mathbb{I}}(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}}), \\ \text{subject to:} & \mathbf{u}_{\mathbb{I}} \text{ solves the fracture propagation PDE for data } q_{\mathbb{I}}, \\ \text{and:} & q_{\mathbb{I}} \text{ lies in an admissible set.} \end{array}\right\}$$

For a rigorous formulation of the model optimal problem, we refer to Section 2.2, and for a rigorous definition, further explanation, and the definition of all spaces and assumptions of this thesis, we refer to Section 2.3.

For completeness, and to recall the most important expressions and standard notation in the context of optimal control problems, let us next give a brief description of the model problem, in accordance with standard literature, e.g. [94, 153]. The control and state belong to a control and function space, which is given in a Banach space setting. For the control, the admissible set demands additional pointwise constraints in the form of box-constraints, i.e. the control is only allowed to have values that are in between an a-priori given upper and lower bound. For a rigorous introduction of all involved function spaces and the admissible set, we refer to Definition 2.3.3 in Chapter 2. The functional $J_{\mathbb{I}}$ is the so-called objective functional, which in this thesis is given in the form of a tracking type functional, combined with a Tikhonov regularization term, cf. Section 2.2. Suitable to the application examples given above, this type of functional is frequently used to model the steering of an optimization process in a way such that the associated state lies as close as possible to an a-priori given, desired state. The standard approach is to first analyze the state equation, i.e. the fracture propagation PDE. If it is uniquely solvable for all $q_{\mathbb{I}}$, i.e. if there exists a unique (associated) state $\mathbf{u}_{\mathbb{I}}$ for every $q_{\mathbb{I}}$ in the corresponding function spaces, it is possible to introduce a solution operator, frequently called the control-to-state operator and denoted by $G_{\mathbb{I}}(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}}$. Then, the model problem is in fact an optimal control problem, instead of just a constrained optimization problem, and by replacing $\mathbf{u}_{\mathbb{I}}$ with $G_{\mathbb{I}}(q_{\mathbb{I}})$ in the objective functional, a reduced formulation $f_{\mathbb{I}}(q_{\mathbb{I}}) := J_{\mathbb{I}}(q_{\mathbb{I}}, G_{\mathbb{I}}(q_{\mathbb{I}}))$ can be introduced. This reduced formulation of the optimal control problem only depends on the variable $q_{\mathbb{I}}$, and can subsequently serve as the basis for the analysis, e.g. when looking at solvability, uniqueness of solutions, optimality conditions, numerical methods, as well as many other aspects.

Note that due to the underlying variational fracture modelling approach, on the one hand the model problem is very flexible. Amongst others, it allows the treatment of controls of a variety of arbitrary fracture paths with changes in topology, and also branching as well as crack nucleation. In this context, the recent works [60, 61] shall be mentioned, where a viscous damage model in a time-continuous setting is investigated w.r.t. necessary optimality conditions. Both the time-continuous approach of [60, 61] and the time discrete approach discussed in this thesis stand in contrast to earlier works that are limited to cracks of fixed length [106], or to prescribed fracture paths [113], or to [57, 91], where a crack propagation in a material is conditioned by controlling the release of the associated energy, but no optimal control in the sense of steering the process towards a desired configuration is achieved. In [3, 130], damage evolution is analyzed using shape optimization methods. In [15, 148], necessary conditions of an optimal control problem of a two-field damage model, and strong stationarity of a nonsmooth coupled damage system are investigated. Let us also mention optimal control problems governed by a so-called free material optimization (FMO) problem, which can be seen as a possible further extension of the model problem of this thesis: In the joint work [83] of the author, D. Khimin, I. Neitzel, N. Simon, T. Wick and W. Wollner some computational experiments for such a problem are conducted as a proof of concept. On the other hand however, again due to the quasilinear coupled phase-field propagation model, the model problem of this thesis has a nonconvex nonlinear structure. This leads to the need for improved regularity, differentiability and other technical results, which makes its analysis nontrivial, and its study challenging. Further, the involvement of several different parameters for the phase-field model and regularizations are of interest, especially when looking at numerical approaches.

Now that the reader has gotten an impression of the optimal control problem we want to investigate, let us give an overview of the goals of this thesis. Along the way, we also put them into context of the current state of research, both of the model problem as well as related works in the corresponding fields, and summarize the structure of this thesis. The main contributions are given in Chapter 3 - 6, with the major results established in Chapter 4 and 6. They are already published for a one time step setting, for simplification, in the authors publications [85, 86] as joint work with I. Neitzel and in [84] as joint work of M. Mohammadi, I. Neitzel and W. Wollner and the author. In this thesis, all notational and technical details are also presented for the multi time step setting (except for Chapter 5). Further, we complement the theoretical results of Chapter 6 by some (up until now) unpublished numerical results.

In the next Chapter 2, we motivate and derive the fracture propagation model, as well as the final optimal control problem that we have already seen in short form above. For reference, the problem setting involving all assumptions and definitions are collated in Section 2.3. Note that some explanations of the used notation and abbreviations are also collected in Appendix A.

In Chapter 3, we collect technical results for the coupled quasilinear PDE that stems from the fracture propagating model, and for the optimal control problem. We start with several technical results for the involved nonlinear phase-field and penalization terms, which are revisited, or established respectively, in Section 3.1. We then restate solvability and (improved) regularity results for the quasilinear PDE from [132, 133]. Further, existence and uniqueness as well as improved regularity for solutions of the linearization of the state equation are recapitulated in Section 3.2. Note that in these two sections, we rely on available results and techniques, again from [132, 133]. As important auxiliary results, the associated control-to-state operator is then investigated w.r.t. Fréchet differentiability and Lipschitz continuity in Section 3.3. Subsequently, differentiability and Lipschitz continuity results of second-order for the reduced functional of the optimal control problem, and its associated Lagrangian functional are established in Section 3.4 and Section 3.5. These results are essential for the main results of the subsequent chapters of this thesis.

The main topic of Chapter 4 is optimality conditions of second-order. In Section 4.1, existence of solutions and first-order necessary optimality conditions for the model problem can be immediately transferred from [132], where these results are established for a very similar problem as the model problem, albeit under slightly different assumptions. Since it is well-known that for nonconvex optimal control problems, optimality conditions of first-order are not sufficient, second-order optimality conditions, notably second-order sufficient conditions (SSCs) are of interest. Generally, SSCs have been a very active research area in recent years ever since they were investigated in the context of optimal control subject to partial differential equations firstly in [71]. In particular, the question of the ”strength” of the required assumptions is often discussed, in the sense that a gap between necessary and sufficient conditions shall be analyzed, and ideally be as small as possible. Further, the concept of two-norm discrepancy, which is initially described for an optimization problem in [97], is the topic of many publications. SSCs for optimal control problems subject to semilinear PDEs with state constraints are examined in [46]. In [37], SSCs for this setting with minimal gap towards the necessary conditions are given. For a more abstract setting, where SSCs are investigated for a class of optimal control problems in Banach spaces w.r.t. improving the result that is expected involving the two-norm discrepancy, see [40]. In the quasilinear setting, SSCs for optimal control problems involving control constraints are given in [36, 39]. Other no-gap SSC results, e.g. for nonsmooth problems and for bang-bang optimal control problems, can be found in [48, 50, 134]. A general framework for optimality conditions of second-order for (reduced) optimal control problems, on which we also rely in the course of action to achieve our results below, is proved in [38]. Finally, for a general overview of second-order sufficient conditions in the context of optimal control, the interested reader is also referred to [44]. As the first major contribution of this thesis, we study second-order optimality conditions, both necessary and sufficient for the fracture propagation optimal control problem. In particular, we prove the prerequisites that allow us to apply the framework from [38] in Proposition 4.2.1. For this, we rely on the (second-order) Fréchet differentiability and Lipschitz continuity of the reduced objective functional presented in Chapter 3. We can then establish necessary, cf. Theorem 4.2.2, as well as (σ-[1]) strongly active sufficient optimality conditions, cf. Theorem 4.2.4 and Corollary 4.3.2. The optimality results involve a minimal gap and do not have a two-norm discrepancy.

In Chapter 5 we investigate the following aspect: We have already argued that for fracture propagation problems, it is inevitable to include some sort of irreversibility of the evolving damage, e.g. in the form of inequality constraints. To obtain our model problem formulation, these constraints subsequently undergo a regularization in the form of a penalization. In the context of regularized optimal control problems, an interesting topic is then the transfer of results back to the original, unregularized problem. As mentioned earlier, the related unregularized fracture problem is an obstacle like problem, therefore the corresponding optimal control problem falls into the category of mathematical programs including complementary constraints (MPCCs). For such problems, first-order and especially second-order optimality conditions, and therewith associated numerical methods and other topics, are challenging due to the lack of

[1] cf. also cf. [70, 152]

smoothness and differentiability of the control-to-state operator, and therefore also of the reduced functional. Similar to the procedure of the model problem, many recent publications use regularization techniques as a first approach, and then establish different stationary concepts, e.g. M, B, C or strong stationarity, cf. [2, 51]. A quick overview and comparison of these concepts is given in [80]. The lack of smoothness, and the approach of investigating generalized derivatives of the control-to-state operator in the context of the obstacle problem is discussed in [137, 138]. Finally, in the overlap between MPCC and SSC research, SSCs for optimal control of the obstacle problem are investigated in [49], and more abstract for optimal control problems governed by variational inequalities in [16, 111]. In [118], a regularized optimal control problem, that is governed by an evolution variational inequality is examined with respect to second-order sufficient conditions. As for the model problem, the convergence of regularized solutions is analyzed with respect to the involved penalization, i.e. the regularization of the irreversibility constraint, in [133]. However, the convergence of dual variables and the recovery of the full associated stationarity system were still open questions. As a further contribution of this thesis these two aspects are investigated. In this context, one important task is to ensure that the solution of the state equation, respectively additionally the adjoint equation for the dual variable convergence, can be bounded independently of the penalization parameter in the corresponding norm. While such a bound is proved for the state equation in [133], for the adjoint equation we ensure such a bound in a suitable space in Chapter 3. Subsequently, we show that the dual variables converge in its respective spaces, and that the limits of both primal and dual variables satisfy a (C-stationarity) optimality condition that corresponds to the associated unpenalized optimal control problem, in Theorem 5.0.1. Note that in this chapter, which presents results from [84] of M. Mohammadi, I. Neitzel and W. Wollner and the author, we restrict the setting to only one time step.

Finally in Chapter 6, we look at the sequential quadratic programming (SQP) method for the optimal control problem. Algorithmic concepts, as well as a space-time formulation and time discretization, with several numerical examples, where a desired phase-field is tracked in the objective functional, are the subject of [102, 103, 104, 105]. An established class of fast and robust solvers for nonlinear optimization problems is the well-known sequential quadratic programming (SQP) method, for which an introduction to the general idea can e.g. be found in [70]. Very briefly, the SQP method can be used to numerically solve nonlinear optimization problems by iteratively solving a sequence of associated quadratic subproblems. As a starting point for the investigation serves [84], where the SQP method for both the regularized and an unregularized problem is described, and a preliminary analysis of the involved regularized quadratic subproblems is conducted under an additional (and strong) local coercivity condition. A-priori error estimates for a linearized fracture control problem, which is closely related to the quadratic subproblems, are analyzed in [128]. SQP methods for optimal control problems that involve semilinear elliptic and parabolic equations and are subject to control constraints have been studied extensively, cf. e.g. [70, 150, 152, 154, 155]. For the latter setting, but with mixed control-state-constraint, the reader is referred to [73, 74]. Furthermore, SQP methods for the Navier-Stokes equation are the subject of [88, 92, 93, 156]. A semilinear phase-field equation is analyzed w.r.t. the SQP formulation and its convergence in [87, 88]. Further, convergence of the SQP method for quasi-linear parabolic optimal control problems (for time-dependent controls) in function space is proved in the recent [96]. In the latter publication, the important feature is that a local L^2-neighborhood can be chosen in the SQP method, instead of an L^∞-neighborhood in the prior literature. As a major contribution of this thesis, we investigate the convergence of the SQP method for the model problem in Section 6.1 - 6.4. We also substantiate our theoretical findings by some numerical results for a simplified problem, which have not been published so far, in Section 6.5. For the convergence proof, we use the meanwhile established concept of strong regularity, and base our analysis on the (weak) σ-strongly active second-order sufficient conditions from Chapter 4. First following the ideas of [152], we prove quadratic convergence of the SQP method for subproblems localized in L^∞ in Theorem 6.3.15, and then secondly follow the ideas of [96] to prove quadratic convergence of the SQP method also for subproblems localized in L^2 in Theorem 6.4.10.

The thesis is concluded by a conclusion and an outlook about further aspects of interest in the context of phase-field fracture optimal control in Chapter 7.

Let us recapitulate that the fracture propagation optimal control problem is challenging in several ways: Firstly, the involved fracture propagation PDE used as a state equation is of quasilinear type, which subsequently makes the model optimal control problem nonconvex. Thus, when analyzing optimality conditions of second-order, the desire of preferably as weak as possible assumptions for second-order conditions makes the analysis more involved. This also plays a major part in the convergence analysis for the SQP method. Further, the coupled structure and the additional involvement of control constraints introduce some difficulties concerning the involved regularities. To investigate optimality conditions, and numerical methods that are based on them, a careful analysis of the involved operators and functionals has to be made w.r.t. second-order differentiability and continuity in suitable, more regular function spaces. Finally from the modelling aspect, the involvement of several physical parameters and their interplay and behavior is not only interesting for the analytical results, but also in the context of obtaining meaningful numerical results and constructing test examples.

2. Modelling optimal control of fracture propagation

The main task of this chapter is to motivate and present the optimal control problem which is analyzed throughout this thesis, and which was outlined as the model problem in the introduction. We start with the derivation of a fracture model that leads to a so-called regularized variational phase-field fracture propagation model, cf. ($C_{\mathbb{I}}^{\gamma,\eta}$). This is an energy minimization problem, and here we incorporate ideas from [31, 64, 75, 107, 119, 121, 122]. Subsequently, we follow [132, 133] and recognize that this fracture propagation model can be reformulated into a coupled quasilinear PDE, cf. ($EL_{\mathbb{I}}^{\gamma,\eta}$). Then, still following [132, 133], the optimal control problem ($NLP_{\mathbb{I}}^{\gamma,\eta}$) is presented by using the fracture propagation problem as a lower-level problem to an additional upper-level tracking type minimization problem.

The final fracture propagation model is able to model the behavior of a brittle material which is subject to an additional load on a Neumann boundary, including the modelling of complex crack patterns, as well as crack nucleation, branching and merging. In this context, brittle materials are understood as materials that, under exposure of stress, fracture without significant prior deformation. These materials comprise e.g. ceramics, concrete and glass, but also certain types of cast iron, if an impeccable material structure is assumed. In the optimal control problem, the boundary load is then used as the control. We also motivate the usage of the PDE formulation of the fracture propagation model below in more detail: In short, when using the energy minimization fracture problem as the lower-level problem, this means that the overall optimal control problem is a bi-level optimization problem. However, with the PDE formulation, we can use it as a state constraint in the lower-level problem, thus we obtain a PDE-constrained optimal control problem, which is a problem class we can tackle. Note that while the upper-level problem is rather standard due to its tracking type objective functional, the more involved fracture propagation problem makes the overall optimal control problem interesting and its analysis nontrivial.

Since in general fracture is one of the most important kinds of failure which a material, a body or a structure can encounter, the topic of modelling and subsequently also of prevention or restraint of fractures is an important area of research in many fields. For an overview over different trends and applications of fracture modelling and damage or fracture mechanics, the interested reader is referred to [161] and [7], as well as the references cited therein. In this chapter, the focus is put on the variational phase-field approach of fracture modelling, its main features and how to use it to govern an optimal control problem. Our starting point is the remarkable milestone for fracture modelling that is given in [75], where "Griffith's criterion for brittle fracture" is stated. It served as the foundation for many further approaches, e.g. in the physics community, see [78, 101, 147], and also the work of [98], the latter dominating the fracture research community for many decades[1]. The foundation for many mathematical (and mechanical) works is [64], which introduces a variational formulation based on the ideas of [75], and is often combined with phase-field methods, cf. [9, 31]. For an overview of the main ideas of this variational approach of fracture, see e.g. [32], and for some applications in the context of multiphysics phase-field fractures see [160]. Current trends in phase-field fracture are also outlined in the recent article [115].

The following sections present the fracture propagation model utilized in this thesis in Section 2.1, as well as the optimal control problem in Section 2.2. We conclude with Section 2.3, where the final optimal control problem setting is recapitulated for further reference, and all assumptions are collected.

2.1 The fracture propagation model

Let us start by only fixing the most necessary notation and assumptions, successively augmenting them where required. The fracture process is investigated on a domain $\Omega \subset \mathbb{R}^2$, which has a boundary $\Gamma = \partial\Omega$, and on a time interval $[0, T]$, for a given final time $T > 0$.

Griffith's criterion for brittle fracture

The starting point of the utilized model is Griffith's criterion for brittle fractures, which is laid in the groundbreaking work [75]. It is recapitulated by many authors, e.g. [30, 32, 47, 62], on which the following introduction is based.

The setting is the following: A two dimensional, bounded domain is filled with "brittle material", i.e. a linear elastic homogeneous and isotropic medium. In this context, isotropic means that the material is uniform in all orientations. A connected crack, which has an a-priori known crack path, and whose length is given by the function $t \mapsto l(t)$ at all times t, is given in the cracked body. The crack is in elastic equilibrium for given time-dependent loads (which are applied slowly such that inertia is negligible) and the crack length, for all times t. This equilibrium idea is frequently called "quasi-staticity". In this section, we denote by $G(t, l)$ the energy release rate at t associated with an infinitesimal advance of a crack of length l along its predefined path at time t, i.e. $G(t, l) = \partial P(t, l)/\partial l$.

[1]As postulated e.g. in [31, page 6] or in [30]

Here, $P(t, l)$ is the potential energy for the load at t, i.e. the energy given through summing bulk energy, surface energy and the load. Further, denote by G_c the surface energy density of the material, a macroscopic material constant, frequently also called "fracture toughness". Intuitively, the surface energy shall be proportional to the number of broken bonds of the material, and therefore proportional to the length of the crack, i.e. $G_c \cdot l(t)$. Then, [75] states that there is competition between surface energy on the crack and restitution of bulk energy away from the crack. Propagation of a crack only occurs when the energy release rate $G(t, l)$ reaches the fracture toughness G_c, and does not if $G < G_c$. As noted in [64, 1. Introduction], the "literature is of various opinion as to what happens whenever $G(t, l) > G_c$; in any case, the propagation is then labeled unstable". Overall, this approach culminates in three properties, that $l(t)$ must obey:

1. Irreversibility: $t \mapsto l(t)$ is monotonically increasing.
2. Griffith's criterion: $G(t, l(t)) \leq G_c$ for all $t \geq 0$.
3. Energy conservation: $G(t, l(t))\partial l(t) = G_c \partial l(t)$ for $t \geq 0$.

Unfortunately, the approach of [75] comes with two disadvantages: It only works for an a-priori known crack path and if the solution $l(t)$ is sufficiently smooth. This, however, cannot be expected in general, as is argued e.g. in [32], and e.g. for kinked paths, cf. [47].

The variational fracture model of Francfort and Marigo

Inspired by the variational viewpoint in the field of image segmentation [129], where an energy conservation idea is used, [64] uses Griffith's criterion as a foundation to develop a variational fracture formulation, cf. also [31, 32]. The total energy is defined there via

$$E(f; u, \mathcal{C}) = \frac{1}{2}\big(\mathbb{C}e(u), e(u)\big)_{\Omega\setminus\mathcal{C}} - (f, u)_\Gamma + G_c \mathcal{H}^{d-1}(\mathcal{C}), \tag{2.1}$$

for all admissible (vector-valued) displacements[2] u, and all fractures $\mathcal{C}$ that lie in a fracture set, shall not intersect any part of the boundary, and be compactly supported in the (two-dimensional) domain Ω. In this context $(\cdot,\cdot)_{\Omega\setminus\mathcal{C}}$ denotes the L^2-inner product on $\Omega\setminus\mathcal{C}$, and $(\cdot,\cdot)_\Gamma$ is the L^2-inner product on the Neumann boundary Γ. There, a traction force f is applied, manifested through the second term in (2.1). In accordance with [75], the first term in (2.1) describes the bulk energy, and the third term in (2.1) describes the surface energy, where G_c is the critical value of the energy restitution rate. In this context, $\mathcal{H}^{d-1}$ is the $d-1$ dimensional Hausdorff-measure [82], which for smooth surfaces and $d = 2$ dimensions, is equivalent to the length of the surface, i.e. in the given case to the length of the crack $\mathcal{C}$. Further, $e(u)$ denotes the symmetric gradient

$$e(u) := \frac{1}{2}\big(\nabla u + \nabla u^T\big),$$

[2] in this thesis the displacements are two-dimensional, but generally also three-dimensional displacements are possible

which is a linear operator. Next, $\mathbb{C} = (\mathbb{C}_{ijkl})^2_{ijkl=1}$ denotes the elasticity tensor, a fourth-order, positive definite material tensor. As in [160, Definition 36], this means there exists a constant $c > 0$ such that for any matrix $\xi = (\xi_{ij})^2_{ij=1}$, ξ being symmetric, and any point $x \subset \Omega$, it holds:

$$c|\xi|^2 \leq \mathbb{C}(x)\xi \colon \xi = \sum_{i,j,k,l=1}^{2} \mathbb{C}_{ijkl}\xi_{ij}\xi_{kl}.$$

For an isotropic, homogeneous and symmetric material, i.e. in particular for brittle materials, the elasticity tensor simplifies to

$$\mathbb{C}e(u) := 2\mu e(u) + \lambda tr(e(u))I,$$

where $\mu, \lambda > 0$ are the so-called Lamé-coefficients, see e.g. [136, Section 3] for a motivation, and where some standard properties of $\mathbb{C}e(u)$ can be found. In this context, tr denotes the trace, which is also a linear operator, cf. Appendix A. Let us only state some of the most important properties of the symmetric gradient and the elasticity tensor, which will be used without further mention, and can be easily verified by direct calculation. For all displacements u, u_1, u_2, it holds

$$\begin{aligned} \mathbb{C}e(u_1) \colon e(u_2) = \mathbb{C}e(u_1) \colon e(u_2), \qquad (\mathbb{C}e(u), e(u)) \geq 0, \\ (tr(e(u))I, e(u)) \geq 0, \qquad (e(u), e(u)) \geq 0, \end{aligned}$$

if all expressions are well-defined. The elasticity operator is widely utilized in the field of linear elasticity theory, which can be used in the context of the analysis and modelling of deformation or strain in elastic and inelastic bodies. An introduction to the numerical approach and further references on this topic can e.g. be found in [33, Chapter 6].

Now, the approach of [64] is to use a monotonically increasing load $f(t) = t \cdot f_0$ in time, for a given initial load $f_0 \subset \Gamma$, which means that f is defined on $\Gamma \times (0, T)$. Subsequently, an evolution law in the sense of quasi-staticity is formulated: The crack $\mathcal{C}(\cdot)$ on $\Omega \times (0, T)$ is an increasing function, which, together with the displacement $u(\cdot)$ on $\Omega^2 \times (0, T)$, has to minimize the total energy $E(f(t); u(t), \mathcal{C}(t))$, cf. (2.1) for every point $t \in (0, T)$ in time, and among all admissible fractures that suffice to an additional condition that respects the irreversibility, i.e. nonhealing condition, of the crack. For more details on this see e.g. [160, Proposition 11], or directly [64, Law 2.9]. This means that in the evolution process, energy is only transferred between bulk and surface energy, and cracks are able to choose their future paths freely without any pre-defined path assumptions. However, using an additional constraint they shall be limited by the previous crack setting. Note that for the two-dimensional setting, cracks can also only be sets of dimension one.

For this kind of problem, the minimality condition is investigated on a global scope. This however leads to some drawbacks, for which [30, page 2 and 3] states "Global minimality of the crack state at each time was key to mathematization of the evolution problem. In physics, however, any minimality postulate is technical convenience rather than the manifestation of a known physical imperative". In particular, [30] states two downsides: Firstly the fact that (negative) force loads in the interior can be problematic, since cutting their support can "prevent the realization of minimality"[3]. Secondly, global minimality might be influenced by distant material properties or geometric features, the minimization process should not be aware of. It is then postulated in [30] that local criteria would seem to be more appropriate. However, even then the force load issues pertain, and crack initiation would be problematic[4]. Further, it is recognized that this might lead to problems in the related context of phase-field regularization, as the appertaining concept of Γ-convergence, both terms being the topic of the next subsection, does not generally imply convergence of local minimizers. For the variational model at hand, existence proofs of a well-posed evolution are established in [55] for a topological setting, in [54] for nonlinear elasticity and in [63] for a setting that is similar to the related Mumford-Shah segmentation problem, where the (sharp) edges of the contours and shapes of objects depicted in a (black and white) picture are formulated as sets. A numerical implementation of the variational fracture model is also the subject of [3].

At this point, note that the force f can also be applied differently, e.g. as a Dirichlet boundary condition. Another possibility is the usage of design variables as data instead of a force f, as e.g. done in the context of free material optimization (FMO), cf. [81]. They correspond to material properties, and are incorporated as coefficients in the nonlinear phase-field operator instead of the elasticity tensor $\mathbb{C}$. The motivation is to model intrinsic properties of the material which change over time through influences as e.g. a change in temperature. Using such a setting to govern an optimal control problem leads to so-called "optimal control problems involving a coefficient control", cf. [146] and the references therein for an abstract setting. In the joint work [83] of D. Khimin, I. Neitzel, N. Simon, T. Wick and W. Wollner and the author, some computational experiments for an optimal control problem governed by an FMO problem are conducted as a proof of concept. Indeed, the numerical examples imply that the susceptibility of the material to fracture propagation is influenced by the changing material properties during the optimization process.

By different modifications of the energy functional (2.1), various other applications in the context of fracture propagation can also be covered: In [112], a computational framework for phase-field fracture models in porous media is presented, where the variational fracture is extended to porous media by employing Biot's theory, cf. [17]. This involves an additional pressure variable, and is also related to the works of [125, 126, 157], which study so-called pressurized fracture problems. The latter are also modelled by incorporating an additional pressure variable, and adding a nonhomogeneous traction force term that acts on the fracture surface into a variational fracture model comparable to (2.1). Similarly, by incorporating time derivatives, one obtains dynamic fracture problems, which are (numerically) investigated in e.g. [8, 25, 26, 89, 121, 122, 145].

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[3] see [30, page 3]

[4] again see [30, page 3]

Ambrosio-Tortorelli regularization and phase-field approach

The energy functional (2.1) involves $\mathcal{C}$, a fracture set that lies in the set of all admissible fractures. This is not only mathematically challenging, since one has to deal with the inherent discontinuities of the displacement and the involvement of the fracture set, but also numerically complex: The changing fracture set has to be resolved for ever time step, which when implementing such problems using e.g. the finite element method means there is a need for constant re-meshing and updating of basis functions.

Similar problems again occur in the context of the theoretical and numerical analysis of the Mumford-Shah functional [129] used in image segmentation. In this context, [10] proposes to circumvent dealing with such sets by regularizing the Hausdorff measure $\mathcal{H}^{d-1}$ by a phase-field approach and then recover the original problem in the sense of Γ-convergence, cf. also [27, 29]. In analogy to this idea, a regularized variational phase-field fracture model is suggested in [31], and studied in [28, 31, 110]. Let us quickly outline this phase-field fracture approach: The sharp crack surface is regularized by smearing it in a transition zone near the crack, through introducing an auxiliary, so-called phase-field variable φ on Ω. In the context of fracture propagation, the phase-field variable can be understood as a damage parameter in the following sense: $\varphi = 1$ indicates the points in the domain Ω where the material is completely sound, $\varphi = 0$ denotes points where the material is broken. A transition zone of thickness ε on either side of the crack surface is given by all points where $0 < \varphi < 1$. Here, the sharp crack jump is replaced by a smooth transition. However, this approach also comes with some disadvantages: In numerical simulations, the interplay between the model and discretization parameters can be challenging, and the transition zone has to be resolved by choosing a sufficiently fine mesh at the corresponding parts of the domain, leading to either potentially high computational costs or the need for an adaptivity scheme, cf. e.g. [89, 117]. Further, the energy functional now turns out to be potentially nonconvex, which might be problematic due to the global minimization approach. Further, note that the limit process has to be done w.r.t. the concept of Γ-convergence when recovering the sharp fracture description, which includes the study of (special) bounded variation ((S)BV-) function spaces, cf. [53], also e.g. [9, 10]. Nevertheless, variational phase-field models are in general a very appealing approach, and we also pursue this approach, since it enables us to use techniques that are established in the field of PDE-constrained optimal control. Note that variational phase-field models are also successfully applied in many other fields, e.g. in material science, cf. [18, 19, 20] or for medical applications, cf. [65, 66] where tumor growth is modelled. The area of image segmentation is also still a very active field of research in this regard, cf. [143]. An overview of phase-field models and their numerical implementations can be found in [56], or in the context of multiphysics fracture problems, again in [160].

Thus, let us conduct the phase-field regularization for (2.1). This means, that for an $\varepsilon \in (0, 1)$, the Hausdorff measure $\mathcal{H}^{d-1}(\mathcal{C})$ is regularized by the

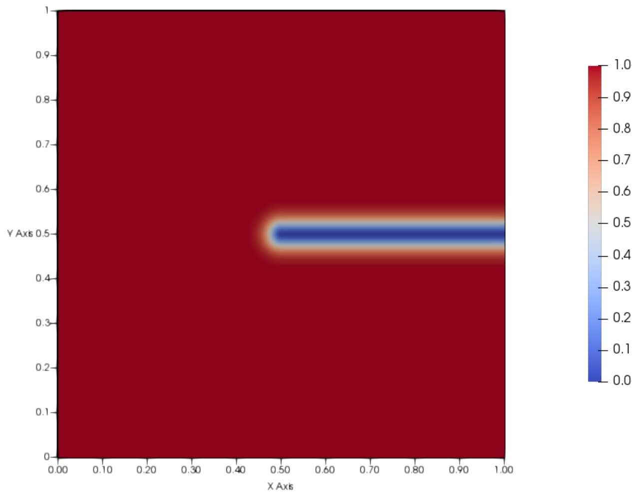

Figure 2.1: Crack modelling using a phase-field approach in a transition zone: A crack $[0.5, 1] \times 0.5$ on the unit square $[0, 1]^2$ is regularized using a phase-field method. The red areas denote $\varphi = 1$, i.e. the completely sound parts of the material, the blue area denotes $\varphi = 0$, i.e. the fracture. There is a transition zone with distance ε around the fracture in which the phase-field variable φ is a smooth function.

regularized fracture functional

$$\frac{1}{2\varepsilon}\|1-\varphi\|^2 + \frac{\varepsilon}{2}\|\nabla\varphi\|^2,$$

where $\|\cdot\|$ denotes the L^2-norm on Ω.

To eliminate the fracture set $\mathcal{C}$ also from the first term in (2.1), in particular to be able to work with the displacement on Ω instead of $\Omega\backslash\mathcal{C} = \Omega\backslash\{x \in \Omega \,|\, \varphi = 0\}$, an additional regularization is needed. Let thus κ be an additional regularization parameter, where $\kappa \ll \varepsilon$, and a coefficient function g be defined via

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

where the latter regularization also has the added benefit that the elastic energy is not degenerated, due to the fact that, for $\varphi \to 0$, the system matrix associated to the bulk energy term remains regular, cf. [160, Remark 26]. Thus, the function g is also frequently called the degradation function, cf. [160, Definition 39]. The overall regularization approach is used also already in [31, 32], and can be justified through Γ convergence results, w.r.t. the limit $\varepsilon \to 0$, which is discussed in [32, 62], or in the context of cohesive fracture, cf. [22, 52], and the references therein.

Overall, this means that the state variable is now given by a pair of two functions $\mathbf{u} = (u, \varphi)$, where u denotes the displacement variable, and φ is the just introduced phase-field variable. Incorporating both regularizations into (2.1), one obtains the regularized total energy

$$E_\varepsilon(f; \mathbf{u}) := \frac{1}{2}\big(g(\varphi)\mathbb{C}e(u), e(u)\big)_\Omega - (f, u)_\Gamma + \frac{G_c \varepsilon}{2}\|\nabla\varphi\|^2 + \frac{G_c}{2\varepsilon}\|1-\varphi\|^2, \quad (2.2)$$

where $(\cdot,\cdot)_\Omega$ is the L^2-inner product on Ω. The identifier Ω is frequently dropped, and $(\cdot,\cdot)$ is used equivalently.

When looking at fracture evolution of brittle materials over time, as one would do in real life applications, a once broken material should not be able to heal and revert readily to its original state. This means that an evolving fracture evolution model over time has to incorporate some kind of irreversibility condition for the broken parts, which tracks the fracture path and prevents its regress. We have already seen above that such evolution laws are incorporated in both [75] and [64]. Other model problems which are subject to an irreversibility condition are studied e.g. in [21] in the context of structural optimization. In [121, 122], a regularized variational fracture model is augmented by a rate-independent formulation, which ensures the local growth of the damage variable[5]. In the context of phase-field formulations, a natural possibility to model an irreversibility constraint is imposed by demanding that the phase-field variable is monotonically decreasing over time, recalling that a lower value of the phase-field variable φ means less integrity of the material at the given point, with brokenness if $\varphi = 0$. Irreversibility of the fracture can therefore be easily modelled by demanding the constraint

$$\varphi(t_1) \geq \varphi(t_2) \quad \text{for all } 0 \leq t_1 \leq t_2 \leq T. \quad (2.3)$$

For the regularized fracture propagation model, again in a quasi-static sense, the following problem setting can be concluded:

> For a given load $f(\cdot)$ on $\Gamma \times (0, T)$, a state pair $\mathbf{u}(\cdot) = (u(\cdot), \varphi(\cdot))$ consisting of a displacement $u(\cdot)$ on $\Omega^2 \times (0, T)$ and a phase-field $\varphi(\cdot)$ on $\Omega \times (0, T)$, is searched, which satisfies
>
> $$\left.\begin{aligned} &\min_{\mathbf{u}(t)} E_\varepsilon(f(t); \mathbf{u}(t)) \quad \text{for all } t \in (0, t), \\ &\text{subject to:} \quad \varphi(t_1) \geq \varphi(t_2) \quad \text{for all } 0 \leq t_1 \leq t_2 \leq T. \end{aligned}\right\} \quad (2.4)$$

Numerically, solution algorithms for these kind of problems are studied in [28, 34] (as alternating minimization, also called staggered solution), [89, 160] (quasi-monolithic), and [68, 108, 158, 159] (monolithic)[6].

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[5] note that in [121, 122] the phase-field variable is defined as *zero* where the material is sound, and as *one* where the material is broken, i.e. switched to the formulation of this thesis

[6] In this context and in plain terms, monolithic roughly means that all equations are solved in a single uniform system, while staggered means that (parts of the) equations are solved in a sequentially way, with quasi-monolithic being a hybrid approach combining the former two.

Time discretization

We recall that for the progress of the fracture over time, a quasi-static approach is used in the fracture problem given through (2.4). This means that the system has to be in equilibrium at all times, i.e. that the regularized total energy functional (2.2) is minimized for the current load f and the associated state $\mathbf{u}$. Further, we recall that the time interval is given by $[0, T]$ for a $T > 0$, and the load $f(\cdot)$ is now given on $\Gamma \times (0, T)$. Similarly, for the state $\mathbf{u}(\cdot) = (u(\cdot), \varphi(\cdot))$, the displacement $u(\cdot)$ is now given on $\Omega^2 \times (0, T)$ and the phase-field $\varphi(\cdot)$ on $\Omega \times (0, T)$. As in [132, 133], also in this thesis a time discrete but spatially continuous model is used, therefore the time interval $(0, T)$ is discretized into $M \in \mathbb{N}$ equidistant time partitions

$$0 = t_0 < t_1 < t_2 < \cdots < t_M = T.$$

The loads are then given by the vector $(f^i)_{i=1}^M$ on Γ^M, and the state by the pair of vectors $\mathbf{u}_{\mathbb{I}} = (\mathbf{u}^i)_{i=1}^M = (u^i, \varphi^i)_{i=1}^M$, with displacement vector $u_{\mathbb{I}} = (u^i)_{i=1}^M$ on $(\Omega^2)^M$ and phase-field vector $\varphi_{\mathbb{I}} = (\varphi^i)_{i=1}^M$ on Ω^M, at the associated time-points t_i. For the chosen time discretization, this means that the irreversibility condition from (2.3) leads to the constraint

$$\varphi^i \leq \varphi^{i-1} \quad \text{for all } i = 1, ..., M, \tag{2.5}$$

where an initial phase-field φ^0 is given, cf. Remark 2.1.1 below.

The quasi-static equilibrium approach in turn means that the discrete formulation of (2.4) then reads:

For given loads $f_{\mathbb{I}} = (f^i)_{i=1}^M$ we look for the minimum of

$$\left.\begin{aligned} &\min_{\mathbf{u}^i} E_\varepsilon(f^i; \mathbf{u}^i) \quad \text{for all } i = 1, ..., M, \\ &\text{subject to:} \quad \varphi^i \leq \varphi^{i-1}. \end{aligned}\right\} \tag{2.6}$$

This means that due to the quasi-static approach, this fracture propagation problem is (a system) of quasilinear elliptic type, and not quasilinear parabolic, despite its purpose of modelling a fracture evolution over time. The (optimal control of) parabolic-type settings involve their own challenges, even if they do not involve the coupled phase-field fracture propagation approach, cf. e.g. [23] and [96]. For a time-continuous approach where a variational fracture propagation governs an optimal control, the reader is also referred to [60, 61].

Viscous approximation

Following [133], an additional term is incorporated into the regularized total energy (2.2), namely the term

$$\frac{\eta}{2} \left\| \varphi^i - \varphi^{i-1} \right\|^2, \tag{2.7}$$

is added for an $\eta \geq 0$. For the time discrete formulation corresponding to (2.6) this leads to the formulation

$$E_\varepsilon^\eta(f^i, \varphi^{i-1}; \mathbf{u}^i) := E_\varepsilon(f^i; \mathbf{u}^i) + \frac{\eta}{2}\left\|\varphi^i - \varphi^{i-1}\right\|^2, \tag{2.8}$$

for all $i = 1, ..., M$, and for a given, initial phase-field φ^0. This is inspired by a regularization technique in rate-independent damage models, cf. [107], where the term from (2.7) corresponds to a potential viscous approximation. Physically, the largeness assumption corresponds to a restriction on the size of permissible time steps. We want to point out that the viscous approximation can also be understood as a penalization of the crack growth, i.e. it can also be seen as some form of penalization for the crack irreversibility constraint. The main point is, that for sufficiently large η the energy functional (2.8) is strictly convex, which also leads to uniqueness of solutions of this energy minimization problem, cf. [133]. It is further essential when establishing differentiability results, and for the (linearized and adjoint, cf. Section 3.2) equations that occur when analyzing the final optimal control problem, which is stated in Section 2.2. Therefore, we in fact demand η to be sufficiently large in Assumption 2.3.11 below. We omit further explanation of the viscous approximation, and refer the reader to [107].

Incorporating this viscous approximation into (2.4), we can formulate the first fracture propagation problem in rigorous form, for which also the state space $V := V_u \times V_\varphi$, where $V_u := H^1(\Omega; \mathbb{R}^2), V_\varphi := H^1(\Omega)$ and the space $L^2(\Gamma)$ is introduced for the boundary force. In this context, we denote product spaces by using an exponent, e.g. $V^M = V \times \cdots \times V$ is the product space of M times V, respectively analogously for $(L^2(\Gamma))^M$. Then the inequality-constrained fracture propagation problem has the following formulation:

Let $\mathbf{u}^0 \in V$, with $\varphi^0 \in [0,1]$, and data $f_{\mathbb{I}} \in (L^2(\Gamma))^M$ be given, find $\mathbf{u}_{\mathbb{I}} \in V^M$ that solves

$$\left.\begin{array}{l} \min\limits_{\mathbf{u}^i} E_\varepsilon^\eta(f^i, \varphi^{i-1}; \mathbf{u}^i) \quad \text{for all } i = 1, ..., M, \\ \text{subject to:} \quad \varphi^i \leq \varphi^{i-1}. \end{array}\right\} \tag{$\mathrm{C}_{\mathbb{I}}^{\eta}$}$$

Remark 2.1.1. *Note that the initial displacement u^0 of the initial state $\mathbf{u}^0$ is not necessary as a datum for ($\mathrm{C}_{\mathbb{I}}^{\gamma,\eta}$). For other fracture propagation approaches, this assumption can however be necessary, e.g. for the modelling of dynamic fractures.*

Without a rigorous argumentation, let us only mention here that its associated stationarity conditions, which in accordance with the notation from [133] we call ($\mathrm{EL}_{\mathbb{I}}^{\eta}$), read:

For every test function $(v^u, v^\varphi) \in V$, given loads $f_{\mathbb{I}} \in (L^2(\Gamma))^M$ and initial phase-field $\varphi^0 \in [0,1]$, any minimizer $\mathbf{u}_{\mathbb{I}} \in V^M$ of $(\mathrm{C}_{\mathbb{I}}^\eta)$ satisfies

$$\left.\begin{aligned} \big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)\big) - (f^i, v^u)_Q &= 0, \\ G_c\varepsilon(\nabla\varphi^i, \nabla v^\varphi) - \frac{G_c}{\varepsilon}(1-\varphi^i, v^\varphi) + \eta(\varphi^i - \varphi^{i-1}, v^\varphi) & \\ +(1-\kappa)(\varphi^i\mathbb{C}e(u^i)\colon e(u^i), v^\varphi) + (\lambda^i, v^\varphi) &= 0, \\ \varphi^i - \varphi^{i-1} &\le 0, \\ \lambda^i &\ge 0, \\ \langle \lambda^i, \varphi^i - \varphi^{i-1}\rangle &= 0, \end{aligned}\right\} \qquad (\mathrm{EL}_{\mathbb{I}}^\eta)$$

for all $i = 1, ..., M$, and Lagrange multipliers $\lambda_{\mathbb{I}} := (\lambda^i)_{i=1}^M \in (V_\varphi^*)^M$, and V_φ^* being the dual space of V_φ.

Note that since the fracture problem $(\mathrm{C}_{\mathbb{I}}^\eta)$ is a minimization problem subject to the irreversibility constraint (2.5), the stationarity conditions $(\mathrm{EL}_{\mathbb{I}}^\eta)$ contain a so-called complementarity condition, given through the last three lines of $(\mathrm{EL}_{\mathbb{I}}^\eta)$. The derivation of such optimality conditions for optimization problems in Banach spaces including state constraints is e.g. explained in [153, Chapter 6]. It involves the Lagrange multiplier rule and leads to so-called Karush-Kuhn-Tucker (KKT) optimality conditions. While the Lagrangian principle is also briefly explained in Section 3.5 below, we only want to mention that in nonlinear programming, KKT conditions are necessary optimality conditions of first-order, and refer the reader to standard literature, e.g. [135, 153] for more information. The resulting optimality system $(\mathrm{EL}_{\mathbb{I}}^\eta)$ is related to the well-known obstacle problem, an optimization problem where for fixed boundary conditions, the associated optimal state is constrained to lie above a given obstacle. It is accompanied by questions of admissibility of the state, and the requirement for constraint qualifications, e.g. Slater's condition. References to classical literature concerning the obstacle problem can be found in [160, Section 2.3], to which the reader is pointed to.

Penalization and regularized fracture propagation problem

Let us recall that for the final model optimal control problem, the fracture propagation problem shall be used to govern an optimal control problem, by adding an outer optimization problem later, see Section 2.2 below. However, due to involvement of inequality conditions in $(\mathrm{C}_{\mathbb{I}}^\eta)$, and subsequently of the complementarity conditions that occur in its stationarity conditions $(\mathrm{EL}_{\mathbb{I}}^\eta)$, such a fracture propagation optimization problem would be a member of a problem class that is called mathematical programs with complementary constraints (MPCC), cf. [13, 123, 124]. Possible challenges, not only for the given problem setting, but in general when dealing with MPCCs, have been stated in Chapter 1. In particular, we recall that the inherent nondifferentiability makes the analysis of (second-order) optimality conditions and numerical methods in the classical sense challenging, mostly because standard constraint qualifications like [139, 163] are not applicable. In [132], a well-known penalization approach that can e.g. be found in [13], is used to eliminate the irreversibility constraint (2.5), at the expense of an additional penalization term. As in [119], a higher-order penalization is used there instead of the standard L^2-approach, that is typically used within the regularization idea of Moreau-Yosida, cf. [99]. Other penalization/regularization approaches for state constraints are the so-called Lavrentiev regularization [120], or [109] which uses a so-called virtual control concept. While the former is a concept to rewrite inequality state constraints into mixed control-state constraints, the latter introduces an additional virtual control, and both have in common that the inequality constraints still involve a state. Another approach frequently used to regularize state constraints are barrier functions, cf. e.g. [144]. For an overview of different approaches, the reader is also referred to [14] and [131]. In any case, a Moreau-Yosida penalization of higher-order is appealing for the given setting since it ensures higher-order regularity and differentiability results rather easily in the context of analyzing second-order conditions and the SQP method. This, as well as potential questions involved with ensuring feasibility of initial values through additional assumptions in e.g. the SQP method, is an advantage for the given problem over e.g. barrier methods. By all means, the penalization term to regularize (2.5) is given, for a penalization parameter $\gamma > 0$ and introducing $(\cdot)^+ := \max(0, \cdot)$, by

$$\frac{\gamma}{4} \left\| (\varphi^i - \varphi^{i-1})^+ \right\|_{L^4}^4, \tag{2.9}$$

where $\|\cdot\|_{L^4}$ denotes the L^4 norm on Ω. Note that it is advisable to choose $\gamma \gg \eta$, in order to ensure that the by physical considerations motivated penalization for the irreversibility dominates the effects of the viscous approximation. Let us now state the regularized fracture problem:

Let $\mathbf{u}^0 = (u^0, \varphi^0) \in V$, with $\varphi^0 \in [0, 1]$ and data $f_{\mathbb{I}} \in (L^2(\Gamma))^M$ be given, find pairs of displacements and phase-fields $\mathbf{u}_{\mathbb{I}} \in V^M$ that solve

$$\min_{\mathbf{u}^i} E_\varepsilon^{\eta,\gamma}(f^i, \varphi^{i-1}; \mathbf{u}^i) := E_\varepsilon^{\eta}(f^i, \varphi^{i-1}; \mathbf{u}^i) + \frac{\gamma}{4} \left\| (\varphi^i - \varphi^{i-1})^+ \right\|_4^4 \tag{$\mathrm{C}_{\mathbb{I}}^{\gamma,\eta}$}$$

for all $i = 1, .., M$, and $\gamma > 0$, $\eta \geq 0$. Note again that only the initial phase-field φ^0 is used, cf. Remark 2.1.1.

At this point, similarly to [133, Section 1], we use the idea proposed in [132, Section 3], and also present the stationarity conditions of the optimization problem ($\mathrm{C}_{\mathbb{I}}^{\gamma,\eta}$). These are given by Euler-Lagrange equations, which are one of the fundamental concepts in the field of calculus of variations, cf. [67]. The Euler-Lagrange equations are a system of second-order equations, that represent necessary optimality conditions of its associated minimization problem. For the regularized fracture problem ($\mathrm{C}_{\mathbb{I}}^{\gamma,\eta}$), we obtain the following formulation:

For all test functions $(v^u, v^\varphi) \in V$, given loads $f_{\mathbb{I}} \in (L^2(\Gamma))^M$, and initial phase-field $\varphi^0 \in [0,1]$, any minimizer $\mathbf{u}_{\mathbb{I}} \in V^M$ of $(\mathrm{C}_{\mathbb{I}}^{\gamma,\eta})$ satisfies

$$\left.\begin{aligned} \big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)\big) - (f^i, v^u)_Q &= 0, \\ G_c\varepsilon(\nabla\varphi^i, \nabla v^\varphi) - \frac{G_c}{\varepsilon}(1-\varphi^i, v^\varphi) + \eta(\varphi^i - \varphi^{i-1}, v^\varphi) & \\ +(1-\kappa)(\varphi^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi) + \gamma([(\varphi^i - \varphi^{i-1})^+]^3, v^\varphi) &= 0, \end{aligned}\right\} \qquad (\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$$

for all $i = 1, .., M$.

It is important to recognize that, in contrast to the model problems of [28, 31, 110, 121], a priori the phase field φ^i, for all $i = 1, ..., M$, is not in L^∞ anymore, since the upper bound induced by (2.5) is not enforced anymore. To ensure well-definedness of the terms in $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ it is proved that $\varphi_{\mathbb{I}} \in (L^\infty(\Omega))^M$ and $\mathbf{u}_{\mathbb{I}}$ is in fact more regular in [132, Corollary 4.2], a result which is revisited in Lemma 3.2.1 below. We want to point out that for η sufficiently large, $(\mathrm{C}_{\mathbb{I}}^{\gamma,\eta})$ is (strictly) convex, and therefore has a unique solution which is given as the solution of $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$. In this case, $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ constitutes both a necessary and sufficient condition for $(\mathrm{C}_{\mathbb{I}}^{\gamma,\eta})$. Note that due to the coupling of the displacement variable u^i and the phase-field variable φ^i for all $i = 1, .., M$, $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ is of quasilinear type. Further, $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ is a system of second-order, elliptic equations.

Let us point out that the overall idea of the penalization approach is to start with the study of $(\mathrm{C}_{\mathbb{I}}^{\gamma,\eta})$, and then to investigate the limit $\gamma \to \infty$ in a later step. Ideally, the solutions then converge to solutions that correspond to the unpenalized optimal control problem $(\mathrm{C}_{\mathbb{I}}^{\eta})$. Respectively, the same analysis can be conducted for $(\mathrm{EL}_{\mathbb{I}}^{\eta})$ and $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$. In fact, restricting the setting to one time step, we see in Chapter 5 that using $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ as governing equation for an outer optimal control problem, when taking the limit w.r.t. the penalization, the limit functions indeed solve the corresponding optimal control problem that is governed by the inequality-constrained fracture problem $(\mathrm{EL}_{\mathbb{I}}^{\eta})$. We do not go into further detail here, and refer the reader to Chapter 5.

2.2 The optimal control problem

To the best of the authors' knowledge, [132] is the first work which added an upper, or outer optimization problem to the regularized variational phase-field fracture model given through $(\mathrm{C}_{\mathbb{I}}^{\gamma,\eta})$ or $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$. This upper level problem consists of an objective functional that is given by a tracking-type functional in combination with a Tikhonov regularization. Additionally to [132], in this thesis we additionally demand box-constraints for the control. For the control space $Q = L^2(\Gamma)$, and Q^M being the M-times product space $Q^M = M \times \cdots \times M$, this then initially leads to a problem formulation that is given by:

Let initial data $\mathbf{u}^0 = (u^0, \varphi^0) \in V$, with $\varphi^0 \in [0,1]$, and the desired displacement $u_{d,\mathbb{I}} = (u_d^i)_{i=1}^M \in (L^2(\Omega))^M$ be given. Find $q_\mathbb{I} = (q^i)_{i=1}^M \in Q_{\text{ad},\mathbb{I}} \subset Q^M$ with associated state pair $\mathbf{u}_\mathbb{I} = (\mathbf{u}^i)_{i=1}^M = ((u^i, \varphi^i))_{i=1}^M \in V^M$ such that

$$\left.\begin{aligned} &\min_{q_\mathbb{I}, \mathbf{u}_\mathbb{I}} && J_\mathbb{I}\big(q_\mathbb{I}, \mathbf{u}_\mathbb{I}\big) := \sum_{i=1}^M \frac{1}{2}\|u^i - u_d^i\|^2_{L^2(\Omega,\mathbb{R}^2)} + \sum_{i=1}^M \frac{\alpha}{2}\|q^i\|_Q^2, \\ &\text{subject to:} && \mathbf{u}_\mathbb{I} \text{ solves } (\mathrm{C}_\mathbb{I}^{\gamma,\eta}) \text{ for data } q_\mathbb{I}, \\ &\text{and:} && q_\mathbb{I} \in Q_{\text{ad},\mathbb{I}}, \end{aligned}\right\} \qquad (\mathrm{P}_\mathbb{I}^{\gamma,\eta})$$

where $0 < \alpha \in \mathbb{R}$, and $Q_{\text{ad},\mathbb{I}} := \{q_\mathbb{I} \in Q^M \mid q_a^i \leq q^i \leq q_b^i \ \ \forall i = 1, ..., M\}$ for given $q_{a,\mathbb{I}}, q_{b,\mathbb{I}} \in (L^\infty(\Omega))^M$.

Let us have a quick look at the objective functional. The first, so-called tracking-type, part of this functional aims to achieve a state, in this case only the displacement part u^i of the state pair $\mathbf{u}^i = (u^i, \varphi^i)$, that lies close to a given, desired displacement u_d^i, for every discrete time step, i.e. for $i = 1, ..., M$. Choosing the desired displacement $u_{d,\mathbb{I}}$ appropriately, the state is therefore steered over time towards a favored configuration. For the second part of the objective function, the nonnegative real number α is called the Tikhonov parameter and the whole term involving α is also called the Tikhonov term. It depicts the cost to be expended in the controlling process, while also serving as a numerical stabilization, which is why this approach is also known under the name "Tikhonov regularization", cf. [44] for further explanation.

Note that $(\mathrm{P}_\mathbb{I}^{\gamma,\eta})$ is a bi-level optimization problem. Following again [132, Section 3], the lower-level problem $(\mathrm{C}_\mathbb{I}^{\gamma,\eta})$ is replaced by its Euler-Lagrange equations formulation $(\mathrm{EL}_\mathbb{I}^{\gamma,\eta})$. This leads to a nonlinear program in a form comparable to standard optimal control problem subject to PDE constraints, which in the context of linear and semilinear PDEs is well-studied, e.g. in [44, 94, 153]. In particular, we obtain:

Let the initial data $\mathbf{u}^0 = (u^0, \varphi^0) \in V$, with $\varphi^0 \in [0,1]$, and the desired displacement $u_{d,\mathbb{I}} \in (L^2(\Omega,\mathbb{R}^2))^M$ be given, find $q_\mathbb{I} \in Q_{\text{ad},\mathbb{I}} \subset Q^M$ with associated state pair $\mathbf{u}_\mathbb{I} \in V^M$ such that

$$\left.\begin{aligned} &\min_{q_\mathbb{I}, \mathbf{u}_\mathbb{I}} && J_\mathbb{I}\big(q_\mathbb{I}, \mathbf{u}_\mathbb{I}\big), \\ &\text{subject to:} && \mathbf{u}_\mathbb{I} \text{ solves } (\mathrm{EL}_\mathbb{I}^{\gamma,\eta}) \text{ for data } q_\mathbb{I}, \\ &\text{and:} && q_\mathbb{I} \in Q_{\text{ad},\mathbb{I}}. \end{aligned}\right\} \qquad (\mathrm{NLP}_\mathbb{I}^{\gamma,\eta})$$

We have already postulated that by utilizing the largeness assumption on η, cf. Assumption 2.3.11 below, existence and uniqueness of solutions of $(\mathrm{EL}_\mathbb{I}^{\gamma,\eta})$ can be ensured, which is addressed in Section 3.2 below. It is then possible to introduce a unique solution operator and a reduced functional, which is essential in the sense that it makes optimal control subject to constraints viable at all, cf. Section 4.1.

At this point, we do not want to repeat the advantages of this approach to model optimal control in the context of fracture propagation over previous ideas, as well as the challenges that come with it. Instead, we refer the reader back to the introductory Chapter 1, where these topics have already been discussed.

2.3 Summary of final problem setting, assumptions and notation

This section recapitulates the problem setting involving all assumptions, introduces some additional notation and serves as a point of reference for the theoretical results in Chapter 3 - 6. In this context, also note the summary of used notation and abbreviations in Appendix A. Let us start by collecting some basic and problem specific assumptions, which have already been made in Section 2.1 and Section 2.2, and which shall hold throughout the rest of this work:

Assumption 2.3.1 (Basic assumptions)**.**

- *The parameters $p > 2$, but close to two, $q := p/2 > 1$, i.e. close to one, as well as $s \in (0, 1/2)$ are given, s.t. $H^{1+s}(\Omega, \mathbb{R}^2) \subset W^{1,p}(\Omega, \mathbb{R}^2)$.*
- *The domain Ω is assumed to be in two spatial dimensions, i.e. $\Omega \in \mathbb{R}^2$.*
- *The boundary $\delta\Omega = \Gamma_D \dot{\cup} \Gamma$ of the domain Ω consists of two parts Γ_D (Dirichlet boundary) and Γ (Neumann boundary) with $\mathcal{H}^{d-1}(\Gamma) \neq 0$ and $\mathcal{H}^{d-1}(\Gamma_D) \neq 0$.*
- *$\Omega \cup \Gamma$ is Gröger regular, cf. [77].*
- *The domain Ω suffices to $W^{2,q}$-regularity for the homogeneous Neumann problem*

$$-\varepsilon \triangle \varphi + \frac{1}{\varepsilon}\varphi = f, \quad \partial_n \varphi = 0 \text{ on } \Gamma, \quad \varphi = 0 \text{ on } \Gamma_D. \tag{2.10}$$

Let us also quickly give the following remark:

Remark 2.3.2. *The final point of Assumption 2.3.1 in particular means that for right-hand sides $f \in L^q(\Omega)$, the solution φ of (2.10) suffices to $\varphi \in W^{2,q}(\Omega)$, c.f. [133, Section 2] where this assumption is initially proposed for the fracture propagation optimal control model problem.*

We continue to introduce some notation used for the involved function spaces and corresponding inner product and norms.

Definition 2.3.3 (Function spaces and norms)**.**

- *Let $H^1_D(\Omega; \mathbb{R}^2) := \{v \in H^1(\Omega; \mathbb{R}^2) \,|\, v = 0 \text{ on } \Gamma_D\}$, respectively for $W^{1,p}_D(\Omega; \mathbb{R}^2)$. Additionally, we define*

$$V_u := H^1_D(\Omega, \mathbb{R}^2), \qquad V_\varphi := H^1(\Omega), \qquad V := V_u \times V_\varphi,$$

$$W_u := W_D^{1,p}(\Omega, \mathbb{R}^2), \qquad W_\varphi := W^{2,q}(\Omega), \qquad W := W_u \times W_\varphi.$$

Further, it holds

$$W^\times := W^{-1,p}(\Omega, \mathbb{R}^2) \times L^q(\Omega).$$

- *The control space Q is given by $Q := L^2(\Gamma)$.*
- *Let $y := (\mathbf{u}, q, \mathbf{z})$ denote a function triple consisting of a state $\mathbf{u}$, a control q and an adjoint state $\mathbf{z}$ (see Chapter 4). The to this triple associated spaces are*

$$Y := W \times Q \times W \qquad \text{and} \qquad Z := W^\times \times Q \times W^\times.$$

In the context of convergence of the SQP method in Chapter 6, additionally also the spaces

$$Y_\infty := W \times L^\infty(\Gamma) \times W \qquad \text{and} \qquad Z_\infty := W^\times \times L^\infty(\Gamma) \times W^\times$$

are used.

- *By $(\cdot,\cdot)$ we denote the L^2-inner product, and by $\|\cdot\|$ the corresponding norm. Further by $(\cdot,\cdot)_Q$ we denote the inner product of the control space $Q := L^2(\Gamma)$, with $\|\cdot\|_Q$ being the corresponding norm.*
- *Let a displacement/phase-field pair $\mathbf{u} = (u, \varphi) \in W$ be given. The norm of the space W is given by*

$$\|\mathbf{u}\|_W = \|(u,\varphi)\|_W = \|u\|_{W_u} + \|\varphi\|_{W_\varphi} := \|u\|_{W^{1,p}(\Omega;\mathbb{R}^2)} + \|\varphi\|_{W^{2,q}(\Omega)},$$

where $\|\cdot\|_{W^{1,p}(\Omega;\mathbb{R}^2)}$ and $\|\cdot\|_{W^{2,q}(\Omega)}$ are the standard Sobolev norms of the corresponding spaces, defined via

$$\|u\|_{W^{1,p}(\Omega;\mathbb{R}^2)} := \sum_{|i|\le 1} \|D^i u\|_{L^p(\Omega;\mathbb{R}^2)}$$
$$\text{and} \quad \|\varphi\|_{W^{2,q}(\Omega)} := \sum_{|i|\le 2} \|D^i \varphi\|_{L^q(\Omega)}.$$

Finally, in this context, $\|\cdot\|_{L^p(\Omega;\mathbb{R}^2)}$ and $\|\cdot\|_{L^q(\Omega)}$ are the standard norms of the corresponding Lebesgue spaces $L^p(\Omega;\mathbb{R}^2)$ and $L^q(\Omega)$.

- *For any Banach-, Hilbert- or Sobolev- space $\mathbb{V}$, the dual space is denoted by $\mathbb{V}^*$. The duality pairing is denoted by $\langle\cdot,\cdot\rangle$, where the spaces are often omitted if obvious from the context.*

We further introduce the following notational convention, which is used throughout this thesis:

Definition 2.3.4 (Time discrete notation for functions and function spaces)**.**

- *Let* $\mathbb{I} := \{1, ..., M\}$*, for an integer* $M \in \mathbb{N}$*.*
- *State and control spaces for multi time step settings are denoted with an exponent, e.g.*

$$V^M = \underbrace{V \times \cdots \times V}_{M \text{ times}} \qquad \text{and} \qquad Q^M = \underbrace{Q \times \cdots \times Q}_{M \text{ times}},$$

  and analogously for other function spaces, like e.g. the ones defined in Definition 2.3.3. Note that the product space $(W \times Q \times W)^M = (W \times Q \times W) \times ... \times (W \times Q \times W)$ *is denoted by* Y^M*. The associated norms are defined analogously to Definition 2.3.3.*

- *The state variable* $\mathbf{u}_{\mathbb{I}}$ *is given by*

$$\begin{aligned}(\mathbf{u}^1, ..., \mathbf{u}^M) = (\mathbf{u}^i)_{i=1}^M = \mathbf{u}_{\mathbb{I}} = (u_{\mathbb{I}}, \varphi_{\mathbb{I}}) &= \big((u^i)_{i=1}^M, (\varphi^i)_{i=1}^M\big) \\ &= \big((u_1, ..., u_M), (\varphi_1, ..., \varphi_M)\big),\end{aligned}$$

  and the control variable $q_{\mathbb{I}}$ *by*

$$q_{\mathbb{I}} = (q^i)_{i=1}^M = (q^1, ..., q^M).$$

  Analogously, the functions $\tilde{\mathbf{u}}_{\mathbb{I}}$*,* $\tilde{\mathbf{u}}_{\mathbb{I},1}$ *and* $\tilde{\mathbf{u}}_{\mathbb{I},2}$ *are introduced.*

- *For (displacement and phase-field pairs of) test functions* $\mathbf{v}_{\mathbb{I}}$ *we use the notation*

$$\begin{aligned}(\mathbf{v}^1, ..., \mathbf{v}^M) = (\mathbf{v}^i)_{i=1}^M = \mathbf{v}_{\mathbb{I}} = (v_{\mathbb{I}}^u, v_{\mathbb{I}}^\varphi) &= \big((v^{u,i})_{i=1}^M, (v^{\varphi,i})_{i=1}^M\big) \\ &= \big((v^{u,1}, ..., v^{u,M}), (v^{\varphi,1}, ..., v^{\varphi,M})\big).\end{aligned}$$

- *For (displacement and phase-field pairs of) function data* $\mathbf{f}_{\mathbb{I}}$*,*

$$\begin{aligned}(\mathbf{f}^1, ..., \mathbf{f}^M) = (\mathbf{f}^i)_{i=1}^M = \mathbf{f}_{\mathbb{I}} = (f_{\mathbb{I}}^u, f_{\mathbb{I}}^\varphi) &= \big((f^{u,i})_{i=1}^M, (f^{\varphi,i})_{i=1}^M\big) \\ &= ((f^{u,1}, ..., f^{u,M}), (f^{\varphi,1}, ..., f^{\varphi,M}))\end{aligned}$$

  is used.

- *For the adjoint functions* $\mathbf{z}_{\mathbb{I}}$*, which occur in the context of optimality conditions cf. Chapter 4, we introduce analogously*

$$\begin{aligned}(\mathbf{z}^1, ..., \mathbf{z}^M) = (\mathbf{z}^i)_{i=1}^M = \mathbf{z}_{\mathbb{I}} = (z_{\mathbb{I}}, \psi_{\mathbb{I}}) &= \big((z^i)_{i=1}^M, (\psi^i)_{i=1}^M\big) \\ &= ((z^1, \psi^1), (z^M, \psi^M)).\end{aligned}$$

- *The desired displacement $u_{d,\mathbb{I}}$ is defined analogously to the displacement function $u_{\mathbb{I}}$.*
- *Finally, for the admissible control set $Q_{ad,\mathbb{I}}$, we define*

$$Q_{ad,\mathbb{I}} := \{q_{\mathbb{I}} \in Q^M \quad | \quad q_a^i \leq q^i \leq q_b^i \quad \text{a.e. on } \Gamma \quad \text{for all } i = 1, .., M\},$$

where $q_{a,\mathbb{I}}, q_{b,\mathbb{I}} \in (L^\infty(\Omega))^M$ are given, s.t. $q_a^i < q_b^i$ a.e. on Γ for all $i = 1, .., M$, cf. also Assumption 2.3.7. This means that the admissible control set is given by so-called box constraints.

In the context of Definition 2.3.4, we make the following remark:

Remark 2.3.5. *Without further mention, we consider all vectors as row or column vectors where needed if obvious from the context. Further, for all functions and their notation, e.g. $\mathbf{u}_{\mathbb{I}}$, is used for both*

$$\mathbf{u}_{\mathbb{I}} = (u_{\mathbb{I}}, \varphi_{\mathbb{I}}) = \big((u^i)_{i=1}^M, (\varphi^i)_{i=1}^M\big) = ((u_1, ..., u_M), (\varphi_1, ..., \varphi_M))$$

and

$$\mathbf{u}_{\mathbb{I}} = \big((u^i, \varphi^i)\big)_{i=1}^M = \big((u^1, \varphi^1), ..., (u^M, \varphi^M)\big).$$

The following facts, which can be found in [153, Chapter 7] and [1], are used frequently without further mention.

Remark 2.3.6.

- *For the choice of p and q, in $d = 2$ spatial dimensions, the embedding theorem of Sobolev and Kondrachov yields*

$$W_u \hookrightarrow V_u, \qquad W_\varphi \hookrightarrow V_\varphi.$$

Moreover, it holds

$$W_u \hookrightarrow L^\infty(\Omega; \mathbb{R}^2), \qquad W_\varphi \hookrightarrow L^\infty(\Omega).$$

- *Due to the definition of $Q_{ad,\mathbb{I}}$, it is immediately clear that all admissible controls suffice to L^∞-regularity.*
- *The trace embedding $L^2(\Gamma) \hookrightarrow W^{-1,p}(\Omega)$ holds and is compact, which holds true due to $p \leq 4$ and Assumption 2.3.1.*

Next, we collect some problem specific assumptions.

Assumption 2.3.7 (Problem setting)**.**

- *The constants $\mathbb{R} \ni \kappa, \gamma > 0$, $1 > \varepsilon > 0$, and $\mathbb{R} \ni \eta \geq 0$ are given, such that $\kappa \gg \varepsilon$. From a modelling point of view, it is suggested that $\eta < \gamma$.*
- *The initial phase-field function $\varphi^0 \in W_\varphi$ s.t. $0 \leq \varphi^0 \leq 1$ is given.*

- *The desired displacement* $u_{d,\mathbb{I}} \in (L^2(\Omega,\mathbb{R}^2))^M$ *is given.*
- *The Tikhonov parameter* $\alpha \in \mathbb{R}$ *is positive, i.e.* $\alpha > 0$.
- *We further recall from Definition 2.3.4 that* $q_{a,\mathbb{I}}, q_{b,\mathbb{I}} \in (L^\infty(\Omega))^M$ *are given, s.t.* $q_a^i < q_b^i$ *a.e. on* Γ *for all* $i = 1,..,M$.
- $\mathbb{C}$ *denotes the rank-4-elasticity tensor. For a proper definition and some properties, cf. Chapter 2.*
- *For the constant* G_c*, w.l.o.g. it holds* $G_c := 1$.

In particular, the physical parameters κ, ε *are assumed to be fixed constants. The penalization parameter* γ *is, with the exception of Chapter 5, also assumed to be a fixed constant.*

Next, to simplify notation and make the technical proofs easier accessible, in most of the theoretical parts of the following chapters the Euler-Lagrange equations are written in a more compact form. In order to do so, we introduce the operators A, R and B.

Definition 2.3.8 (Operators A, R, B)**.** *Let the parameters* $\kappa, \varepsilon, \gamma > 0, \eta \geq 0$ *be given as in Assumption 2.3.7. The operators* A, R*, and* B*, are given, for previous phase-field function* $\varphi^{i-1} \in V_\varphi$*, and test functions* $\mathbf{v} = (v^u, v^\varphi) \in V$*, as*

- *the nonlinear phase-field operator* $A\colon V \times V_\varphi \supset W \times W_\varphi \to V^*$*, defined by*

$$\begin{aligned}\big\langle A(\mathbf{u}^i, \varphi^{i-1}), \mathbf{v}\big\rangle := {} & \big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)\big) \\ & + G_c\varepsilon\big(\nabla\varphi^i, \nabla v^\varphi\big) - \frac{G_c}{\varepsilon}\big(1-\varphi^i, v^\varphi\big) \\ & + \eta\big(\varphi^i - \varphi^{i-1}, v^\varphi\big) \\ & + (1-\kappa)\big(\varphi^i\mathbb{C}e(u^i) : e(u^i), v^\varphi\big),\end{aligned}$$

  recalling g *as the quadratic degradation function* $g(x) := (1-\kappa)x^2 + \kappa$.

- *the penalization operator* $R\colon V_\varphi \to V_\varphi^*$*, defined by*

$$\big\langle R(\varphi^i, \varphi^{i-1}; \gamma), v^\varphi\big\rangle := \gamma\big([(\varphi^i - \varphi^{i-1})^+]^3, v^\varphi\big).$$

- *the control-action operator on the Neumann boundary* Γ*,* $B\colon Q \to V^*$*, defined by*

$$\big\langle Bq^i, \mathbf{v}\big\rangle := \big(q^i, v^u\big)_Q.$$

Let us make two remarks concerning the operators introduced in Definition 2.3.8.

Remark 2.3.9. *Note that the operators A and R are later also considered as mappings in the spaces $W^\times$ and $L^q(\Omega)$, and that by definition it holds $W^\times \hookrightarrow V^*$, and $L^q(\Omega) \hookrightarrow V_\varphi^*$. In either way, test functions $\mathbf{v} \in V$ can be used. The operator B is also used as a mapping into the more regular space $W^\times$, i.e. $B\colon Q \to W^\times$, which is well-defined due to Remark 2.3.6.*

Remark 2.3.10. *Note that the notation for the nonlinear phase-field operator A and the penalization operator R are slightly different to the definition made in [84, 85, 86]: There, a one time step model, i.e. $M = 1$, is investigated, where the initial phase-field $\varphi^- := \varphi^0$ is a given, a-priori known function, for which the corresponding assumptions as in Assumption 2.3.7 hold. For the discrete multi time step model, the previous phase-field variable φ^- is now incorporated into the respective operators.*

With Definition 2.3.8, we rewrite the model optimal control problem $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$ into the following compact problem formulation:

Let Assumption 2.3.1 and Assumption 2.3.7 hold, then

$$\left.\begin{aligned} \min_{q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}},\ \mathbf{u}_{\mathbb{I}} \in V^M} \quad & \sum_{i=1}^{M} \frac{1}{2}\|u^i - u_d^i\|^2_{L^2(\Omega,\mathbb{R}^2)} + \sum_{i=1}^{M} \frac{\alpha}{2}\|q^i\|_Q^2, \\ \text{subject to:} \quad & A(\mathbf{u}^i, \varphi^{i-1}) + R(\varphi^i, \varphi^{i-1}; \gamma) = Bq^i \quad \text{for all } i = 1, ..., M. \end{aligned}\right\}$$

Note that by Definition 2.3.8, the involved partial differential equation is the same as $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ from Section 2.1, and the just stated optimal control problem is in fact the same problem as $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$. For most of our analysis, we use this representation of the model optimal control problem $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$.

This section is closed with the following essential assumption, that is expected to hold throughout our entire analysis.

Assumption 2.3.11 (Viscous approximation)**.** *Let $\eta \geq 0$ be chosen large enough, such that all results in Chapter 3 are applicable.*

At this point, the focus shall quickly be put on the importance of Assumption 2.3.11 for the analysis of the model problem. The assumption stems from [86, 133] and is inspired by [107]. We frequently utilize results that are based on these works. In particular, Assumption 2.3.11 ensures both unique solvability of $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$, and the associated linearized PDE, see Chapter 3, and subsequently also the differentiability and Lipschitz results for the associated solution operators. Most of the auxiliary properties showed for the control-to-state operator, and subsequently of the to $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$ associated reduced functional depend on a sufficiently big η. Note that in [86, Section 3], some more details on the dependence of η on $\varepsilon, 1/\varepsilon$ and κ can be found, cf. also the proof of Lemma 3.2.3

below. At this point, it is important to point out again that for all theoretical results of Chapter 3, 4 and 6, all physical parameters remain fixed, as assumed in Assumption 2.3.7. The exception is Chapter 5, where we look at the limit of the penalization parameter γ, leaving every physical parameter but γ fixed. In this context, note that for a similar optimal problem a trivial kernel assumption is used in [132], instead of Assumption 2.3.11. We refer to Section 3.2, where the setting of [132] is outlined.

3. Analysis of the control-to-state operator, the reduced functional and the Lagrangian functional

This chapter lays the technical foundations needed to investigate (second-order) optimality conditions and the SQP method in the later chapters. In particular, we start by presenting norm bounds as well as differentiability and Lipschitz continuity results for the operators A and R. Further, we present solvability results for the state equation ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$), its linearization and adjoint. The main contributions are the differentiability and Lipschitz continuity results, in particular the Lipschitz results of second-order, for the solution operator of ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$) as well as the reduced functional and the Lagrangian of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) in Section 3.3, 3.4 and 3.5. For the case $M = 1$, i.e. the one time step setting, these second-order results are investigated in the joint works [85, 86] of the author and I. Neitzel. Note that for the results concerning the operators A and R, we rely on techniques from [132, 133] to extend available preliminary results from the same publications. Furthermore, the solvability result for ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$) can be adopted as it stands from [132, 133]. As for the existence and improved regularity results for solutions of the linearization and the adjoint of the state equation, similar ideas as for the state equation, in particular also involving a viscous approximation Assumption 2.3.11, cf. [107], are utilized. Again for $M = 1$, i.e. the one time step setting, a rigorous proof for the results involving the linearization of the state equation can be found in the joint work [86] of I. Neitzel and the author. We also want to point out, that the presented results for the linearization of the state equation are already used in [84, 128, 132][1].

Throughout our analysis, we emphasize where the multi time step setting from ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) requires a more careful analysis as opposed to the one time step setting from [85, 86]. At this point, we further want to point out that the improved regularity, differentiability and Lipschitz continuity of the solution operator, and the reduced objective as well as the Lagrangian functional proved below are nontrivial tasks, that involve an in-depth analysis of the structure of the involved operators A and R and the coupled structure of ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$).

[1] under slightly different assumptions, see the paragraph below (3.75) on page 67

Let us give a quick outline of the course of action and the main results: We start with an analysis of norm bounds and differentiability and Lipschitz results for the nonlinear phase-field operator A and the penalization operator R, as well as their linearized and adjoint counterparts in Section 3.1. We can then ensure solvability and improved regularity of solutions for both the state equation ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$) and its linearization in Section 3.2 and introduce the associated solution operators. Subsequently, (second-order) Fréchet differentiability and (second-order) Lipschitz continuity in improved Banach spaces of the solution operator are established in Section 3.3. Finally, we transfer the corresponding results to the (reduced) functional and the Lagrangian of the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) in Section 3.4 and Section 3.5.

3.1 Preliminary technical results for the operators A and R

This section collects some auxiliary results for the operators A and R, which are used throughout the entire thesis. The techniques utilized stem for the most part from [132, 133]. Most of these results are already used for the one time step setting in [85, 86] of the author and I. Neitzel. The main difference for the multi time step setting $M > 1$ lies in the added appearance of involved functions depending also on the time steps $i-1$ and $i+1$. In particular, some additional caution has to be taken care of when working with the adjoint operators, in particular the operators R_{l*} and R_{b*}. For convenience, we revisit all used techniques in detail, adapt them to the notation of this thesis and state all results explicitly in citable form.

Let us first point back to the definition of the operators A, R and B from Definition 2.3.8, and introduce the linearized operators A_l and R_l: Let $\mathbf{u}^i = (u^i, \varphi^i) \in W$ and $\varphi^{i-1} \in W_\varphi$ be given, we define the linear operators $A_l(\mathbf{u}^i)\colon V \times V_\varphi \to V^*$ and $R_l(\varphi^i, \varphi^{i-1}; \gamma)\colon V_\varphi \times V_\varphi \to V_\varphi^*$, for test functions $\mathbf{v} = (v^u, v^\varphi) \in V$, via:

$$
\begin{aligned}
\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}\big\rangle := {}& \big(g(\varphi^i)\mathbb{C}e(\tilde{u}^i), e(v^u)\big) \\
& + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i)\tilde{\varphi}^i, e(v^u)\big) \\
& + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) : e(\tilde{u}^i), v^\varphi\big) \\
& + (1-\kappa)\big(\tilde{\varphi}^i \mathbb{C}e(u^i) : e(u^i), v^\varphi\big) \\
& + \varepsilon\big(\nabla\tilde{\varphi}^i, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(\tilde{\varphi}^i, v^\varphi\big) \\
& + \eta\big(\tilde{\varphi}^i - \tilde{\varphi}^{i-1}, v^\varphi\big), \qquad (3.1) \\
\big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^\varphi\big\rangle := {}& 3\gamma\big([(\varphi^i - \varphi^{i-1})^+]^2(\tilde{\varphi}^i - \tilde{\varphi}^{i-1}), v^\varphi\big). \qquad (3.2)
\end{aligned}
$$

Note that, in comparison to A, A_l does not depend on φ^{i-1} anymore. Therefore the dependence is dropped to ease notation, i.e. $A_l(\mathbf{u}^i)$ is defined for given $\mathbf{u}^i \in W$, and not for given pair $(\mathbf{u}^i, \varphi^{i-1}) \in W \times W_\varphi$. Further, as in Remark 2.3.9,

A_l and R_l can be also used as mappings from $W \times W_\varphi$ into $W^\times$, respectively from $W_\varphi \times W_\varphi$ into $L^q(\Omega)$, and for either way test functions $\mathbf{v} \in V$ are applicable. We frequently also use $A_l(\mathbf{u}^i)\colon W \times W_\varphi \to W^\times$ as a mapping from the more regular space $W \hookrightarrow V$, and $R'(\varphi^i, \varphi^{i-1}; \gamma)\colon W_\varphi \times W_\varphi \to L^q(\Omega)$, respectively.

Let us continue by introducing the bilinear operator $A_b(\mathbf{u}^i)\colon W \times W \to V^*$, for given $\mathbf{u}^i \in W$, which for all test functions $\mathbf{v} = (v^u, v^\varphi) \in V$ is defined via

$$\begin{aligned} \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{v}\big\rangle := {} & 2(1-\kappa)\big(\varphi^i \mathbb{C} e(\tilde{u}_1^i)\tilde{\varphi}_2^i, e(v^u)\big) \\ & + 2(1-\kappa)\big(\tilde{\varphi}_2^i \mathbb{C} e(u^i)\tilde{\varphi}_1^i, e(v^u)\big) \\ & + 2(1-\kappa)\big(\varphi^i \mathbb{C} e(\tilde{u}_2^i)\tilde{\varphi}_1^i, e(v^u)\big) \\ & + 2(1-\kappa)\big(\tilde{\varphi}_2^i \mathbb{C} e(u^i)\colon e(\tilde{u}_1^i), v^\varphi\big) \\ & + 2(1-\kappa)\big(\varphi^i \mathbb{C} e(\tilde{u}_2^i)\colon e(\tilde{u}_1^i), v^\varphi\big) \\ & + 2(1-\kappa)\big(\tilde{\varphi}_1^i \mathbb{C} e(\tilde{u}_2^i)\colon e(u^i), v^\varphi\big), \end{aligned} \tag{3.3}$$

as well as the bilinear operator $R_b(\varphi^i, \varphi^{i-1}; \gamma)\colon\ (W_\varphi \times W_\varphi) \times (W_\varphi \times W_\varphi) \to V_\varphi^*$, which is defined for given $\varphi^i, \varphi^{i-1} \in W_\varphi$ and all test functions $v^\varphi \in V$, by:

$$\begin{aligned} & \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], v^\varphi\big\rangle \\ & \quad := 6\gamma\big([(\varphi^i - \varphi^{i-1})^+](\tilde{\varphi}_1^i - \tilde{\varphi}_1^{i-1})(\tilde{\varphi}_2^i - \tilde{\varphi}_2^{i-1}), v^\varphi\big). \end{aligned} \tag{3.4}$$

Again as in Remark 2.3.9, A_b and R_b can be also used as mappings from $W \times W$ into $W^\times$, respectively from $(W_\varphi \times W_\varphi) \times (W_\varphi \times W_\varphi)$ into $L^q(\Omega)$, and for either way test functions $\mathbf{v} \in V$ are applicable. Let us collect some further properties of A_b in the following remark.

Remark 3.1.1.

- *The operator A_b, for fixed i, is in fact the same as the operator A'' of [85, 86], since it only involves the current time step i. In particular similar to A_l, A_b is also independent of the previous time step $i-1$, both for the linearization and both directions. We again drop this dependence for better readability. The bilinear form A_b is therefore a mapping from $W \times W$, and not from $(W \times W_\varphi) \times (W \times W_\varphi)$.*

- *Note that the operator A_b, is well-defined for functions $\mathbf{u}^i, \tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i, \mathbf{v}$ as long as at least two of the four functions are in the space W, and the other functions being in the space V.*

- *For the operator R_b, for fixed i, in comparison to the operator R'' from [85, 86], the previous phase-field directions $\tilde{\varphi}_1^{i-1}$ and $\tilde{\varphi}_2^{i-1}$ now occur in the definition of R_b. This has to be taken care of in the investigation.*

Next, recalling the notation defined in Definition 2.3.4, we additionally introduce the auxiliary (adjoint) operators $A_{l*}(\mathbf{u}^i)\colon\ V \times V_\varphi \to V^*$, and

$R_{l*}(\varphi^i;\varphi^{i-1},\varphi^{i+1})\colon V_\varphi \times V_\varphi \to V_\varphi^*$. These are defined, for test functions $\mathbf{v} = (v^u, v^\varphi) \in V$, by:

$$\begin{aligned}\big\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i,\psi^{i+1}),\mathbf{v}\big\rangle := &\big(g(\varphi^i)\mathbb{C}e(z^i),e(v^u)\big)\\ &+2(1-\kappa)\big(\varphi^i\mathbb{C}e(u^i)\colon e(z^i),v^\varphi\big)\\ &+2(1-\kappa)\big(\varphi^i\mathbb{C}e(u^i)\psi^i,e(v^u)\big)\\ &+(1-\kappa)\big(\psi^i\mathbb{C}e(u^i)\colon e(u^i),v^\varphi\big)\\ &+\varepsilon\big(\nabla\psi^i,\nabla v^\varphi\big)+\frac{1}{\varepsilon}\big(\psi^i,v^\varphi\big)\\ &+\eta\big(\psi^i-\psi^{i+1},v^\varphi\big),\end{aligned} \tag{3.5}$$

and

$$\begin{aligned}&\big\langle R_{l*}(\varphi^i,\varphi^{i-1},\varphi^{i+1};\gamma)(\psi^i,\psi^{i+1}),v^\varphi\big\rangle\\ &:=3\gamma\big([(\varphi^i-\varphi^{i-1})^+]^2\psi^i-[(\varphi^{i+1}-\varphi^i)^+]^2\psi^{i+1},v^\varphi\big).\end{aligned} \tag{3.6}$$

The definitions are motivated by the fact that

$$\sum_{i=1}^M\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i,\tilde{\varphi}^{i-1}),\mathbf{z}^i\big\rangle=\sum_{i=1}^M\big\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i,\psi^{i+1}),\tilde{\mathbf{u}}^i\big\rangle \tag{3.7}$$

and

$$\sum_{i=1}^M\big\langle R_l(\varphi^i,\varphi^{i-1};\gamma)(\tilde{\varphi}^i,\tilde{\varphi}^{i-1}),\psi^i\big\rangle=\sum_{i=1}^M\big\langle R_{l*}(\varphi^i,\varphi^{i-1},\varphi^{i+1};\gamma)(\psi^i,\psi^{i+1}),\tilde{\varphi}^i\big\rangle \tag{3.8}$$

hold true for all $\mathbf{u}_\mathbb{I},\mathbf{z}_\mathbb{I},\tilde{\mathbf{u}}_\mathbb{I}$. For simplification of the notation, we set

$$\psi^{M+1}:=0,\quad \varphi^{M+1}:=0,\quad \tilde{\varphi}^0:=0. \tag{3.9}$$

Let us point out that in comparison to [85, 86], for $M>1$ we have to be more careful due to the involvement of succeeding time steps:

Remark 3.1.2. *The operators A_{l*} and R_{l*} in particular contain the succeeding time step ψ^{i+1}, and in fact R_{l*} depends additionally on the time steps $i-1,i$, and $i+1$ in the phase-field variable. This introduces the need for some additional calculations when looking at norm bounds and Lipschitz results, as seen below. Further, the linearized operators A_{l*} and R_{l*} are not self-adjoint, which stands in contrast to their one time step counterparts A' and R' from [85, 86]. However, it holds $A'(\mathbf{u})\tilde{\mathbf{u}}=A_l(\mathbf{u})(\tilde{\mathbf{u}},0)$ and $R'(\varphi;\gamma)\tilde{\varphi}=R_l(\varphi,\varphi^0;\gamma)(\tilde{\varphi},0)$, for which self-adjointness holds true.*

Let us conclude with the introduction of the operators A_{b*} and R_{b*}: Similarly to the operators A_{l*} and R_{l*} from (3.5) and (3.6), we introduce them as the adjoint counterparts (w.r.t. the second direction) of the operators A_b and R_b: Firstly, for all $\mathbf{u}^i, \tilde{\mathbf{u}}^i \in W$ the operator $A_{b*}(\mathbf{u}^i, \tilde{\mathbf{u}}^i)\colon W \to V^*$ is given, for all test functions $\mathbf{v}^i \in V$, via

$$\begin{aligned}\big\langle A_{b*}(\mathbf{u}^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i, \mathbf{v}^i\big\rangle = {}& 2(1-\kappa)\big(\varphi^i \mathbb{C} e(\tilde{u}^i) \colon e(z^i), v^{\varphi,i}\big) \\ &+ 2(1-\kappa)\big(\tilde{\varphi}^i \mathbb{C} e(u^i) \colon e(z^i), v^{\varphi,i}\big) \\ &+ 2(1-\kappa)\big(\varphi^i \mathbb{C} e(z^i)\tilde{\varphi}^i, e(v^{u,i})\big) \\ &+ 2(1-\kappa)\big(\psi^i \mathbb{C} e(u^i) \colon e(\tilde{u}^i), v^{\varphi,i}\big) \\ &+ 2(1-\kappa)\big(\varphi^i \mathbb{C} e(\tilde{u}^i)\psi^i, e(v^{u,i})\big) \\ &+ 2(1-\kappa)\big(\tilde{\varphi}^i \mathbb{C} e(u^i)\psi^i, e(v^{u,i})\big). \end{aligned} \tag{3.10}$$

In particular, due to the fact that A_b is not dependent on any functions of the previous (or succeeding) time steps $i-1$ and $i+1$, this definition is immediately motivated through:

$$\begin{aligned}\sum_{i=1}^{M} \big\langle A_{b*}(\mathbf{u}^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i, \mathbf{v}^i\big\rangle &= \sum_{i=1}^{M} \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}^i, \mathbf{v}^i], \mathbf{z}^i\big\rangle \\ &= \sum_{i=1}^{M} \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}^i, \mathbf{z}^i], \mathbf{v}^i\big\rangle, \end{aligned} \tag{3.11}$$

which holds for all $\mathbf{u}_{\mathbb{I}}, \tilde{\mathbf{u}}_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}} \in W^M$ and all test functions $\mathbf{v}_{\mathbb{I}} \in V^M$. Note that the second equality directly follows from the linearity of A_b in all four entries $\mathbf{u}^i, \tilde{\mathbf{u}}^i, \mathbf{z}^i$ and $\mathbf{v}^i$. Finally, for all $\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1} \in W_\varphi$ the operator $R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1})\colon W_\varphi \times W_\varphi \to V_\varphi^*$, is defined for all test functions $v^{\varphi,i} \in V_\varphi$:

$$\begin{aligned}&\big\langle R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^{\varphi,i}\big\rangle \\ &\quad = 6\gamma\big([(\varphi^i - \varphi^{i-1})^+](\tilde{\varphi}^i - \tilde{\varphi}^{i-1})\psi^i - [(\varphi^{i+1} - \varphi^i)^+](\tilde{\varphi}^{i+1} - \tilde{\varphi}^i)\psi^{i+1}, v^{\varphi,i}\big), \end{aligned} \tag{3.12}$$

which is motivated due to

$$\begin{aligned}&\sum_{i=1}^{M} \big\langle R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}), \mathbf{v}^i\big\rangle \\ &\quad = \sum_{i=1}^{M} \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), (v^{\varphi,i}, v^{\varphi,i-1})], \psi^i\big\rangle, \end{aligned} \tag{3.13}$$

where $\varphi_{\mathbb{I}}, \tilde{\varphi}_{\mathbb{I}}, \psi_{\mathbb{I}} \in W_\varphi^M$, φ^0 is a given function, $\tilde{\varphi}^0, \tilde{\varphi}^{M+1}, \psi^{M+1} := 0$ for notational concurrence, cf. (3.9), and all test functions $v_{\mathbb{I}}^{\varphi} \in V^M$, where we set $v^{\varphi,0} = 0$.

The operators A_{b*} and R_{b*} are also useful to express optimality conditions in the context of the linear-quadratic subproblems occurring in the analysis of the

SQP method, see Chapter 6 below. While A_{b*} is only dependent on the current time step i, R_{b*} again depends on functions of the time steps $i-1, i$, and $i+1$. The same properties as for the operator R_{l*} hold true, cf. Remark 3.1.2.

We are now in a position to start with auxiliary results for the operators A, A_l, A_b and A_{b*}. In particular, we can show the following norm bounds:

Lemma 3.1.3. *There exist constants* $0 < c(\kappa, \varepsilon, \eta, \|\mathbf{u}^i\|_W, \|\mathbf{u}^{i-1}\|_W)$, $c(\kappa, \varepsilon, \eta, \|\mathbf{u}^i\|_W)$, $c(\kappa, \varepsilon, \eta, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})$, $c(\kappa) \in \mathbb{R}$, *such that for all* $\mathbf{u}_{\mathbb{I}}, \tilde{\mathbf{u}}_{\mathbb{I}}, \tilde{\mathbf{u}}_{j,\mathbb{I}} \in W^M$, *where* $j = 1, 2$, *it holds*

$$\begin{aligned} \|A(\mathbf{u}^i, \varphi^{i-1})\|_{W^\times} &\le c(\kappa, \varepsilon, \eta, \|\mathbf{u}^i\|_W, \|\mathbf{u}^{i-1}\|_W) \\ &\le c(\kappa, \varepsilon, \eta, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}), \end{aligned} \tag{3.14}$$

$$\begin{aligned} \|A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1})\|_{W^\times} &\le c(\kappa, \varepsilon, \eta, \|\mathbf{u}^i\|_W)\big(\|\tilde{\mathbf{u}}^i\|_W + \|\tilde{\mathbf{u}}^{i-1}\|_W\big) \\ &\le c(\kappa, \varepsilon, \eta, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \end{aligned} \tag{3.15}$$

$$\begin{aligned} \big\|A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i]\big\|_{W^\times} &\le c(\kappa)\|\tilde{\mathbf{u}}_2^i\|_W\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W \\ &\le c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}. \end{aligned} \tag{3.16}$$

It further holds, for all $\mathbf{z}_{\mathbb{I}} \in W^M$,

$$\begin{aligned} \|A_{b*}(\mathbf{u}^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i\|_{W^\times} &\le c(\kappa)\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}^i\|_W\|\mathbf{z}^i\|_W \\ &\le c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}, \end{aligned} \tag{3.17}$$

$$\begin{aligned} \big|\big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i\big\rangle\big| &\le c(\kappa)\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W\|\tilde{\mathbf{u}}_2^i\|_W\|\mathbf{z}^i\|_W \\ &\le c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}. \end{aligned} \tag{3.18}$$

Proof. All bounds are established similarly to the estimations conducted in e.g. [132, Lemma 5.1]. For the convenience of the reader, we present the course of action in detail.

1. Recall the definition of A from Definition 2.3.8 and estimate term-wise: In the $W^{1,p}(\Omega;\mathbb{R}^2)$-norm, using the triangle inequality and the Sobolev-embedding $W_\varphi \hookrightarrow L^\infty(\Omega;\mathbb{R}^2)$ yields

$$\begin{aligned} \|g(\varphi^i)\mathbb{C}e(u^i)\|_{L^p(\Omega;\mathbb{R}^2)} &= \|(1-\kappa)(\varphi^i)^2\mathbb{C}e(u^i) + \kappa\mathbb{C}e(u^i)\|_{L^p(\Omega;\mathbb{R}^2)} \\ &\le c(\kappa)\|(\varphi^i)^2\mathbb{C}e(u^i)\|_{L^p(\Omega;\mathbb{R}^2)} \\ &\quad + c(\kappa)\|\mathbb{C}e(u^i)\|_{L^p(\Omega;\mathbb{R}^2)} \\ &\le c(\kappa)\|\varphi^i\|_{L^\infty(\Omega)}^2\|u^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)} \\ &\quad + c(\kappa)\|u^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)} \\ &\le c(\kappa)\|\varphi^i\|_{W_\varphi}\|u^i\|_{W_u} + c(\kappa)\|u^i\|_{W_u} \\ &\le c(\kappa)\|\mathbf{u}^i\|_W^3 + c(\kappa)\|\mathbf{u}^i\|_W \\ &\le c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_W^3 + c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_W, \end{aligned}$$

where we also used

$$\|\varphi^i\|_{W_\varphi}, \|u^i\|_{W_u} \le \|\varphi^i\|_{W_\varphi} + \|u^i\|_{W_u} \le \|\mathbf{u}^i\|_W \le \|\mathbf{u}_\mathbb{I}\|_{W^M},$$

see the definition of the W norm, cf. Definition 2.3.3, and the multi time step definition of the functions in Definition 2.3.4. Next, using the L^p-embedding $L^2(\Omega) \hookrightarrow L^q(\Omega)$ (recalling $q > 1$ but close, thus $q < 2$), and the Sobolev embedding $W_\varphi \hookrightarrow V_\varphi$, it holds

$$\begin{aligned}
\|\varepsilon\nabla\varphi^i\|_{L^q(\Omega;\mathbb{R}^2)} &\le c(\varepsilon)\|\nabla\varphi^i\|_{L^2(\Omega;\mathbb{R}^2)} \le c(\varepsilon)\|\varphi^1\|_{V_\varphi} \le c(\varepsilon)\|\varphi^i\|_{W_\varphi} \\
&\le c(\varepsilon)\|\mathbf{u}^i\|_W \le c(\varepsilon)\|\mathbf{u}_\mathbb{I}\|_{W^M}, \\
\Big\|\frac{1}{\varepsilon}(1-\varphi^i)\Big\|_{L^q(\Omega} &\le c(\varepsilon^{-1})\|\varphi^i\|_{L^\infty(\Omega;\mathbb{R}^2)} \le c(\varepsilon^{-1})\|\varphi^i\|_{W_\varphi} \\
&\le c(\varepsilon^{-1})\|\mathbf{u}^i\|_W \le c(\varepsilon^{-1})\|\mathbf{u}_\mathbb{I}\|_{W^M}, \\
\|\eta(\varphi^i - \varphi^{i-1})\|_{L^q(\Omega)} &\le c(\eta)\|\varphi^i - \varphi^{i-1}\|_{L^\infty} \\
&\le c(\eta)\|\varphi^i\|_{L^\infty(\Omega)} + c(\eta)\|\varphi^{i-1}\|_{L^\infty(\Omega)} \\
&\le c(\eta)\|\varphi^i\|_{W_\varphi} + c(\eta)\|\varphi^{i-1}\|_{W_\varphi} \\
&\le c(\eta)\|\mathbf{u}^i\|_W + c(\eta)\|\mathbf{u}^{i-1}\|_W \\
&\le c(\eta)\|\mathbf{u}_\mathbb{I}\|_{W^M}.
\end{aligned}$$

Finally, for the remaining term in A, similarly to above, additionally using Hölder's inequality for $\frac{1}{q} = \frac{1}{p} + \frac{1}{p}$, it holds

$$\begin{aligned}
\|(1-\kappa)\varphi^i\mathbb{C}e(u^i) \colon e(u^i)\|_{L^q(\Omega)} &\le c(\kappa)\|\varphi^i\|_{L^\infty(\Omega;\mathbb{R}^2)}\|u^i\|^2_{W^{1,p}(\Omega;\mathbb{R}^2)} \\
&\le c(\kappa)\|\varphi^i\|_{W_\varphi}\|u^i\|^2_{W_u} \\
&\le c(\kappa)\|\mathbf{u}^i\|^3_W \le c(\kappa)\|\mathbf{u}_\mathbb{I}\|^3_{W^M}.
\end{aligned}$$

Combining all estimates, (3.14) holds true.

2. Recall the definition of A_l from (3.1). Analogously to the first point, the following estimates hold:

$$\begin{aligned}
\|g(\varphi^i)\mathbb{C}e(\tilde{u}^i)\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa)\|\mathbf{u}^i\|^2_W\|\tilde{\mathbf{u}}^i\|_W + c(\kappa)\|\tilde{\mathbf{u}}^i\|_W \\
&\le c(\kappa)\|\mathbf{u}_\mathbb{I}\|^2_{W^M}\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M} + c(\kappa)\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M}, \\
\|2(1-\kappa)\varphi^i\mathbb{C}e(u^i)\tilde{\varphi}^i\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa)\|\mathbf{u}^i\|^2_W\|\tilde{\mathbf{u}}^i\|_W \\
&\le c(\kappa)\|\mathbf{u}_\mathbb{I}\|^2_{W^M}\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M}, \\
\|2(1-\kappa)\varphi^i\mathbb{C}e(u^i) \colon e(\tilde{u}^i)\|_{L^q(\Omega)} &\le c(\kappa)\|\mathbf{u}^i\|^2_W\|\tilde{\mathbf{u}}^i\|_W \\
&\le c(\kappa)\|\mathbf{u}_\mathbb{I}\|^2_{W^M}\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M}, \\
\|(1-\kappa)\tilde{\varphi}^i\mathbb{C}e(u^i) \colon e(u^i)\|_{L^q(\Omega)} &\le c(\kappa)\|\mathbf{u}^i\|^2_W\|\tilde{\mathbf{u}}^i\|_W \\
&\le c(\kappa)\|\mathbf{u}_\mathbb{I}\|^2_{W^M}\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M}, \\
\|\varepsilon\nabla\tilde{\varphi}^i\|_{L^q(\Omega,\mathbb{R}^2)} &\le c(\varepsilon)\|\tilde{\mathbf{u}}^i\|_W \le c(\varepsilon)\|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M},
\end{aligned}$$

$$
\begin{aligned}
\left\|\frac{1}{\varepsilon}\tilde{\varphi}^i\right\|_{L^q(\Omega)} &\leq c(\varepsilon^{-1})\|\tilde{\mathbf{u}}^i\|_W \leq c(\varepsilon^{-1})\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M},\\
\|\eta(\tilde{\varphi}^i-\tilde{\varphi}^{i-1})\|_{L^q(\Omega)} &\leq c(\eta)\|\tilde{\mathbf{u}}^i\|_W + c(\eta)\|\tilde{\mathbf{u}}^{i-1}\|_W\\
&\leq c(\eta)\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M},
\end{aligned}
$$

and the result from (3.15) can easily be concluded.

3. Recall the definition of A_b from (3.3). Again, analogously to the first point the following estimates hold:

$$
\begin{aligned}
\|2(1-\kappa)\varphi^i\mathbb{C}e(\tilde{u}_1^i)\tilde{\varphi}_2^i\|_{L^p(\Omega;\mathbb{R}^2)} &\leq c(\kappa)\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W\|\tilde{\mathbf{u}}_2^i\|_W\\
&\leq c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M},\\
\|2(1-\kappa)\tilde{\varphi}_2^i\mathbb{C}e(u^i)\colon e(\tilde{u}_1^i)\|_{L^q(\Omega)} &\leq c(\kappa)\|\tilde{\mathbf{u}}_2^i\|_W\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W\\
&\leq c(\kappa)\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}.
\end{aligned}
$$

The other terms are estimated in the same way, overall the $W^{\times}$-norm estimate follows.

4. Recalling the definition of A_{b*} from (3.10), one can see that the terms are the same as in A_b. The estimate therefore follows in the same way as in point 3.

5. The estimate (3.18) follows similarly to the third point: Using Hölder's inequality for $1 \geq \frac{1}{p} + \frac{1}{p}$, it immediately follows

$$
\begin{aligned}
&\big(2(1-\kappa)\varphi^i\mathbb{C}e(\tilde{u}_1^i)\tilde{\varphi}_2^i, e(z^i)\big)\\
&\quad\leq c(\kappa)\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W\|\mathbf{z}_1^i\|_W\|\tilde{\mathbf{u}}_2^i\|_W\\
&\quad\leq c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M},\\
&\big(2(1-\kappa)\tilde{\varphi}_2^i\mathbb{C}e(u^i)\colon e(\tilde{u}_1^i), \psi^i\big)\\
&\quad\leq c(\kappa)\|\tilde{\varphi}_2^i\|_{L^\infty(\Omega)}\|u^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|\tilde{u}_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|\psi^i\|_{L^\infty(\Omega)}\\
&\quad\leq c(\kappa)\|\tilde{\varphi}_2^i\|_{W_\varphi}\|u^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|\tilde{u}_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|\psi^i\|_{W_\varphi}\\
&\quad\leq c(\kappa)\|\tilde{\mathbf{u}}_2^i\|_W\|\mathbf{u}^i\|_W\|\tilde{\mathbf{u}}_1^i\|_W\|\mathbf{z}^i\|_W\\
&\quad\leq c(\kappa)\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}.
\end{aligned}
$$

The other terms are estimated in the same way, which concludes the proof.

□

We now turn towards Fréchet differentiability of the operators A, A_l and A_{l*} in the improved Banach space setting:

Lemma 3.1.4.

1. *The operator A from Definition 2.3.8 is Fréchet differentiable from $W \times W_\varphi$ into $W^\times$, i.e. it holds*

$$A(\mathbf{u}^i + \mathbf{du}^i; \varphi^{i-1} + d\varphi^{i-1}) - A(\mathbf{u}^i; \varphi^{i-1}) = A_l(\mathbf{u}^i)(\mathbf{du}^i, d\varphi^{i-1}) + o(\|\mathbf{du}^i\|_W + \|d\varphi^{i-1}\|_{W_\varphi}).$$

2. *Let $\mathbf{du}_1^i \in W, d\varphi_1^{i-1} \in W_\varphi$, then the operator $A_l(\cdot)(\mathbf{du}_1^i, d\varphi_1^{i-1})$ from* (3.1) *is Fréchet differentiable from W into $W^\times$, i.e. it holds*

$$\begin{aligned} &A_l(\mathbf{u}^i + \mathbf{du}_2^i)(\mathbf{du}_1^i, d\varphi_1^{i-1}) - A_l(\mathbf{u}^i)(\mathbf{du}_1^i, d\varphi^{i-1}) \\ &\quad = A_b(\mathbf{u}^i)[\mathbf{du}_1^i, \mathbf{du}_2^i] + o(\|\mathbf{du}_2^i\|_W). \end{aligned}$$

   In combination with 1*, this means that the operator A is twice Fréchet differentiable in the corresponding spaces.*

3. *Let $\mathbf{z}^i \in W, \psi^{i+1} \in W_\varphi$, then the operator $A_{l*}(\cdot)(\mathbf{z}^i, \psi^{i+1})$ from* (3.5) *is Fréchet differentiable from W into $W^\times$, i.e. it holds*

$$A_{l*}(\mathbf{u}^i + \mathbf{du}^i)(\mathbf{z}^i, \psi^{i+1}) - A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) = A_{b*}(\mathbf{u}^i, \mathbf{du}^i)\mathbf{z}^i + o(\|\mathbf{du}^i\|_W).$$

4. *Let $\mathbf{u}^i \in W$, then the operator $A_{l*}(\mathbf{u}^i)(\cdot^i, \cdot^{i+1})$ from* (3.5) *is Fréchet differentiable from $W \times W_\varphi$ into $W^\times$, i.e. it holds*

$$\begin{aligned} &A_{l*}(\mathbf{u}^i)(\mathbf{z}^i + \mathbf{dz}^i, \psi^{i+1} + d\psi^{i+1}) - A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) \\ &\quad = A_{l*}(\mathbf{u}^i)(\mathbf{dz}^i, d\psi^{i+1}) + o(\|\mathbf{dz}^i\|_W + \|d\psi^{i+1}\|_{W_\varphi}). \end{aligned}$$

Proof. The proofs of 1 and 2 are already given along the way of [86, Proof of Proposition 3.3], and are revisited in detail for the convenience of the reader. The proofs of 3 and 4 then immediately follow from the structure of A_{l*}.

1. Let $\mathbf{u}^i, \mathbf{du}^i \in W$, $\varphi^{i-1}, d\varphi^{i-1} \in W_\varphi$ and $\mathbf{v} \in V$, recalling the definition of A from Definition 2.3.8 and utilizing the linearity of $e(u)$ and $\mathbb{C}e(u)$, as well as the symmetry of the inner products of these operators, it holds

$$\begin{aligned} &\big\langle A(\mathbf{u}^i + \mathbf{du}^i, \varphi^{i-1} + d\varphi^{i-1}), \mathbf{v}\big\rangle \\ &\quad = \big(g(\varphi^i + d\varphi^i)\mathbb{C}e(u^i + du^i), e(v^u)\big) + \varepsilon\big(\nabla(\varphi^i + d\varphi^i), \nabla v^\varphi\big) \\ &\qquad - \frac{1}{\varepsilon}\big(1 - (\varphi^i - d\varphi^i), v^\varphi\big) + \eta\big(\varphi^i + d\varphi^i - (\varphi^{i-1} + d\varphi^{i-1}), v^\varphi\big) \\ &\qquad + (1-\kappa)\big((\varphi^i + d\varphi^i)\mathbb{C}e(u^i + du^i) : e(u^i + du^i), v^\varphi\big) \\ &\quad = \big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)) + (g(\varphi^i)\mathbb{C}e(du^i), e(v^u)\big) \end{aligned}$$

$$
\begin{aligned}
&+ 2(1-\kappa)\big(\varphi^i d\varphi^i \mathbb{C}e(u^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i d\varphi^i \mathbb{C}e(du^i), e(v^u)\big) \\
&+ (1-\kappa)\big((d\varphi^i)^2 \mathbb{C}e(u^i + du^i), e(v^u)\big) + \varepsilon\big(\nabla\varphi^i, \nabla v^\varphi\big) + \varepsilon\big(\nabla d\varphi^i, \nabla v^\varphi\big) \\
&- \frac{1}{\varepsilon}\big(1-\varphi^i, v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi^i, v^\varphi\big) + \eta\big(\varphi^i - \varphi^{i-1}, v^\varphi\big) + \eta\big(d\varphi^i - d\varphi^{i-1}, v^\varphi\big) \\
&+ (1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du^i) \colon e(u^i), v^\varphi\big) \\
&+ (1-\kappa)\big(\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big) + (1-\kappa)\big(d\varphi^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi\big) \\
&+ 2(1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(u^i), v^\varphi\big) + (1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big) \\
=& \big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)\big) + \varepsilon\big(\nabla\varphi^i, \nabla v^\varphi\big) - \frac{1}{\varepsilon}\big(1-\varphi^i, v^\varphi\big) \qquad (3.19) \\
&+ \eta\big(\varphi^i - \varphi^{i-1}, v^\varphi\big) + (1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi\big) \qquad (3.20) \\
&+ \big(g(\varphi^i)\mathbb{C}e(du^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du^i) \colon e(u^i), v^\varphi\big) \qquad (3.21) \\
&+ \varepsilon\big(\nabla d\varphi^i, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi^i, v^\varphi\big) + \eta\big(d\varphi^i - d\varphi^{i-1}, v^\varphi\big) \qquad (3.22) \\
&+ (1-\kappa)\big(d\varphi^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi\big) + 2(1-\kappa)\big(\varphi^i d\varphi^i \mathbb{C}e(u^i), e(v^u)\big) \qquad (3.23) \\
&+ 2(1-\kappa)\big(\varphi^i d\varphi^i \mathbb{C}e(du^i), e(v^u)\big) + (1-\kappa)\big((d\varphi^i)^2 \mathbb{C}e(u^i + du^i), e(v^u)\big) \qquad (3.24) \\
&+ (1-\kappa)\big(\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big) + 2(1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(u^i), v^\varphi\big) \qquad (3.25) \\
&+ (1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big) \qquad (3.26) \\
=& \big\langle A(\mathbf{u}^i; \varphi^{i-1}), \mathbf{v}\big\rangle + \big\langle A_l(\mathbf{u}^i)(\mathbf{du}^i, d\varphi^{i-1}), \mathbf{v}\big\rangle + \big\langle \mathrm{rem}_A(\mathbf{u}^i, \mathbf{du}^i), \mathbf{v}\big\rangle,
\end{aligned}
$$

where one recognizes that to obtain the last equality, the first two lines (3.19)-(3.20) of the second-to-last equality can be expressed by the operator $A(\mathbf{u}^i; \varphi^{i-1})$, the following three lines (3.21)-(3.23) by the linearized operator $A_l(\mathbf{u}^i)(\mathbf{du}^i, d\varphi^{i-1})$, and the remainder $\mathrm{rem}_A(\mathbf{u}^i, \mathbf{du}^i)$ was introduced, which is given by (3.24)-(3.26), i.p.

$$
\begin{aligned}
\big\langle \mathrm{rem}_A(\mathbf{u}^i, \mathbf{du}^i), \mathbf{v}\big\rangle := \;& 2(1-\kappa)\big(\varphi^i d\varphi^i \mathbb{C}e(du^i), e(v^u)\big) \\
&+ (1-\kappa)\big((d\varphi^i)^2 \mathbb{C}e(u^i), e(v^u)\big) \\
&+ (1-\kappa)\big((d\varphi^i)^2 \mathbb{C}e(du^i), e(v^u)\big) \\
&+ (1-\kappa)\big(\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big) \\
&+ 2(1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(u^i), v^\varphi\big) \\
&+ (1-\kappa)\big(d\varphi^i \mathbb{C}e(du^i) \colon e(du^i), v^\varphi\big). \qquad (3.27)
\end{aligned}
$$

Recall the regularities $u^i, du^i \in W^{1,p}(\Omega; \mathbb{R}^2)$, and $\varphi^i, d\varphi^i \in W^{2,q}(\Omega) \hookrightarrow C(\bar{\Omega}) \hookrightarrow L^\infty(\Omega)$, which holds since $q = p/2 > 1$ in $N = 2$ dimensions. To estimate the remainder $\mathrm{rem}_A(\mathbf{u}^i, \mathbf{du}^i)$, for the first three terms of (3.27) it thus immediately holds, analogously to the estimations done in the proof of Lemma 3.1.3,

$$
\|2(1-\kappa)\varphi^i d\varphi^i \mathbb{C}e(du^i)\|_{L^p(\Omega;\mathbb{R}^2)} \le c(\kappa)\|\mathbf{u}^i\|_W \|\mathbf{du}^i\|_W^2 \le c(\mathbf{u}^i)\|\mathbf{du}^i\|_W^2,
$$

$$
\begin{aligned}
\|(1-\kappa)(d\varphi^i)^2\mathbb{C}(u^i)\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa)\|\mathbf{du}^i\|_W^2\|\mathbf{u}^i\|_W \le c(\mathbf{u}^i)\|\mathbf{du}^i\|_W^2,\\
\|(1-\kappa)(d\varphi^i)^2\mathbb{C}(du^i)\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa)\|\mathbf{du}^i\|_W^3 \le c(\mathbf{du}^i)\|\mathbf{du}^i\|_W^2,
\end{aligned}
$$

for a constant $c(\mathbf{u}^i) = 2\max(c, \|\mathbf{u}^i\|_W) < \infty$ and a constant $c(\mathbf{du}^i) = 3\max(c, \|\mathbf{du}^i\|_W) < \infty$. For the last three terms of the remainder $\mathrm{rem}_A(\mathbf{u}, \mathbf{d}^{\mathbf{u}})$ from (3.27), one obtains for the same $c(\mathbf{u}^i) < \infty$ and $c(\mathbf{du}^i) < \infty$ as above,

$$
\begin{aligned}
\|(1-\kappa)\varphi\mathbb{C}e(du^i) : e(du^i)\|_{L^q(\Omega)} &\le c(\kappa, \mathbf{u}^i)\|\mathbf{du}^i\|_W^2,\\
\|2(1-\kappa)d\varphi^i\mathbb{C}e(du^i) : e(u^i)\|_{L^q(\Omega)} &\le c(\kappa, \mathbf{u}^i)\|\mathbf{du}^i\|_W^2,\\
\|(1-\kappa)d\varphi^i\mathbb{C}e(du^i) : e(du^i)\|_{L^q(\Omega)} &\le c(\kappa, \mathbf{du}^i)\|\mathbf{du}^i\|_W^2.
\end{aligned}
$$

Thus, $\mathrm{rem}_A(\mathbf{u}^i, \mathbf{du}^i)$ suffices to (note that since the φ^{i-1}-terms occur only linearly in A, the remainder is independent of any $i-1$-terms, nevertheless we add the $\|d\varphi^{i-1}\|_{W_\varphi}$-term in the denominator),

$$
\begin{aligned}
&\|rem_A(\mathbf{u}^i, \mathbf{du}^i)\|_{W^\times} / \big(\|\mathbf{du}^i\|_W + \|d\varphi^{i-1}\|_{W_\varphi}\big) \to 0\\
&\quad \text{for} \quad \big(\|\mathbf{du}^i\|_W + \|d\varphi^{i-1}\|_{W_\varphi}\big) \to 0.
\end{aligned}
$$

Note that well-definedness of all terms involved in $A(\mathbf{u}^i, \varphi^{i-1})$ and $A_l(\mathbf{u}^i)(\mathbf{du}^i, d\varphi^{i-1})$ in $W^\times$ is clear from Lemma 3.1.3, thus A is differentiable from $W \times W_\varphi$ into $W^\times$.

2. Let $\mathbf{u}^i, \mathbf{du}^i_j \in W$ for $j = 1, 2$, and $\mathbf{v} \in V$, analogously to above we calculate

$$
\begin{aligned}
&\big\langle A_l(\mathbf{u}^i + \mathbf{du}^i_2)(\mathbf{du}^i_1, d\varphi_1^{i-1}), \mathbf{v}\big\rangle\\
&\quad = \big(g(\varphi^i + d\varphi^i_2)\mathbb{C}e(du^i_1), e(v^u)\big)\\
&\qquad + 2(1-\kappa)\big((\varphi^i + d\varphi^i_2)\mathbb{C}e(u^i + du^i_2) \colon e(du^i_1), v^\varphi\big)\\
&\qquad + \varepsilon\big(\nabla d\varphi^i_1, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi^i_1, v^\varphi\big) + \eta\big(d\varphi^i_1 - d\varphi^{i-1}_1, v^\varphi\big)\\
&\qquad + (1+\kappa)\big(d\varphi^i_1\mathbb{C}e(u^i + du^i_2) \colon e(u^i + du^i_2), v^\varphi\big)\\
&\qquad + 2(1-\kappa)\big((\varphi^i + d\varphi^i_2)\mathbb{C}e(u^i + du^i_2)d\varphi^i_1, e(v^u)\big)\\
&\quad = \big(g(\varphi^i)\mathbb{C}e(du^i_1), e(v^u)\big)\\
&\qquad + 2(1-\kappa)\big(\varphi^i d\varphi^i_2\mathbb{C}e(du^i_1), e(v^u)\big)\\
&\qquad + (1-\kappa)\big((d\varphi^i_2)^2\mathbb{C}e(du^i_1), e(v^u)\big)\\
&\qquad + 2(1-\kappa)\big(\varphi\mathbb{C}e(u^i + du^i_2) \colon e(du^i_1), v^\varphi\big)\\
&\qquad + 2(1-\kappa)\big(d\varphi^i_2\mathbb{C}e(u^i + du^i_2) \colon e(du^i_1), v^\varphi\big)\\
&\qquad + \varepsilon\big(\nabla d\varphi^i_1, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi^i_1, v^\varphi\big) + \eta\big(d\varphi^i_1 - d\varphi^{i-1}_1, v^\varphi\big)\\
&\qquad + (1+\kappa)\big(d\varphi^i_1\mathbb{C}e(u^i) \colon e(u^i + du^i_2), v^\varphi\big)\\
&\qquad + (1+\kappa)\big(d\varphi^i_1\mathbb{C}e(du^i_2) \colon e(u^i + du^i_2), v^\varphi\big)
\end{aligned}
$$

$$
\begin{aligned}
&+ 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i + du_2^i) d\varphi_1^i, e(v^u)\big) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(u^i + du_2^i) d\varphi_1^i, e(v^u)\big) \\
= &\big(g(\varphi^i)\mathbb{C}e(du_1^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i d\varphi_2^i \mathbb{C}e(du_1^i), e(v^u)\big) \\
&+ (1-\kappa)\big((d\varphi_2^i)^2 \mathbb{C}e(du_1^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) \colon e(du_1^i), v^\varphi\big) \\
&+ 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du_2^i) \colon e(du_1^i), v^\varphi\big) + 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(u^i) \colon e(du_1^i), v^\varphi\big) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) \colon e(du_1^i), v^\varphi\big) \\
&+ \varepsilon\big(\nabla d\varphi_1^i, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi_1^i, v^\varphi\big) + \eta\big(d\varphi_1^i - d\varphi_1^{i-1}, v^\varphi\big) \\
&+ (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(u^i) : e(u^i), v^\varphi\big) + (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(u^i) \colon e(du_2^i), v^\varphi\big) \\
&+ (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(du_2^i) \colon e(u^i), v^\varphi\big) + (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(du_2^i) \colon e(du_2^i), v^\varphi\big) \\
&+ 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) d\varphi_1^i, e(v^u)\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(u^i) d\varphi_1^i, e(v^u)\big) + 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big) \\
= &\big(g(\varphi^i)\mathbb{C}e(du_1^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) \colon e(du_1^i), v^\varphi\big) \qquad (3.28) \\
&+ \varepsilon\big(\nabla d\varphi_1^i, \nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(d\varphi_1^i, v^\varphi\big) + \eta\big(d\varphi_1^i - d\varphi_1^{i-1}, v^\varphi\big) \qquad (3.29) \\
&+ (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(u^i) \colon e(u^i), v^\varphi\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(u^i) d\varphi_1^i, e(v^u)\big) \qquad (3.30) \\
&+ 2(1-\kappa)\big(\varphi^i d\varphi_2^i \mathbb{C}e(du_1^i), e(v^u)\big) + 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du_2^i) \colon e(du_1^i), v^\varphi\big) \qquad (3.31) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(u^i) \colon e(du_1^i), v^\varphi\big) + 2(1+\kappa)\big(d\varphi_1^i \mathbb{C}e(u^i) \colon e(du_2^i), v^\varphi\big) \qquad (3.32) \\
&+ 2(1-\kappa)\big(\varphi^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big) + 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(u^i) d\varphi_1^i, e(v^u)\big) \qquad (3.33) \\
&+ (1-\kappa)\big((d\varphi_2^i)^2 \mathbb{C}e(du_1^i), e(v^u)\big) + (1+\kappa)\big(d\varphi_1^i \mathbb{C}e(du_2^i) \colon e(du_2^i), v^\varphi\big) \qquad (3.34) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big) + 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big) \qquad (3.35) \\
= &\big\langle A_l(\mathbf{u}^i)(\mathbf{du}_1^i, d\varphi_1^{i-1}), \mathbf{v}\big\rangle + \big\langle A_b(\mathbf{u}^i)[\mathbf{du}_1^i, \mathbf{du}_2^i], \mathbf{v}\big\rangle \\
&+ \big\langle \mathrm{rem}_{A_l}(\mathbf{du}_1^i, \mathbf{du}_2^i), \mathbf{v}\big\rangle,
\end{aligned}
$$

where one recognizes that the first three lines (3.28)-(3.30) of the second-to-last equality can be expressed by the operator $A_l(\mathbf{u}^i)(\mathbf{du}_1^i, d\varphi_1^{i-1})$, and the following four lines (3.31)-(3.33) by the operator $A_b(\mathbf{u}^i)[\mathbf{du}_1^i, \mathbf{du}_2^i]$. Note that the symmetry property $\mathbb{C}e(u_1) : e(u_2) = \mathbb{C}e(u_2) : e(u_1)$, c.f. Chapter 2, is used to obtain the second to last equality. Further, the remainder $\mathrm{rem}_{A_l}(\mathbf{du}_1^i, \mathbf{du}_2^i)$ was introduced, which is given by the last two lines (3.34)-(3.35), i.e.

$$
\begin{aligned}
\big\langle \mathrm{rem}_{A_l}(\mathbf{du}_1^i, \mathbf{du}_2^i), \mathbf{v}\big\rangle := &+ (1-\kappa)\big((d\varphi_2^i)^2 \mathbb{C}e(du_1^i), e(v^u)\big) \\
&+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) : e(du_1^i), v^\varphi\big)
\end{aligned}
$$

$$+ (1-\kappa)\big(d\varphi_1^i \mathbb{C}e(du_2^i) : e(du_2^i), v^\varphi\big)$$
$$+ 2(1-\kappa)\big(d\varphi_2^i \mathbb{C}e(du_2^i) d\varphi_1^i, e(v^u)\big).$$

Well-definedness in $W^\times$ of all terms involved in $A_l(\mathbf{u}^i)(\mathbf{du}_1^i, d\varphi_1^{i-1})$ and $A_b(\mathbf{u}^i)[\mathbf{du}_1^i, \mathbf{du}_2^i]$ is again clear by Lemma 3.1.3 from the given regularities. To estimate the terms in the remainder $\mathrm{rem}_{A_l}(\mathbf{du}_1^i, \mathbf{du}_2^i)$, for a constant $c(\mathbf{du}_1^i) = \max(c, \|\mathbf{du}_1^i\|_W) < \infty$, it again follows as in Lemma 3.1.3, that

$$\begin{aligned}
\|(1-\kappa)(d\varphi_2^i)^2 \mathbb{C}e(du_1^i)\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa, \mathbf{du}_1^i)\|\mathbf{du}_2^i\|_W^2, \\
\|2(1-\kappa) d\varphi_2^i \mathbb{C}e(du_2^i) d\varphi_1^i\|_{L^p(\Omega;\mathbb{R}^2)} &\le c(\kappa, \mathbf{du}_1^i)\|\mathbf{du}_2^i\|_W^2, \\
\|2(1-\kappa) d\varphi_2^i \mathbb{C}e(du_2^i) : e(du_1^i)\|_{L^q(\Omega)} &\le c(\kappa, \mathbf{du}_1^i)\|\mathbf{du}_2^i\|_W^2, \\
\|(1-\kappa) d\varphi_1^i \mathbb{C}e(du_2^i) : e(du_2^i)\|_{L^q(\Omega)} &\le c(\kappa, \mathbf{du}_1^i)\|\mathbf{du}_2^i\|_W^2.
\end{aligned}$$

Thus, similarly to above it holds

$$\|\mathrm{rem}_{A_l}(\mathbf{du}_1^i, \mathbf{du}_2^i)\|_{W^\times} / \|\mathbf{du}_2^i\|_W \to 0 \quad \text{for} \quad \|\mathbf{du}_2^i\|_W \to 0,$$

therefore $A'(\cdot)(\mathbf{du}_1^i, d\varphi_1^{i-1})$ is differentiable from W into $W^\times$.

3. This follows analogously to the proof of the previous point 2.
4. The operator A_{l*} is linear in $(\mathbf{z}^i, \psi^{i+1})$, thus the differentiability result is clear, and the representation of the derivative follows analogously to point 2.

□

Let us conclude the analysis of the operator A, and its associated linearized and adjoint operators with the following continuity results:

Lemma 3.1.5. *There exist constants* $0 < c(\kappa, \varepsilon, \eta, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})$, $c(\kappa) \in \mathbb{R}$, *such that for all* $\mathbf{u}_{j,\mathbb{I}}, \tilde{\mathbf{u}}_{j,\mathbb{I}} \in W^M$, $j = 1, 2$ *and* $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M$, *it holds,*

$$\begin{aligned}
&\big\|A(\mathbf{u}_1^i, \varphi_1^{i-1}) - A(\mathbf{u}_2^i, \varphi_2^{i-1})\|_{W^\times} \\
&\quad \le c(\kappa, \varepsilon, \eta, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, && (3.36) \\
&\big\|A_l(\mathbf{u}_1^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}) - A_l(\mathbf{u}_2^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1})\big\|_{W^\times} \\
&\quad \le c(\kappa)\big(\|\mathbf{u}_1^i\|_W + \|\mathbf{u}_2^i\|_W\big)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \|\tilde{\mathbf{u}}^i\|_W && (3.37) \\
&\quad \le c(\kappa)\big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, && (3.38) \\
&\big\|A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i]\big\|_{W^\times} \\
&\quad \le c(\kappa)\|\tilde{\mathbf{u}}_1^i\|_W \|\tilde{\mathbf{u}}_2^i\|_W \|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W && (3.39) \\
&\quad \le c(\kappa)\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{2,\mathbb{I}}\|_{W^M}, && (3.40)
\end{aligned}$$

for all $i = 1, ..., M$. *In particular, the mapping* $\mathbf{u}^i \mapsto A'(\mathbf{u}^i)$ *is continuous from* W *into* $\mathcal{L}(W \times W_\varphi, W^\times)$, *and the mapping* $\mathbf{u}^i \mapsto A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}^i, \cdot]$ *is continuous from* W *into* $\mathcal{L}(W, W^\times)$.

Let further $\mathbf{z}_{\mathbb{I}} \in W^M$*, then*

$$\begin{aligned}
&\big\|A_{l*}(\mathbf{u}_1^i)(\mathbf{z}^i,\psi^{i+1}) - A_{l*}(\mathbf{u}_2^i)(\mathbf{z}^i,\psi^{i+1})\|_{W^\times} \\
&\quad \le c(\kappa)\big(\|\mathbf{u}_1^i\|_W + \|\mathbf{u}_2^i\|_W\big)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\|\mathbf{z}^i\|_W \\
&\quad \le c(\kappa)\big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}, \qquad (3.41)\\
&\big\|A_{b*}(\mathbf{u}_1^i,\tilde{\mathbf{u}}^i)\mathbf{z}^i - A_{b*}(\mathbf{u}_2^i,\tilde{\mathbf{u}}^i)\mathbf{z}^i\|_{W^\times} \\
&\quad \le c(\kappa)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\|\tilde{\mathbf{u}}^i\|_W\|\mathbf{z}^i\|_W \\
&\quad \le c(\kappa)\|\mathbf{u}_{1,\mathbb{I}} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}. \qquad (3.42)
\end{aligned}$$

Proof. Again, the proofs of (3.36)-(3.40) are given along the way of [86, Section 3.1 and 3.2], and are revisited in detail for the convenience of the reader. The proofs of (3.41) and (3.42) then again can be followed from the structure of A_{l*} and A_{b*}.

1. Recalling the definition of A from Definition 2.3.8, the difference is explicitly given in weak form, for all $(v^u, v^\varphi) = \mathbf{v} \in V$, by

$$\begin{aligned}
&\big\langle A(\mathbf{u}_1^i,\varphi_1^{i-1}) - A(\mathbf{u}_2^i,\varphi_2^{i-1}),\mathbf{v}\big\rangle \\
&\quad = \big(g(\varphi_1^i)\mathbb{C}e(u_1^i) - g(\varphi_2^i)\mathbb{C}e(u_2^i), e(v^u)\big) \qquad (3.43)\\
&\qquad + \varepsilon\big(\nabla\varphi_1^i - \nabla\varphi_2^i,\nabla v^\varphi\big) + \frac{1}{\varepsilon}\big(\varphi_1 - \varphi_2, v^\varphi\big) \qquad (3.44)\\
&\qquad + \eta\big(\varphi_1^i - \varphi_2^i, v^\varphi\big) - \eta\big(\varphi_1^{i-1} - \varphi_2^{i-1}, v^\varphi\big) \qquad (3.45)\\
&\qquad + (1-\kappa)\big(\varphi_1\mathbb{C}e(u_1^i) : e(u_1^i) - \varphi_2\mathbb{C}e(u_2^i) : e(u_2^i), v^\varphi\big). \qquad (3.46)
\end{aligned}$$

   Calculate term-wise in the respective W_u and W_φ norms. The same techniques as in the proof of Lemma 3.1.3 can be used: Starting with (3.43), adding and subtracting the term $g(\varphi_2^i)\mathbb{C}e(u_1^i)$, and then using the Lipschitz continuity of $g(\cdot)$, yields:

$$\begin{aligned}
&\big\|g(\varphi_1^i)\mathbb{C}e(u_1^i) - g(\varphi_2^i)\mathbb{C}e(u_2^i)\big\|_{L^p(\Omega;\mathbb{R}^2)} \\
&\quad = \|(g(\varphi_1^i) - g(\varphi_2^i))\mathbb{C}e(u_1^i) + g(\varphi_2^i)\mathbb{C}e(u_1^i - u_2^i)\big\|_{L^p(\Omega;\mathbb{R}^2)} \\
&\quad \le c(\kappa)\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)}\|u_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)} \\
&\qquad + c(\kappa)\|\varphi_2^i\|_{L^\infty(\Omega)}\|u_1^i - u_2^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)} \\
&\quad \le c(\kappa)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\|\mathbf{u}_1^i\|_W + c(\kappa)\|\mathbf{u}_2^i\|_W\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \\
&\quad \le c(\kappa)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + c(\kappa)\|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},
\end{aligned}$$

   where the same inequalities and ideas as in Lemma 3.1.3 were used. For the terms in (3.44) and (3.45) it also immediately follows

$$\begin{aligned}
\|\varepsilon(\nabla\varphi_1^i - \nabla\varphi_2^i)\|_{L^2(\Omega;\mathbb{R}^2)} &\le c(\varepsilon)\|\varphi_1^i - \varphi_2^i\|_{V_\varphi} \le c(\varepsilon)\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} \\
&\le c(\varepsilon)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \le c(\varepsilon)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \\
\Big\|\frac{1}{\varepsilon}(\varphi_1^i - \varphi_2^i)\Big\|_{L^q(\Omega)} &\le c(\varepsilon^{-1})\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)} \le c(\varepsilon^{-1})\|\varphi_1^i - \varphi_2^i\|_{W_\varphi}
\end{aligned}$$

$$
\begin{aligned}
&\leq c(\varepsilon^{-1})\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \leq c(\varepsilon^{-1})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},\\
\big\|\eta(\varphi_1^i - \varphi_2^i)\big\|_{L^q(\Omega)} &\leq c(\eta)\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)} \leq c(\eta)\|\varphi_1^i - \varphi_2^i\|_{W_\varphi}\\
&\leq c(\eta)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \leq c(\eta)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},\\
\big\|\eta(\varphi_1^{i-1} - \varphi_2^{i-1})\big\|_{L^q(\Omega)} &\leq c(\eta)\|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{L^\infty(\Omega)}\\
&\leq c(\eta)\|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\\
&\leq c(\eta)\|\mathbf{u}_1^{i-1} - \mathbf{u}_2^{i-1}\|_W\\
&\leq c(\eta)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}.
\end{aligned}
$$

Finally, for the term in (3.46), we add and subtract the terms $\varphi_2^i \mathbb{C}e(u_1^i) : e(u_1^i)$ and $\varphi_2^i \mathbb{C}e(u_2^i) : e(u_1^i)$, and then again as in Lemma 3.1.3, it holds

$$
\begin{aligned}
&\big\|(1-\kappa)\big(\varphi_1 \mathbb{C}e(u_1^i) : e(u_1^i) - \varphi_2^i \mathbb{C}e(u_2^i) : e(u_2^i)\big)\big\|_{L^q(\Omega)}\\
&\quad\leq c(\kappa)\big\|(\varphi_1^i - \varphi_2^i)\mathbb{C}e(u_1^i) : e(u_1^i) + \varphi_2^i \mathbb{C}e(u_1^i - u_2^i) : e(u_1^i)\\
&\qquad\qquad + \varphi_2^i \mathbb{C}e(u_2^i) : e(u_1^i - u_2^i)\big\|_{L^q(\Omega)}\\
&\quad\leq c(\kappa)\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)}\|u_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|u_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\\
&\qquad + c(\kappa)\|\varphi_2^i\|_{L^\infty(\Omega)}\|u_1^i - u_2^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|u_1^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\\
&\qquad + c(\kappa)\|\varphi_2^i\|_{L^\infty(\Omega)}\|u_2^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\|u_1^i - u_2^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\\
&\quad\leq c(\kappa)\|\varphi_1^i - \varphi_2^i\|_{W_\varphi}\|u_1^i\|_{W_u}\|u_1^i\|_{W_u} + c(\kappa)\|\varphi_2^i\|_{W_\varphi}\|u_1^i - u_2^i\|_{W_u}\|u_1^i\|_{W_u}\\
&\qquad + c(\kappa)\|\varphi_2^i\|_{W_\varphi}\|u_2^i\|_{W_u}\|u_1^i - u_2^i\|_{W_u}\\
&\quad\leq c(\kappa)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\|\mathbf{u}_1^i\|_W\|\mathbf{u}_1^i\|_W + c(\kappa)\|\mathbf{u}_2^i\|_W\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\|\mathbf{u}_1^i\|_W\\
&\qquad + c(\kappa)\|\mathbf{u}_2^i\|_W\|\mathbf{u}_2^i\|_W\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W\\
&\quad\leq c(\kappa)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1}\|_{W^M}\\
&\qquad + c(\kappa)\|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1}\|_{W^M}\\
&\qquad + c(\kappa)\|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}.
\end{aligned}
$$

Combining all estimates leads to the result in (3.36).

2. Recalling the definition of A_l from (3.1), the difference is explicitly given in weak form, for all $(v^u, v^\varphi) = \mathbf{v} \in V$, by

$$
\begin{aligned}
&\big\langle A_l(\mathbf{u}_1^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}) - A_l(\mathbf{u}_2^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}\big\rangle\\
&\quad= \big((g(\varphi_1^i) - g(\varphi_2^i))\mathbb{C}e(\tilde{u}^i), e(v^u)\big) &(3.47)\\
&\qquad + 2(1-\kappa)\big((\varphi_1^i \mathbb{C}e(u_1^i) - \varphi_2^i \mathbb{C}e(u_2^i)) : e(\tilde{u}^i), v^\varphi\big) &(3.48)\\
&\qquad + (1-\kappa)\big(\tilde{\varphi}^i(\mathbb{C}e(u_1^i) : e(u_1^i) - \mathbb{C}e(u_2^i) : e(u_2^i)), v^\varphi\big) &(3.49)\\
&\qquad + 2(1-\kappa)\big((\varphi_1^i \mathbb{C}e(u_1^i) - \varphi_2^i \mathbb{C}e(u_2^i))\tilde{\varphi}^i, e(v^u)\big). &(3.50)
\end{aligned}
$$

Calculate term-wise in the respective W_u and W_φ norms. The same techniques as in the proof of Lemma 3.1.3 can be used: Starting with

(3.47), exploiting the Lipschitz continuity of $g(\cdot)$ yields

$$\begin{aligned}\left\|\big(g(\varphi_1^i)-g(\varphi_2^i)\big)\mathbb{C}e(\tilde{u}^i)\right\|_{L^p(\Omega;\mathbb{R}^2)} &\leq c(\kappa)\|\varphi_1^i-\varphi_2^i\|_{L^\infty(\Omega)}\|\tilde{u}^i\|_{W^{1,p}(\Omega;\mathbb{R}^2)}\\ &\leq c(\kappa)\|\mathbf{u}_1^i-\mathbf{u}_2^i\|_W\|\tilde{\mathbf{u}}^i\|_W.\end{aligned}$$

For (3.48), adding and subtracting the term $\varphi_2^i\mathbb{C}e(u_1^i):e(\tilde{u}^i)$, again as in Lemma 3.1.3, it holds

$$\begin{aligned}&\left\|2(1-\kappa)\Big(\big(\varphi_1^i\mathbb{C}e(u_1^i)-\varphi_2^i\mathbb{C}e(u_2^i)\big):e(\tilde{u}^i)\Big)\right\|_{L^q(\Omega)}\\ &\quad\leq c(\kappa)\left\|\big((\varphi_1^i-\varphi_2^i)\mathbb{C}e(u_1^i)+\varphi_2^i\mathbb{C}e(u_1^i-u_2^i)\big):e(\tilde{u}^i)\right\|_{L^q(\Omega)}\\ &\quad\leq c(\kappa)\|\mathbf{u}_1^i-\mathbf{u}_2^i\|_W\|\mathbf{u}_1^i\|_W\|\tilde{\mathbf{u}}^i\|_W+c(\kappa)\|\mathbf{u}_2^i\|_W\|\mathbf{u}_1^i-\mathbf{u}_2^i\|_W\|\tilde{\mathbf{u}}^i\|_W.\end{aligned}$$

The terms in (3.49) and (3.50) are estimated in the same way, combining all estimates leads to the result stated in (3.37).

3. Recalling the definition of A_b from (3.3), the difference is given in weak form for all test functions $\mathbf{v}\in V$ by

$$\begin{aligned}&\big\langle A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i,\tilde{\mathbf{u}}_2^i]-A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i,\tilde{\mathbf{u}}_2^i],\mathbf{v}\big\rangle\\ &\quad=2(1-\kappa)\big(\tilde{\varphi}_2^i\mathbb{C}e(u_1^i-u_2^i)\tilde{\varphi}_1^i,e(v^u)\big)\\ &\qquad+2(1-\kappa)\big(\tilde{\varphi}_2^i\mathbb{C}e(\tilde{u}_1^i)(\varphi_1^i-\varphi_2^i),e(v^u)\big)\\ &\qquad+2(1-\kappa)\big(\tilde{\varphi}_2^i\mathbb{C}e(u_1^i-u_2^i):e(\tilde{u}_1^i),v^\varphi\big)\\ &\qquad+2(1-\kappa)\big((\varphi_1^i-\varphi_2^i)\mathbb{C}e(\tilde{u}_2^i)\tilde{\varphi}_1^i,e(v^u)\big)\\ &\qquad+2(1-\kappa)\big(\tilde{\varphi}_1^i\mathbb{C}e(\tilde{u}_2^i):e(u_1^i-u_2^i),v^\varphi\big)\\ &\qquad+2(1-\kappa)\big((\varphi_1^i-\varphi_2^i)\mathbb{C}e(\tilde{u}_2^i):e(\tilde{u}_1^i),v^\varphi\big).\end{aligned}$$

The remainder of the proof works in the same way as in step 1, estimating the terms in the $W^{1,p}(\Omega;\mathbb{R}^2)$-norm and the $L^q(\Omega)$-norm in the same way as in the proof of Lemma 3.1.3. These estimations closely follow also e.g. [86, Proof of Lemma 3.9].

4. The continuity of the mapping $\mathbf{u}^i\mapsto A_l(\mathbf{u}^i)$ follows in the following way: Let $\mathbf{u}_1^i,\mathbf{u}_2^i\in W$, then

$$\begin{aligned}&\big\|A_l(\mathbf{u}_1^i)-A_l(\mathbf{u}_2^i)\big\|_{\mathcal{L}(W\times W_\varphi,W^\times)}\\ &\quad=\sup_{(\|\tilde{\mathbf{u}}\|_W+\|\tilde{\varphi}^{i-1}\|_{W_\varphi})=1}\big\|A_l(\mathbf{u}_1^i)(\tilde{\mathbf{u}}^i,\tilde{\varphi}^{i-1})-A_l(\mathbf{u}_2^i)(\tilde{\mathbf{u}}^i,\tilde{\varphi}^{i-1})\big\|_{W^\times}\\ &\quad\leq\sup_{(\|\tilde{\mathbf{u}}\|_W+\|\tilde{\varphi}^{i-1}\|_{W_\varphi})=1}c(\kappa)\big(\|\mathbf{u}_1^i\|_W+\|\mathbf{u}_2^i\|_W\big)\|\mathbf{u}_1^i-\mathbf{u}_2^i\|_W\|\tilde{\mathbf{u}}^i\|_W\\ &\quad\leq 2c(\kappa)\max\big(\|\mathbf{u}_1^i\|_W,\|\mathbf{u}_2^i\|_W\big)\|\mathbf{u}_1^i-\mathbf{u}_2^i\|_W,\end{aligned}$$

where (3.37) is used. The constant $c(\kappa)\max(\|\mathbf{u}_1^i\|_W, \|\mathbf{u}_2^i\|_W)$ is bounded for $\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \to 0$, since $\mathbf{u}_2^i \in W$ and $\|\mathbf{u}_1^i\| = \|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W + \|\mathbf{u}_2^i\|_W$ by the triangle inequality. This now immediately means that

$$\|A_l(\mathbf{u}_1^i) - A_l(\mathbf{u}_2^i)\|_{\mathcal{L}(W\times L_\varphi, W^\times)} \to 0 \quad \text{for} \quad \|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \to 0,$$

which proves the desired result.

5. The continuity of the mapping $\mathbf{u}^i \mapsto A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}^i, \cdot]$ follows in the following way: Let $\mathbf{u}_1^i, \mathbf{u}_2^i, \tilde{\mathbf{u}}_1^i \in W$, then

$$\begin{aligned}
&\big\|A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \cdot] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i, \cdot]\big\|_{\mathcal{L}(W,W^\times)} \\
&\quad = \sup_{\|\tilde{\mathbf{u}}_2^i\|_W=1} \big\|A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i]\big\|_{W^\times} \\
&\quad \le \sup_{\|\tilde{\mathbf{u}}_2^i\|_W=1} c(\kappa)\|\tilde{\mathbf{u}}_1^i\|_W \|\tilde{\mathbf{u}}_2^i\|_W \|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \\
&\quad \le c(\kappa)\|\tilde{\mathbf{u}}_1^i\|_W \|\mathbf{u}_1^i - \mathbf{u}_2^1\|_W,
\end{aligned}$$

where (3.39) is used. The constant $c(\kappa)\|\tilde{\mathbf{u}}_1^i\|_W$ is bounded by assumption. Thus

$$\begin{aligned}
&\|A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \cdot] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i, \cdot]\|_{\mathcal{L}(W,W^\times)} \to 0 \\
&\qquad \text{for} \qquad \|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \to 0,
\end{aligned}$$

which proves the desired result.

6. Recalling the definition of A_{l*} from (3.5), the difference is explicitly given in weak form, for all $(v^u, v^\varphi) = \mathbf{v} \in V$, by

$$\begin{aligned}
&\big\langle A_{l*}(\mathbf{u}_1^i)(\mathbf{z}^i, \psi^{i+1}) - A_{l*}(\mathbf{u}_2^i)(\mathbf{z}^i, \psi^{i+1}), \mathbf{v}\big\rangle \\
&\quad = \big((g(\varphi_1^i) - g(\varphi_2^i))\mathbb{C}e(z^i), e(v^u)\big) \\
&\qquad + 2(1-\kappa)\big((\varphi_1^i \mathbb{C}e(u_1^i) - \varphi_2^i \mathbb{C}e(u_2^i)) \colon e(z^i), v^\varphi\big) \\
&\qquad + (1-\kappa)\big(\psi^i(\mathbb{C}e(u_1^i) : e(u_1^i) - \mathbb{C}e(u_2^i) \colon e(u_2^i)), v^\varphi\big) \\
&\qquad + 2(1-\kappa)\big((\varphi_1^i \mathbb{C}e(u_1^i) - \varphi_2^i \mathbb{C}e(u_2^i))\psi^i, e(v^u)\big),
\end{aligned}$$

but these are the same terms as in step 2. The estimations in the $W^{1,p}(\Omega;\mathbb{R}^2)$ and $L^q(\Omega)$ norm work completely analogously.

7. Recalling the definition of A_{b*} from (3.10), the difference is given in weak form for all test functions $\mathbf{v} \in V$ by

$$\begin{aligned}
&\big\langle A_{b*}(\mathbf{u}_1^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i - A_{b*}(\mathbf{u}_2^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i, \mathbf{v}\big\rangle \\
&\quad = 2(1-\kappa)((\varphi_1^i - \varphi_2^i)\mathbb{C}e(\tilde{u}^i) \colon e(z^i), v^\varphi) \\
&\qquad + 2(1-\kappa)(\tilde{\varphi}^i \mathbb{C}e(u_1^i - u_2^i) \colon e(z^i), v^\varphi) \\
&\qquad + 2(1-\kappa)((\varphi_1^i - \varphi_2^i)\mathbb{C}e(z^i)\tilde{\varphi}^i, e(v^u))
\end{aligned}$$

$$
\begin{aligned}
&+ 2(1-\kappa)(\psi^i \mathbb{C} e(u_1^i - u_2^i) : e(\tilde{u}^i), v^\varphi) \\
&+ 2(1-\kappa)((\varphi_1^i - \varphi_2^i)\mathbb{C} e(\tilde{u}^i)\psi^i, e(v^u)) \\
&+ 2(1-\kappa)(\tilde{\varphi}^i \mathbb{C} e(u_1^i - u_2^i)\psi^i, e(v^u)).
\end{aligned}
$$

The remainder of the proof works in the same way as in step 2, and hence as in step 1, estimating the terms in the $W^{1,p}(\Omega;\mathbb{R}^2)$-norm and the $L^q(\Omega)$-norm in the same way as in the proof of Lemma 3.1.3.

□

Next, let us look at the penalization operator R. We establish norm bounds, differentiability and continuity results as above for the operators A, A_l etc. Note that due to the nonlinear structure of R, the coupling of functions of the previous, current and succeeding time steps $i-1$, i and $i+1$ is now more involved: While we can estimate them analogously to the functions of the time step i in the operators R_l and R_b, some additional steps are necessary for the analysis of the desired properties, in particular for the differentiability and Lipschitz results, in the operators R_{l*} and R_{b*}. We start again with some norm bounds:

Lemma 3.1.6. *There exist constants* $0 < c(\gamma, \|\varphi_{\mathbb{I}}\|_{W_\varphi^M})$*,* $c(\gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})\|\mathbf{u}_{\mathbb{I}}\|_{W^M}$*,* $c(\gamma) \in \mathbb{R}$*, such that for all* $\varphi_{\mathbb{I}}, \tilde{\varphi}_{\mathbb{I}}, \tilde{\varphi}_{j,\mathbb{I}} \in W_\varphi^M$*, where* $j = 1, 2$*, it holds*

$$
\begin{aligned}
&\|R(\varphi^i, \varphi^{i-1};\gamma)\|_{L^q(\Omega)} \\
&\quad \le c(\gamma, \|\varphi_{\mathbb{I}}\|_{W_\varphi^M})\|\varphi_{\mathbb{I}}\|_{W_\varphi^M} \le c(\gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})\|\mathbf{u}_{\mathbb{I}}\|_{W^M}, \qquad (3.51)\\
&\|R_l(\varphi^i, \varphi^{i-1};\gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1})\|_{L^q(\Omega)} \\
&\quad \le c(\gamma, \|\varphi_{\mathbb{I}}\|_{W_\varphi^M})\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \le c(\gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \qquad (3.52)\\
&\|R_b(\varphi^i, \varphi^{i-1};\gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})]\|_{L^q(\Omega)} \\
&\quad \le c(\gamma)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{1,\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{2,\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \le c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}. \qquad (3.53)
\end{aligned}
$$

It further holds, for all $\psi_{\mathbb{I}} \in W_\varphi^M$*,*

$$
\begin{aligned}
&\|R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1};\gamma)(\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
&\quad \le c(\gamma)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M}\|\psi_{\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \le c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}, \qquad (3.54)\\
&\left|\left\langle R_b(\varphi^i, \varphi^{i-1};\gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i\right\rangle\right| \\
&\quad \le c(\gamma)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{1,\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{2,\mathbb{I}}\|_{W_\varphi^M}\|\psi_{\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \le c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}. \qquad (3.55)
\end{aligned}
$$

Proof. Again, the bounds are established analogously the estimations conducted in e.g. [132, Lemma 5.1].

1. We recall the definition of R from Definition 2.3.8. Estimating in the $L^q(\Omega)$-norm, we obtain using the continuity of $[(\cdot)^+]^3$ and the Sobolev-embedding $W_\varphi \hookrightarrow L^\infty(\Omega) \hookrightarrow L^q(\Omega)$, for $q = \frac{p}{2} > 1$, but close to one,

$$\begin{aligned}
&\|\gamma[(\varphi^i - \varphi^{i-1})^+]^3\|_{L^q(\Omega)} \\
&\quad \leq \|\gamma[(\varphi^i - \varphi^{i-1})^+]^3\|_{L^\infty(\Omega)} \\
&\quad \leq c\big(\gamma, \|\varphi^i\|_{L^\infty(\Omega)}, \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\varphi^i\|_{L^\infty(\Omega)} + \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\quad \leq c\big(\gamma, \|\varphi^i\|_{W_\varphi}, \|\varphi^{i-1}\|_{W_\varphi}\big)\big(\|\varphi^i\|_{W_\varphi} + \|\varphi^{i-1}\|_{W_\varphi}\big) \\
&\quad \leq c(\gamma, \|\varphi_{\mathbb{I}}\|_{W_\varphi^M})\|\varphi_{\mathbb{I}}\|_{W_\varphi^M} \leq c(\gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M})\|\mathbf{u}_{\mathbb{I}}\|_{W^M}.
\end{aligned}$$

2. Recall the definition of R_l from (3.2). Analogously to above, now using the continuity of $[(\cdot)^+]^2$, it holds

$$\begin{aligned}
&\|3\gamma[(\varphi^i - \varphi^{i-1})^+]^2(\tilde{\varphi}^i - \tilde{\varphi}^{i-1})\|_{L^q(\Omega)} \\
&\quad \leq c\big(\gamma, \|\varphi^i\|_{L^\infty(\Omega)}, \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\varphi^i\|_{L^\infty(\Omega)} + \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\qquad\quad \cdot \big(\|\tilde{\varphi}^i\|_{L^\infty(\Omega)} + \|\tilde{\varphi}^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\quad \leq c\big(\gamma, \|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\big)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \leq c\big(\gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}.
\end{aligned}$$

3. Recall the definition of R_b from (3.4). Again, analogously to the first point, we estimate

$$\begin{aligned}
&\|6\gamma[(\varphi^i - \varphi^{i-1})^+](\tilde{\varphi}_1^i - \tilde{\varphi}_1^{i-1})(\tilde{\varphi}_2^i - \tilde{\varphi}_2^{i-1})\|_{L^q(\Omega)} \\
&\quad \leq c(\gamma)\big(\|\varphi^i\|_{L^\infty(\Omega)} + \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\tilde{\varphi}_1^i\|_{L^\infty(\Omega)} + \|\tilde{\varphi}_1^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\qquad \cdot \big(\|\tilde{\varphi}_2^i\|_{L^\infty(\Omega)} + \|\tilde{\varphi}_2^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\quad \leq c(\gamma)\big(\|\varphi^i\|_{W_\varphi} + \|\varphi^{i-1}\|_{W_\varphi}\big)\big(\|\tilde{\varphi}_1^i\|_{W_\varphi} + \|\tilde{\varphi}_1^{i-1}\|_{W_\varphi}\big) \\
&\qquad \cdot \big(\|\tilde{\varphi}_2^i\|_{W_\varphi} + \|\tilde{\varphi}_2^{i-1}\|_{W_\varphi}\big) \\
&\quad \leq c(\gamma)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{1,\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{2,\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \leq c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}.
\end{aligned}$$

4. Recall the definition of R_{b*} from (3.12), we estimate

$$\begin{aligned}
&\|6\gamma([(\varphi^i - \varphi^{i-1})^+](\tilde{\varphi}^i - \tilde{\varphi}^{i-1})\psi^i - [(\varphi^{i+1} - \varphi^i)^+](\tilde{\varphi}^{i+1} - \tilde{\varphi}^i)\psi^{i+1})\|_{L^q(\Omega)} \\
&\quad \leq c(\gamma)\big(\|\varphi^i\|_{L^\infty(\Omega)} + \|\varphi^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\qquad \cdot \big(\|\tilde{\varphi}^i\|_{L^\infty(\Omega)} + \|\tilde{\varphi}^{i-1}\|_{L^\infty(\Omega)}\big)\|\psi^i\|_{L^\infty(\Omega)} \\
&\qquad + c(\gamma)\big(\|\varphi^{i+1}\|_{L^\infty(\Omega)} + \|\varphi^i\|_{L^\infty(\Omega)}\big) \\
&\qquad \cdot \big(\|\tilde{\varphi}^{i+1}\|_{L^\infty(\Omega)} + \|\tilde{\varphi}^i\|_{L^\infty(\Omega)}\big)\|\psi^{i+1}\|_{L^\infty(\Omega)} \\
&\quad \leq c(\gamma)\big(\|\varphi^i\|_{W_\varphi} + \|\varphi^{i-1}\|_{W_\varphi}\big)\big(\|\tilde{\varphi}^i\|_{W_\varphi} + \|\tilde{\varphi}^{i-1}\|_{W_\varphi}\big)\|\psi^i\|_{W_\varphi} \\
&\qquad + c(\gamma)\big(\|\varphi^{i+1}\|_{W_\varphi} + \|\varphi^i\|_{W_\varphi}\big)\big(\|\tilde{\varphi}^{i+1}\|_{W_\varphi} + \|\tilde{\varphi}^i\|_{W_\varphi}\big)\|\psi^{i+1}\|_{W_\varphi}
\end{aligned}$$

$$\leq c(\gamma)\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M}\|\psi_{\mathbb{I}}\|_{W_\varphi^M}$$
$$\leq c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}.$$

5. The estimate (3.55) follows similarly to the third point. It immediately follows

$$\begin{aligned}
&\Big(6\gamma[(\varphi^i-\varphi^{i-1})^+](\tilde{\varphi}_1^i-\tilde{\varphi}_1^{i-1})(\tilde{\varphi}_2^i-\tilde{\varphi}_2^{i-1}),\psi^i\Big)\\
&\quad\leq c(\gamma)\big(\|\varphi^i\|_{L^\infty(\Omega)}+\|\varphi^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\tilde{\varphi}_1^i\|_{L^\infty(\Omega)}+\|\tilde{\varphi}_1^{i-1}\|_{L^\infty(\Omega)}\big)\\
&\qquad\cdot\big(\|\tilde{\varphi}_2^i\|_{L^\infty(\Omega)}+\|\tilde{\varphi}_2^{i-1}\|_{L^\infty(\Omega)}\big)\|\psi^i\|_{L^\infty(\Omega)}\\
&\quad\leq c(\gamma)\big(\|\varphi^i\|_{W_\varphi}+\|\varphi^{i-1}\|_{W_\varphi}\big)\big(\|\tilde{\varphi}_1^i\|_{W_\varphi}+\|\tilde{\varphi}_1^{i-1}\|_{W_\varphi}\big)\\
&\qquad\cdot\big(\|\tilde{\varphi}_2^i\|_{W_\varphi}+\|\tilde{\varphi}_2^{i-1}\|_{W_\varphi}\big)\|\psi^i\|_{W_\varphi}\\
&\quad\leq c_\gamma\|\varphi_{\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{1,\mathbb{I}}\|_{W_\varphi^M}\|\tilde{\varphi}_{2,\mathbb{I}}\|_{W_\varphi^M}\|\psi_{\mathbb{I}}\|_{W_\varphi^M}\\
&\quad\leq c_\gamma\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{1,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M},
\end{aligned}$$

which concludes the proof.

□

Similarly to Lemma 3.1.4, we can then turn towards Fréchet differentiability. For the operators R, R_l and R_{l*}, we establish the following result in improved Banach spaces:

Lemma 3.1.7.

1. *The operator R from Definition 2.3.8 is Fréchet differentiable from $W_\varphi \times W_\varphi$ into L^q, i.e. it holds*

$$\begin{aligned}
&R(\varphi^i+d\varphi^i,\varphi^{i-1}+d\varphi^{i-1};\gamma)-R(\varphi^i,\varphi^{i-1};\gamma)\\
&\quad=R_l(\varphi^i,\varphi^{i-1};\gamma)(d\varphi^i,d\varphi^{i-1})+o(\|d\varphi^i\|_{W_\varphi}+\|d\varphi^{i-1}\|_{W_\varphi}).
\end{aligned}$$

2. *Let $d\varphi_1^i, d\varphi_1^{i-1} \in W_\varphi$, then the operator $R_l(\cdot^i, \cdot^{i-1};\gamma)(d\varphi_1^i, d\varphi_1^{i-1})$ is Fréchet differentiable from $W_\varphi \times W_\varphi$ into L^q, i.e. it holds*

$$\begin{aligned}
&R_l(\varphi^i+d\varphi_2^i,\varphi^{i-1}+d\varphi_2^{i-1};\gamma)(d\varphi_1^i,d\varphi_1^{i-1})\\
&\qquad-R_l(\varphi^i,\varphi^{i-1};\gamma)(d\varphi_1^i,d\varphi_1^{i-1})\\
&\quad=R_b(\varphi^i,\varphi^{i-1};\gamma)[(d\varphi_1^i,d\varphi_1^{i-1}),(d\varphi_2^i,d\varphi_2^{i-1})]\\
&\qquad+o(\|d\varphi_2^i\|_{W_\varphi}+\|d\varphi_2^{i-1}\|_{W_\varphi}).
\end{aligned}$$

In combination with 1, this means that the operator R is twice Fréchet differentiable from $W_\varphi \times W_\varphi$ into L^q.

3. *Let $\psi^i, \psi^{i+1} \in W_\varphi$, then the operator $R_{l*}(\cdot^i, \cdot^{i-1}, \cdot^{i+1};\gamma)(\psi^i, \psi^{i+1})$ from* (3.6) *is Fréchet differentiable from $W_\varphi \times W_\varphi \times W_\varphi$ into $L^q(\Omega)$, i.e. it holds*

$$R_{l*}(\varphi^i+d\varphi^i,\varphi^{i-1}+d\varphi^{i-1},\varphi^{i+1}+d\varphi^{i+1};\gamma)(\psi^i,\psi^{i+1})$$

$$
\begin{aligned}
&\quad - R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i-1}) \\
&= R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\quad + o(\|d\varphi^i\|_{W_\varphi} + \|d\varphi^{i-1}\|_{W_\varphi} + \|d\varphi^{i+1}\|_{W_\varphi}).
\end{aligned}
$$

4. *Let $\varphi^i, \varphi^{i-1}, \varphi^{i+1} \in W_\varphi$, then the operator $R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\cdot^i, \cdot^{i+1})$ from* (3.6) *is Fréchet differentiable from $W_\varphi \times W_\varphi$ into $L^q(\Omega)$, i.e. it holds*

$$
\begin{aligned}
&R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i + d\psi^i, \psi^{i+1} + d\psi^{i+1}) \\
&\qquad - R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\quad = R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(d\psi^i, d\psi^{i+1}) + o(\|d\psi^i\|_{W_\varphi} + \|d\psi^{i+1}\|_{W_\varphi}).
\end{aligned}
$$

Proof. Again as in Lemma 3.1.4, the proofs of 1 and 2 are given along the way of [86, Proof of Proposition 3.3], and are revisited in detail for the convenience of the reader. In the proof of 3 the functions from the previous and succeeding time step $i-1$ and $i+1$ now occur, which we have to be taken care of. The proof of 4 again immediately follows from the structure of R_{l*}.

1. Let $\varphi^i, \varphi^{i-1}, d\varphi^i, d\varphi^{i-1} \in W_\varphi$ and $v^\varphi \in V_\varphi$. By Fréchet differentiability of the Nemytskii operator $[(\cdot)^+]^3$, it holds

$$
\begin{aligned}
&\big\langle R(\varphi^i + d\varphi^i, \varphi^i + d\varphi^{i-1}; \gamma), v^\varphi \big\rangle \\
&\quad = \gamma\big(\big[(\varphi^i + d\varphi^i - (\varphi^{i-1} + d\varphi^{i-1}))^+\big]^3, v^\varphi\big) \\
&\quad = \gamma\big(\big[(\varphi^i - \varphi^{i-1})^+\big]^3, v^\varphi\big) + 3\gamma\big(\big[(\varphi^i - \varphi^{i-1})^+\big]^2(d\varphi^i - d\varphi^{i-1}), v^\varphi\big) \\
&\qquad + \big\langle rem_R(\varphi^i, \varphi^{i-1}, d\varphi^i, d\varphi^{i-1}), v^\varphi \big\rangle \\
&\quad = \big\langle R(\varphi^i, \varphi^{i-1}; \gamma), v^\varphi \big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(d\varphi^i, d\varphi^{i-1}), v^\varphi \big\rangle \\
&\qquad + \big\langle rem_R(\varphi^i, \varphi^{i-1}, d\varphi^i, d\varphi^{i-1}), v^\varphi \big\rangle,
\end{aligned}
$$

where $\|rem_R(\varphi^i, \varphi^{i-1}, d\varphi^i, d\varphi^{i-1})\|_{L^q(\Omega)} / \ \big(\|d\varphi^i\|_{W_\varphi} + \|d\varphi^{i-1}\|_{W_\varphi}\big) \to 0$ for $\big(\|d\varphi^i\|_{W_\varphi} + \|d\varphi^{i-1}\|_{W_\varphi}\big) \to 0$. The well-definedness of all terms is clear by the given regularities, since $\varphi^i, \varphi^{i-1}, d\varphi^i, d\varphi^{i-1} \in W_\varphi \hookrightarrow L^\infty(\Omega)$.

2. Let $\varphi^i, \varphi^{i-1}, d\varphi^i_j, d\varphi^{i-1}_j \in W_\varphi$, for $j = 1, 2$, and $v^\varphi \in V_\varphi$. Again, by Fréchet differentiability of the Nemytskii operator $[(\cdot)^+]^2$, it holds

$$
\begin{aligned}
&\big\langle R_l(\varphi^i + d\varphi^i_2, \varphi^{i-1} + d\varphi^{i-1}_2; \gamma)(d\varphi^i_1, d\varphi^{i-1}_1), v^\varphi \big\rangle \\
&\quad = 3\gamma\big(\big[(\varphi^i + d\varphi^i_2 - (\varphi^{i-1} + d\varphi^{i-1}_2))^+\big]^2(d\varphi^i_1 - d\varphi^{i-1}_1), v^\varphi\big) \\
&\quad = 3\gamma\big(\big[(\varphi^i - \varphi^{i-1})^+\big]^2(d\varphi^i_1 - d\varphi^{i-1}_1), v^\varphi\big) \\
&\qquad + 6\gamma\big(\big[(\varphi^i - \varphi^{i-1})^+\big](d\varphi^i_2 - d\varphi^{i-1}_2)(d\varphi^i_1 - d\varphi^{i-1}_1), v^\varphi\big) \\
&\qquad + \big\langle \mathrm{rem}_{R_l}(\varphi^i, \varphi^{i-1}, d\varphi^i_1, d\varphi^{i-1}_1, d\varphi^i_2, d\varphi^{i-1}_2), v^\varphi \big\rangle \\
&\quad = \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(d\varphi^i_1, d\varphi^{i-1}_1), v^\varphi \big\rangle \\
&\qquad + \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(d\varphi^i_1, d\varphi^{i-1}_1), (d\varphi^i_2, d\varphi^{i-1}_2)], v^\varphi \big\rangle
\end{aligned}
$$

$$+ \left\langle \mathrm{rem}_{R_l}(\varphi^i, \varphi^{i-1}, d\varphi_1^i, d\varphi_1^{i-1}, d\varphi_2^i, d\varphi_2^{i-1}), v^\varphi \right\rangle,$$

where again it holds $\|\mathrm{rem}_{R_l}(\varphi^i, \varphi^{i-1}, d\varphi_1^i, d\varphi_1^{i-1}, d\varphi_2^i, d\varphi_2^{i-1})\|_{L^q(\Omega)} / \big(\|d\varphi_2^i\|_{W_\varphi} + \|d\varphi_2^{i-1}\|_{W_\varphi}\big) \to 0$ for $\big(\|d\varphi_2^i\|_{W_\varphi} + \|d\varphi_2^{i-1}\|_{W_\varphi}\big) \to 0$. The assumed regularities again immediately ensure well-definedness for all involved terms.

3. Let $\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i-1} \in W_\varphi$, and $v^\varphi \in V_\varphi$. By Fréchet differentiability of the Nemytskii operator $[(\cdot)^+]^2$, it holds

$$\begin{aligned}
&\left\langle R_{l*}(\varphi^i + d\varphi^i, \varphi^{i-1} + d\varphi^{i-1}, \varphi^{i+1} + d\varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^\varphi \right\rangle \\
&\quad = 3\gamma\big([(\varphi^i + d\varphi^i) - (\varphi^{i-1} + d\varphi^{i-1})^+]^2 \psi^i \\
&\qquad\qquad - [(\varphi^{i+1} + d\varphi^{i+1} - (\varphi^i + d\varphi^i))^+]^2 \psi^{i+1}, v^\varphi\big) \\
&\quad = 3\gamma\big([(\varphi^i - \varphi^{i-1})^+]^2 \psi^i - [(\varphi^{i+1} - \varphi^i)^+]^2 \psi^{i+1}, v^\varphi\big) \\
&\qquad + 6\gamma\big([(\varphi^i - \varphi^{i-1})^+](d\varphi^i - d\varphi^{i-1})\psi^i \\
&\qquad\qquad - [(\varphi^{i+1} - \varphi^i)](d\varphi^{i+1} - d\varphi^i)\psi^{i+1}, v^\varphi\big) \\
&\qquad + \left\langle rem_{R_{l*}}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i+1}), v^\varphi \right\rangle \\
&\quad = \left\langle R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1} l\gamma)(\psi^i, \psi^{i+1}), v^\varphi \right\rangle \\
&\qquad + \left\langle R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^\varphi \right\rangle \\
&\qquad + \left\langle rem_{R_{l*}}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i+1}), v^\varphi \right\rangle,
\end{aligned}$$

where again it holds $\|rem_{R_{l*}}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, d\varphi^i, d\varphi^{i-1}, d\varphi^{i+1})\|_{L^q(\Omega)} / \big(\|d\varphi^i\|_{W_\varphi} + \|d\varphi^{i-1}\|_{W_\varphi} + \|d\varphi^{i+1}\|_{W_\varphi}\big) \to 0$ for $\big(\|d\varphi^i\|_{W_\varphi} + \|d\varphi^{i-1}\|_{W_\varphi} + \|d\varphi^{i+1}\|_{W_\varphi}\big) \to 0$. The assumed regularities again immediately ensure well-definedness of all involved terms.

4. The operator R_{l*} is linear in (ψ^i, ψ^{i+1}), thus the differentiability result is clear, and the representation of the derivative follows analogously to point 2.

□

Finally, analogously to Lemma 3.1.5, we show the following continuity results:

Lemma 3.1.8. *There exist constants* $0 < c(\gamma, \|\varphi_{\mathbb{I},1}\|_{W_\varphi^M}, \|\varphi_{\mathbb{I},2}\|_{W_\varphi^M})$, $c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})$, $c(\gamma) \in \mathbb{R}$, *such that for all* $\mathbf{u}_{j,\mathbb{I}}, \tilde{\mathbf{u}}_{j,\mathbb{I}} \in W^M$, $j = 1, 2$, $\tilde{\mathbf{u}}_{\mathbb{I}}$, *and* $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M$, *it holds,*

$$\begin{aligned}
&\big\|R(\varphi_1^i, \varphi_i^{i-1}; \gamma) - R(\varphi_2^i, \varphi_2^{i-1}; \gamma)\|_{L^q(\Omega)} \\
&\quad \le c(\gamma, \|\varphi_{\mathbb{I},1}\|_{W_\varphi^M}, \|\varphi_{\mathbb{I},2}\|_{W_\varphi^M})\|\varphi_{\mathbb{I},1} - \varphi_{\mathbb{I},2}\|_{W_\varphi^M} \\
&\quad \le c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \qquad (3.56) \\
&\big\|R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1})\big\|_{L^q(\Omega)} \\
&\quad \le c(\gamma, \|\varphi_{\mathbb{I},1}\|_{W_\varphi^M}, \|\varphi_{\mathbb{I},2}\|_{W_\varphi^M})\|\varphi_{\mathbb{I},1} - \varphi_{\mathbb{I},2}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M}
\end{aligned}$$

$$\leq c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \tag{3.57}$$

$$\begin{aligned}
&\big\|\big[R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big][(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})]\|_{L^q(\Omega)} \\
&\quad \leq c(\gamma)\|\varphi_{\mathbb{I},1} - \varphi_{\mathbb{I},2}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I},1}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I},2}\|_{W_\varphi^M} \\
&\quad \leq c(\gamma)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M},
\end{aligned} \tag{3.58}$$

for all $i = 1, ..., M$. In particular, the mapping $(\varphi^i, \varphi^{i-1}) \mapsto R_l(\varphi^i, \varphi^{i-1}; \gamma)$ is continuous from $W_\varphi \times W_\varphi$ into $\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))$, and the mapping $(\varphi^i, \varphi^{i-1}) \mapsto R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), \cdot]$ is continuous from $W_\varphi \times W_\varphi$ into $\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))$.

Let further $\mathbf{z}_{\mathbb{I}} \in W^M$, then

$$\begin{aligned}
&\big\|R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) - R_{l*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \gamma)(\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
&\quad \leq c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M},
\end{aligned} \tag{3.59}$$

$$\begin{aligned}
&\big\|[R_{b*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)\big](\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
&\quad \leq \|\varphi_{\mathbb{I},1} - \varphi_{\mathbb{I},2}\|_{W_\varphi^M}\|\tilde{\varphi}_{\mathbb{I}}\|_{W_\varphi^M}\|\psi_{\mathbb{I}}\|_{W_\varphi^M} \\
&\quad \leq c(\gamma)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}.
\end{aligned} \tag{3.60}$$

Proof. Again, the proofs of (3.56)-(3.58) are given along the way of [86, Section 3.1 and 3.2]. The only difference are the additional occurring functions from the previous time step $i-1$. We again revisit this for the convenience of the reader. In the proofs of (3.59) and (3.60), due to the structure of R_{l*}, a coupling in the time steps i, $i-1$ and $i+1$ occurs.

1. Recalling the weak definition of R from Definition 2.3.8, the difference is explicitly given in weak form, for all $v^\varphi \in V$, by

$$\begin{aligned}
&\big\langle R(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R(\varphi_2^i, \varphi_2^{i-1}; \gamma), v^\varphi \big\rangle \\
&\quad = \big(\gamma\big([(\varphi_1^i - \varphi_1^{i-1})^+]^3 - [(\varphi_2^i - \varphi_2^{i-1})^+]^3\big), v^\varphi\big).
\end{aligned}$$

   Calculating the L^q-norm, and exploiting the Lipschitz continuity of $[(\cdot)^+]^3$, analogously to the techniques in Lemma 3.1.6, it holds

$$\begin{aligned}
&\big\|\gamma\big([(\varphi_1^i - \varphi_1^{i-1})^+]^3 - [(\varphi_2^i - \varphi_2^{i-1})^+]^3\big)\big\|_{L^q(\Omega)} \\
&\quad \leq c(\gamma, \|\varphi_1^i\|_{L^\infty(\Omega)}, \|\varphi_1^{i-1}\|_{L^\infty(\Omega)}, \|\varphi_2^i\|_{L^\infty(\Omega)}, \|\varphi_2^{i-1}\|_{L^\infty(\Omega)}) \\
&\qquad \cdot \big(\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\quad \leq c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi}) \\
&\qquad \cdot \big(\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\big) \\
&\quad \leq c(\gamma, \|\varphi_{\mathbb{I},1}\|_{W_\varphi^M}, \|\varphi_{\mathbb{I},2}\|_{W_\varphi^M})\|\varphi_{\mathbb{I},1} - \varphi_{\mathbb{I},2}\|_{W_\varphi^M} \\
&\quad \leq c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}.
\end{aligned}$$

2. Recalling the weak definition of R_l from (3.2), the difference is explicitly given in weak form, for all $v^\varphi \in V_\varphi$, by

$$\begin{aligned}&\big\langle R_l(\varphi_1^i,\varphi_1^{i-1};\gamma)(\tilde\varphi^i,\tilde\varphi^{i-1}) - R_l(\varphi_2^i,\varphi_2^{i-1};\gamma)(\tilde\varphi^i,\tilde\varphi^{i-1}), v^\varphi\big\rangle\\ &\quad = \big(3\gamma\big([(\varphi_1^i-\varphi_1^{i-1})^+]^2 - [(\varphi_2^i-\varphi_2^{i-1})^+]^2\big)(\tilde\varphi^i-\tilde\varphi^{i-1}), v^\varphi\big).\end{aligned}$$

Thus, calculating in the L^q-norm, exploiting the Lipschitz continuity of $[(\cdot)^+]^2$, the triangle inequality and the Sobolev-embedding $W_\varphi \hookrightarrow L^\infty(\Omega)$, it holds

$$\begin{aligned}&\Big\|3\gamma\big([(\varphi_1^i-\varphi_1^{i-1})^+]^2 - [(\varphi_2^i-\varphi_2^{i-1})^+]^2\big)(\tilde\varphi^i-\tilde\varphi^{i-1})\Big\|_{L^q(\Omega)}\\ &\le c(\gamma, \|\varphi_1^i\|_{L^\infty(\Omega)}, \|\varphi_1^{i-1}\|_{L^\infty(\Omega)}, \|\varphi_2^i\|_{L^\infty(\Omega)}, \|\varphi_2^{i-1}\|_{L^\infty(\Omega)})\\ &\quad\cdot\big(\|\varphi_1^i-\varphi_2^i\|_{L^\infty(\Omega)} + \|\varphi_1^{i-1}-\varphi_2^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\tilde\varphi^i\|_{L^\infty(\Omega)} + \|\tilde\varphi^{i-1}\|_{L^\infty(\Omega)}\big)\\ &\le c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi})\\ &\quad\cdot\big(\|\varphi_1^i-\varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1}-\varphi_2^{i-1}\|_{W_\varphi}\big)\big(\|\tilde\varphi^i\|_{W_\varphi} + \|\tilde\varphi^{i-1}\|_{W_\varphi}\big) \qquad (3.61)\\ &\le c(\gamma, \|\varphi_{\mathbb{I},1}\|_{W_\varphi^M}, \|\varphi_{\mathbb{I},2}\|_{W_\varphi^M})\|\varphi_{\mathbb{I},1}-\varphi_{\mathbb{I},2}\|_{W_\varphi^M}\|\tilde\varphi_{\mathbb{I}}\|_{W_\varphi^M}\\ &\le c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1}-\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I}}\|_{W^M}.\end{aligned}$$

3. Recalling the definition of R_b from (3.4), the difference is explicitly given in weak form for all test functions $v^\varphi \in V_\varphi$, by

$$\begin{aligned}&\big\langle\big[R_b(\varphi_1^i,\varphi_1^{i-1};\gamma) - R_b(\varphi_2^i,\varphi_2^{i-1};\gamma)\big][(\tilde\varphi_1^i,\tilde\varphi_1^{i-1}),(\tilde\varphi_2^i,\tilde\varphi_2^{i-1})], v^\varphi\big\rangle\\ &\quad = 6\gamma\Big(\big([(\varphi_1^i-\varphi_1^{i-1})^+] - [(\varphi_2^i-\varphi_2^{i-1})^+]\big)(\tilde\varphi_1^i-\tilde\varphi_1^{i-1})(\tilde\varphi_2^i-\tilde\varphi_2^{i-1}), v^\varphi\Big).\end{aligned}$$

By Lipschitz continuity of $[(\cdot)^+]$ and similarly to the first step, it holds

$$\begin{aligned}&\|6\gamma\big([(\varphi_1^i-\varphi_1^{i-1})^+] - [(\varphi_2^i-\varphi_2^{i-1})^+]\big)(\tilde\varphi_1^i-\tilde\varphi_1^{i-1})(\tilde\varphi_2^i-\tilde\varphi_2^{i-1})\|_{L^q(\Omega)}\\ &\quad\le c(\gamma)\big(\|\varphi_1^i-\varphi_2^i\|_{L^\infty(\Omega)} + \|\varphi_1^{i-1}-\varphi_2^{i-1}\|_{L^\infty(\Omega)}\big)\\ &\qquad\cdot\big(\|\tilde\varphi_1^i\|_{L^\infty(\Omega)} + \|\tilde\varphi_1^{i-1}\|_{L^\infty(\Omega)}\big)\big(\|\tilde\varphi_2^i\|_{L^\infty(\Omega)} + \|\tilde\varphi_2^{i-1}\|_{L^\infty(\Omega)}\big)\\ &\quad\le c(\gamma)\big(\|\varphi_1^i-\varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1}-\varphi_2^{i-1}\|_{W_\varphi}\big)\\ &\qquad\cdot\big(\|\tilde\varphi_1^i\|_{W_\varphi} + \|\tilde\varphi_1^{i-1}\|_{W_\varphi}\big)\big(\|\tilde\varphi_2^i\|_{W_\varphi} + \|\tilde\varphi_2^{i-1}\|_{W_\varphi}\big) \qquad (3.62)\\ &\quad\le c(\gamma)\|\varphi_{1,\mathbb{I}}-\varphi_{2,\mathbb{I}}\|_{W_\varphi^M}\|\tilde\varphi_{\mathbb{I},1}\|_{W_\varphi^M}\|\tilde\varphi_{2,\mathbb{I}}\|_{W_\varphi^M}\\ &\quad\le c(\gamma)\|\mathbf{u}_{1,\mathbb{I}}-\mathbf{u}_{2,\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\tilde{\mathbf{u}}_{2,\mathbb{I}}\|_{W^M}.\end{aligned}$$

4. The continuity as a mapping $(\varphi^i,\varphi^{i-1}) \mapsto R_l(\varphi^i,\varphi^{i-1};\gamma)$ follows in the following way: Let $\varphi_1^i,\varphi_1^{i-1},\varphi_2^i,\varphi_2^{i-1} \in W_\varphi$, then

$$\begin{aligned}&\big\|R_l(\varphi_1^i,\varphi_1^{i-1};\gamma) - R_l(\varphi_2^i,\varphi_2^{i-1};\gamma)\big\|_{\mathcal{L}(W_\varphi\times W_\varphi, L^q(\Omega))}\\ &\quad = \sup_{(\|\tilde\varphi^i\|_{W_\varphi}+\|\tilde\varphi^{i-1}\|_{W})=1} \big\|R_l(\varphi_1^i,\varphi_1^{i-1};\gamma)(\tilde\varphi^i,\tilde\varphi^{i-1})\end{aligned}$$

$$
\begin{aligned}
&\qquad\qquad - R(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1})\big\|_{L^q(\Omega)} \\
\leq &\sup_{(\|\tilde{\varphi}^i\|_{W_\varphi} + \|\tilde{\varphi}^{i-1}\|_W) = 1} c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi}) \\
&\qquad\qquad \cdot \big(\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\big) \\
&\qquad\qquad \cdot \big(\|\tilde{\varphi}^i\|_{W_\varphi} + \|\tilde{\varphi}^{i-1}\|_{W_\varphi}\big) \\
\leq & \, c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi}) \\
&\quad \cdot \big(\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\big),
\end{aligned}
$$

where (3.61) is used in the fist inequality, and the constant

$$
c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi})
$$

is again bounded for $\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_2^{i-1} - \varphi_2^{i-1}\|_{W_\varphi} \to 0$, due to $\varphi_1^i, \varphi_1^{i-1}, \varphi_2^i, \varphi_2^{i-1} \in W_\varphi$ and the triangle inequality, as in step 3 of the proof of Lemma 3.1.5. Thus

$$
\begin{aligned}
\|R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)\|_{\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))} \to 0 \\
\text{for} \qquad \|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_2^{i-1} - \varphi_2^{i-1}\|_{W_\varphi} \to 0,
\end{aligned}
$$

which proves the desired result.

5. The continuity of the mapping

$$
(\varphi^i, \varphi^{i-1}) \mapsto R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), \cdot]
$$

follows in the following way: Let $\varphi_1^i, \varphi_1^{i-1}\varphi_2^i, \varphi_2^{i-1}, \tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1} \in W_\varphi$ be given, then

$$
\begin{aligned}
&\big\|R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), \cdot] \\
&\qquad - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), \cdot]\big\|_{\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))} \\
&= \sup_{(\|\tilde{\varphi}_2^i\|_{W_\varphi} + \|\tilde{\varphi}_2^{i-1}\|_{W_\varphi}) = 1} \big\|R_b(\varphi_1^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})] \\
&\qquad\qquad - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})]\big\|_{L^q(\Omega)} \\
&\leq \sup_{(\|\tilde{\varphi}_2^i\|_{W_\varphi} + \|\tilde{\varphi}_2^{i-1}\|_{W_\varphi}) = 1} c(\gamma)\big(\|\tilde{\varphi}_1^i\|_{W_\varphi} + \|\tilde{\varphi}_1^{i-1}\|_{W_\varphi}\big) \\
&\qquad\qquad \cdot \big(\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\big) \\
&\qquad\qquad \cdot \big(\|\tilde{\varphi}_2^i\|_{W_\varphi} + \|\tilde{\varphi}_2^{i-1}\|_{W_\varphi}\big) \\
&\leq c(\gamma)\big(\|\tilde{\varphi}_1^i\|_{W_\varphi} + \|\tilde{\varphi}_1^{i-1}\|_{W_\varphi}\big)\big(\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi}\big),
\end{aligned}
$$

where (3.62) is used. The constant $c(\gamma)\big(\|\tilde{\varphi}_1^i\|_{W_\varphi} + \|\tilde{\varphi}_1^{i-1}\|_{W_\varphi}\big)$ is bounded by assumption. Thus

$$
\|R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), \cdot]
$$

$$- R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), \cdot]\|_{\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))} \to 0$$
$$\text{for} \quad \|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi} \to 0,$$

which proves the desired result.

6. Recalling the definition of R_{l*} from (3.6), the difference is explicitly given in weak form, for all $v^\varphi \in V_\varphi$, by

$$\begin{aligned}
&\big\langle R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}; \gamma)(\psi^i, \psi^{i+1}) - R_{l*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^\varphi \big\rangle \\
&\quad = \big(3\gamma\big([(\varphi_1^i - \varphi_1^{i-1})^+]^2 - [(\varphi_2^i - \varphi_2^{i-1})^+]^2\big)\psi^i \\
&\qquad\quad - 3\gamma\big([(\varphi_1^{i+1} - \varphi_1^i)^+]^2 - [(\varphi_2^{i+1} - \varphi_2^i)^+]^2\big)\psi^{i+1}, v^\varphi\big).
\end{aligned}$$

Analogously to step 2, it now holds

$$\begin{aligned}
&\|\big(3\gamma\big([(\varphi_1^i - \varphi_1^{i-1})^+]^2 - [(\varphi_2^i - \varphi_2^{i-1})^+]^2\big)\psi^i \\
&\qquad\quad - 3\gamma\big([(\varphi_1^{i+1} - \varphi_1^i)^+]^2 - [(\varphi_2^{i+1} - \varphi_2^i)^+]^2\big)\psi^{i+1}, v^\varphi\big)\|_{L^q(\Omega)} \\
&\quad \le c(\gamma, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_1^{i-1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}, \|\varphi_2^{i-1}\|_{W_\varphi}) \\
&\qquad\quad \cdot (\|\varphi_1^i - \varphi_2^i\|_{W_\varphi} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{W_\varphi})\|\psi^i\|_{W_\varphi} \\
&\qquad + c(\gamma, \|\varphi_1^{i+1}\|_{W_\varphi}, \|\varphi_1^i\|_{W_\varphi}, \|\varphi_2^{i+1}\|_{W_\varphi}, \|\varphi_2^i\|_{W_\varphi}) \\
&\qquad\qquad \cdot (\|\varphi_1^{i+1} - \varphi_2^{i+1}\|_{W_\varphi} + \|\varphi_1^i - \varphi_2^i\|_{W_\varphi})\|\psi^{i+1}\|_{W_\varphi} \\
&\quad \le c(\gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M}.
\end{aligned}$$

7. Recalling the definition of R_{b*} from (3.12), the difference is given in weak form for all test functions $v^\varphi \in V_\varphi$ by

$$\begin{aligned}
&\big\langle R_{b*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^\varphi \big\rangle \\
&\quad = 6\gamma\Big(\big([(\varphi_1^i - \varphi_1^{i-1})^+] - [(\varphi_2^i - \varphi_2^{i-1})^+]\big)(\tilde{\varphi}^i - \tilde{\varphi}^{i-1})\psi^i \\
&\qquad\quad - \big([(\varphi_1^{i+1} - \varphi_1^i)^+] - [(\varphi_2^{i+1} - \varphi_2^i)^+]\big)(\tilde{\varphi}^{i+1} - \tilde{\varphi}^i)\psi^{i+1}, v^\varphi\Big).
\end{aligned}$$

By Lipschitz continuity of $[(\cdot)^+]$ and similarly to the second step, and hence as in step 1, we estimate

$$\begin{aligned}
&\Big\|6\gamma\big(\big([(\varphi_1^i - \varphi_1^{i-1})^+] - [(\varphi_2^i - \varphi_2^{i-1})^+]\big)(\tilde{\varphi}^i - \tilde{\varphi}^{i-1})\psi^i \\
&\qquad - \big([(\varphi_1^{i+1} - \varphi_1^i)^+] - [(\varphi_2^{i+1} - \varphi_2^i)^+]\big)(\tilde{\varphi}^{i+1} - \tilde{\varphi}^i)\psi^{i+1}\big)\Big\|_{L^q(\Omega)} \\
&\quad \le c(\gamma)\big(\|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)} + \|\varphi_1^{i-1} - \varphi_2^{i-1}\|_{L^\infty(\Omega)}\big) \\
&\qquad\quad \cdot \big(\|\tilde{\varphi}^i\|_{L^\infty(\Omega)} + \|\tilde{\varphi}^{i-1}\|_{L^\infty(\Omega)}\big)\|\psi^i\|_{L^\infty(\Omega)} \\
&\qquad + c(\gamma)\big(\|\varphi_1^{i+1} - \varphi_2^{i+1}\|_{L^\infty(\Omega)} + \|\varphi_1^i - \varphi_2^i\|_{L^\infty(\Omega)}\big) \\
&\qquad\quad \cdot \big(\|\tilde{\varphi}^{i+1}\|_{L^\infty(\Omega)} + \|\tilde{\varphi}^i\|_{L^\infty(\Omega)}\big)\|\psi^{i+1}\|_{L^\infty(\Omega)}
\end{aligned}$$

$$\le c(\gamma)\|\varphi_{1,\mathbb{I}} - \varphi_{2,\mathbb{I}}\|_{W_\varphi^M} \|\tilde{\varphi}_\mathbb{I}\|_{W_\varphi^M} \|\psi_\mathbb{I}\|_{W_\varphi^M}$$
$$\le c(\gamma)\|\mathbf{u}_{1,\mathbb{I}} - \mathbf{u}_{2,\mathbb{I}}\|_{W^M} \|\tilde{\mathbf{u}}_\mathbb{I}\|_{W^M} \|\mathbf{z}_\mathbb{I}\|_{W^M}.$$

□

3.2 Solvability and regularity of the state equation and its linearization

Now, using the definition of the operators A, R and B from Definition 2.3.8, we can recall the Euler-Lagrange equation ($\mathrm{EL}_\mathbb{I}^{\gamma,\eta}$) from Section 2.1. It reads

$$A(\mathbf{u}^i, \varphi^{i-1}) + R(\varphi^i, \varphi^{i-1}; \gamma) = Bq^i, \tag{3.63}$$

for all $i = 1, ..., M$, and can be formulated in weak form, for all test functions $\mathbf{v} = (v^u, v^\varphi) \in V$, by

$$\big\langle A(\mathbf{u}^i, \varphi^{i-1}), \mathbf{v}\big\rangle + \big\langle R(\varphi^i, \varphi^{i-1}; \gamma), v^\varphi\big\rangle = \big\langle Bq^i, \mathbf{v}\big\rangle, \tag{3.64}$$

again for all $i = 1, ..., M$. This can finally equivalently be expressed, for all test functions $\mathbf{v}_\mathbb{I} \in V^M$, as

$$\sum_{i=1}^{M} \Big[\big\langle A(\mathbf{u}^i, \varphi^{i-1}), \mathbf{v}^i\big\rangle + \big\langle R(\varphi^i, \varphi^{i-1}; \gamma), v^{\varphi,i}\big\rangle\Big] = \sum_{i=1}^{M} \big\langle Bq^i, \mathbf{v}^i\big\rangle. \tag{3.65}$$

Let us point out again that a related (system of) nonlinear partial differential equation(s) is analyzed in [132], where the difference to the PDE at hand is that [132] does not include the viscous approximation, i.e. $\eta \equiv 0$. In [132], it is pointed out that coupled quasilinear partial differential equations of such a type cannot be investigated in the Hilbert space setting $V := V_u \times V_\varphi = H_D^1(\Omega; \mathbb{R}^2) \times H^1(\Omega)$, cf. Definition 2.3.3, since the involved terms are not well-defined in these spaces. This can e.g. be seen since for $\mathbf{u}^i = (u^i, \varphi^i) \in V$, and test functions $v^u \in V_u$, the term $\big(g(\varphi^i)\mathbb{C}e(u^i), e(v^u)\big)$ is not in $L^1(\Omega)$. It is therefore necessary to look at solvability in more regular spaces. Solvability of the PDE without viscous approximation in $(V \cap (W^{1,p}(\Omega; \mathbb{R}^2) \times L^\infty(\Omega)))^M$ is thus proved in [132, Lemma 4.1 and Corollary 4.2].

In [133], for the same setting as in this thesis, i.e. involving the viscous approximation and under Assumption 2.3.11, Assumption 2.3.1 and Assumption 2.3.7, unique solvability and improved regularity of the solution in the space $W := W_u \times W_\varphi = W_D^{1,p}(\Omega; \mathbb{R}^2) \times W^{2,q}(\Omega)$, for $p > 2$, and $q = \frac{p}{2} > 1$ for ($\mathrm{EL}_\mathbb{I}^{\gamma,\eta}$), or equivalently (3.63) is proved. Let us collect this result and state it for further use:

Lemma 3.2.1. *Let $\eta \ge 0$ be sufficiently large. Let $\varphi^0 \in W_\varphi$, $\varphi^0 \in [0, 1]$, then for every $q_\mathbb{I} \in Q^M$, ($\mathrm{EL}_\mathbb{I}^{\gamma,\eta}$), or equivalently* (3.63)-(3.65)*, has a unique weak solution $\mathbf{u}_\mathbb{I} \in W^M$, such that in particular $\varphi^i \in L^\infty(\Omega)$, as well as $\varphi^i \in [0, 1]$, for* *all* $i = 1, .., M$*. Further, it holds* $u_{\mathbb{I}} \in (H^{1+s}(\Omega, \mathbb{R}^2))^M$*, and for all* $i = 1, .., M$ *the following stability properties hold:*

$$\|u^i\|_{W_u} \leq c\|q^i\|_Q, \tag{3.66}$$

$$\|\varphi^i\|_{W_\varphi} \leq c\big(1 + \|q^i\|_Q^2 + \gamma\|[(\varphi^i - \varphi^{i-1})^+]^3\|_{L^q(\Omega)}^2 + \eta\|\varphi^i - \varphi^{i-1}\|_{L^q(\Omega)}\big) \tag{3.67}$$

$$\leq c\big(1 + \|q^i\|_Q^2 + \|\frac{1}{\varepsilon} + \varepsilon\triangle\varphi^{i-1}\|_{L^q(\Omega)}\big) \tag{3.68}$$

$$\leq c\Big(M + \|q_{\mathbb{I}}\|_{Q^M}^2 + \|\varphi^0\|_{W_\varphi}\Big), \tag{3.69}$$

$$\|u^i\|_{H^{1+s}(\Omega,\mathbb{R}^2)} \leq \tilde{c}\|q^i\|_Q, \tag{3.70}$$

for constants $c > 0$*, and some* $\tilde{c} = \tilde{c}(\kappa, M, \|q_{\mathbb{I}}\|_{Q^M}^2, \|\varphi^0\|_{W_\varphi})$*, i.e.* $\tilde{c}$ *only depends on* κ *and the right-hand side of* (3.69)*.*

Proof. The result, which uses ideas from [79, 90, 132, 133], is given in [133, Section 1 and Section 2]. The norm estimates are proved in [133, Corollary 4.1]. □

Consequently, we can introduce the control-to-state operator via

$$G_{\mathbb{I}} \colon Q^M \to W^M, \qquad G_{\mathbb{I}}(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}}. \tag{3.71}$$

In this context, $G_{\mathbb{I}}$ is understood as the mapping of the data $q_{\mathbb{I}} \in Q^M$ to the vector of solution function pairs of displacement and phase-field functions $\mathbf{u}_{\mathbb{I}} = (u_{\mathbb{I}}, \varphi_{\mathbb{I}}) \in W^M$ of $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$, or equivalently (3.63)-(3.65) for all $i = 1, .., M$.

The next task is to discuss a linearized partial differential equation, that emerges in the context of differentiability of $G_{\mathbb{I}}$ and then subsequently in the optimality conditions of $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$, cf. Chapter 4 below. For this, we recall the definitions of A_l and R_l from (3.1) and (3.2), and assume $\mathbf{u}_{\mathbb{I}} \in W^M$, $\varphi^0 \in W_\varphi$, $\mathbf{f}_{\mathbb{I}} \in V^M$. For a concurrent notation, also set $\tilde{\varphi}^0 := 0$, cf. (3.9). The linearized partial differential equation is introduced in the following three equivalent forms: Firstly, look for a solution $\tilde{\mathbf{u}}_{\mathbb{I}} \in V^M$ of the system

$$A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}) + R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}) = \mathbf{f}^i, \tag{3.72}$$

for all $i = 1, .., M$, which in weak form can be formulated, for all test functions $\mathbf{v} = (v^u, v^\varphi) \in V$, by

$$\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}\big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^\varphi\big\rangle = \big\langle \mathbf{f}^i, \mathbf{v}\big\rangle, \tag{3.73}$$

again for all $i = 1, ..., M$. Finally, this is equivalent to: For all test functions $\mathbf{v}_{\mathbb{I}} \in V^M$, look for the solution $\tilde{\mathbf{u}}_{\mathbb{I}} \in V^M$ of

$$\sum_{i=1}^M \Big[\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}^i\big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^{\varphi,i}\big\rangle\Big] = \sum_{i=1}^M \big\langle \mathbf{f}^i, \mathbf{v}^i\big\rangle. \tag{3.74}$$

The linearized equation (3.72)-(3.74) is formally motivated as the derivative of the nonlinear PDE (3.63)-(3.65), cf. Lemma 3.2.3 below, and $\tilde{\varphi}^0$ serves as a placeholder of the derivative of the a-priori given starting value φ^0, which is constant in the derivation process. For the chosen notation, we make the following assumption concerning the 0-th time step, which shall hold throughout the entire analysis.

Assumption 3.2.2. *For the function $\tilde{\varphi}^0$, which occurs in the definition of the linearized equation* (3.72)-(3.74)*, we set $\tilde{\varphi}^0 := 0$.*

Next, let us also give a brief overview of the state of the art for the linearized PDE (3.72)-(3.74). We start again with the setting of [132], which we recall does not involve a viscous approximation, i.e. $\eta \equiv 0$. Under the assumption $\mathbf{u}_{\mathbb{I}} \in (V \cap (W^{1,p}(\Omega;\mathbb{R}^2) \times L^\infty(\Omega))^M$, it is proved in [132, Lemma 5.1] that

$$\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, 0), \cdot^i \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, 0), \cdot^{\varphi,i} \right\rangle + c(\tilde{\varphi}^i, \cdot^{\varphi,i})_{s,2} \tag{3.75}$$

is coercive on $V \times V_\varphi$, for an $s \in [0,1]$ such that $H^s(\Omega) \hookrightarrow L^r(\Omega)$ for $\frac{1}{p} + \frac{1}{2} + \frac{1}{r} = 1$, which in turn means that

$$\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, 0), \cdot^i \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, 0), \cdot^{\varphi,i} \right\rangle$$

is in particular also Fredholm of index zero. Subsequently, in [132] the system of linearized PDEs is expressed in matrix form through a matrix $\mathcal{A}\colon V^M \to V^M$ that has $A_l(\mathbf{u}^i) + R_l(\varphi^i, \varphi^{i-1}; \gamma)$ on the diagonal, and $3\gamma[(\varphi^i - \varphi^{i-1})^+]^2$ on the subdiagonal. This matrix is again Fredholm of index zero, cf. [132, Corollary 5.5], and by assuming additionally that $\mathcal{A}$ has a trivial kernel, i.e. $\ker(\mathcal{A}) = \{0\}$, both $\mathcal{A}$ and $\mathcal{A}^*$ are isomorphisms, cf. [132, Theorem 6.1]. Note that this trivial kernel assumption holds e.g. under the assumption that $\|\mathbf{u}^i\|_W$ is sufficiently small for all $i = 1, ..., M$, cf. [132, Lemma 5.2, Remark 5.3]. We have already seen in Section 2.1, that [133] proposes to use an idea of [107] to incorporate a viscous approximation term, cf. (2.7), into the fracture propagation model. Choosing η sufficiently large, cf. Assumption 2.3.11, coercivity of (3.75) can be ensured, even after dropping the trivial kernel assumption. The reason is that the last term of (3.75) can be absorbed into the (from the viscous approximation stemming additional) term $\eta(\tilde{\varphi}^i, \cdot^{\varphi,i})$. This means that the left-hand side of (3.72) is in fact coercive under Assumption 2.3.11. The Lax-Milgram lemma can therefore be utilized, and unique solvability in $V^M \times V^M$ can be ensured. Further, it is possible to establish improved regularity in the space W^M. This was presented for the case $M = 1$, i.e. the one time step linearized equation in [84, Section 2.2, Proposition 2.1] of M. Mohammadi, I. Neitzel, W. Wollner and the author. A rigorous proof for $M = 1$ is also given in [86, Lemma 3.2] of I. Neitzel and the author. For $M > 1$, we obtain:

Lemma 3.2.3. *Let $\eta \geq 0$ be sufficiently large, $\mathbf{u}_{\mathbb{I}} \in W^M$, $\varphi^0 \in W_\varphi$ be given, and recall that $\tilde{\varphi}^0 = 0$, cf. Assumption 3.2.2. Then for every $\mathbf{f}_{\mathbb{I}} \in (V^*)^M$,* *there exists a unique solution* $\tilde{\mathbf{u}}_{\mathbb{I}} \in V^M$ *to* (3.72)-(3.74) *for all* $i = 1, ..., M$*, that satisfies the stability property*

$$\|\tilde{u}^i\|_{V_u} + \|\tilde{\varphi}^i\|_{V_\varphi} \leq \tilde{c}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M}, \tag{3.76}$$

for some $0 < \tilde{c} := \tilde{c}(\eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$*, and all* $i = 1, .., M$*. If further* $\mathbf{f}_{\mathbb{I}} \in (W^\times)^M \hookrightarrow (V^*)^M$*, then additionally* $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M$*, and it holds,*

$$\|\tilde{u}^i\|_{W_u} + \|\tilde{\varphi}^i\|_{W_\varphi} \leq c\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}, \tag{3.77}$$

for some $0 < c := c(\eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$*, and all* $i = 1, .., M$*. Note that the constant* c *depends on* $\|\mathbf{u}_{\mathbb{I}}\|_{W^M}$*, as well as positive powers thereof.*

Proof. We apply the ideas of [107, 132, 133], combining them with an induction argument. We argue iteratively, showing unique solvability in the space V^M and (3.76) in a first step (1a) and (1b), and then the improved regularity in a second step (2a) and (2b).

(1a) For $i = 1$, the task is to solve

$$A_l(\mathbf{u}^1)(\tilde{\mathbf{u}}^1, \tilde{\varphi}^0) + R_l(\varphi^1, \varphi^0; \gamma)(\tilde{\varphi}^1, \tilde{\varphi}^0) = \mathbf{f}^1, \tag{3.78}$$

for given $\mathbf{u}^1 \in W, \varphi^0 \in W_\varphi$, $\tilde{\varphi}^0 = 0$ and $\mathbf{f}^1 \in V^*$. We prove that the bilinear form induced by $\langle A_l(\mathbf{u}^1)(\cdot^i, 0), (\cdot^i, 0)\rangle$ is coercive. We immediately see from the definition (3.1) of A_l that there is only one possibly nonnegative term. As hinted in the paragraph immediately above this lemma, this term in fact can be absorbed by the viscous approximation term in the following way: Let $r \in (2, \infty)$, such that $\frac{1}{r} + \frac{1}{p} = \frac{1}{2}$, which means that i.p. $\tilde{\varphi}^i \in H^1 \hookrightarrow L^r$. Therefore, using Hölder's and Young's inequality for a $\delta_1 > 0$ yields

$$\begin{aligned} &4(1-\kappa)\big(\varphi^i \mathbb{C} e(u^i), \tilde{\varphi}^i e(\tilde{u}^i)\big) \\ &\quad \geq -4(1-\kappa)\|\varphi^i\|_{L^\infty(\Omega)}\|u^i\|_{W_u}\left(\frac{1}{\delta_1}\|\tilde{\varphi}^i\|_{L^r}^2 + \delta_1\|\tilde{u}^i\|_{V_u}^2\right). \end{aligned} \tag{3.79}$$

Due to $r > 0$, the Gagliardo-Nirenberg inequality and again Young's inequality ensure

$$\begin{aligned} \|\tilde{\varphi}^i\|_{L^r}^2 &\leq \tilde{c}(\Omega)^2\left(\|\nabla\tilde{\varphi}^i\|_{L^2}^{\frac{r-2}{2}}\|\tilde{\varphi}^i\|_{L^2}^{\frac{2}{r}}\right)^2 \\ &\leq c(\Omega)\delta_2\|\nabla\tilde{\varphi}^i\|_{L^2}^2 + c(\Omega)C(\delta_2)\|\tilde{\varphi}^i\|_{L^2}^2, \end{aligned}$$

for a $\delta_2 > 0$ and exponents $\frac{r}{r-2}$ and $\frac{r}{2}$. Then, continuing in (3.79) leads to

$$\begin{aligned} &4(1-\kappa)\big(\varphi^i \mathbb{C} e(u^i), \tilde{\varphi}^i e(\tilde{u}^i)\big) \\ &\quad \geq -c(\kappa, \Omega)\|\mathbf{u}^i\|_W^2\left(\delta_1\|\tilde{u}\|_{V_u}^2 + \frac{\delta_2}{\delta_1}\|\nabla\tilde{\varphi}^i\|_{L^2} + C(\delta_1, \delta_2)\|\tilde{\varphi}^i\|_{L^2}^2\right), \end{aligned}$$

for a constant $C(\delta_1,\delta_2)>0$. We omit the remaining estimations, since they are similar to [132, Lemma 5.1], and immediately conclude that overall

$$\begin{aligned}
&\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i,0),\tilde{\mathbf{u}}^i\right\rangle\\
&\quad\geq\left(\kappa c_{korn}-\delta_1 c(\kappa)\|\mathbf{u}^i\|_W^2\right)\|\tilde{u}^i\|_{V_u}^2\\
&\qquad+\left(\varepsilon-\frac{\delta_2}{\delta_1}c(\kappa,\Omega)\|\mathbf{u}^i\|_W^2\right)\|\nabla\tilde{\varphi}^i\|_{L^2}^2\\
&\qquad+\left(C(\varepsilon)+\eta-C(\delta_1,\delta_2)c(\kappa,\Omega)\|\mathbf{u}^i\|_W^2\right)\|\tilde{\varphi}^i\|_{L^2}^2,
\end{aligned}\tag{3.80}$$

where Korn's inequality of the second kind for zero boundary functions with $c_{korn}>0$ is used. Now, due to $\varepsilon>0$ being an a-priori fixed number, it is possible to choose $\delta_1>0$ small enough such that $\kappa c_{korn}-\delta_1 c(\kappa)\|\mathbf{u}^i\|_W^2>0$, and subsequently $\delta_2>0$ small such that $\varepsilon-\frac{\delta_2}{\delta_1}c(\kappa,\Omega)\|\mathbf{u}^i\|_W^2>0$. Finally, for $\eta>0$ sufficiently large, it is possible to bound the right-hand side of (3.80) from below by $c(\|\tilde{u}^i\|_{V_u}^2+\|\tilde{\varphi}^i\|_{V_\varphi}^2)$ for a $c>0$. Further, R_l suffices to the nonnegativity condition

$$\begin{aligned}
\left\langle R_l(\varphi^1,\varphi^0;\gamma)(\tilde{\varphi}^1,0),\tilde{\varphi}^1\right\rangle&=3\gamma([(\varphi^1-\varphi^0)^+]^2\tilde{\varphi}^1,\tilde{\varphi}^1)\\
&\geq 0\quad\forall\tilde{\varphi}^1\in V_\varphi\times V_\varphi.
\end{aligned}\tag{3.81}$$

Overall, unique solvability of (3.78) in V, as well as

$$\|\tilde{u}^1\||_{V_u}+\|\tilde{\varphi}^1\|_{V_\varphi}\leq c(\eta)\|\mathbf{f}^1\|_{V^*},\tag{3.82}$$

now follows by the Lax-Milgram lemma, for a $0<c(\eta)\in\mathbb{R}$.

(1b) For $i=2$, the task is to solve

$$A_l(\mathbf{u}^2)(\tilde{\mathbf{u}}^2,\tilde{\varphi}^1)+R_l(\varphi^2,\varphi^1;\gamma)(\tilde{\varphi}^2,\tilde{\varphi}^1)=\mathbf{f}^2,$$

for given $\mathbf{u}^2\in W,\varphi^1\in W_\varphi$, and the $\tilde{\varphi}^1\in V_\varphi$ from the step (1a), as well as $\mathbf{f}^2\in V^*$. This can be written in weak form, cf. (3.1) and (3.2), for all test functions $\mathbf{v}\in V$, as

$$\begin{aligned}
&\big(g(\varphi^2)\mathbb{C}e(\tilde{u}^2),e(v^u)\big)+2(1-\kappa)\big(\varphi^2\mathbb{C}e(u^2)\tilde{\varphi}^2,e(v^u)\big)\\
&+2(1-\kappa)\big(\varphi^2\mathbb{C}e(u^2)\colon e(\tilde{u}^2),v^\varphi\big)+(1-\kappa)\big(\tilde{\varphi}^2\mathbb{C}e(u^2)\colon e(u^2),v^\varphi\big)\\
&+\varepsilon(\nabla\tilde{\varphi}^2,\nabla v^\varphi)+\frac{1}{\varepsilon}(\tilde{\varphi}^2,v^\varphi)+\eta(\tilde{\varphi}^2,v^\varphi)+3\gamma([(\varphi^2-\varphi^1)^+]^2\tilde{\varphi}^2,v^\varphi)\\
&=(f^{u,2},v^u)+(f^{\varphi,2},v^\varphi)+\eta(\tilde{\varphi}^1,v^\varphi)+3\gamma([(\varphi^2-\varphi^1)^+]^2\tilde{\varphi}^1,v^\varphi).
\end{aligned}\tag{3.83}$$

For $\eta\geq 0$ again sufficiently large, depending on the constants η,κ, the domain Ω and $\|\mathbf{u}^2\|_W$, the left-hand side of (3.83) constitutes the sum of a coercive and a nonnegative operator, identical to the case of step (1a). The right-hand side lies in V^*, due to $\varphi^2,\varphi^1\in L^\infty(\Omega),\tilde{\varphi}^1\in V_\varphi^*$, and the assumption on $\mathbf{f}^2$. Again unique solvability of (3.83) follows by the Lax-Milgram lemma, and also using (3.82) yields

$$\begin{aligned}\|\tilde{u}^2\|_{V_u} + \|\tilde{\varphi}^2\|_{V_\varphi} &\leq c(\eta)\big(\|\mathbf{f}^2\|_{V^*} + c(\eta)c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|^2_{W^M}\|\tilde{\varphi}^1\|_{V_\varphi^*}\big)\\ &\leq c(\eta)\big(\|\mathbf{f}^2\|_{V^*} + c(\eta)c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|^2_{W^M}\|\mathbf{f}^1\|_{V^*}\big).\end{aligned}$$

By induction, the existence result is then concluded for all $i = 3, .., M$, and there exists some $\tilde{c}$ as stated such that (3.76) holds true. Note that it holds $0 \leq \eta < \infty$, and η is chosen as the largest necessary one of every step $i = 1, ..., M$.

Next, the improved regularity result is proved:

(2a) Starting again with $i = 1$, using the test functions $(0, v^\varphi) \in V$ and $(v^u, 0) \in V$ in (3.73), it holds after rearranging

$$\begin{aligned}\varepsilon(\nabla\tilde{\varphi}^1, \nabla v^\varphi) + \frac{1+\varepsilon\eta}{\varepsilon}(\tilde{\varphi}^1, v^\varphi) =& -2(1-\kappa)\big(\varphi^1\mathbb{C}e(u^1) : e(\tilde{u}^1), v^\varphi\big)\\ & -(1-\kappa)\big(\tilde{\varphi}^1\mathbb{C}e(u^1) : e(u^1), v^\varphi\big)\\ & -3\gamma([(\varphi^1-\varphi^0)^+]^2\tilde{\varphi}^1, v^\varphi)\\ & +(f^{\varphi,1}, v^\varphi) \qquad =: (\tilde{g}^{\varphi,1}, v^\varphi),\end{aligned} \tag{3.84}$$

$$\begin{aligned}\big(g(\varphi^1)\mathbb{C}e(\tilde{u}^1), e(v^u)\big) =& -2(1-\kappa)\big(\varphi^1\mathbb{C}e(u^1)\tilde{\varphi}^1, e(v^u)\big)\\ & +(f^{u,1}, v^u) \qquad := (\tilde{g}^{u,1}, v^u).\end{aligned} \tag{3.85}$$

The function $\tilde{g}^{\varphi,1}$, the right-hand side of (3.84) respectively, can now be estimated in the same way as e.g. in [132, Lemma 5.2], [86, Lemma 3.2] cf. also Lemma 3.1.3. In particular, using (3.76) in the second inequality, this leads to:

$$\begin{aligned}\|\tilde{g}^{\varphi,1}\|_{L^{r'}} &\leq 2c(\kappa)\|\mathbf{u}^1\|^2_W\|\tilde{u}^1\|_{V_u} + c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|^2_{W^M}\|\tilde{\varphi}^1\|_{V_\varphi} + c\|f^{\varphi,i}\|_{V_\varphi}\\ &\leq c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|^2_{W^M}\tilde{c}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M} + c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|^2_{W^M}\tilde{c}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M}\\ &\quad + c\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M}\\ &\leq \tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M},\end{aligned} \tag{3.86}$$

for an $r' \in (1,2), 1 = \frac{1}{r'} + \frac{1}{r}$, where $r \in (2,\infty), \frac{1}{2} = \frac{1}{r} + \frac{1}{p}$ recalling $p > 2$ as in Definition 2.3.3, and for a $0 < \tilde{c}_{\varphi,1} := c(\tilde{c}, \eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$. By standard elliptic regularity results, cf. e.g. [153, Theorem 4.7 and Chapter 7.2.1], from (3.84) it holds $\tilde{\varphi}^1 \in H^1(\Omega) \cup L^\infty(\Omega)$, as well as

$$\|\tilde{\varphi}^1\|_{L^\infty(\Omega)} \leq \tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M}. \tag{3.87}$$

Now, using (3.87), we find from (3.85),

$$\|\tilde{g}^{u,1}\|_{L^p(\Omega,\mathbb{R}^2)} \leq c(\kappa)\|\mathbf{u}^1\|^2_W\|\tilde{\varphi}^1\|_{L^\infty(\Omega)} + \|f^{u,1}\|_{W^{-1,p}(\Omega;\mathbb{R}^2)}$$

$$\le c(\kappa)\tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(V^*)^M} + c\|\mathbf{f^1}\|_{W^\times}$$
$$\le \tilde{c}_{u,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M},$$

for a $0 < \tilde{c}_{u,1} := c(\eta, \tilde{c}_{\varphi,1}) \in \mathbb{R}$. From (3.85), by [90, Proposition 1.1] we can conclude $\tilde{u}^1 \in W_u$ and

$$\|\tilde{u}^1\|_{W_u} \le \tilde{c}_{u,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}. \tag{3.88}$$

Note that, at this point, using $\mathbf{f}^1 \in W^\times$, in particular $f^{\varphi,1} \in L^q(\Omega)$, and the W_u regularity of $\tilde{u}^1$ as well as the $L^\infty(\Omega)$ regularity of $\tilde{\varphi}^1$, it is in fact possible to improve the estimate (3.86) by choosing $r' = q = \frac{p}{2}$. In particular, it holds

$$\begin{aligned}\|\tilde{g}^{\varphi,1}\|_{L^q(\Omega)} &\le c(\kappa)\|\mathbf{u}^1\|_W^2\,\tilde{c}_{u,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M} + c(\kappa)\|\mathbf{u}^1\|_W^2 + \tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M} \\ &\quad + c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}^2\tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M} + c\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M} \\ &\le \tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M},\end{aligned}$$

for some $0 < \tilde{c}_{\varphi,1} := c(\kappa, \tilde{c}_{u,1}, \tilde{c}_{\varphi,1}, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$. As in [79, Section 7, Corollary 2], making use of the $W^{2,q}$-regularity of Ω from Definition 2.3.3, we can conclude $\tilde{\varphi} \in W_\varphi$, as well as

$$\|\tilde{\varphi}^1\|_{W_\varphi} \le \tilde{c}_{\varphi,1}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}. \tag{3.89}$$

Combining this with (3.88) now means that there exists some constant $0 < \tilde{c}_1 := c(c(\eta), \kappa, \eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$, such that

$$\|\tilde{u}^1\|_{W_u} + \|\tilde{\varphi}^1\|_{W_\varphi} \le \tilde{c}_1\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M},$$

which proves the claim for $i = 1$.

(2b) For $i = 2$, again using the test functions $(0, v^\varphi) \in V$, and $(v^u, 0) \in V$ respectively, it holds

$$\begin{aligned}\varepsilon(\nabla\tilde{\varphi}^2, \nabla v^\varphi) + \frac{1+\varepsilon\eta}{\varepsilon}(\tilde{\varphi}^2, v^\varphi) =& -2(1-\kappa)\big(\varphi^2\mathbb{C}e(u^2)\colon e(\tilde{u}^2), v^\varphi\big) \\ & - (1-\kappa)\big(\tilde{\varphi}^2\mathbb{C}e(u^2)\colon e(u^2), v^\varphi\big) \\ & - 3\gamma([(\varphi^2-\varphi^0)^+]^1\tilde{\varphi}^2, v^\varphi) \\ & + \eta(\tilde{\varphi}^1, v^\varphi) + 3\gamma([(\varphi^2-\varphi^1)^+]^2\tilde{\varphi}^1, v^\varphi) \\ & + (f^{\varphi,2}, v^\varphi) \qquad =: (\tilde{g}^{\varphi,2}, v^\varphi), \\ \big(g(\varphi^2)\mathbb{C}e(\tilde{u}^2), e(v^u)\big) =& -2(1-\kappa)\big(\varphi^2\mathbb{C}e(u^1)\tilde{\varphi}^2, e(v^u)\big) \\ & + (f^{u,2}, v^u) \qquad := (\tilde{g}^{u,2}, v^u).\end{aligned}$$

Analogously to the estimates in (3.87), (3.88) and (3.89), one can incorporate the two additional terms into the $L^\infty(\Omega)$- and W_φ-norm estimate of $\tilde{g}^{\varphi,2}$, to obtain, for constants $0 < \tilde{c}_{\varphi,2} := c(c(\eta), \kappa, \eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}, 0 < \tilde{c}_{u,2} := c(\eta, \tilde{c}_{\varphi,2}) \in \mathbb{R}$,

$$\|\tilde{\varphi}^2\|_{W_\varphi} \le \tilde{c}_{\varphi,2}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M},$$

$$\|\tilde{u}^2\|_{W_u} \leq \tilde{c}_{u,2}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}.$$

Note that the $\tilde{\varphi}^1$ terms can be captured by the terms $\tilde{c}_{\varphi,2}\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}$, through (3.89). Overall, there exists a $0 < \tilde{c}_2 := c(c(\eta), \kappa, \eta, \gamma, \|\mathbf{u}_{\mathbb{I}}\|_{W^M}) \in \mathbb{R}$ such that

$$\|\tilde{u}^2\|_{W_u} + \|\tilde{\varphi}^2\|_{W_\varphi} \leq \tilde{c}_2\|\mathbf{f}_{\mathbb{I}}\|_{(W^\times)^M}.$$

By induction, the result can be concluded for all $i = 3, ..., M$, and there again exists some c as stated such that (3.77) follows.

□

We conclude this subsection with two quick remarks. Firstly, all operators and solution spaces already include homogeneous Dirichlet boundary conditions on Γ_D, and we can also include Neumann boundary conditions for the data $\mathbf{f}_{\mathbb{I}}$, by setting $\mathbf{f}^i = B\tilde{q}_i \in W^\times \hookrightarrow V^*$, cf. Remark 2.3.6. Secondly, let us quickly put the focus at only the first time step, respectively only one time step for given φ^0. In particular, we have proved along the way that in this case we can also obtain bounds that do not involve a dependence on γ, which we state for later use.

Lemma 3.2.4. *Let $\eta \geq 0$ be sufficiently large, $\mathbf{u} \in W$ and $\varphi^0 \in W_\varphi$ be given. For every $\mathbf{f} = (f^u, f^\varphi) \in V^*$, there exists a unique solution $\tilde{\mathbf{u}} \in V$ to*

$$\left\langle A_l(\mathbf{u})(\tilde{\mathbf{u}}, 0), \mathbf{v}\right\rangle + \left\langle R_l(\varphi, \varphi^0; \gamma)(\tilde{\varphi}, 0), v^\varphi\right\rangle = \left\langle \mathbf{f}, \mathbf{v}\right\rangle \quad \forall \mathbf{v} \in V \tag{3.90}$$

and it holds

$$\|\tilde{u}\|_{V_u} + \|\tilde{\varphi}\|_{V_\varphi} \leq c\|\mathbf{f}\|_{V^*}, \tag{3.91}$$

for a $c > 0$ independently of γ. If we further assume $\mathbf{f} \in W^\times \hookrightarrow V^*$, then the solution $\tilde{\mathbf{u}}$ of (3.90) is in the space W and the estimate

$$\|\tilde{u}\|_{W_u} + \|\tilde{\varphi}\|_{W_\varphi} \leq c\|\mathbf{f}\|_{W^\times} \tag{3.92}$$

holds, where the dependence of the constant $c = c(\mathbf{u}, \varphi^-, \eta, \gamma, \kappa, \varepsilon) > 0$ is a dependence on positive integer powers of the norm $\|\mathbf{u}\|_W$.

Finally, let additionally $u \in H^{1+s}(\Omega)$ and $s \in (0, 1/2)$ as in Assumption 2.3.1 such that $s > \frac{p-2}{p}$. Then it additionally holds

$$\|\tilde{u}\|_{W_u} \leq c\|\mathbf{f}\|_{W^\times}, \tag{3.93}$$

for a $c = c(\mathbf{u}, \varphi^-, \eta, \kappa, \varepsilon)$ dependent on positive integer powers of the norm $\|\mathbf{u}\|_W$, but independently of γ.

While the first two statements (3.91) and (3.92) are proved in [86, Lemma 3.2], and also already stated in [84], the bound (3.93) has not been published before. Note that even restricting the setting to one time step, we obtain the dependence of c on γ on the right-hand side of (3.92) for the pair $\tilde{\mathbf{u}} = (\tilde{u}, \tilde{\varphi})$ in the space W, similarly to both bounds (3.76) and (3.92) for the multi time step model (i.e. for both V^M and W^M). This point is also taken up shortly in Chapter 5 and Chapter 7.

Proof. Existence of a unique solution as well as (3.91) were proved in step (1a) of the above proof of Lemma 3.2.3: The coercivity constant $0 < c$ on the right-hand side of (3.80) ultimately depends on the entities $c_{korn}, \kappa, \eta, \|\mathbf{u}\|_W, \|\mathbf{u}\|_W^2$ and Ω, in particular it can be chosen independently of γ. Due to the analogous positivity result (3.81) of the operator R_l, it is clear that the left-hand side of (3.78) is coercive with coercivity constant independently of γ.

Next, the bound (3.92) directly follows from step (2a). Here, we want to again point out that the term in the third line of the right-hand side of (3.84) is potentially dependent on γ in the L^q-norm.

For the final γ-independent bound, we revisit the proof of step (2a) again: Similarly, we test (3.90) with $(v^u, 0) \in V$, and obtain the linearized displacement equation

$$\big(g(\varphi)\mathbb{C}e(\tilde{u}), e(v^u)\big) = -2(1-\kappa)(\varphi\mathbb{C}e(u)\tilde{\varphi}, e(v^u)) + (f^u, v^u) \quad \forall\, v^u \in V_u. \tag{3.94}$$

Directly applying [90, Proposition 1.1], $\tilde{u}$ suffices to a bound in $W^{1,p}$ depending on the right-hand side of (3.94), if the right-hand side can be bounded in the space $W^{-1,p}$. By assumption $f^u \in W^{-1,p}(\Omega;\mathbb{R}^2)$, and exploiting the additional regularity $u \in H^{1+s}(\Omega;\mathbb{R}^2)$, it can be showed that the term $\varphi\mathbb{C}e(u)\tilde{\varphi}$ can be bounded in $L^p(\Omega)$ independently of γ: We recall the standard Sobolev embedding for $\Omega \in \mathbb{R}^2$, which ensures $H^{1+s}(\Omega) \hookrightarrow W^{1,t}(\Omega)$, for a $t \leq \frac{2}{1-s}$. Also using the assumption $u \in H^{1+s}(\Omega;\mathbb{R}^2)$, this means there exists a t as stated such that

$$\|u\|_{W^{1,t}(\Omega)} \leq c\|u\|_{H^{1+s}(\Omega)} \leq c, \tag{3.95}$$

for a c independently of γ. Note that due to $s \in (0, 1/2)$, the upper bound on t lies in the interval $(2, 4)$.

Secondly, by (3.91), it holds $\tilde{\varphi} \in H^1(\Omega)$, and again by the Sobolev embedding for $\Omega \in \mathbb{R}^2$ there exists an $r \in (1, \infty)$ such that

$$\|\tilde{\varphi}\|_{L^r(\Omega)} \leq c\|\tilde{\varphi}\|_{H^1(\Omega)} \leq c, \tag{3.96}$$

again for a c independent of γ. It is therefore possible to show that the first term on the right-hand side of (3.94) can be estimated independently of γ, i.e. we check that the above choice of t and r is applicable when utilizing Hölder's inequality, to show that $\varphi\mathbb{C}e(u)\tilde{\varphi} \in L^p(\Omega)$. Recalling $\varphi \in L^\infty(\Omega)$, it remains to show that $\mathbb{C}e(u)\tilde{\varphi} \in L^p(\Omega)$ independently of γ. The following Hölder exponent calculation holds true:

$$\frac{1}{p} \geq \frac{1}{t} + \frac{1}{r} \quad \Rightarrow \quad \frac{1}{r} \leq \frac{1}{p} - \frac{1}{t} \leq \frac{1}{p} - \frac{1-s}{2} = \frac{2-p+ps}{2p},$$

i.e. $r \geq \frac{2p}{2-p+ps}$. Recalling $p > 2$, the denominator has to be positive, i.e.

$$2 - p + ps > 0 \quad \Rightarrow \quad s > \frac{p-2}{p}.$$

Thus there exists an $\epsilon_s > 0$ small, such that $s = \frac{p-2}{p} + \epsilon_s$. The choice $r \geq \frac{2}{\epsilon_s}$ and $t \leq \frac{2}{1-s} = \frac{2p}{2-p\epsilon_s}$ is now applicable for the above Sobolev embeddings and the assumed regularities of u and $\tilde{\varphi}_\gamma$. Overall,

$$\|\varphi \mathbb{C} e(u) \tilde{\varphi}\|_{L^p(\Omega)} \leq c \|\varphi\|_{L^\infty(\Omega)} \|u\|_{W^{1,t}(\Omega)} \|\tilde{\varphi}\|_{L^r(\Omega)} \leq c$$

for a c independently of γ, utilizing (3.95) and (3.96). □

3.3 Analysis of the control-to-state operator

The next task is to investigate several essential properties of the control-to-state operator $G_{\mathbb{I}}$ from (3.71). In particular, we are interested in second-order differentiability and Lipschitz results. We start with a differentiability result for control-to-state operator $G_{\mathbb{I}}$ of the multi time state equation $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$ defined in (3.71), analogously to the joint work [86, Proof of Proposition 3.3] of the author and I. Neitzel.

Proposition 3.3.1. *Let Assumption 2.3.11 hold. The control-to-state operator $G_{\mathbb{I}}$ is twice continuously Fréchet differentiable from Q^M into W^M. For the first derivative, we obtain $G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}} = \tilde{\mathbf{u}}_{\mathbb{I}}$, where $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M$ is the unique weak solution to*

$$\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v} \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^\varphi \right\rangle = (\tilde{q}^i, v^u)_Q, \qquad (3.97)$$

for all $i = 1, ..., M$ and all test functions $\mathbf{v} \in V$, and where $G(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}}$. For notational purposes, it is understood that $\tilde{\varphi}^0 := 0$, cf. Assumption 3.2.2.

For the second derivative, we find $G''_{\mathbb{I}}(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] = \mathring{\mathbf{u}}_{\mathbb{I}}$, where $\mathring{\mathbf{u}}_{\mathbb{I}} \in W^M$ is the unique weak solution to

$$\begin{aligned} &\left\langle A_l(\mathbf{u}^i)(\mathring{\mathbf{u}}^i, \mathring{\varphi}^{i-1}), \mathbf{v} \right\rangle + \left\langle R_l(\varphi^i; \varphi^{i-1}; \gamma)(\mathring{\varphi}^i, \mathring{\varphi}^{i-1}), v^\varphi \right\rangle \\ &\quad = -\left\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{v} \right\rangle - \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], v^\varphi \right\rangle, \quad (3.98) \end{aligned}$$

for all $i = 1, ..., M$ and all test functions $\mathbf{v} \in V$, and where $G_{\mathbb{I}}(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}}$, as well as $G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j} = \tilde{\mathbf{u}}_{\mathbb{I},j}$ for $j = 1, 2$. For notational purposes, it is again understood that $\mathring{\varphi}^0, \tilde{\varphi}_j^0 := 0$, for $j = 1, 2$.

Proof. To prove the statement, an implicit function theorem, cf. [162, Theorem 4.B] is utilized. Due to the structure of the nonlinear partial differential equation $(\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta})$, cf. i.p. (3.65), we introduce the operator $T_{\mathbb{I}} : Q^M \times W^M \mapsto (W^\times)^M$, for all $\mathbf{v}_{\mathbb{I}} \in V^M$, via

$$\left\langle T_{\mathbb{I}}(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}}), \mathbf{v}_{\mathbb{I}} \right\rangle = \sum_{i=1}^{M} \Big[\left\langle A(\mathbf{u}^i \varphi^{i-1}); \mathbf{v}^i \right\rangle + \left\langle R(\varphi^i, \varphi^{i-1}; \gamma), v^{\varphi,i} \right\rangle - \left\langle Bq^i, \mathbf{v}^i \right\rangle \Big].$$

The aim is to show that the mapping $T_{\mathbb{I}}$, simply being the sum over all time steps i, is continuously Fréchet differentiable from $Q^M \times W^M$ into $(W^\times)^M$, with derivative, in weak formulation for all $\mathbf{v}_{\mathbb{I}} \in V^M$, being

$$\left\langle T'_{\mathbb{I}}(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}})(\tilde{q}_{\mathbb{I}}, \tilde{\mathbf{u}}_{\mathbb{I}}), \mathbf{v}_{\mathbb{I}} \right\rangle$$

$$= \sum_{i=1}^{M} \Big[\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}^i \big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^{\varphi,i} \big\rangle - \big\langle B\tilde{q}^i, \mathbf{v}^i \big\rangle \Big]. \tag{3.99}$$

This follows from continuous Fréchet differentiability of the operators A, R and B in its corresponding spaces, which have been proved rigorously in Lemma 3.1.4 and Lemma 3.1.7. The continuity of the mappings $\mathbf{u}^i \mapsto A_l(\mathbf{u}^i)$ from W into $\mathcal{L}(W \times W_\varphi, W^\times)$ and $(\varphi^i, \varphi^{i-1}) \to R_l(\varphi^i, \varphi^{i-1}; \gamma)$ from $W_\varphi \times W_\varphi$ into $\mathcal{L}(W_\varphi \times W_\varphi, L^q(\Omega))$ has been proved in Lemma 3.1.5 and Lemma 3.1.8. Lastly, the continuous differentiability result is clear for the linear operator B.

Therefore, the derivative $T'_{\mathbb{I},\mathbf{u}_\mathbb{I}} \colon W^M \mapsto (W^\times)^M$ of $T_\mathbb{I}$ w.r.t. the state variable $\mathbf{u}_\mathbb{I}$ is also immediately given by

$$\big\langle T'_{\mathbb{I},\mathbf{u}_\mathbb{I}}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})\tilde{\mathbf{u}}_\mathbb{I}, \mathbf{v}_\mathbb{I} \big\rangle := \sum_{i=1}^{M} \Big[\big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}^i \big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^{\varphi,i} \big\rangle \Big],$$

and setting $\mathbf{f}_\mathbb{I} = (B\tilde{q}_\mathbb{I}, 0) \in (W^\times)^M$, $T'_{\mathbb{I},\mathbf{u}_\mathbb{I}}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})\tilde{\mathbf{u}}_\mathbb{I} = B\tilde{q}_\mathbb{I}$ is uniquely solvable in W^M by Lemma 3.2.3, which makes the mapping $T'_{\mathbb{I},\mathbf{u}_\mathbb{I}}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})$ invertible.

Finally, note that by Lemma 3.2.1 there exists a unique $\mathbf{u}_\mathbb{I} \in W^M$, for every $q_\mathbb{I} \in Q^M$ that satisfies $T_\mathbb{I}(q_\mathbb{I}, \mathbf{u}_\mathbb{I}) = 0$. The implicit function theorem can now be applied, thus the operator $G_\mathbb{I}$ is Fréchet differentiable from Q^M into W^M, with derivative $G'_\mathbb{I}(q_\mathbb{I})\tilde{q}_\mathbb{I} = \tilde{\mathbf{u}}_\mathbb{I}$ given by (3.97).

For the second derivative, introduce the operator

$$\tilde{T}_\mathbb{I}(q_\mathbb{I}, \mathbf{u}_\mathbb{I}) = T'_\mathbb{I}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})(\tilde{q}_{\mathbb{I},1}, \tilde{\mathbf{u}}_{\mathbb{I},1}) \colon Q^M \times W^M \mapsto (W^\times)^M,$$

with $T'_\mathbb{I}$ being defined as in (3.99). The mapping $\tilde{F}$ is again continuously Fréchet differentiable from $Q^M \times W^M$ into $(W^\times)^M$, with derivative, in weak formulation for all $\mathbf{v}_\mathbb{I} \in V^M$,

$$\big\langle \tilde{T}'_\mathbb{I}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})(\tilde{q}_{\mathbb{I},2}, \tilde{\mathbf{u}}_{\mathbb{I},2}) \big\rangle = \sum_{i=1}^{M} \Big[\big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{v}^i \big\rangle + \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], v^{\varphi,i} \big\rangle \Big].$$

The continuous Fréchet differentiability result of $\tilde{T}_\mathbb{I}$ follows from continuous Fréchet differentiability of the operators A_l and R_l in its corresponding spaces, and is again performed in Lemma 3.1.4, Lemma 3.1.7, Lemma 3.1.5 and Lemma 3.1.8. The second-order differentiability result of $G_\mathbb{I}$ from Q^M into W^M now follows again from [162, Theorem 4.B]. The partial differential equation (3.98) follows by implicit differentiation using the product rule, and setting $\tilde{T}'_\mathbb{I}(q_\mathbb{I}, \mathbf{u}_\mathbb{I})(\tilde{q}_{\mathbb{I},2}, \tilde{\mathbf{u}}_{\mathbb{I},2}) = 0$, noting that the second derivative of B is zero. □

Let us quickly put the focus on the second derivative $G''_{\mathbb{I}}$ of the control-to-state operator $G_{\mathbb{I}}$, and its associated partial differential equation (3.98).

Corollary 3.3.2. *For every $q_{\mathbb{I}}, \tilde{q}_{\mathbb{I},j} \in Q^M$, $j = 1, 2$, with associated $G_{\mathbb{I}}(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}} \in W^M$, $G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j} = \tilde{\mathbf{u}}_{\mathbb{I},j}$, and $\mathring{\varphi}^0 = 0$, cf. Assumption 3.2.2, the PDE given through* (3.98) *has a unique weak solution $\mathring{\mathbf{u}}_{\mathbb{I}} \in W^M$, that satisfies the stability property*

$$\|\mathring{u}^i\|_{W_u} + \|\mathring{\varphi}^i\|_{W_\varphi} \leq c\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},$$

for some constant $c = c(\eta, \kappa, \gamma, \|q_{\mathbb{I}}\|_{Q^M}) > 0$ and all $i = 1, ..., M$.

Proof. Set $\mathbf{f}_{\mathbb{I}}$ with $\mathbf{f}^i = -A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i] - R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})]$, for all $i = 1, .., M$. Using the assumed regularities of $\mathbf{u}_{\mathbb{I}}, \tilde{\mathbf{u}}_{\mathbb{I},j}$, $j = 1, 2$, from Lemma 3.1.3 and Lemma 3.1.6, it immediately follows

$$\begin{aligned}\|\mathbf{f}^i\|_{W^\times} &\leq c(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} + c(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \\ &\leq c(\kappa, \gamma, \|q_{\mathbb{I}}\|_{Q^M})\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},\end{aligned}$$

where for the second inequality the norm estimates from Lemma 3.2.1 and Lemma 3.2.3 were used. Thus it holds $\mathbf{f}_{\mathbb{I}} \in (W^\times)^M$, and again Lemma 3.2.3 can be utilized, which concludes the proof. □

Next, we establish Lipschitz continuity of the operators $G_{\mathbb{I}}, G'_{\mathbb{I}}$ and $G''_{\mathbb{I}}$, working analogously to [86, Lemma 3.6, 3.8 and 3.9], where this is proved for $M = 1$. This is an essential auxiliary result since it transfers to the (reduced) functional of ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$), on which the analysis of second-order optimality conditions is based upon.

Lemma 3.3.3. *For every $0 < \rho \in \mathbb{R}$ and $q_{\mathbb{I},j} \in Q^M$, $j = 1, 2$, such that $\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \leq \rho$, there exists a constant $c = c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho) > 0$ such that*

$$\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M},$$

where $\mathbf{u}_{\mathbb{I},j} = G_{\mathbb{I}}(q_{\mathbb{I},j})$.

Proof. By Proposition 3.3.1, the control-to-state operator $G_{\mathbb{I}}$ is continuously Fréchet differentiable from Q^M into W^M. Using the mean value inequality, cf. [116, Section 7.3, Proposition 2], for a $t \in [0, 1]$ it holds

$$\begin{aligned}\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} &= \|G_{\mathbb{I}}(q_{\mathbb{I},1}) - G_{\mathbb{I}}(q_{\mathbb{I},2})\|_{W^M} \\ &\leq \|G'_{\mathbb{I}}\big(q_{\mathbb{I},2} - t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)\|_{\mathcal{L}(Q^M, W^M)}\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \\ &\leq \sup_{\|\tilde{q}_{\mathbb{I}}\|_{Q^M}=1} \|G'_{\mathbb{I}}\big(q_{\mathbb{I},2} - t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)\tilde{q}_{\mathbb{I}}\|_{W^M}\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}.\end{aligned}$$

Let $W^M \ni \mathbf{u}_{\mathbb{I},t} := G_{\mathbb{I}}\big(q_{\mathbb{I},2} - t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)$ and $W \ni \tilde{\mathbf{u}}_{\mathbb{I},t} := G'_{\mathbb{I}}\big(q_{\mathbb{I},2} - t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)\tilde{q}_{\mathbb{I}}$, for any $t \in [0, 1]$. By Lemma 3.2.1, it thus follows, for a $\tilde{c}_1 :=$

$\tilde{c}_1(\kappa, M, \rho, \|q_{\mathbb{I},2}\|_{Q^M}, \|\varphi^0\|_{W_\varphi})$ independent of t and the direction $(q_{\mathbb{I},1} - q_{\mathbb{I},2})$, that

$$\|\mathbf{u}_{\mathbb{I},t}\|_{W^M} \leq \tilde{c}_1.$$

Now, setting $\mathbf{f}_{\mathbb{I}} = (B\tilde{q}_{\mathbb{I}}, 0) \in (W^\times)^M$, by Lemma 3.2.3, for a $\tilde{c}_2 := \tilde{c}_2(\eta, \gamma, M, \tilde{c}_1)$, it holds

$$\|\tilde{\mathbf{u}}_{\mathbb{I},t}\|_{W^M} \leq \tilde{c}_2 \|\tilde{q}_{\mathbb{I}}\|_{Q^M}.$$

Combining all estimates concludes the result. □

Lemma 3.3.4. *Let $\tilde{q}_{\mathbb{I}} \in Q^M$ be given. For every $0 < \rho \in \mathbb{R}$ and $q_{\mathbb{I},j} \in Q^M$, $j = 1, 2$, such that $\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \leq \rho$, there exists a constant $c = c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho) > 0$ such that*

$$\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \|\tilde{q}_{\mathbb{I}}\|_{Q^M},$$

where $\tilde{\mathbf{u}}_{\mathbb{I},j} = G'_{\mathbb{I}}(q_{\mathbb{I},j})\tilde{q}_{\mathbb{I}}$.

Proof. By Proposition 3.3.1, the operator $G_{\mathbb{I}}$ is twice continuously Fréchet differentiable from Q^M into W^M. Analogously to the proof of Lemma 3.3.3, for a $t \in [0, 1]$, it holds

$$\begin{aligned}
&\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \\
&\quad \leq \|G'_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I}} - G'_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I}}\|_{W^M} \\
&\quad \leq \|G''_{\mathbb{I}}\big(q_{\mathbb{I},2} + t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)\tilde{q}_{\mathbb{I}}\|_{\mathcal{L}(Q^M, W^M)} \|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \\
&\quad \leq \sup_{\|\tilde{q}_{\mathbb{I},2}\|_{Q^M}=1} \|G''_{\mathbb{I}}\big(q_{\mathbb{I},2} + t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)[\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},2}]\|_{W^M} \|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

For any $t \in [0, 1]$, set $W^M \ni \mathring{\mathbf{u}}_{\mathbb{I},t} := G''_{\mathbb{I}}\big(q_{\mathbb{I},2} + t(q_{\mathbb{I},1} - q_{\mathbb{I},2})\big)[\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},2}]$ and utilizing Corollary 3.3.2 yields, for a $\tilde{c} = \tilde{c}(\eta, \kappa, \gamma, M, \rho, \|q_{\mathbb{I},2}\|_{Q^M})$ independent of t and the direction $(q_{\mathbb{I},1} - q_{\mathbb{I},2})$,

$$\|\mathring{\mathbf{u}}_{\mathbb{I},t}\|_{W^M} \leq \tilde{c}\|\tilde{q}_{\mathbb{I}}\|_{Q^M} \|\tilde{q}_{\mathbb{I},2}\|_{Q^M}.$$

The assertion now follows from collecting all estimates. □

As the previous results, also the following lemma, showing a Lipschitz result for the second-derivative of the control-to-state operator, follows analogously as in the one time step setting from [86]. We have seen that up until now, establishing our results also for $M > 1$ were only slight adaptions, mainly introducing some additional notation and taking care of the involved previous $i-1$-time steps, cf. Section 3.1. However, let us point out that it is in fact important to choose the notation carefully, as e.g. can be seen when looking at Lipschitz continuity results for G'':

Lemma 3.3.5. *Let $\tilde{q}_{\mathbb{I},j} \in Q^M$, $j = 1, 2$ be given. For every $0 < \rho \in \mathbb{R}$ and $q_{\mathbb{I},j} \in Q^M$, $j = 1, 2$, such that $\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \leq \rho$, there exists a constant $c = c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho, M)$ such that*

$$\|\mathring{\mathbf{u}}_{\mathbb{I},1} - \mathring{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},$$

where $\mathring{\mathbf{u}}_{\mathbb{I},1} = G''_{\mathbb{I}}\big(q_{\mathbb{I},1}\big)[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}]$ and $\mathring{\mathbf{u}}_{\mathbb{I},2} = G''_{\mathbb{I}}\big(q_{\mathbb{I},2}\big)[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}]$.

Proof. Let $\mathring{\mathbf{u}}_{\mathbb{I},1}$ and $\mathring{\mathbf{u}}_{\mathbb{I},1}$ be as assumed. For clarification, we recall Definition 2.3.4, and set the following notation for the solutions of (3.63), (3.72), respectively, for different data $q_{\mathbb{I},j}, \tilde{q}_{\mathbb{I},j}$, $j = 1, 2$,

$$\begin{aligned}
G_{\mathbb{I}}(q_{\mathbb{I},1}) &=: \mathbf{u}_{\mathbb{I},1} = (\mathbf{u}_1^1, ..., \mathbf{u}_1^M),\\
G_{\mathbb{I}}(q_{\mathbb{I},2}) &=: \mathbf{u}_{\mathbb{I},2} = (\mathbf{u}_2^1, ..., \mathbf{u}_2^M),\\
G'_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I},1} &=: \tilde{\mathbf{u}}_{\mathbb{I},1,1} = (\tilde{\mathbf{u}}_{1,1}^1, ..., \tilde{\mathbf{u}}_{1,1}^M),\\
G'_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I},1} &=: \tilde{\mathbf{u}}_{\mathbb{I},1,2} = (\tilde{\mathbf{u}}_{1,2}^1, ..., \tilde{\mathbf{u}}_{1,2}^M),\\
G'_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I},2} &=: \tilde{\mathbf{u}}_{\mathbb{I},2,1} = (\tilde{\mathbf{u}}_{2,1}^1, ..., \tilde{\mathbf{u}}_{2,1}^M),\\
G'_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I},2} &=: \tilde{\mathbf{u}}_{\mathbb{I},2,2} = (\tilde{\mathbf{u}}_{2,2}^1, ..., \tilde{\mathbf{u}}_{2,2}^M).
\end{aligned}$$

The function $\mathring{\mathbf{u}}_{\mathbb{I},1}$ then satisfies, for all $i = 1, ..., M$,

$$\begin{aligned}
&A_l(\mathbf{u}_1^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1}) + R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma)(\mathring{\varphi}_1^i, \mathring{\varphi}_1^{i-1})\\
&\quad = - A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_{1,1}^i, \tilde{\mathbf{u}}_{2,1}^i] - R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_{1,1}^i, \tilde{\varphi}_{1,1}^{i-1}), (\tilde{\varphi}_{2,1}^i, \tilde{\varphi}_{2,1}^{i-1})], \qquad (3.100)
\end{aligned}$$

while the function $\mathring{\mathbf{u}}_{\mathbb{I},2}$ satisfies, for all $i = 1, ..., M$,

$$\begin{aligned}
&A_l(\mathbf{u}_2^i)(\mathring{\mathbf{u}}_2^i, \mathring{\varphi}_2^{i-1}) + R_l(\varphi_2^i; \varphi_2^{i-1}; \gamma)(\mathring{\varphi}_2^i, \mathring{\varphi}_2^{i-1})\\
&\quad = - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,2}^i, \tilde{\mathbf{u}}_{2,2}^i] - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_{1,2}^i, \tilde{\varphi}_{1,2}^{i-1}), (\tilde{\varphi}_{2,2}^i, \tilde{\varphi}_{2,2}^{i-1})], \qquad (3.101)
\end{aligned}$$

where $\tilde{\varphi}_{1,j}^0, \tilde{\varphi}_{2,j}^0 = 0$, $j = 1, 2$, cf. Assumption 3.2.2. Taking the difference of (3.100) and (3.101), due to linearity of A_l and R_l for $\mathring{\mathbf{u}}^i$, $\mathring{\varphi}^i$ and $\mathring{\varphi}^{i-1}$ cf. (3.1) and (3.2), yields for all $i = 1, ..., M$, the partial differential equation

$$\begin{aligned}
&A_l(\mathbf{u}_2^i)(\mathring{\mathbf{u}}_1^i - \mathring{\mathbf{u}}_2^i, \mathring{\varphi}_1^{i-1} - \mathring{\varphi}_2^{i-1}) + R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\mathring{\varphi}_1^i - \mathring{\varphi}_2^i, \mathring{\varphi}_1^{i-1} - \mathring{\varphi}_2^{i-1})\\
&\quad = - \big(A_l(\mathbf{u}_1^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1}) - A_l(\mathbf{u}_2^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1})\big)\\
&\qquad - \big(R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma)(\mathring{\varphi}_1^i, \mathring{\varphi}_1^{i-1}) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\mathring{\varphi}_1^i, \mathring{\varphi}_1^{i-1})\big)\\
&\qquad - \big(A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_{1,1}^i, \tilde{\mathbf{u}}_{2,1}^i] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,2}^i, \tilde{\mathbf{u}}_{2,2}^i]\big)\\
&\qquad - \big(R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_{1,1}^i, \tilde{\varphi}_{1,1}^{i-1}), (\tilde{\varphi}_{2,1}^i, \tilde{\varphi}_{2,1}^{i-1})]\\
&\qquad\quad - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_{1,2}^i, \tilde{\varphi}_{1,2}^{i-1}), (\tilde{\varphi}_{2,2}^i, \tilde{\varphi}_{2,2}^{i-1})]\big). \qquad (3.102)
\end{aligned}$$

We want to utilize Lemma 3.2.3, thus the right-hand sides of (3.102) needs to be estimated in the $W^\times$-norm. The first difference of the right-hand side of (3.102) is estimated, using Lemma 3.1.5, via

$$\|A_l(\mathbf{u}_1^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1}) - A_l(\mathbf{u}_2^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1})\|_{W^\times}$$

$$\leq c(\kappa)\big(\|\mathbf{u}_1^i\|_W + \|\mathbf{u}_2^i\|_W\big)\|\mathbf{u}_1^i - \mathbf{u}_2^i\|_W \|\mathring{\mathbf{u}}_1^i\|_W.$$

Continuing the estimation, utilizing Lemma 3.2.1, Corollary 3.3.2 as well as Lemma 3.3.3, yields

$$\begin{aligned}
&\|A_l(\mathbf{u}_1^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1}) - A_l(\mathbf{u}_2^i)(\mathring{\mathbf{u}}_1^i, \mathring{\varphi}_1^{i-1})\|_{W^\times} \\
&\quad \leq c(\kappa)\big(\tilde{c}\|q_{\mathbb{I},1}\|_{Q^M} + \tilde{c}\|q_{\mathbb{I},2}\|_{Q^M}\big) c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},1}\|_{Q^M} \\
&\qquad \cdot c(\eta, \kappa, \gamma, \|q_{\mathbb{I},1}\|_{Q^M})\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

Note that the constant $\tilde{c} := \max(c(\eta, \gamma, \|\mathbf{u}_{\mathbb{I},1}\|_{W^M}), c(\eta, \gamma, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M}))$ is implied by (3.77). Due to the triangle inequality $\|q_{\mathbb{I},1}\|_{Q^M} = \|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} + \rho$, the constant $\tilde{c}$ and $c(\eta, \kappa, \gamma, \|q_{\mathbb{I},1}\|_{Q^M})$ can in fact be expressed via a $c = c(\eta, \kappa, \gamma, \|q_{\mathbb{I},2}\|_{Q^M}, \rho)$. Here, notice that for the last inequality the dependence of c on some constants is dropped, and we only keep track of the constants we are interested in. For the difference in the R_l term, analogously it follows

$$\begin{aligned}
&\|R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma)(\mathring{\varphi}_1^i, \mathring{\varphi}_1^{i-1}) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\mathring{\varphi}_1^i, \mathring{\varphi}_1^{i-1})\|_{L^q(\Omega)} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

For the differences in the A_b-terms, rearranging using the linearity of A_b in all three entries as well as Lemma 3.1.3, similarly to above we conclude

$$\begin{aligned}
&\big\|A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_{1,1}^i, \tilde{\mathbf{u}}_{2,1}^i] - A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,2}^i, \tilde{\mathbf{u}}_{2,2}^i]\big\|_{W^\times} \\
&\quad \leq \big\|A_b(\mathbf{u}_1^i - \mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,1}^i, \tilde{\mathbf{u}}_{2,1}^i]\|_{W^\times} + \big\|A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,1}^i - \tilde{\mathbf{u}}_{1,2}^i, \tilde{\mathbf{u}}_{2,1}^i]\|_{W^\times} \\
&\qquad + \big\|A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_{1,2}^i, \tilde{\mathbf{u}}_{2,1}^i - \tilde{\mathbf{u}}_{2,2}^i]\big\|_{W^\times} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

As mentioned in Remark 3.1.1, A_b can be identified by the A''-terms in [86, Equation (43) of the proof of Lemma 3.9], so alternatively this estimate can also be followed in the same way as in [86, Proof of Lemma 3.9].

For the differences in the R_b-terms, we calculate

$$\begin{aligned}
&\big\| - R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_{1,1}^i, \tilde{\varphi}_{1,1}^{i-1}), (\tilde{\varphi}_{2,1}^i, \tilde{\varphi}_{2,1}^{i-1})] \\
&\qquad + R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_{1,2}^i, \tilde{\varphi}_{1,2}^{i-1}), (\tilde{\varphi}_{2,2}^i, \tilde{\varphi}_{2,2}^{i-1})]\big\|_{L^q(\Omega)} \\
&\quad = \big\|\big(R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)[(\tilde{\varphi}_{1,1}^i, \tilde{\varphi}_{1,1}^{i-1}), (\tilde{\varphi}_{2,1}^i, \tilde{\varphi}_{2,1}^{i-1})]\big\|_{L^q(\Omega)} \\
&\qquad + \big\|R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_{1,1}^i - \tilde{\varphi}_{1,2}^i, \tilde{\varphi}_{1,1}^{i-1} - \tilde{\varphi}_{1,2}^{i-1}), (\tilde{\varphi}_{2,1}^i, \tilde{\varphi}_{2,1}^{i-1})]\big\|_{L^q(\Omega)} \\
&\qquad + \big\|R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_{1,2}^i, \tilde{\varphi}_{1,2}^{i-1}), (\tilde{\varphi}_{2,1}^i - \tilde{\varphi}_{2,2}^i, \tilde{\varphi}_{2,1}^{i-1} - \tilde{\varphi}_{2,2}^{i-1})]\big\|_{L^q(\Omega)} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},
\end{aligned}$$

where we used (3.58) from Lemma 3.1.8, as well as Lemma 3.1.6, and then continued the estimate in the same way as for the first term of (3.102).

Combining all equations, the right-hand side of (3.102) can be estimated. We now can use Lemma 3.2.3, which yields

$$\|\mathring{\mathbf{u}}_1^i - \mathring{\mathbf{u}}_2^i\|_W \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},$$

which holds for all $i = 1, ..., M$, and concludes the proof. □

Let us conclude the analysis of the nonlinear fracture propagation Euler-Lagrange equation ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$) and its solution operator $G_{\mathbb{I}}$ with the following remark:

Remark 3.3.6. *In the context of optimal control, the controls $q_{\mathbb{I}}$ are subject to the constraint $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}} \subset Q^M$, where $Q_{ad,\mathbb{I}}$ is defined as in Definition 2.3.3. In particular, this means that $Q_{ad,\mathbb{I}}$ is bounded, therefore for all $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ we in fact obtain global Lipschitz continuity results.*

3.4 Analysis of the (reduced) objective functional

This section covers differentiability and Lipschitz continuity results of the (reduced) objective functional of the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$). For $M = 1$, i.e. for the one time step model, these results are published in [86, Section 3.2 and Section 3.3] by the author and I. Neitzel. We present them here also for $M > 1$, i.e. the multi time step ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$). In this context, some additional caution is necessary due to the coupling in time through the involvement of both the previous and the successive time step in the adjoint operators A_{l*} and R_{l*}. Again, we rely on the auxiliary results of the operators A_{l*} and R_{l*} from Section 3.1.

Let us introduce the reduced functional associated to the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$): Using the control-to-state operator $G_{\mathbb{I}}$ from (3.71), we obtain a reduced objective functional formulation

$$f_{\mathbb{I}} \colon Q^M \to \mathbb{R}, \qquad f_{\mathbb{I}}(q_{\mathbb{I}}) := J_{\mathbb{I}}(q_{\mathbb{I}}, G_{\mathbb{I}}(q_{\mathbb{I}})), \tag{3.103}$$

implicitly using that W^M is embedded in $(L^2(\Omega, \mathbb{R}^2) \times L^2(\Omega))^M$.

Due to the structure of the objective functional, involving a tracking type functional and a Tikhonov regularization term, the results for $G_{\mathbb{I}}, G'_{\mathbb{I}}$, and $G''_{\mathbb{I}}$ from Section 3.3 can be transferred to $f_{\mathbb{I}}, f'_{\mathbb{I}}$ and $f''_{\mathbb{I}}$. A rather straight-forward differentiability result directly follows for the reduced objective functional $f_{\mathbb{I}}$.

Corollary 3.4.1. *Let Assumption 2.3.11 hold, let $q_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},j} \in Q^M$, for $j = 1, 2$. The reduced functional f from* (3.103) *is twice Fréchet differentiable from Q^M into $\mathbb{R}$. The first derivative is given by*

$$f'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}} := \sum_{i=1}^{M}(u^i - u_d^i, \tilde{u}^i) + \sum_{i=1}^{M}\alpha(q^i, \tilde{q}^i)_Q, \tag{3.104}$$

where $\mathbf{u}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})$ *and* $\tilde{\mathbf{u}}_{\mathbb{I}} = G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}}$.

The second derivative is given by

$$f''_{\mathbb{I}}(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] = \sum_{i=1}^{M} \Big[(\tilde{u}_2^i, \tilde{u}_1^i) + (u^i - u_d^i, \mathring{u}^i)\Big] + \sum_{i=1}^{M} \alpha(\tilde{q}_2^i, \tilde{q}_1^i)_Q, \qquad (3.105)$$

where $\mathbf{u}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})$, $\tilde{\mathbf{u}}_{\mathbb{I},j} = G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j}$, *for* $j = 1, 2$, *and* $\mathring{\mathbf{u}} = G''_{\mathbb{I}}(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}]$.

Proof. This immediately follows from Proposition 3.3.1 and the chain rule. □

Lipschitz continuity results for the reduced functional $f_{\mathbb{I}}$ and its derivatives $f'_{\mathbb{I}}$ and $f''_{\mathbb{I}}$ are now obtained as a consequence of Lemma 3.3.3, Lemma 3.3.4 and Lemma 3.3.5.

Lemma 3.4.2. *Let* $\tilde{q}_{\mathbb{I},j} \in Q^M$, $j = 1, 2$, *be given. For every* $0 < \rho \in \mathbb{R}$ *and* $q_{\mathbb{I},j} \in Q^M$, *for* $j = 1, 2$, *such that* $\max(\|q_{\mathbb{I},1}\|_{Q^M}, \|q_{\mathbb{I},2}\|_{Q^M}, \|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}) \leq \rho$, *there exists a constant* $c = c(\rho, M) > 0$ *such that*

$$\Big|f_{\mathbb{I}}(q_{\mathbb{I},1}) - f_{\mathbb{I}}(q_{\mathbb{I},2})\Big| \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}, \qquad (3.106)$$

$$\Big|f'_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I},1} - f'_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I},1}\Big| \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}, \qquad (3.107)$$

$$\Big|f''_{\mathbb{I}}(q_{\mathbb{I},1})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] - f''_{\mathbb{I}}(q_{\mathbb{I},2})[\tilde{q}_{\mathbb{I},1}.\tilde{q}_{\mathbb{I},2}]\Big| \leq c\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M}. \qquad (3.108)$$

Proof. We work analogously to [86, Proof of Lemma 3.10]. Let $q_{\mathbb{I},j}, \tilde{q}_{\mathbb{I},j}$, $j = 1, 2$, be as stated, and let

$$G_{\mathbb{I}}(q_{\mathbb{I},1}) = \mathbf{u}_{\mathbb{I},1} = (\mathbf{u}_1^1, ..., \mathbf{u}_1^M), \qquad G_{\mathbb{I}}(q_{\mathbb{I},2}) = \mathbf{u}_{\mathbb{I},2} = (\mathbf{u}_2^1, ..., \mathbf{u}_2^M).$$

Using the definition (3.103) of $f_{\mathbb{I}}$, we calculate

$$\begin{aligned}
&\Big|f_{\mathbb{I}}(q_{\mathbb{I},1}) - f_{\mathbb{I}}(q_{\mathbb{I},1})\Big| \\
&\quad = \Bigg|\frac{1}{2}\sum_{i=1}^{M}\Big[(u_1^i - u_2^i, u_1^i) + (u_1^i - u_2^i, u_2^i) - 2(u_1^i - u_2^i, u_d^i)\Big] \\
&\qquad\qquad + \frac{\alpha}{2}\sum_{i=1}^{M}\Big[(q_1^i - q_2^i, q_1^i) + (q_1^i - q_2^i, q_2^i)\Big]\Bigg| \\
&\quad \leq c\sum_{i=1}^{M}\Big[\|u_1^i - u_2^i\|_{W_u}\|u_1^i\|_{W_u} + \|u_1^i - u_2^i\|_{W_u}\|u_2^i\|_{W_u} \\
&\qquad\qquad + \|u_1^i - u_2^i\|_{W_u}\|u_d^i\|_{L^2(\Omega;\mathbb{R}^2)} + \|q_1^i - q_2^i\|_Q\|q_1^i\|_Q + \|q_1^i - q_2^i\|_Q\|q_2^i\|_Q\Big] \\
&\quad \leq cMc(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|q_{\mathbb{I},1}\|_{Q^M} \\
&\qquad + cMc(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}\|q_{\mathbb{I},2}\|_{Q^M} \\
&\qquad + cMc(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \\
&\qquad + cM\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}(\|q_{\mathbb{I},1}\|_{Q^M} + \|q_{\mathbb{I},2}\|_{Q^M})
\end{aligned}$$

$$\leq c(M, \|q_{\mathbb{I},1}\|_{Q^M}, \|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M},$$

where Lemma 3.2.1 and Lemma 3.3.3 were utilized, and $c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)$ is the constant from Lemma 3.3.3. Note further that the multi time step function definition, cf. Definition 2.3.4, is used.

For the first derivative $f'_{\mathbb{I}}$, let us additionally introduce the notation (which is the same notation as in the proof of Lemma 3.3.5),

$$G_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I},1} = \tilde{\mathbf{u}}_{\mathbb{I},1,1} = (\tilde{\mathbf{u}}^1_{1,1}, ..., \tilde{\mathbf{u}}^M_{1,1}), \qquad G_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I},1} = \tilde{\mathbf{u}}_{\mathbb{I},1,2} = (\tilde{\mathbf{u}}^1_{1,2}, ..., \tilde{\mathbf{u}}^M_{1,2}),$$

and, using the representation (3.104) of $f'_{\mathbb{I}}$, we calculate

$$\begin{aligned}
&\left|\big(f'_{\mathbb{I}}(q_{\mathbb{I},1}) - f'_{\mathbb{I}}(q_{\mathbb{I},2})\big)\tilde{q}_{\mathbb{I},1}\right| \\
&= \Bigg| \sum_{i=1}^M \Big[(u^i_1 - u^i_2, \tilde{u}^i_{1,1}) + (u^i_2, \tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}) - (u^i_d, \tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}) \Big] \\
&\qquad + \alpha \sum_{i=1}^M \Big[(q^i_1 - q^i_2, \tilde{q}^i_1) + (q^i_2, \tilde{q}^i_1 - \tilde{q}^i_2) \Big] \Bigg| \\
&\leq c \sum_{i=1}^M \Big[\|u^i_1 - u^i_2\|_{W_u} \|\tilde{u}^i_{1,1}\|_{W_u} + \|u^i_2\|_{W_u} \|\tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}\|_{W_u} \\
&\qquad + \|u^i_d\|_{L^2(\Omega;\mathbb{R}^2)} \|\tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}\|_{W_u} + \|q^i_1 - q^i_2\|_Q \|\tilde{q}^i_1\|_Q + \|q^i_2\|_Q \|\tilde{q}^i_1 - \tilde{q}^i_2\|_Q \Big] \\
&\leq c(M, \|q_{\mathbb{I},1}\|_{Q^M}, \|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \|\tilde{q}_{\mathbb{I},1}\|_{Q^M},
\end{aligned}$$

similarly to above, also additionally utilizing Lemma 3.2.3 and Lemma 3.3.4.

Finally, introduce additionally the notation (which again is the same notation as in the proof of Lemma 3.3.5),

$$\begin{aligned}
G_{\mathbb{I}}(q_{\mathbb{I},1})\tilde{q}_{\mathbb{I},2} &= \tilde{\mathbf{u}}_{\mathbb{I},2,1} = (\tilde{\mathbf{u}}^1_{2,1}, ..., \tilde{\mathbf{u}}^M_{2,1}), \\
G_{\mathbb{I}}(q_{\mathbb{I},2})\tilde{q}_{\mathbb{I},2} &= \tilde{\mathbf{u}}_{\mathbb{I},2,2} = (\tilde{\mathbf{u}}^1_{2,2}, ..., \tilde{\mathbf{u}}^M_{2,2}), \\
G_{\mathbb{I}}(q_{\mathbb{I},1})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] &= \mathring{\mathbf{u}}_{\mathbb{I},1} = (\mathring{\mathbf{u}}^1_1, ..., \mathring{\mathbf{u}}^M_1), \\
G_{\mathbb{I}}(q_{\mathbb{I},2})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] &= \mathring{\mathbf{u}}_{\mathbb{I},2} = (\mathring{\mathbf{u}}^1_2, ..., \mathring{\mathbf{u}}^M_2),
\end{aligned}$$

which, in combination with the representation (3.105) of $f''_{\mathbb{I}}$, leads to

$$\begin{aligned}
&\left| f''_{\mathbb{I}}(q_{\mathbb{I},1})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] - f''_{\mathbb{I}}(q_{\mathbb{I},2}[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] \right| \\
&= \Bigg| \sum_{i=1}^M \Big[(\tilde{u}^i_{2,1} - \tilde{u}^i_{2,2}, \tilde{u}^i_{1,1}) + (\tilde{u}^i_{2,2}, \tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}) \\
&\qquad + (u^i_1 - u^i_2, \mathring{u}^i_1) + (u^i_2, \mathring{u}^i_1 - \mathring{u}^i_2) - (u^i_d, \mathring{u}^i_1 - \mathring{u}^i_2) \Big] \Bigg| \\
&\leq c \sum_{i=1}^M \Big[\|\tilde{u}^i_{2,1} - \tilde{u}^i_{2,2}\|_{W_u} \|\tilde{u}^i_{1,1}\|_{W_u} + \|\tilde{u}^i_{2,2}\|_{W_u} \|\tilde{u}^i_{1,1} - \tilde{u}^i_{1,2}\|_{W_u}
\end{aligned}$$

$$+ \|u_1^i - u_2^i\|_{W_u} \|\mathring{u}_1^i\|_{W_u} + \|u_2^i\|_{W_u} \|\mathring{u}_1^i - \mathring{u}_2^i\|_{W_u}$$
$$+ \|u_d^i\|_{W_u} \|\mathring{u}_1^i - \mathring{u}_2^i\|_{W_u} \Big]$$
$$\leq c(M, \|q_{\mathbb{I},1}\|_{Q^M}, \|q_{\mathbb{I},2}\|_{Q^M}, \rho) \|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \|\tilde{q}_{\mathbb{I},1}\|_{Q^M} \|\tilde{q}_{\mathbb{I},2}\|_{Q^M},$$

again similarly to above, also additionally using Corollary 3.3.2 as well as Lemma 3.3.5. This concludes the proof. □

To conclude the analysis of the preliminary technical results of the reduced functional f, we also take a quick look at explicit representations of $f'_{\mathbb{I}}$ and $f''_{\mathbb{I}}$, which requires the introduction of a so-called adjoint equation. We omit further explanations of the meaning of adjoint equations until Section 4.1, where they occur in the context of first-order necessary optimality conditions. This connection however is not important at this point.

Recalling the operators $A_{l,*}$ and $R_{l,*}$ from (3.5) and (3.6), the backwards-in-time adjoint partial differential equation, is closely related to the linearized equation (3.72). We introduce it in its three equivalent forms, for given $\mathbf{u}_{\mathbb{I}} \in W^M$, $\varphi^0 \in W_\varphi$, data $\mathbf{f}_{\mathbb{I},adj} \in (W^\times)^M$, and (3.9): Firstly, for all $i = 1, ..., M$, solve for $\mathbf{z}_{\mathbb{I}} \in V^M$ the system

$$A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) = \mathbf{f}^i_{adj}, \tag{3.109}$$

which in weak form can be formulated, for all test functions $\mathbf{v} = (v^u, v^\varphi) \in V$, by

$$\big\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}), \mathbf{v} \big\rangle + \big\langle R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^\varphi \big\rangle = \big\langle \mathbf{f}^i_{adj}, \mathbf{v} \big\rangle. \tag{3.110}$$

Finally, this is equivalent to: For all test functions $\mathbf{v}_{\mathbb{I}} \in V^M$ look for the solution $\mathbf{z}_{\mathbb{I}} \in V^M$ of

$$\sum_{i=1}^{M} \Big[\big\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}), \mathbf{v}^i \big\rangle + \big\langle R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), v^{\varphi,i} \big\rangle \Big]$$
$$= \sum_{i=1}^{M} \big\langle \mathbf{f}^i_{adj}, \mathbf{v}^i \big\rangle. \tag{3.111}$$

The corresponding solvability result is then a corollary of Lemma 3.2.3.

Corollary 3.4.3. *Let $\mathbf{u}_{\mathbb{I}} \in W^M, \varphi^0 \in W_\varphi$ be given, and $\psi^{M+1} := 0$. Then for every $\mathbf{f}_{\mathbb{I},adj} \in (W^\times)^M$, there exists a unique solution $\mathbf{z}_{\mathbb{I}} \in W^M$ to* (3.109)*, that satisfies the stability property*

$$\|z^i\|_{W_u} + \|\psi^i\|_{W_\varphi} \leq c \|\mathbf{f}_{adj,\mathbb{I}}\|_{(W^\times)^M}, \tag{3.112}$$

for all $i = 1, ..., M$, and the constant c from Equation (3.77)*.*

Proof. Looking at the operators A_{l*} and R_{l*}, we see that except for the terms involving $\tilde{\varphi}^{i-1}$, respectively ψ^{i+1}, they are the same as A_l and R_l. These terms occur linearly, and the operators A_{l*} and R_{l*} are now dependent on the successive time steps instead of the previous. The proof therefore works analogously to the proof of Lemma 3.2.3, just backwards in time. This means that the starting point is $i = M$, which then works in the same way as in steps (1a) and (2a) of the proof of Lemma 3.2.3. The other steps are then made inductively for $i = M-1, .., 1$, in the same way as in the steps (1b) and (2b) in the proof of the same lemma. □

Again similarly to Lemma 3.2.4, let us quickly restrict the setting to one time step. We have already seen in Remark 3.1.2, that the operators A_{l*} and R_{l*} are then self-adjoint. Thus, we can directly apply Lemma 3.2.4 to obtain the following result for the solution of the one time step adjoint equation, in particular with a γ-independent bound in V. This is utilized in Chapter 5.

Corollary 3.4.4. *Let $\mathbf{u} \in W$ and $\varphi^0 \in W_\varphi$ be given. For every $\mathbf{f}_{adj} \in V$, there exists a unique solution $\mathbf{z} \in V$ to*

$$\big\langle (A_{l*}(\mathbf{u}))(\mathbf{z}, 0), \mathbf{v} \big\rangle + \big\langle (R_{l*}(\varphi, \varphi^0; \gamma))(\psi, 0), v^\varphi \big\rangle = \big\langle \mathbf{f}_{adj}, v^\varphi \big\rangle \quad \forall \mathbf{v} \in V, \quad (3.113)$$

and it holds

$$\|z\|_{V_u} + \|\psi\|_{V_\varphi} \leq c\|\mathbf{f}\|_V, \quad (3.114)$$

where $c > 0$ is the constant from (3.91)*. Analogously to the the bounds from* (3.92) *and* (3.93)*, we can also bound (z, ψ) in W (with a c depending on γ) and z in W_u (with a c independently of γ).*

Next, let us additionally establish an auxiliary result for later use. In particular, we show a Lipschitz result for the adjoint equation for specific given right-hand sides. After rigorously introducing the adjoint equation associated to ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) below in Section 4.1, it will become clear that we in fact prove a Lipschitz result for the solution of this adjoint equation, already here.

Corollary 3.4.5. *Let $0 < \rho \in \mathbb{R}$ arbitrary, and $q_{\mathbb{I},j} \in Q^M$ such that $\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \leq \rho$, and $W^M \ni \mathbf{u}_{\mathbb{I},j} = G_{\mathbb{I}}(q_{\mathbb{I},j})$, $j = 1, 2$. Further, let $\mathbf{z}_{\mathbb{I},j} \in W^M$ be the solutions to*

$$A_{l*}(\mathbf{u}_j^i)(\mathbf{z}_j^i, \psi_j^{i+1}) + R_{l*}(\varphi_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}; \gamma)(\psi_j^i, \psi_j^{i+1}) = u_j^i - u_d^i, \quad (3.115)$$

for all $i = 1, ..., M$. Then there exists a constant $0 < c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho) \in \mathbb{R}$ such that

$$\|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M} \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}$$

Proof. The difference $\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}$ fulfills for all $i = 1, ..., M$,

$$A_{l*}(\mathbf{u}_1^i)\big((\mathbf{z}_1^i, \psi_1^{i+1}) - (\mathbf{z}_2^i, \psi_2^{i+1})\big) + R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}; \gamma)\big((\psi_1^i, \psi_1^{i+1}) - (\psi_2^i, \psi_2^{i+1})\big)$$

$$= u_1^i - u_2^i + \big(A_{l*}(\mathbf{u}_2^i) - A_{l*}(\mathbf{u}_1^i)\big)(\mathbf{z}_2^i, \psi_2^{i+1})$$
$$+ \big(R_{l*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \gamma) - R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}; \gamma)\big)(\psi_2^i, \psi_2^{i+1}). \tag{3.116}$$

Before we estimate the terms on the right-hand side of (3.116), we want to point out that it is clear that $\|\mathbf{u}_{\mathbb{I},j}\|_{W^M} \leq c\|q_{\mathbb{I},j}\|_{Q^M}$ by Lemma 3.2.1, and therefore $\|\mathbf{z}_{\mathbb{I}.j}\|_W \leq c(\|\mathbf{u}_{\mathbb{I},j}\|_{W^M} + 1) \leq c(\|q_{\mathbb{I},j}\|_{Q^M} + 1)$ by Corollary 3.4.3.

Now, by Lemma 3.3.3 and for all $i = 1, ..., M$, it holds

$$\|u_1^i - u_2^i\|_{W^\times} \leq \|u_1^i - u_2^i\|_W \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}. \tag{3.117}$$

By Lemma 3.1.5 and then using the triangle inequality as well as (3.117) and the right-hand side estimates for $\|\mathbf{u}_{\mathbb{I},j}\|_{W^M}, \|\mathbf{z}_{\mathbb{I},j}\|_{W^M}$ given in the paragraph below (3.116), we obtain

$$\begin{aligned}
&\|\big(A_{l*}(\mathbf{u}_2^i) - A_{l*}(\mathbf{u}_1^i)\big)(\mathbf{z}_2^i, \psi_2^{i+1})\|_{W^\times} \\
&\quad \leq c\big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I},2}\|_{W^M} \\
&\quad \leq c\big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + 2\|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I},2}\|_{W^M} \\
&\quad \leq c\big(\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} + 2\|q_{\mathbb{I},2}\|_{Q^M}\big)\big(\|q_{\mathbb{I},2}\|_{Q^M} + 1\big)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

Analogously, using Lemma 3.1.8, we obtain

$$\begin{aligned}
&\|\big(R_{l*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \gamma) - R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}; \gamma)\big)(\psi_2^i, \psi_2^{i+1})\|_{L^q(\Omega)} \\
&\quad \leq c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

Therefore the right-hand side of (3.116) can be estimated in the $W^\times$-norm by $c(\|q_{\mathbb{I},2}\|_{Q^M}, \rho)\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M}$, thus the statement follows immediately by applying Corollary 3.4.3. □

We can now come back to the reduced objective functional $f_{\mathbb{I}}$ and its derivatives: The first derivative $f_{\mathbb{I}}'$ and the second derivative $f_{\mathbb{I}}''$ of the reduced objective functional $f_{\mathbb{I}}$, cf. (3.104), (3.105) and (3.103), can equivalently be expressed in the following form.

Corollary 3.4.6. *The first derivative $f_{\mathbb{I}}'$ from* (3.104) *of the reduced functional $f_{\mathbb{I}}$ from* (3.103) *can equivalently be expressed by*

$$f_{\mathbb{I}}'(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}} = \sum_{i=1}^{M}(B^*\mathbf{z}^i + \alpha q^i, \tilde{q}^i)_Q, \tag{3.118}$$

where $\mathbf{u}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})$, and $\mathbf{z}_{\mathbb{I}} \in W^M$ is the weak solution to (3.115) *for all $i = 1, ..., M$ and data $\mathbf{f}_{adj,\mathbb{I}}$ such that $\mathbf{f}_{adj}^i = (u^i - u_d^i, 0)$, for all $i = 1, ..., M$.*

The second derivative $f_{\mathbb{I}}''$ from (3.105) *of the reduced functional $f_{\mathbb{I}}$ from* (3.103) *can equivalently be expressed by*

$$f_{\mathbb{I}}''(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] = \sum_{i=1}^{M}\Big[(\tilde{u}_1^i, \tilde{u}_2^i) + \alpha(\tilde{q}_2^i, \tilde{q}_1^i)_Q - \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i\big\rangle$$

$$- \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \right\rangle \Big], \quad (3.119)$$

where again $G_{\mathbb{I}}(q_{\mathbb{I}}) = \mathbf{u}_{\mathbb{I}} \in W^M$, $G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j}$, for $j = 1, 2$, and $\mathbf{z}_{\mathbb{I}} \in W^M$ is the weak solution to (3.115) *for all $i = 1, ..., M$ and data $\mathbf{f}_{adj,\mathbb{I}}$ such that $\mathbf{f}^i_{adj} = (u^i - u^i_d, 0)$, for all $i = 1, ..., M$.*

Proof. Firstly, note that by Corollary 3.4.3, $\mathbf{z}_{\mathbb{I}} \in W^M$ is the unique solution of (3.109), since $\mathbf{f}^i_{adj} = (u^i - u^i_d, 0) \in W^\times$ holds true due to $u_{d,\mathbb{I}} \in (L^2(\Omega; \mathbb{R}^2))^M$ and $u_{\mathbb{I}} \subset (L^2(\Omega; \mathbb{R}^2))^M$, the latter following immediately from $\mathbf{u}_{\mathbb{I}} \in W^M$. Further, by Lemma 3.2.3, there exists a unique solution $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M$ to

$$\sum_{i=1}^{M} \Big[\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{v}^i \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), v^{\varphi,i} \right\rangle \Big]$$
$$= \sum_{i=1}^{M} \left\langle \tilde{q}^i, B^* \mathbf{v}^i \right\rangle_Q, \quad (3.120)$$

for all test functions $\mathbf{v}_{\mathbb{I}} \in V^M$, since $(B\tilde{q}^i, 0) \hookrightarrow W^\times$, due to $\tilde{q}_{\mathbb{I}} \in Q^M$. It is therefore possible to test (3.120) with $\mathbf{z}_{\mathbb{I}} \in W^M \hookrightarrow V^M$, to obtain

$$\sum_{i=1}^{M} \Big[\left\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{z}^i \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), \psi^i \right\rangle \Big] = \sum_{i=1}^{M} \left\langle \tilde{q}^i, B^* \mathbf{z}^i \right\rangle_Q, \quad (3.121)$$

and to use the test function $\tilde{\mathbf{u}}_{\mathbb{I}} \in W^M \hookrightarrow V^M$ for the equation that $\mathbf{z}_{\mathbb{I}}$ fulfills, which leads to

$$\sum_{i=1}^{M} \Big[\left\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}), \tilde{\mathbf{u}}^i \right\rangle + \left\langle R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), \tilde{\varphi}^i \right\rangle \Big]$$
$$= \sum_{i=1}^{M} (u^i - u^i_d, \tilde{u}^i). \quad (3.122)$$

By writing out the sum of the left-hand side of (3.121) and (3.122), it is clear that the left-hand sides of both equations are the same. In fact, this is precisely the motivation for the operators A_{l*} and R_{l*} from (3.7) and (3.8). We conclude

$$\sum_{i=1}^{M} (u^i - u^i_d, \tilde{u}^i) = \sum_{i=1}^{M} \left\langle \tilde{q}^i, B^* \mathbf{z}^i \right\rangle_Q,$$

and inserting this into (3.104) immediately leads to to the first statement of the lemma, cf. (3.118).

For the representation of the second derivative $f''_{\mathbb{I}}$, we recall from Corollary 3.3.2 that there exists a unique solution $\mathring{\mathbf{u}}_{\mathbb{I}} \in W^M$ to

$$\sum_{i=1}^{M} \Big[\left\langle A_l(\mathbf{u}^i)(\mathring{\mathbf{u}}^i, \mathring{\varphi}^{i-1}), \mathbf{v}^i \right\rangle + \left\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\mathring{\varphi}^i, \mathring{\varphi}^{i-1}), v^{\varphi,i} \right\rangle \Big]$$

$$= \sum_{i=1}^{M} \Big[- \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{v}^i \big\rangle$$

$$- \big\langle R_b(\varphi^i;, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], v^{\varphi,i} \big\rangle \Big], \tag{3.123}$$

for all test functions $\mathbf{v}_{\mathbb{I}} \in V^M$, and where $\tilde{\mathbf{u}}_{\mathbb{I}} = G'_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j}$, for $j = 1, 2$. Now, testing (3.123) with $\mathbf{z}_{\mathbb{I}} \in W^M \hookrightarrow V^M$, we obtain

$$\sum_{i=1}^{M} \Big[\big\langle A_l(\mathbf{u}^i)(\mathring{\mathbf{u}}^i, \mathring{\varphi}^{i-1}), \mathbf{z}^i \big\rangle + \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\mathring{\varphi}^i, \mathring{\varphi}^{i-1}), \psi^i \big\rangle \Big]$$

$$= - \sum_{i=1}^{M} \Big[\big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i \big\rangle$$

$$+ \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \big\rangle \Big]. \tag{3.124}$$

Further, it is again possible to use the test function $\mathring{\mathbf{u}}_{\mathbb{I}} \in W^M \hookrightarrow V^M$ for the equation that $\mathbf{z}_{\mathbb{I}}$ satisfies, which yields

$$\sum_{i=1}^{M} \Big[\big\langle A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}), \mathring{\mathbf{u}}^i \big\rangle + \big\langle R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}), \mathring{\varphi}^i \big\rangle \Big]$$

$$= \sum_{i=1}^{M} (u^i - u_d^i, \mathring{u}^i). \tag{3.125}$$

Similarly, as in the case above for the first derivative, the left-hand sides of both (3.125) and (3.124) are equal, thus

$$\sum_{i=1}^{M} (u^i - u_d^i, \mathring{u}^i) = - \sum_{i=1}^{M} \Big[\big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i \big\rangle$$

$$+ \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \big\rangle \Big],$$

which immediately leads to (3.119). □

3.5 Analysis of the Lagrangian functional

In this section, we look at the Lagrangian functional. The Lagrangian is used later in the context of SQP method, and shares many properties with the reduced functional. For $M = 1$, i.e. the one time step setting, the Lagrangian is investigated in [85, Section 3.2 and 3.3] by I. Neitzel and the author. In this section, we establish the results also for $M > 1$, i.e. for the to $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$ associated Lagrangian. The motivation for the Lagrangian functional stems from the context of the well-known Lagrangian principle, cf. e.g. [153, Section 2.10]. In the given context, this approach means that the equality constraints in

($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), which are given through the Euler-Lagrange equations ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$), are eliminated by including them into the functional, using so-called Lagrangian multipliers.

Recalling the notation for function triples $y_{\mathbb{I}} = (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}})$ introduced in Definition 2.3.3 and Definition 2.3.4, the Lagrangian functional associated to ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) is defined via

$$\begin{aligned}
&\mathcal{L}_{\mathbb{I}}\colon\ Y^M \to \mathbb{R},\\
&\mathcal{L}_{\mathbb{I}}(y_{\mathbb{I}}) := J_{\mathbb{I}}(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}}) - \sum_{i=1}^{M} \Big[\big\langle A(\mathbf{u}^i, \varphi^{i-1}), \mathbf{z}^i \big\rangle + \big\langle R(\varphi^i, \varphi^{i-1}; \gamma), \psi^i \big\rangle - \big\langle Bq^i, \mathbf{z}^i \big\rangle \Big]\\
&\quad = \sum_{i=1}^{M} \Big[\frac{1}{2} \|u^i - u_d^i\|^2 + \frac{\alpha}{2} \|q^i\|_Q^2\\
&\qquad - \big\langle A(\mathbf{u}^i, \varphi^{i-1}), \mathbf{z}^i \big\rangle - \big\langle R(\varphi^i, \varphi^{i-1}; \gamma), \psi^i \big\rangle + \big\langle Bq^i, \mathbf{z}^i \big\rangle \Big], \quad (3.126)
\end{aligned}$$

where $\mathbf{z}_{\mathbb{I}} \in W^M$ is the so-called Lagrangian multiplier, and $J_{\mathbb{I}}$ is the objective functional of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), cf. ($\mathrm{P}_{\mathbb{I}}^{\gamma,\eta}$). It is well known that the Lagrangian multiplier corresponds to the associated adjoint state, which is introduced in the context of optimality conditions below, for which we again refer to Section 4.1.

We are interested in second-order differentiability results of the Lagrangian $\mathcal{L}_{\mathbb{I}}$. Before differentiability is analyzed, let us clarify some notation, which holds throughout the entire thesis:

Notation 3.5.1. *The second derivative $\mathcal{L}_{\mathbb{I}}''$ of the Lagrangian functional $\mathcal{L}_{\mathbb{I}}$ is always understood with respect to the function pair $(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})$. It is denoted by*

$$\begin{aligned}
&\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})]\\
&\quad := \mathcal{L}_{\mathbb{I}\,(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}),(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})}''(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1} \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})].
\end{aligned}$$

Now, the differentiability and Lipschitz results of $f_{\mathbb{I}}$ from Section 3.4 transfer to the Lagrangian $\mathcal{L}_{\mathbb{I}}$. In particular, it holds:

Corollary 3.5.2. *The Lagrangian functional $\mathcal{L}_{\mathbb{I}}$ is twice continuously Fréchet differentiable from $W^M \times Q^M$ into $\mathbb{R}$. The second derivative can be expressed via*

$$\begin{aligned}
&\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})]\\
&\quad = \sum_{i=1}^{M} \Big[(\tilde{u}_1^i, \tilde{u}_2^i)_{L^2(\Omega;\mathbb{R}^2)} + \alpha(\tilde{q}_1^i, \tilde{q}_2^i)_Q - \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i \big\rangle\\
&\qquad - \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \big\rangle \Big].
\end{aligned}$$

For $\tilde{\mathbf{u}}_{\mathbb{I},j} = G_{\mathbb{I}}'(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},j}$, $j = 1, 2$, as well as $\mathbf{u}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})$, and $\mathbf{z}_{\mathbb{I}}$ satisfying (3.115), *it thus holds*

$$\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] = f_{\mathbb{I}}''(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}]. \quad (3.127)$$

Proof. An easy calculation, using the Fréchet differentiability results of A, R, A_l and R_l, cf. Lemma 3.1.4 and Lemma 3.1.7, leads to

$$\begin{aligned}\mathcal{L}'_{\mathbb{I}}(y_{\mathbb{I}})(\tilde{\mathbf{u}}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}) = \sum_{i=1}^{M} \Big[&(u^i - u_d^i, \tilde{u}^i) + \alpha(q^i, \tilde{q}^i)_Q \\ &- \big\langle A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i, \tilde{\varphi}^{i-1}), \mathbf{z}^i \big\rangle + \big\langle B\tilde{q}^i, \mathbf{z}^i \big\rangle \\ &- \big\langle R_l(\varphi^i, \varphi^{i-1}; \gamma)(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), \psi^i \big\rangle \Big],\end{aligned}$$

and subsequently also to

$$\begin{aligned}&\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] \\ &= \sum_{i=1}^{M} \Big[(\tilde{u}_1^i, \tilde{u}_2^i) + \alpha(\tilde{q}_1^i, \tilde{q}_2^i)_Q - \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i \big\rangle \\ &\qquad - \big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \big\rangle \Big].\end{aligned}$$

The second statement now follows directly from the representation of $f''_{\mathbb{I}}$ from Corollary 3.4.6. □

On the one hand, Lipschitz continuity of $\mathcal{L}''_{\mathbb{I}}$ could now be followed immediately from (3.127) and Lemma 3.4.2. On the other hand, we are also interested in a Lipschitz continuity result of $\mathcal{L}''_{\mathbb{I}}$ w.r.t the involved functions $\mathbf{u}_{\mathbb{I}}$ and $\mathbf{z}_{\mathbb{I}}$, for which we can explicitly track the Lipschitz constant.

Lemma 3.5.3. *There exists a constant* $0 < c := c(\kappa, \gamma, M) \in \mathbb{R}$*, such that for all* $y_{\mathbb{I},j} \in Y^M$ *and all* $(\tilde{\mathbf{u}}_{\mathbb{I},j}, \tilde{q}_{\mathbb{I},j}) \in W^M \times Q^M$*, where* $j = 1, 2$*, it holds*

$$\begin{aligned}&\big|\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I},1}) - \mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I},2})\big|[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] \\ &\le c\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\Big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},2}\|_{W^M}\Big) \\ &\qquad \cdot \Big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},2} - \mathbf{z}_{\mathbb{I},1}\|_{W^M}\Big).\end{aligned}$$

Proof. We work analogously to [85, Proposition 3.8]. A quick calculation verifies:

$$\begin{aligned}&\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I},1}) - \mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I},2})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] \\ &= \sum_{i=1}^{M} \Big[\big\langle A_b(\mathbf{u}_2^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}_2^i \big\rangle - \big\langle A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}_1^i \big\rangle \\ &\qquad + \big\langle R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi_2^i \big\rangle \\ &\qquad - \big\langle R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi_1^i \big\rangle \Big] \\ &= \sum_{i=1}^{M} \Big[\big\langle \big(A_b(\mathbf{u}_2^i) - A_b(\mathbf{u}_1^i)\big)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}_2^i \big\rangle + \big\langle A_b(\mathbf{u}_1^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}_2^i - \mathbf{z}_1^i \big\rangle \\ &\qquad + \big\langle \big(R_b(\varphi_2^i, \varphi_2^{i-1}; \gamma) - R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)\big)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi_2^i \big\rangle\end{aligned}$$

$$+ \left\langle R_b(\varphi_1^i, \varphi_1^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi_2^i - \psi_1^i \right\rangle \Big]$$

Now, utilizing the results of Lemma 3.1.3, Lemma 3.1.5, Lemma 3.1.6 and Lemma 3.1.8 yields

$$\begin{aligned}
&\left|\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I},1}) - \mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I},2})\right| [(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] \\
&\quad \leq Mc(\kappa) \|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \|\mathbf{z}_{\mathbb{I},2}\|_{W^M} \\
&\qquad + Mc(\kappa) \|\mathbf{u}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \|\mathbf{z}_{\mathbb{I},2} - \mathbf{z}_{\mathbb{I},1}\|_{W^M} \\
&\qquad + Mc(\gamma) \|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \|\mathbf{z}_{\mathbb{I},2}\|_{W^M} \\
&\qquad + Mc(\gamma) \|\mathbf{u}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \|\mathbf{z}_{\mathbb{I},2} - \mathbf{z}_{\mathbb{I},1}\|_{W^M} \\
&\quad \leq c(\kappa, \gamma, M) \Big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},2}\|_{W^M} \Big) \|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \\
&\qquad \cdot \Big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},2} - \mathbf{z}_{\mathbb{I},1}\|_{W^M} \Big),
\end{aligned}$$

and the statement follows immediately. □

Lemma 3.5.4. *There exists a constant $0 < c := c(\kappa, \gamma, M) \in \mathbb{R}$ such that for all $y_{\mathbb{I}} \in Y$ and all $(\tilde{\mathbf{u}}_{\mathbb{I},j}, \tilde{q}_{\mathbb{I},j}) \in W^M \times Q^M$, $j = 1, 2$, it holds*

$$\begin{aligned}
&\left|\mathcal{L}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1})] - \mathcal{L}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})]\right| \\
&\quad \leq c \|\mathbf{u}_{\mathbb{I}}\|_{W^M} \|\mathbf{z}_{\mathbb{I}}\|_{W^M} \Big(\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} + \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \Big) \|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \\
&\qquad + c \Big(\|\tilde{q}_{\mathbb{I},1}\|_{Q^M} + \|\tilde{q}_{\mathbb{I},2}\|_{Q^M} \Big) \|\tilde{q}_{\mathbb{I},1} - \tilde{q}_{\mathbb{I},2}\|_{Q^M}.
\end{aligned}$$

Proof. Again, analogously to [85, Proposition 3.8], a quick calculation verifies:

$$\begin{aligned}
&\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},1})] - \mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2}), (\tilde{\mathbf{u}}_{\mathbb{I},2}, \tilde{q}_{\mathbb{I},2})] \\
&\quad = \sum_{i=1}^{M} \Big[\|\tilde{u}_1^i\| - \|\tilde{u}_2^i\| + \alpha\big(\|\tilde{q}_1^i\|_Q - \|\tilde{q}_2^i\|_Q\big) \\
&\qquad\qquad + \left\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_2^i, \tilde{\mathbf{u}}_2^i], \mathbf{z}^i \right\rangle - \left\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_1^i], \mathbf{z}^i \right\rangle \\
&\qquad\qquad + \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1})], \psi^i \right\rangle \\
&\qquad\qquad - \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1})], \psi^i \right\rangle \Big] \\
&\quad = \sum_{i=1}^{M} \Big[\|\tilde{u}_1^i\| - \|\tilde{u}_2^i\| + \alpha\big(\|\tilde{q}_1^i\|_Q - \|\tilde{q}_2^i\|_Q\big) \\
&\qquad\qquad + \left\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_2^i, \tilde{\mathbf{u}}_2^i - \tilde{\mathbf{u}}_1^i], \mathbf{z}^i \right\rangle \\
&\qquad\qquad + \left\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_2^i - \tilde{\mathbf{u}}_1^i, \tilde{\mathbf{u}}_1^i], \mathbf{z}^i \right\rangle \\
&\qquad\qquad + \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1}), (\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1}) - (\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1})], \psi^i \right\rangle \\
&\qquad\qquad + \left\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_2^i, \tilde{\varphi}_2^{i-1}) - (\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1}), (\tilde{\varphi}_1^i, \tilde{\varphi}_1^{i-1})], \psi^i \right\rangle \Big]. \qquad (3.128)
\end{aligned}$$

Now, utilizing the Lipschitz continuity of the squared norms, as well as Lemma 3.1.3 and Lemma 3.1.6, yields

$$\begin{aligned}
&\big|\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},1},\tilde{q}_{\mathbb{I},1}),(\tilde{\mathbf{u}}_{\mathbb{I},1},\tilde{q}_{\mathbb{I},1})] - \mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},2},\tilde{q}_{\mathbb{I},2}),(\tilde{\mathbf{u}}_{\mathbb{I},2},\tilde{q}_{\mathbb{I},2})]\big| \\
&\quad \leq Mc\big(\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M} + \|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\big)\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M} \\
&\qquad + Mc\Big(\|\tilde{q}_{\mathbb{I},1}\|_{Q^M} + \|\tilde{q}_{\mathbb{I},2}\|_{Q^M}\Big)\|\tilde{q}_{\mathbb{I},1} - \tilde{q}_{\mathbb{I},2}\|_{Q^M} \\
&\qquad + Mc(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M} \\
&\qquad + Mc(\kappa)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M} \\
&\qquad + Mc(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M} \\
&\qquad + Mc(\gamma)\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},1}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M},
\end{aligned}$$

again, the statement follows immediately.

□

Note that both Lemma 3.5.3 and Lemma 3.5.4 hold true with estimates that involve the V^M-norm for the directions, i.e. $\|\tilde{\mathbf{u}}_{\mathbb{I},j}\|_{V^M}$, $j = 1, 2$, and the difference in the directions $\|\tilde{\mathbf{u}}_{\mathbb{I},1} - \tilde{\mathbf{u}}_{\mathbb{I},2}\|_{V^M}$, cf. [85, Proposition 3.8] for the equivalent result in the one time step setting. However, such a result is not necessary for the subsequent chapters, and to avoid further additional notation we omit these results here.

4. Second-order necessary and sufficient optimality conditions

This chapter is concerned with the first main results of this thesis: Second-order optimality conditions for the phase-field fracture optimal control problem ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$). In particular, we prove second-order necessary conditions in Theorem 4.2.2 and second-order sufficient conditions, which do not involve a two-norm discrepancy, in Theorem 4.2.4. These necessary and sufficient conditions involve only a minimal gap. We subsequently also establish so-called σ-strongly active second-order sufficient conditions in Corollary 4.3.2, which are slightly stronger and which are needed later for Chapter 6. For $M = 1$, i.e. the one time step model, both necessary and sufficient second-order optimality conditions are published as joint work [86] of the author and I. Neitzel, and σ-strongly active second-order sufficient conditions are previously used in the joint work [85] of the author and I. Neitzel. To prove our main results, we show that a general theorem concerning second-order optimality conditions from [38] can be applied. Here, the technical results proved in Chapter 3 are utilized. Note that σ-strongly active second-order sufficient conditions are a known technique in the convergence analysis of the SQP method, and have been introduced in the context of sequential quadratic programming (SQP) in [70, 152].

Let us start with an introduction into (first- and second-order) optimality conditions, following the exposition in [44, Section 1 and Section 2]. From calculus, the following facts for optimization problems in the vector space $\mathbb{R}^n$ are well-known: Let $\mathcal{F}\colon \mathbb{R}^n \mapsto \mathbb{R}$ be a differentiable function, then for all local minima $\bar{x}$ the first-order necessary condition

$$\mathcal{F}'(\bar{x}) = 0 \tag{4.1}$$

has to be satisfied. If the function is twice differentiable, then the Hessian matrix $\mathcal{F}''(\bar{x})$ has to be positive semi-definite, i.e.

$$x^T \mathcal{F}''(\bar{x}) x \geq 0 \qquad \forall\, x \in \mathbb{R}^n, \tag{4.2}$$

where x^T denotes the transpose of the vector x. Due to the involvement of the Hessian, (4.2) constitutes a second-order condition, in particular a second-order necessary condition. In return, we can also give a (second-order) sufficient condition: If $\bar{x}$ satisfies both $F'(\bar{x}) = 0$ and the Hessian is positive definite, i.e. if it holds

$$x^T F''(\bar{x})x > 0 \qquad \forall\, x \in \mathbb{R}^n \backslash \{0\}, \tag{4.3}$$

then $\bar{x}$ is indeed a local minimum of F, and not a maximum or a saddle-point. Note that this means in particular that if the function F is (strictly) convex, then the first-order necessary condition is already a sufficient condition. As stated on [44, page 10], it is important that for the finite dimensional setting the condition (4.3) is equivalent to the existence of some $c > 0$ such that

$$x^T F''(\bar{x})x \geq c\|x\|^2_{\mathbb{R}^n}. \tag{4.4}$$

Still following [44], let us continue with optimality conditions of optimization problems in function space: As of now, let $\mathbb{V}$ be a generic Banach Space. Let the (reduced) objective functional $\tilde{F} : \mathbb{V} \to \mathbb{R}$ be continuously (Fréchet) differentiable in $\mathbb{V}$ on the domain Ω, not necessarily the same domain as in Assumption 2.3.1. Let us further use $v \in \mathbb{V}$ as the control, and $\bar{v} \in \mathbb{V}$ as the optimal control. The model problem is then of the form $\min \tilde{F}(v)$, s.t. $v \in \mathbb{V}$ and similarly to (4.1), first-order necessary conditions are given by

$$\tilde{F}'(\bar{v}) = 0. \tag{4.5}$$

Subsequently, a second-order sufficient condition, see [44, Theorem 3.4], is proved in [35]: Let us additionally assume that $\tilde{F}$ is twice continuously (Fréchet) differentiable in a neighborhood of $\bar{v}$. If $\bar{v}$ satisfies the first-order necessary condition (4.5) and there exists a $c > 0$ such that

$$\tilde{F}''(\bar{v})[v, v] \geq c\|v\|^2_V \qquad \forall v \in \mathbb{V}, \tag{4.6}$$

i.e. $\tilde{F}''(\bar{v})$ satisfies a coercivity condition for the space $\mathbb{V}$, then $\bar{v}$ is a strict local optimal solution[1].

Let us cite [44, page 12], which states that [44, Theorem 3.4], respectively (4.6), "[...] might create the impression that the theory of second-order conditions is fairly analogous to that in finite dimensions. This expectation is wrong, because the celebrated *two-norm discrepancy* occurs in many problems of interest". This is first recognized by [97], which describes the difficulty that for many optimization problems, a coercivity condition like (4.6) does not hold in the same space in which the reduced functional is twice (Fréchet) differentiable. At this point, let us put on record that for $(\mathrm{NLP}^{\gamma,\eta}_{\mathbb{I}})$, we have already seen in Corollary 3.4.1 that the reduced functional $f_{\mathbb{I}}$ is twice (Fréchet) differentiable in Q^M, i.e. in L^2. The space Q^M is also the space a coercivity condition like (4.6) can be expected, see Remark 4.2.5 below. Therefore this so-called two-norm discrepancy does not occur in the second-order sufficient conditions we prove below in Theorem 4.2.4 for the phase-field optimal control problem $(\mathrm{NLP}^{\gamma,\eta}_{\mathbb{I}})$. However, for many other problems, the reduced functional is twice Fréchet differentiable only in a stronger

[1] For the definition of local optimal solutions in this context, see e.g. Definition 4.1.2

norm, e.g. the L^∞-norm, while the coercivity condition holds in a weaker norm like e.g. the L^2-norm. The resulting gap between the two norms is then called the two-norm gap. This means that while in finite dimensions this does not pose any problems due to the well-known norm equivalence, in the infinite dimensional setting it is important to be careful when choosing the involved norms, as can e.g. be seen for some quick and too formal calculations in [40, Example 1.2]. In [40], it is subsequently proved that many results that one might expect initially only in the (stronger) L^∞-sense can be extended to hold also in the (weaker) L^2-setting. In particular, [40] establishes strict local optimality for an abstract optimal control problem setting. This result e.g. covers elliptic optimal control problems subject to Neumann and Dirichlet boundary controls, in the L^2-sense through a quadratic growth condition in L^2-neighborhoods under some additional conditions, even if the problem is subject to the two-norm discrepancy. Similarly, a quasilinear parabolic optimal control problem setting is analyzed in [96] w.r.t. tightening the involved two-norm gap for the associated SSCs of [23]. Besides the aspect of the two-norm discrepancy, we again point out that the equivalence of (4.3) and (4.4) is important in the finite dimensional case. As we see in Remark 4.2.5, it is possible to show a similar property if certain conditions are satisfied, as e.g. for the setting of ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$).

Since the model problem ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$) involves the admissible set $Q_{\text{ad},\mathbb{I}}$, let us also add control constraints to the model optimization problem $\min \tilde{F}(v)$. Let a convex, closed and nonempty admissible set $\mathbb{V}_{\text{ad}}$ be given such that $\mathbb{V}_{\text{ad}} \subset \mathbb{V}$. In particular, we assume that the admissible set is given by control box constraints

$$\mathbb{V}_{\text{ad}} = \{v \in \mathbb{V} \quad | \quad v_a(x) \leq v(x) \leq v_b(x) \quad \text{ for a.e. } x \in \Omega\}$$

for some threshold functions v_a, v_b with $v_a(x) \leq v_b(x)$ for all $x \in \Omega$, similarly to the admissible set $Q_{\text{ad},\mathbb{I}}$ from Definition 2.3.4. We follow [44, Section 3.3], and point out that clearly a first-order necessary condition of the form (4.5) cannot hold anymore for the optimal control problem $\min \tilde{F}(v)$, s.t. $v \in \mathbb{V}_{\text{ad}}$. Instead, it is a standard approach to formulate first-order necessary conditions via a so-called variational inequality in the form

$$\tilde{F}'(\bar{v})(v - \bar{v}) \geq 0 \qquad \forall v \in \mathbb{V}_{\text{ad}}. \tag{4.7}$$

Note that subsequently, it is also common to rewrite the optimality condition (4.7) into a KKT type condition. At this point, we omit this step, but for an example of a KKT type condition, e.g. for ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$), we refer to Lemma 4.1.3 below. Now, by the minimum principle [43], cf. also [153, Section 4.10], it is possible to conclude from (4.7) that $\bar{v}$ is already determined on the (active) set

$$\tilde{A}_0(x) := \{x \in \Omega \quad | \quad |\tilde{F}'(\bar{v}(x))| > 0\}, \tag{4.8}$$

cf. also [153, Equation (4.99)]. Second-order necessary conditions are therefore especially of interest on the complement of this set. Still following the reasoning of [44, Section 3.3] and [153, Section 4.10], we can define a cone of critical directions $\tilde{C}_0(\bar{v})$, see [153, page 245], of all $h \in \mathbb{V}$ such that

$$\begin{cases} h(x) = 0 & x \in \tilde{A}_0(x), \\ h(x) \geq 0 & x \notin \tilde{A}_0(x) \text{ and } \bar{v}(x) = v_a(x), \\ h(x) \leq 0 & x \notin \tilde{A}_0(x) \text{ and } \bar{v}(x) = v_b(x). \end{cases}$$

A second-order necessary condition for $\min \tilde{F}(v),$ s.t. $v \in \mathbb{V}_{\text{ad}}$ is then given in [153, Theorem 4.27] by

$$\tilde{F}''(\bar{v})[h, h] \geq 0 \qquad \forall h \in \tilde{C}_0(\bar{v}). \tag{4.9}$$

Subsequently, for sufficient conditions of second-order, the cone $\tilde{C}(\bar{v})$ can be introduced similarly to [153, Equation (4.102)], via

$$\tilde{C}(\bar{v}) := \{v \in \mathbb{V} \quad | \quad v(x) \geq 0 \text{ if } v(x) = v_a(x) \\ \text{and } v(x) \leq 0 \text{ if } v(x) = v_b(x)\}.$$

A second-order sufficient condition is then be given by: There exists a $c > 0$ such that

$$\tilde{F}''(\bar{v})[v, v] \geq c\|v\|_{\mathbb{V}}^2 \qquad \forall v \in \tilde{C}(\bar{v}). \tag{4.10}$$

However, [153, Remark on page 247] claims that sufficient conditions like (4.10) are "[...] too restrictive". The reason is the gap between the cone $\tilde{C}(\bar{v})$ of the second-order sufficient conditions and the cone $\tilde{C}_0(\bar{v})$ of the second-order necessary conditions. On the one hand, it is appealing to keep this gap as close as possible. On the other hand, in the context of the analysis of numerical methods, second-order sufficient conditions involving directions in a cone like $\tilde{C}(\bar{v})$, or even on the whole control set $\mathbb{V}$, are widely used as assumptions, as stated on [153, page 247]. While one reason for such a choice is that the convergence analysis of numerical methods can be more involved when cones are involved, another reason to widen the aforementioned gap can be seen when looking at the SQP method in Chapter 6: There, we have to use slightly different second-order sufficient conditions than the ones with the smallest gap attainable for $(\text{NLP}_{\mathbb{I}}^{\gamma,\eta})$, because we need to ensure that for each iteration step of the SQP method, the directions of the succeeding step must again satisfy the corresponding SSC. If the cone of critical directions is too small these succeeding directions might not lie therein anymore. To rectify this issue in the context of SQP methods for optimal control problems with semilinear PDEs, [152] proposes to introduce so-called σ-strongly second-order sufficient conditions, on which we also base our SQP convergence proof in Chapter 6 on. In general, the larger the set of possible directions is chosen, the stronger the SSCs are. SSCs involving the directions from the whole control space $\mathbb{V}$ are SSCs in the strongest sense, and the closer the cone of critical directions is chosen towards the cone from the necessary conditions, e.g. by involving sign conditions or so-called (strongly-) active constraints, cf. [45], the weaker the SSCs become. The interested reader is also referred to [24], where the gap between second-order necessary and sufficient conditions is further elaborated.

Next, let us give a brief literature overview in the context of (second-order optimality conditions of) PDE constrained optimal control problems: The first studied problems in e.g. [114] are (quadratic) optimal control problems involving linear PDEs. Due to the linearity of the involved PDEs, most of these problems are convex and therefore the established first-order necessary conditions are also sufficient. As a consequence, second-order conditions are not of particular interest. However, second-order conditions come into focus when optimal control problems with semilinear and quasilinear PDEs are investigated. Here, combinations of different constraints and settings are involved, e.g. for optimal control problems governed by elliptic and parabolic partial differential equations with additional box constraints on the control variable, cf. e.g. [94, 153]. Optimal control problems with state constraints are e.g. analyzed in [37, 41, 46], and second-order optimality conditions for a nonlinear optimal control problem in function space restricted by equality and inequality constraints are established in [42]. For an extended overview of second-order conditions in different settings and their applications, let us refer to [44] and the comprehensive reference list given therein. Let us point out that if both the local minimum is given analytically and the definiteness of the second derivative of the reduced objective functional can be checked analytically, then the basic ideas from calculus can be transferred also to the infinite dimensional PDE constrained optimal control setting, as stated on [44, page 8]. Unfortunately, only for a very limited amount of academic examples analytical solutions can be given, cf. e.g. [100, 127]. Concurrently, for solutions that are only given approximately as e.g. the result of numerical methods, the verification of second-order sufficient conditions is both a difficult task and can also be carried out only for some cases, see [141]. Nevertheless, the importance of second-order sufficient conditions is emphasized again on [44, page 8]: "[...] second-order conditions develop their power mainly as theoretical assumptions. They ensure stability of optimal solutions with respect to perturbations of the problems such as finite element discretizations". The stability w.r.t. perturbations is also an essential tool in the convergence analysis of many numerical algorithms. Let us revisit this aspect in Chapter 6, where we investigate the convergence of the SQP method.

Let us conclude this introduction by giving an overview of the course of action and the main results of this chapter. We have already seen a quick overview and motivation for second-order optimality conditions in this introduction. Before we can come to second-order optimality conditions of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), it is essential to look at existence and first-order necessary optimality results. These are already established results, and are recapitulated in Section 4.1 – under a slight adaption to the setting of this thesis – from [132]. In Section 4.2, we then show second-order necessary optimality conditions in Theorem 4.2.2 and second-order sufficient conditions in Theorem 4.2.4. In particular, Theorem 4.2.2 is showed for directions that lie in the critical cone $C(\bar{q}_{\mathbb{I}})$, cf. (4.16), analogously to the necessary conditions (4.9) of the above model problem with a comparable critical cone. For the proof, a significant part of the work has already been done in Section 3.4 by showing the technical prerequisites which allow us to utilize a general second-order optimality condition result from [38]. For Theorem 4.2.4, we assume a (strict) positivity condition for $f''_{\mathbb{I}}(\bar{q})$ for all directions in $C(\bar{q}_{\mathbb{I}})\backslash\{0\}$, cf. (4.18), and prove a quadratic growth condition that does not involve the two-norm discrepancy, i.e. a local optimality result in the Hilbert space L^2. Again, we show that we can apply a general second-order optimality condition result from [38]. Note that as explained in Remark 4.2.5 this means in particular that overall the gap between the necessary and sufficient conditions is minimal. Finally, we have already hinted that in the context of the SQP method for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) in Chapter 6, we have to rely on slightly stronger SSCs than the one proved in Section 4.2. In Section 4.3, we take up on this idea, which originally stems from [70, 152], and also establish so-called σ-strongly second-order sufficient conditions for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$).

4.1 Revisiting existence of solutions and first-order necessary conditions of the optimal control problem

We can now finally turn our focus back to the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$). The start are solvability and first-order necessary conditions, that originally are showed for a to ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) related problem in [132]. The main differences in the state equation between [132] and the setting of this thesis, cf. ($\mathrm{EL}_{\mathbb{I}}^{\gamma,\eta}$), is outlined in Section 3.2. Furthermore, in [132] no control constraints are involved in the optimal control problem, i.e. $Q_{ad,\mathbb{I}} := Q^M$. Let us point out again that for $M = 1$, i.e. one time step setting of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), solvability and first-order necessary conditions are also given in the joint work [86] of I. Neitzel and the author, also by a slight adaption of the results of [132].

We start with the following standard procedure: In (3.103), we have already stated the reduced functional $f_{\mathbb{I}}$, using the solution operator $G_{\mathbb{I}}$ from (3.71). Recall that, as throughout the whole thesis, we expect Assumption 2.3.11 to hold, i.e. the viscous approximation parameter η being sufficiently large. Subsequently, the reduced form of the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) can be introduced:

$$\min_{q_{\mathbb{I}}\in Q_{\mathrm{ad},\mathbb{I}}} f_{\mathbb{I}}(q_{\mathbb{I}}), \qquad (\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}})$$

where $f_{\mathbb{I}}$ is the reduced objective functional originally from (3.103).

The first result is a global existence result for solutions to ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), or equivalently ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}}$).

Proposition 4.1.1. *There exists at least one global minimizer $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$, with associated optimal state $\bar{\mathbf{u}}_{\mathbb{I}} \in W^M$, to* $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}})$.

Proof. The proof works in the same way as [132, Theorem 4.3], on which also [86, Theorem 4.1] relies for the case $M = 1$: The admissible set $Q_{\mathrm{ad},\mathbb{I}}$ is a bounded, closed and convex subset of $(L^2(\Gamma))^M$. Further, for $k \to \infty$, and minimizing sequence $\{q_{\mathbb{I},k}\} \subset Q_{\mathrm{ad},\mathbb{I}}$, the associated sequence of states $\{(u_{\mathbb{I},k}, \varphi_{\mathbb{I},k})\}$ is bounded in W^M by Lemma 3.2.1. Standard theory can now be applied, cf. [153, Teorem 2.14] or [94, Theorem 1.45]. □

Although the tracking type terms in the objective functional are of convex structure, due to the nonlinear state equation, the overall problem is nonconvex. It is therefore of interest to characterize local solutions of $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}})$.

Definition 4.1.2. *A control $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ is called a local minimizer of* $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}})$ *in the sense of L^2, if there exists a radius $r > 0$ such that*

$$f_{\mathbb{I}}(\bar{q}_{\mathbb{I}}) \leq f_{\mathbb{I}}(q_{\mathbb{I}}) \quad \forall\, q_{\mathbb{I}} \in Q_{ad,\mathbb{I}} \quad \textit{with} \quad \|\bar{q}_{\mathbb{I}} - q_{\mathbb{I}}\|_{Q^M} \leq r.$$

Every local minimizer $\bar{q}_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}$, with associated optimal state $\bar{\mathbf{u}}_{\mathbb{I}} = G_{\mathbb{I}}(\bar{q}_{\mathbb{I}})$, satisfies the first-order optimality conditions of $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta,\mathrm{red}})$ given by the following lemma.

Lemma 4.1.3. *If $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ is a local minimizer with associated state $\bar{\mathbf{u}}_{\mathbb{I}} \in W^M$, there exists an adjoint state $\bar{\mathbf{z}}_{\mathbb{I}} = (\bar{z}_{\mathbb{I}}, \bar{\psi}_{\mathbb{I}}) \in W^M$ such that*

$$A(\bar{\mathbf{u}}^i; \bar{\varphi}^{i-1}) + R(\bar{\varphi}^i; \bar{\varphi}^{i-1}, \gamma) = B\bar{q}^i \quad \forall i = 1, ..., M, \quad \Big\} \qquad (\mathrm{EL}^{\gamma,\eta})$$

$$\left.\begin{aligned} &A_{l*}(\bar{\mathbf{u}}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) + R_{l*}(\bar{\varphi}^i; \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) \\ &\quad = \bar{u}^i - u_d^i \quad \forall i = 1, ..., M, \end{aligned}\right\} \qquad (\mathrm{AE}^{\gamma,\eta})$$

$$\left(B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i, q^i - \bar{q}^i\right)_Q \geq 0 \quad \forall i = 1, ..., M \text{ and } \forall\, q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}. \quad \Big\} \qquad (\mathrm{VE}^{\gamma,\eta})$$

Proof. The reduced objective functional $f_{\mathbb{I}}$ is Fréchet differentiable by Corollary 3.4.1. By standard methods, e.g. used also in [132, Theorem 6.1] or [86, Lemma 4.3], the KKT system $(\mathrm{EL}^{\gamma,\eta})$, $(\mathrm{AE}^{\gamma,\eta})$ and $(\mathrm{VE}^{\gamma,\eta})$ then follows directly from the optimality condition (4.7) and Corollary 3.4.6. □

Note in particular, that the adjoint state $\bar{\mathbf{z}}_{\mathbb{I}} := (\bar{z}_{\mathbb{I}}, \bar{\psi}_{\mathbb{I}})$ satisfies (3.109) for $\mathbf{f}_{\mathbb{I}}$, where $\mathbf{f}_{adj}^i = (\bar{u}^i - u_d^i, 0) \in (W^\times)^M$, or equivalently (3.115), for $i = 1, ..., M$, which is precisely why the analysis of this equation is conducted earlier in Section 3.4. From now on, these equations are simply called the (system of) adjoint equation(s). The function $z_{\mathbb{I}}$ is also called the adjoint displacement, and $\psi_{\mathbb{I}}$ the adjoint phase-field, respectively. For (unique) solvability of the adjoint equation $(\mathrm{AE}^{\gamma,\eta})$ and regularity of the solutions $\mathbf{z}_{\mathbb{I}}$ we refer to Corollary 3.4.3.

4.2 Second-order optimality conditions with minimal gap

In this section, we show the main results of this chapter, second-order necessary optimality conditions and second-order sufficient optimality conditions with minimal gap. We utilize the abstract second-order optimality results [38, Theorem 2.3] and [38, Theorem 2.5], for which we have to verify the assumptions stated in [38, Assumption (A2)]. We want to point out that these results would also cover the case where a two-norm discrepancy is involved, which however shall not be used here. For $M = 1$, all properties of [38, Assumption (A2)] are verified in [86, Theorem 4.4] by the author and I. Neitzel, and for $M > 1$ we can analogously show the following:

Proposition 4.2.1. *The reduced functional $f_{\mathbb{I}}$ from* (3.103) *satisfies the properties of [38, Assumption (A2)]. This means that $f_{\mathbb{I}}$ satisfies:*

- *There exists an open subset $\mathbb{A} \subset Q^M$ covering $Q_{ad,\mathbb{I}}$, such that $f_{\mathbb{I}}(q_{\mathbb{I}}) \colon \mathbb{A} \to \mathbb{R}$ is of class C^2.*
- *There exist constants $0 < r$, $0 < \mathbb{M}_j$, $j = 1, 2$, such that it holds for all $q_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2} \in Q^M$ and $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}} \cap \|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq r$, that*

$$|f_{\mathbb{I}}'(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}}| \leq \mathbb{M}_1 \|\tilde{q}_{\mathbb{I}}\|_{Q^M}, \tag{4.11}$$

$$|f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2})| \leq \mathbb{M}_2 \|\tilde{q}_{\mathbb{I},1}\|_{Q^M} \|\tilde{q}_{\mathbb{I},2}\|_{Q^M}. \tag{4.12}$$

- *For every $\epsilon > 0$ there exists a $\delta > 0$ such that for all $q_{\mathbb{I},1}, q_{\mathbb{I},2} \in \{\tilde{q}_{\mathbb{I}} \in Q^M \mid \|\bar{q}_{\mathbb{I}} - \tilde{q}_{\mathbb{I}}\|_{Q^M} \leq r\}$, and $\tilde{q}_{\mathbb{I}} \in Q^M$ it holds:*

$$\|q_{\mathbb{I},1} - q_{\mathbb{I},2}\|_{Q^M} < \delta \quad \Rightarrow \quad \begin{cases} |[f_{\mathbb{I}}'(q_{\mathbb{I},1}) - f_{\mathbb{I}}'(q_{\mathbb{I},2})]\tilde{q}_{\mathbb{I}}| \leq \epsilon \|\tilde{q}_{\mathbb{I}}\|_{Q^M}, \\ |[f_{\mathbb{I}}''(q_{\mathbb{I},1}) - f_{\mathbb{I}}''(q_{\mathbb{I},2})](\tilde{q}_{\mathbb{I}})^2| \leq \epsilon \|\tilde{q}_{\mathbb{I}}\|_{Q^M}^2. \end{cases}$$

- *The quadratic form given through $\tilde{q}_{\mathbb{I}} \mapsto f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2$, as a mapping from Q^M into $\mathbb{R}$, is a Legendre form, i.e.*

  (1) If $\tilde{q}_{\mathbb{I},k} \rightharpoonup \tilde{q}_{\mathbb{I}}$ in Q^M as $k \to \infty$, then $f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2 \leq \liminf_{k\to\infty} f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2$.

  (2) If additionally $\lim_{k\to\infty} f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 = f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2$, then $\|\tilde{q}_{\mathbb{I}} - \tilde{q}_{\mathbb{I},k}\|_{Q^M} \to 0$.

Before we give the proof let us give some additional information: For [38, Assumption (A2)], due to the differentiability and Lipschitz results for $f_{\mathbb{I}}$ in Q^M from Section 3.4, indeed all norms can be chosen in the L^2-sense. Further, the requirement that the linear- and bilinear forms associated to the first and second derivative of the reduced functional are continuously extensible to L^2 and $L^2 \times L^2$ is correct. Similarly, continuity of the mappings $f_{\mathbb{I}}'(q_{\mathbb{I}})$ and $f_{\mathbb{I}}''(q_{\mathbb{I}})$ from L^∞ to the spaces of the linear/bilinear forms indeed holds true for the reduced functional $f_{\mathbb{I}}$, due to the L^2-continuity results proved in Lemma 3.4.2.

Proof. First, note that by Corollary 3.4.1, the reduced functional $f_{\mathbb{I}}$ is twice Fréchet differentiable from Q^M into $\mathbb{R}$. Further, using the results from Corollary 3.4.6, Lemma 3.2.3 and Corollary 3.4.3, the bounds from (4.11) and (4.12) are satisfied. By Lemma 3.4.2 it is also clear that $f_{\mathbb{I}}'$ and $f_{\mathbb{I}}''$ are Lipschitz continuous in Q^M for all $\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2} \in Q^M$ and in a neighborhood of $\bar{q}_{\mathbb{I}}$.

Secondly, the tracking-type objective functional $J_{\mathbb{I}}$ results in a Legendre form $\mathcal{Q} : \tilde{q} \mapsto f_{\mathbb{I}}''(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2$ from Q^M into $\mathbb{R}$. Here, in comparison to the one time-step setting, we have to put in some additional work. Note that by the regularity of the control-to-state operator $G_{\mathbb{I}}$ from (3.71) and the adjoint equation (3.109), from Lemma 3.2.1 and Corollary 3.4.3 respectively, it holds $\mathbf{u}_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}}$ in W^M. Due to the compact embeddings $L^2(\Gamma) \hookrightarrow W^{-1,p}(\Omega)$ and $W \hookrightarrow V$, cf. Remark 2.3.6, in combination with Lemma 3.2.3, the state $\tilde{\mathbf{u}}_{\mathbb{I},k} = G_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},k}$ converges strongly in at least V^M to $\tilde{\mathbf{u}}_{\mathbb{I}}$. Therefore, for all $i = 1, ..., M$, for $k \to \infty$, the strong convergence results

$$\begin{aligned}
&\big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}_k^i, \tilde{\mathbf{u}}_k^i], \mathbf{z}^i \big\rangle \to \big\langle A_b(\mathbf{u}^i)[\tilde{\mathbf{u}}^i, \tilde{\mathbf{u}}^i], \mathbf{z}^i \big\rangle, \\
&\big\langle R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}_k^i, \tilde{\varphi}_k^{i-1}), (\tilde{\varphi}_k^i, \tilde{\varphi}_k^{i-1})], \psi^i \big\rangle \\
&\ \to R_b(\varphi^i, \varphi^{i-1}; \gamma)[(\tilde{\varphi}^i, \tilde{\varphi}^{i-1}), (\tilde{\varphi}^i, \tilde{\varphi}^{i-1})], \psi^i \big\rangle, \\
&\text{and} \quad \|\tilde{u}_k^i\|^2 \to \|\tilde{u}^i\|^2
\end{aligned}$$

hold. Further, due to the weak lower semi-continuity of the norm $\|\cdot\|_Q^2$, it immediately holds

$$\|\tilde{q}^i\|_Q^2 \le \lim \inf_{k\to\infty} \|\tilde{q}_k^i\|_Q^2. \tag{4.13}$$

Combining the limit considerations from above and the structure of $f_{\mathbb{I}}$ being a sum of M time steps, weak lower semi-continuity of $f_{\mathbb{I}}''(q_{\mathbb{I}})$, and therefore *(1)* of the fourth point is clear.

Next, assume that $\lim_{k\to\infty} f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 = f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2$, which using (3.127) yields

$$\begin{aligned}
0 &= \lim_{k\to\infty} \Big(f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 - f_{\mathbb{I}}''(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2 \Big) \\
&= \lim_{k\to\infty} \Big(\mathcal{L}_{\mathbb{I}}(y_{\mathbb{I}})(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I},k})^2 - \mathcal{L}_{\mathbb{I}}(y_{\mathbb{I}})(\tilde{\mathbf{u}}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}})^2 \Big),
\end{aligned} \tag{4.14}$$

where $y_{\mathbb{I}} = (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}})$ with $\mathbf{u}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})$ and $\mathbf{z}_{\mathbb{I}}$ satisfying (3.115), and again $\tilde{\mathbf{u}}_{\mathbb{I}} = G_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}}$ as well as $\tilde{\mathbf{u}}_{\mathbb{I},k} = G_{\mathbb{I}}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I},k}$. Recall that $\tilde{\mathbf{u}}_{\mathbb{I},k} \to \tilde{\mathbf{u}}_{\mathbb{I}}$ strongly in at least V^M, therefore all terms in (3.128) except for the ones involving $\tilde{q}^i$ and $\tilde{q}_k^i$ are zero, and for (4.14) to hold true, it has to hold

$$\lim_{k\to\infty} \sum_{i=1}^{M} \|\tilde{q}_k^i\|_Q^2 - \|\tilde{q}^i\|_Q^2 = 0. \tag{4.15}$$

But now, due to the weak convergence of $q_{\mathbb{I},k}$ and the weak lower semi-continuity from (4.13), this means that for every $i = 1, ..., M$ it holds

$$\|\tilde{q}^i\|_Q^2 \le \lim \inf_{k\to\infty} \|\tilde{q}_k^i\|_Q^2 = \lim_{k\to\infty} \|\tilde{q}_k^i\|_Q^2$$

and thus $0 \le \lim_{k\to\infty} \|\tilde{q}_k^i\|_Q^2 - \|\tilde{q}^i\|_Q^2$. Therefore, from (4.15) it has to hold $\|\tilde{q}_k^i\|_Q^2 = \|\tilde{q}^i\|_Q^2$ for all $i = 1, ..., M$, and thus $\|\tilde{q}_{\mathbb{I}} - \tilde{q}_{\mathbb{I},k}\|_{Q^M} \to 0$.

Overall, all properties have been showed, and the proof is concluded. □

Before we can apply [38, Theorem 2.3], we also have to look at the cone of critical directions. For the one time step setting, it is clear that the cone of critical directions used in [86, Section 4] is applicable by [38, Remark 2.4]. Due to the structure of $Q_{\text{ad},\mathbb{I}}$ being box-constraints in M directions, or dimensions respectively, the cone from [86, Section 4] can now easily be generalized towards

$$C(\bar{q}_{\mathbb{I}}) = \left\{ \tilde{q}_{\mathbb{I}} \in Q^M \mid \forall i = 1, ..., M, \begin{cases} \tilde{q}^i(x) \ge 0 \text{ if } & \bar{q}^i(x) = q_a^i(x), \\ \tilde{q}^i(x) \le 0 \text{ if } & \bar{q}^i(x) = q_b^i(x), \\ \tilde{q}^i(x) = 0 \text{ if } & 0 \neq B^*\bar{\mathbf{z}}^i(x) + \alpha \bar{q}^i(x) \end{cases} \right\}. \tag{4.16}$$

To come back to the introduction of this chapter, we see the sign-conditions in the first two lines, and the strongly active constraint set in the third line, reminding ourselves that the expression $B^*\bar{\mathbf{z}}^i + \alpha q^i$ stems from the variational inequality ($\text{VE}^{\gamma,\eta}$).

As for the one time step model, cf. [86, Theorem 4.4] of I. Neitzel and the author, the following first main theorem, second-order necessary optimal conditions, then immediately follows from [38].

Theorem 4.2.2. *Let $\bar{q}_{\mathbb{I}} \in Q_{ad}^M$ be a locally optimal control of* ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$). *Then, it holds*

$$f_{\mathbb{I}}''(\bar{q}_{\mathbb{I}})[\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}] \ge 0 \qquad \forall \tilde{q}_{\mathbb{I}} \in C(\bar{q}_{\mathbb{I}}). \tag{4.17}$$

Proof. By Proposition 4.2.1, we can apply [38, Theorem 2.3] for ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$) with the cone $C(\bar{q}_{\mathbb{I}})$ from (4.16). This directly proves the statement. □

For the second main theorem, we show second-order sufficient optimal conditions that do not involve a two-norm discrepancy, analogously to [38, Equation (2.6) in Theorem 2.5]. For $M = 1$, i.e. the one time step setting, SSCs are established in [86, Theorem 4.6] as joint work of the author and I. Neitzel. For the case $M > 1$, i.e. for ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$), we make the following SSC assumption.

Assumption 4.2.3 (Second-order sufficient condition (SSC))**.** *let $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$, with associated state $\bar{\mathbf{u}}_{\mathbb{I}} \in W^M$ and associated adjoint state $\bar{\mathbf{z}}_{\mathbb{I}} \in W^M$, satisfy the first-order necessary conditions given in Lemma 4.1.3. Now, assume that*

$$f_{\mathbb{I}}''(\bar{q}_{\mathbb{I}})[\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}] > 0 \qquad \forall \tilde{q}_{\mathbb{I}} \in C(\bar{q}_{\mathbb{I}}) \backslash \{0\}. \tag{4.18}$$

The following quadratic growth condition can then be established:

Theorem 4.2.4. *Let $\bar{q}_{\mathbb{I}}$, with associated state $\bar{\mathbf{u}}_{\mathbb{I}}$ and associated adjoint state $\bar{\mathbf{z}}_{\mathbb{I}}$, satisfy Assumption 4.2.3. Then, there exist constants $\epsilon > 0$ and $c > 0$ such that the quadratic growth condition*

$$f_{\mathbb{I}}(q_{\mathbb{I}}) \geq f_{\mathbb{I}}(\bar{q}_{\mathbb{I}}) + c\|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|^2_{Q^M}$$

holds for every $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ with $\|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq \epsilon$. This means that $\bar{q}_{\mathbb{I}}$ is a locally optimal control of $(\mathrm{NLP}^{\gamma,\eta}_{\mathbb{I}})$ *in the sense of L^2.*

Proof. By assumption, $\bar{q}_{\mathbb{I}}$ satisfies the first-order necessary optimality conditions from Lemma 4.1.3, i.e. also the variational inequality of [38, Equation (2.3)]. Further, by Proposition 4.2.1, the prerequisites [38, (A2) on page 3] of [38, Theorem 2.5] are fulfilled. Applying [38, Theorem 2.5] concludes the proof. □

We can also equivalently write the SSC from Assumption 4.2.3 into the well-known form of a coercivity condition:

Remark 4.2.5 (Equivalence of positivity and coercivity condition)**.** *Under the properties of Proposition 4.2.1, the positivity condition from Assumption 4.2.3 is equivalent to the coercivity condition:*

$$\exists c_{SSC} > 0 \qquad \text{such that} \qquad f''_{\mathbb{I}}(\bar{q})[\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}] \geq c_{SSC}\|\tilde{q}_{\mathbb{I}}\|^2_{Q^M} \quad \forall \tilde{q}_{\mathbb{I}} \in C(\bar{q}_{\mathbb{I}}). \quad (4.19)$$

We have outlined in the introduction of this chapter, that in the finite dimensional setting many issues we have to deal with do not occur: For example, the equivalence of the positivity and the coercivity condition is immediately clear. For the infinite dimensional setting, a proof for the equivalence of (4.19) *and* (4.18) *is first given in [38, Remark 2.6]. Let us recapitulate the proof: Assume that* (4.18) *does not hold, then*

$$\forall\, k \geq 1 \quad \exists\, \tilde{q}_{\mathbb{I},k} \in C(\bar{q}_{\mathbb{I}}) \quad \text{such that} \quad f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 < \frac{1}{k}\|\tilde{q}_{\mathbb{I},k}\|^2_{Q^M}.$$

W.l.o.g. let $\tilde{q}_{\mathbb{I},k} := \tilde{q}_{\mathbb{I},k}/\|\tilde{q}_{\mathbb{I},k}\|_{Q^M}$, then $f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 < \frac{1}{k}$. Taking a subsequence, denoted also by $\tilde{q}_{\mathbb{I},k}$, we have $\tilde{q}_{\mathbb{I},k} \rightharpoonup \tilde{q}_{\mathbb{I}}$ in Q^M. This ensures $\tilde{q}_{\mathbb{I}} \in C(\bar{q}_{\mathbb{I}})$, since $C(\bar{q}_{\mathbb{I}})$ is closed and convex in Q^M. Further since $f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})$ is a Legendre form, by (4.19) *we obtain*

$$\begin{aligned} c_{SSC}\|\tilde{q}_{\mathbb{I}}\|^2_{Q^M} \leq f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2 \leq \liminf_{k\to 0} f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 &\leq \limsup_{k\to 0} f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 \\ &\leq \limsup_{k\to 0} \frac{1}{k} = 0, \end{aligned}$$

which immediately implies $\tilde{q}_{\mathbb{I}} = 0$ and thus it has to hold that $f''_{\mathbb{I}}(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I},k})^2 \to 0$, hence $\|\tilde{q}_{\mathbb{I},k}\|_2 \to 0$, which contradicts $\|\tilde{q}_{\mathbb{I},k}\|_{Q^M} = 1$. Finally, the reverse implication, i.e. (4.19) *implies* (4.18)*, is evident.*

Let us conclude by again pointing out the following important property, cf [86, Remark 4.7]: Comparing the necessary conditions from (4.17) and the sufficient conditions from (4.18), or equivalently (4.19), one sees that the gap between them is small. To the best of knowledge of the author, this gap is minimal in the sense that no closer result can be achieved.

4.3 σ-strongly active second-order sufficient conditions

We have already motivated in the introduction that in the context of (convergence proofs of) numerical methods, SSCs play an important role. In Chapter 6, we investigate the convergence of one numerical method, the SQP method, for ($\text{NLP}_{\mathbb{I}}^{\gamma,\eta}$). In this context, we cannot rely on the SSCs of Assumption 4.2.3, as they might be too weak. In many situations like Chapter 6, second-order sufficient conditions that are (slightly) stronger are required, and in this section we look at so called σ-strongly second-order sufficient conditions. For problems involving semilinear PDEs, these are studied in e.g. [153, Section 4.10.5] and the references therein. In the context of SQP methods they are also used in e.g. [70, 96, 152, 156]: As explained before, the reason is that all iteration directions have to stay feasible, i.e. lie in the same cone of critical directions. This does not hold true for e.g. the SSCs from Theorem 4.2.4. Mathematically, a small parameter $\sigma > 0$ bounds the strongly active set away from zero, which allows for small perturbations in the stability analysis involved in the SQP convergence analysis. We do not go into more detail at this point and refer the reader to Section 6.2.2. Without further ado, we introduce the σ-active set, which in accordance with [152, Section 3], is given by: Let $\mathbb{R} \ni \sigma > 0$,

$$\mathcal{I}(\sigma) := \big\{ x \in \Gamma \;\big|\; |B^*\bar{\mathbf{z}}^i + \alpha \bar{q}^i| \geq \sigma \quad \text{for all } i = 1, ..., M \big\}, \tag{4.20}$$

where $(\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$ is a local optimal triple, cf. Section 4.1. We can then define the cone of ($\sigma-$)critical directions via

$$C_\sigma(\bar{q}_{\mathbb{I}}) := \{ \tilde{q}_{\mathbb{I}} \in Q^M \;\mid\; \tilde{q}_{\mathbb{I}}(x) = 0 \;\text{ on }\; \mathcal{I}(\sigma) \}. \tag{4.21}$$

Let us point out that in comparison to the cone $C(\bar{q}_{\mathbb{I}})$ from (4.16), the cone $C_\sigma(\bar{q}_{\mathbb{I}})$ does not involve any sign conditions. Note that in particular, for every $\sigma > 0$, the inclusion

$$C(\bar{q}_{\mathbb{I}}) \subset C_\sigma(\bar{q}_{\mathbb{I}}) \tag{4.22}$$

holds. This assures that the σ-strongly active second-order sufficient conditions from Assumption 4.3.1 immediately below are (slightly) stronger than the (strongly active) second-order sufficient conditions from Assumption 4.2.3. In [85, Assumption 3.3] of the author and I. Neitzel, σ-strongly active second-order sufficient conditions are stated for $M = 1$, i.e. for the one time step setting. For $M > 1$, we analogously make the following assumption:

Assumption 4.3.1 (σ-strongly active second-order sufficient conditions)**.** *Let $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ and the associated function triple $(\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}}) \in Y^M$ fulfill the first-order necessary conditions that have been given in Lemma 4.1.3. There exist constants $\sigma > 0$ and $c_{SSC} > 0$ such that*

$$f_{\mathbb{I}}''(\bar{q}_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2 \geq c_{SSC} \|\tilde{q}_{\mathbb{I}}\|_{Q^M}^2 \quad \textit{for all} \quad \tilde{q}_{\mathbb{I}} \in C_\sigma(\bar{q}_{\mathbb{I}}).$$

Note that due to Corollary 3.5.2, Assumption 4.3.1 can also equivalently be expressed in a in the literature more popular form involving the Lagrangian: Let $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}}) \in Y^M$ fulfill the first-order necessary conditions of Lemma 4.1.3, then there exists constants $\sigma > 0$ and $c_{SSC} > 0$ such that

$$\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I}}, \tilde{q}_{\mathbb{I}})] \geq c_{SSC} \|\tilde{q}_{\mathbb{I}}\|^2_{Q^M} \quad \forall \tilde{q}_{\mathbb{I}} \in C_\sigma(\bar{q}_{\mathbb{I}}),\ \tilde{\mathbf{u}}_{\mathbb{I}} = G'_{\mathbb{I}}\big(\bar{q}_{\mathbb{I}}\big)\tilde{q}_{\mathbb{I}}. \quad (4.23)$$

Now finally, due to the inclusion (4.22), it immediately follows from Theorem 4.2.4 that a quadratic growth condition also holds under Assumption 4.3.1.

Corollary 4.3.2. *Let $\bar{q}_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$, with associated state $\bar{\mathbf{u}}_{\mathbb{I}} \in W^M$ and adjoint state $\bar{\mathbf{z}}_{\mathbb{I}} \in W^M$, fulfill Assumption 4.3.1. There exist constants $\epsilon > 0$ and $c > 0$ such that the quadratic growth condition*

$$f_{\mathbb{I}}(q_{\mathbb{I}}) \geq f_{\mathbb{I}}(\bar{q}_{\mathbb{I}}) + c\|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|^2_{Q^M}$$

holds for all $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ with $\|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq \epsilon$. This means that $\bar{q}_{\mathbb{I}}$ is a strict local optimal control in the sense of L^2, and no two-norm gap is involved.

5. Modelling of fracture irreversibility: Recovering complementarity constraints in the penalization limit

The main topic of this chapter is the investigation of the behavior of solutions of an optimal control problem governed by a regularized fracture propagation model, like ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), with respect to taking the penalization limit $\gamma \to \infty$. In this chapter, we restrict the model problem to one time step only, i.e. set $M = 1$. The state space is then V, W respectively, and the control space is Q, cf. Definition 2.3.3. Furthermore, no control constraints are incorporated, i.e. the set of admissible controls is $Q_{\mathrm{ad},\mathbb{I}} = Q$. Overall, this leads to the model problem (NLP^{γ}) stated below. As the main result Theorem 5.0.1, we prove that the dual variables of this problem converge in suitable function spaces, and that subsequently the limits of primal and dual variables in fact satisfy a C-stationarity system. This is an already published result in the joint work [84] of the author and M. Mohammadi, I. Neitzel and W. Wollner. It builds upon, incorporates essential ideas of, and extends results from [133], where convergence of primal variables, i.e. optimal control and optimal state, w.r.t. the penalization parameter γ to their limit is showed. Note further that in the proof we adapt ideas used in [119], where the penalization limit of an obstacle constrained optimal control problem is investigated.

Let us define the one time step problem formulation of this chapter by:

Find an optimal control $q_\gamma \in Q$ with associated state $\mathbf{u}_\gamma = (u_\gamma, \varphi_\gamma) \in V$ satisfying

$$\left.\begin{aligned} &\min_{q,\mathbf{u}} J(q,\mathbf{u}) := \frac{1}{2}\|u - u_d\|_{L^2(\Omega;\mathbb{R}^2)} + \frac{\alpha}{2}\|q\|_Q^2, \\ &\text{subject to:} \quad A(\mathbf{u},\varphi^-) + R(\varphi,\varphi^-;\gamma) = Bq, \end{aligned}\right\} \qquad (\mathrm{NLP}^{\gamma})$$

where Assumption 2.3.1 and Assumption 2.3.7 hold true, with $\varphi^- := \varphi^0$, i.e. $\varphi^- \in W^{2,q}$, $\varphi^- \in [0,1]$, as well as $u_d \in L^2(\Omega)$ given.

Note that in accordance with [84, 133], we denote the optimal controls, states and adjoint states associated to the penalized problem (NLP$^\gamma$) with an index γ, to make it clear that the dependence on the penalization parameter is of interest and explicitly tracked, i.e. q_γ, $\mathbf{u}_\gamma = (u_\gamma, \varphi_\gamma)$ and $\mathbf{z}_\gamma = (z_\gamma, \psi_\gamma)$. In this context, φ^- is a given phase-field function.

Let us also state the unpenalized fracture optimal control problem, cf. Section 2.1: Using (EL$^\eta$), the one time step equivalent of (EL$^\eta_{\mathbb{I}}$), as a constraint for the tracking type functional $J(q, \mathbf{u})$, we obtain the problem formulation

$$\left.\begin{aligned} &\min_{q,\mathbf{u}} J(q, \mathbf{u}), \\ &\text{subject to: } \mathbf{u} \text{ solves (EL}^\eta\text{) for data } q, \end{aligned}\right\} \tag{NLP$^{\mathrm{VI}}$}$$

with

$$\begin{aligned} A(\mathbf{u}, \varphi^-) + \lambda &= Bq && \text{in } V^*, \\ \lambda &\geq 0 && \text{in } V_\varphi^*, \\ \varphi &\leq \varphi^- && \text{a.e. in } \Omega, \\ \langle \lambda, \varphi - \varphi^- \rangle &= 0, \end{aligned} \tag{EL$^\eta$}$$

where $\lambda \in V_\varphi^*$. We also implicitly used that $(0, \lambda) \in (V_u^* \times V_\varphi^*) \subset V^*$.

We have already mentioned that problems like (NLP$^{\mathrm{VI}}$) fall into the category of mathematical problems with complementarity constraints, often abbreviated MPCCs. Some of the aspects involved with the analysis of MPCCs have been discussed earlier in Chapter 1 and 2 and we refer the reader to the references stated there. For (NLP$^{\mathrm{VI}}$), the Lagrange technique suggests that the associated (formal) first-order necessary optimality conditions are given by Clarke- or commonly called C-stationary conditions, which are stated in (5.7) on page 111 below. These are first-order necessary optimality conditions involving complementarity constraints and sign conditions, which hold in the $V - V^*$ duality sense. In comparison to e.g. more rigorous first-order optimality conditions given by the strong stationarity concept, C-stationary conditions do not involve conditions that hold quasi-everywhere, i.e. up to a set of capacity zero, as stated on [119, page A925]. We do not go into further details on stationarity systems, and refer the interested reader to [80, 142].

In [133] convergence of the primal variables is established, and it is also showed that the limit functions then satisfy the equations (5.7a)-(5.7d) of the C-stationarity system (5.7). We want to point out that [133] proves this for a multi time step setting as in (NLP$^{\gamma,\eta}_{\mathbb{I}}$), which immediately includes the one time step setting of this chapter. Using this in combination with the γ-independent bounds for the adjoint state $\mathbf{z}_\gamma$ proved in Corollary 3.4.4, we establish the main result of this chapter in Theorem 5.0.1: We can tend to the limit in the dual variables and prove their weak convergence. Subsequently, the remaining parts of the limit optimality system, cf. (5.7e)-(5.7j), are showed.

Let us start by recalling some important preliminaries, as well as already established results from the literature we rely on. Firstly, we want to refer to Assumption 2.3.1 (basic assumptions) and Assumption 2.3.7 (problem setting specific assumptions), as well as the viscous approximation Assumption 2.3.11, which shall hold throughout this chapter. Note also that the operators A and R from Definition 2.3.8 slightly differ from the notation of both [84] and [133], cf. Remark 2.3.10. Secondly, it is clear from [133], cf. Lemma 3.2.1, that the one time step state equation

$$A(\mathbf{u}_\gamma, \varphi^-) + \lambda_\gamma = Bq_\gamma \tag{EL$^\gamma$}$$

is uniquely solvable, and the solution $\mathbf{u}_\gamma$ is bounded uniformly in γ in both V and W. As in [133], to depict the operator $R(\varphi_\gamma, \varphi^-; \gamma)$ we also introduce the variable

$$\lambda_\gamma := \gamma[(\varphi_\gamma - \varphi^-)^+]^3. \tag{5.1}$$

We recall that such a term is introduced to regularize the irreversibility condition, which for one time step is the inequality constraint $\varphi^- \leq \varphi$, see also Section 2.1. However, after the regularization the inequality is not strictly enforced anymore. The term λ_γ then describes the violation of this constraint.

Note that in fact the norm bounds of $\mathbf{u}_\gamma$ already rely on a constraint violation estimate for λ_γ, which is used to conclude (3.68) from (3.67), cf. Lemma 3.2.1. Let us therefore also quickly look at available norm estimates for λ_γ: In [133, Lemma 3.2], it is proved that $\lambda_\gamma \in L^1(\Omega) \cap H^1(\Omega)^*$ with uniform norm bounds in γ. Subsequently in [133, Lemma 3.8] it is showed that $\lambda_\gamma \in L^q(\Omega)$ with bound

$$\|\lambda_\gamma\|_{L^q(\Omega)} \leq c \left\| \frac{1}{\varepsilon} + \varepsilon \triangle \varphi^- \right\|_{L^q(\Omega)} \tag{5.2}$$

holding true for a constant $c > 0$ independent of γ, where $q = \frac{p}{2} > 1$ as in Assumption 2.3.1. The proof of (5.2) relies on the fact that both φ^- and φ_γ are positive and λ_γ is non negative. This is ensured by assumption, and [132, Lemma 4.1 and Corollary 4.2], cf. again Lemma 3.2.1, as well as the definition of λ_γ, cf. (5.1), respectively.

Further, we state a convergence result for the primal variables of (NLP$^\gamma$) from [133, Theorem 5.2][1]: Let $\bar{q} \in Q$ be an isolated minimum of (NLP$^{\mathrm{VI}}$), and assume that the corresponding state $\bar{\mathbf{u}}, \bar{\lambda}$ is the unique solution to (EL$^\eta$). Then, for γ sufficiently large, there exists a sequence q_γ of local minimizers of (NLP$^\gamma$), with associated state $\mathbf{u}_\gamma$ satisfying (EL$^\gamma$), such that

$$q_\gamma \to \bar{q} \qquad \text{in} \quad Q, \tag{5.3}$$

$$\mathbf{u}_\gamma \to \bar{\mathbf{u}} \qquad \text{in} \quad V \cap (H^{1+s}(\Omega; \mathbb{R}^2) \times C^{0,\alpha}(\Omega)). \tag{5.4}$$

[1]Again, we want to point out that [133] proved their results for a multi time step setting as in (NLP$_{\mathbb{I}}^{\gamma,\eta}$), which immediately includes the one time step setting of this chapter.

Next, let us emphasize that when restricting ourselves to the one time step setting, we work with the operators $A_l(\mathbf{u})(\cdot,0)$ and $R_l(\varphi,\varphi^-,\gamma)(\cdot,0)$, which are self adjoint, cf. Remark 3.1.2. By Corollary 3.4.4, we obtain unique solvability of the to (NLP$^\gamma$) associated one time step adjoint equation

$$A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma,0) + R_{l*}(\varphi_\gamma,\varphi^-,0;\gamma)(\psi_\gamma,0) = u_\gamma - u_d. \qquad (\mathrm{AE}^\gamma)$$

The solution $\mathbf{z}_\gamma = (z_\gamma,\psi_\gamma) \in V$ can be bounded γ-independently in V, see (3.112). In this context, we utilize $\mathbf{u}_\gamma \in W, \varphi^- \in W_\varphi$ and $(u_\gamma - u_d, 0) \in V^*$.

Finally, existence of solutions of (NLP$^\gamma$) and first-order optimality conditions now follow immediately from standard theory, cf. the results proved in Chapter 4, recalling that the difference towards (NLP$^{\gamma,\eta}_{\mathbb{I}}$) is simply the lack of control constraints, and the restriction towards one time step. In particular, and analogously to Section 4.1, any local minimizer $(q_\gamma,\mathbf{u}_\gamma) \in Q \times W$ of (NLP$^\gamma$), together with the associated adjoint state $\mathbf{z}_\gamma \in V$, and the auxiliary variables $\lambda_\gamma, \mu_\gamma \in V_\varphi^*$, $\theta_\gamma \in V_\varphi$, has to satisfy

$$\begin{aligned}
A(\mathbf{u}_\gamma,\varphi^-) + \lambda_\gamma &= B(q_\gamma) && \text{in } V^*, && (5.5a)\\
\lambda_\gamma &= R(\varphi_\gamma,\varphi^-;\gamma) && \text{in } V_\varphi^*, && (5.5b)\\
A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma,0) &= u_\gamma - u_d - \mu_\gamma && \text{in } V^*, && (5.5c)\\
B^*\mathbf{z}_\gamma + \alpha q_\gamma &= 0 && \text{in } V^*, && (5.5d)\\
\psi_\gamma - \theta_\gamma &= 0 && \text{in } V_\varphi, && (5.5e)\\
\mu_\gamma - R_{l*}(\varphi_\gamma,\varphi^-,0;\gamma)(\theta_\gamma,0) &= 0 && \text{in } V_\varphi^*. && (5.5f)
\end{aligned}$$

The optimality system (5.5) has previously also been stated in [84, (FON$^\gamma$)], and the improved regularity $\mathbf{u}_\gamma \in W$, $\lambda_\gamma \in L^q(\Omega)$ holds true due to the results of [133] stated above. Note further that although the variables $\lambda_\gamma, \mu_\gamma$ and θ_γ seem redundant, in accordance to [84, 119] they were introduced as they have meaning as multipliers for the limit. Of course, they could easily be eliminated.

We already know from [133] that when taking the limit γ to infinity, we can recover all isolated local minimizers of (NLP$^{\mathrm{VI}}$). In particular, existence of a convergent sequence q_γ of local minimizers of (NLP$^\gamma$) is ensured, cf. (5.3). Adapting the ideas of [119], where the penalization limit of an optimal control problem of an obstacle problem is investigated, we are now in a position to prove the main theorem of this chapter, which is published in [84, Theorem 3.1] as joint work of M. Mohammadi, I. Neitzel, W. Wollner and the author.

Theorem 5.0.1. *Let $q_\gamma \to \bar{q}$ be a convergent sequence of local minimizers of* (NLP$^\gamma$) *for $\gamma \to \infty$. Up to selecting a subsequence, the following convergences hold true:*

$$\begin{aligned}
\mathbf{u}_\gamma &\to \bar{\mathbf{u}} && \textit{in} \quad V, && (5.6a)\\
u_\gamma &\to \bar{u} && \textit{in} \quad W_u && (5.6b)\\
\varphi_\gamma &\rightharpoonup \bar{\varphi} && \textit{in} \quad W_\varphi, && (5.6c)
\end{aligned}$$

$$
\begin{aligned}
\lambda_\gamma &\to \bar\lambda && \textit{in} \quad V_\varphi^*, && (5.6d)\\
\mathbf{z}_\gamma &\rightharpoonup \bar{\mathbf{z}} && \textit{in} \quad V, && (5.6e)\\
\mu_\gamma &\rightharpoonup \bar\mu && \textit{in} \quad V_\varphi^*, && (5.6f)\\
\theta_\gamma &\rightharpoonup \bar\theta && \textit{in} \quad V_\varphi. && (5.6g)
\end{aligned}
$$

Furthermore, any such limit satisfies the C-stationary optimality system

$$
\begin{aligned}
A(\bar{\mathbf{u}},\varphi^-) + \bar\lambda &= B(\bar q) && \textit{in } V^*, && (5.7a)\\
\bar\lambda &\geq 0 && \textit{in } V_\varphi^*, && (5.7b)\\
\bar\varphi &\leq \varphi^- && \textit{a.e. in } \Omega, && (5.7c)\\
\langle \bar\lambda, \bar\varphi - \varphi^- \rangle &= 0 && && (5.7d)\\
A_{l*}(\bar{\mathbf{u}})(\bar{\mathbf{z}},0) &= \bar u - u_d - \bar\mu && \textit{in } V^*, && (5.7e)\\
B^*\bar{\mathbf{z}} + \alpha\bar q &= 0 && \textit{in } V^*, && (5.7f)\\
\bar\psi - \bar\theta &= 0, && \textit{in } V_\varphi, && (5.7g)\\
\langle \bar\theta, \bar\lambda \rangle &= 0, && && (5.7h)\\
\langle \bar\mu, \bar\varphi - \varphi^- \rangle &= 0, && && (5.7i)\\
\langle \bar\theta, \bar\mu \rangle &\geq 0. && && (5.7j)
\end{aligned}
$$

Proof. The convergence results (5.6a)-(5.6c) are proved in [133, Corolary 3.10]. Further, it is proved there that the limit functions satisfy (5.7a)-(5.7d). Then $\lambda_\gamma \to \bar\lambda$ in V_φ^*, i.e. (5.6d), follows from (5.6a)-(5.6c) and (5.7a).

As for the convergence of the dual variables and the limits in the adjoint (5.7e) and gradient (5.7f) equation as well as the complementary slackness conditions (5.7h)-(5.7j), the starting point is the weak convergence of the adjoint state $\mathbf{z}_\gamma = (z_\gamma, \psi_\gamma)$ in V: After eliminating the variables μ_γ and θ_γ by inserting (5.5f) and (5.5e) into the adjoint equation (5.5c), one obtains

$$
A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma, 0) + R_{l*}(\varphi_\gamma, \varphi^-, 0; \gamma)(\psi_\gamma, 0) = u_\gamma - u_d.
$$

We recall that the operators $A_l(\mathbf{u})(\cdot,0)$ and $R_l(\varphi,\varphi^-;\gamma)(\cdot,0)$ are self-adjoint for the one time step setting, see Remark 3.1.2. Further, in the proof of Lemma 3.2.3, coercivity (3.80) of $A_l(\mathbf{u})(\cdot,0)$ and nonnegativity (3.81) of $R_l(\varphi,\varphi^-;\gamma)(\cdot,0)$ were showed. Now, using the test function $\mathbf{z}_\gamma$, we obtain

$$
\big\langle A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma,0), \mathbf{z}_\gamma \big\rangle + \big\langle R_{l*}(\varphi_\gamma,\varphi^-,0;\gamma)(\psi_\gamma,0), \psi_\gamma \big\rangle = \langle u_\gamma - u_d, z_\gamma \rangle,
$$

which then ensures

$$
\|\mathbf{z}_\gamma\|_V \leq \frac{1}{c} \|u_\gamma - u_d\|_{V_u^*}, \tag{5.8}
$$

for a $c > 0$ independently of γ. We skip further details on the other constants c depends on, and refer to the right-hand side of (3.80) for more details. Note that to obtain (6.53) we also utilize $u_\gamma \in W_u \hookrightarrow V_u \hookrightarrow V_u^*$ independently of γ, which directly follows from the solution result for (EL$^\gamma$) and $u_d \in L^2(\Omega) \hookrightarrow V_u^*$ by assumption. As a consequence $\mathbf{z}_\gamma$ is bounded independently of γ in V and there exists a subsequence that converges weakly to some limit $\bar{\mathbf{z}}$ in V, establishing (5.6e). From (5.6b) and (5.6c), one easily obtains $A_l(\mathbf{u}_\gamma) - A_l(\bar{\mathbf{u}}) \to 0$ in $L(V, V^*)$, hence it also holds

$$A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma, 0) \rightharpoonup A_{l*}(\bar{\mathbf{u}})(\bar{\mathbf{z}}, 0) \quad \text{in } V^*.$$

Now, again by (5.6b) we have in particular $u_\gamma \to \bar{u}$ in $W_u \hookrightarrow V_u^*$, and both the convergence claim (5.6f) of μ_γ and the limit equation (5.7e) follow by

$$\mu_\gamma = u_\gamma - u_d - A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma, 0) \rightharpoonup \bar{u} - u_d - A_{l*}(\bar{\mathbf{u}})(\bar{\mathbf{z}}, 0) =: \bar{\mu} \quad \text{in } V_\varphi^*. \tag{5.9}$$

Due to (5.5e), i.e. $\theta_\gamma = \psi_\gamma$, the weak convergence (5.6g) of θ_γ to $\bar{\theta} = \bar{\psi}$, cf. (5.7g), is directly obtained. It is therefore possible to pass to the limit in the gradient equation (5.5d), which immediately leads to (5.7f). Up until now, all convergence claims from the theorem are proved, and it was showed that (5.7a)-(5.7g) are satisfied, which means it remains to prove the complementary slackness conditions (5.7h)-(5.7j). Let the set $\mathcal{A} := \{x \in \Omega \mid \varphi_\gamma > \varphi^-\}$ be given, then from the definition of λ_γ one calculates

$$|\langle \lambda_\gamma, \theta_\gamma \rangle| = \left| \int_{\mathcal{A}} \gamma [(\varphi_\gamma - \varphi^-)^+]^3 \theta_\gamma \, dx \right| \leq \|\lambda_\gamma\|_{L^q(\mathcal{A})} \|\theta_\gamma\|_{L^{q'}(\mathcal{A})}. \tag{5.10}$$

Due to (5.2), λ_γ can be bounded in the L^q-norm by a constant independently of γ, in particular this also implies a uniform bound for $\|\lambda_\gamma\|_{L^q(\mathcal{A})}$. Next, due to (5.8) and (5.5e), it holds $\theta_\gamma \in H^1 \hookrightarrow L^{q'}$ for any $q' \in (1, \infty)$. Due to (5.6a), i.e. i.p. $\varphi_\gamma \to \bar{\varphi}$ in V_φ, and (5.7c), it holds $|\mathcal{A}| \to 0$ for $\gamma \to \infty$, and therefore

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

Overall, from (5.10) it follows

$$|\langle \lambda_\gamma, \theta_\gamma \rangle| \leq C \|\theta_\gamma\|_{L^{q'}(\mathcal{A})} \to 0 \quad \text{for} \quad \gamma \to \infty. \tag{5.11}$$

Now, from (5.11), (5.6g) and (5.6d), we obtain

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

hence (5.7h) holds. Next, using the definition of μ_γ, as well as (5.11), it holds

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

which proves (5.7i), since the limit can also be taken on the left-hand side due to (5.6f) and $\varphi_\gamma \to \bar{\varphi}$ in V_φ, cf. (5.6a).

Finally, it remains to prove (5.7j). To start, note that by definition of μ_γ, it immediately holds

$$\langle \mu_\gamma, \theta_\gamma \rangle = 3 \int_\Omega \gamma [(\varphi_\gamma - \varphi^-)^+]^2 \theta_\gamma^2 \, dx \geq 0, \tag{5.12}$$

and that by the same arguments as in (5.9), it holds

$$\big\langle \big(A_{l*}(\mathbf{u}_\gamma) - A_{l*}(\bar{\mathbf{u}})\big)(\bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle \to 0 \quad \text{for} \quad \gamma \to \infty. \tag{5.13}$$

Next, test both (5.5c) and (5.7e) with $\mathbf{z}_\gamma - \bar{\mathbf{z}}$, and subtract the equations to obtain

$$\begin{aligned} \langle \mu_\gamma - \bar{\mu}, \theta_\gamma - \bar{\theta} \rangle &= \langle \mu_\gamma - \bar{\gamma}, \psi_\gamma - \bar{\psi} \rangle \\ &= \langle u_\gamma - \bar{u}, z_\gamma - \bar{z} \rangle - \big\langle A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma, 0) - A_{l*}(\bar{\mathbf{u}})(\bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle \\ &= \langle u_\gamma - \bar{u}, z_\gamma - \bar{z} \rangle - \big\langle A_{l*}(\mathbf{u}_\gamma)(\mathbf{z}_\gamma - \bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle \\ &\quad - \big\langle \big(A_{l*}(\mathbf{u}_\gamma) - A_{l*}(\bar{\mathbf{u}})\big)(\bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle \\ &\leq \langle u_\gamma - \bar{u}, z_\gamma - \bar{z} \rangle - \big\langle \big(A_{l*}(\mathbf{u}_\gamma) - A_{l*}(\bar{\mathbf{u}})\big)(\bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle, \end{aligned} \tag{5.14}$$

where again coercivity of A_{l*}, see the remarks above (5.8), is used to obtain the last inequality.

Overall, a quick calculation using (5.12) and (5.14) now shows,

$$\begin{aligned} \langle \bar{\mu}, \bar{\theta} \rangle &= \langle \bar{\mu}, \theta_\gamma \rangle + \langle \mu_\gamma, \bar{\theta} \rangle - \langle \mu_\gamma, \theta_\gamma \rangle + \langle \mu_\gamma - \bar{\mu}, \theta_\gamma - \bar{\theta} \rangle \\ &\leq \langle \bar{\mu}, \theta_\gamma \rangle + \langle \mu_\gamma, \bar{\theta} \rangle + \langle u_\gamma - \bar{u}, z_\gamma - \bar{z} \rangle \\ &\quad - \big\langle \big(A_{l*}(\mathbf{u}_\gamma) - A_{l*}(\bar{\mathbf{u}})\big)(\bar{\mathbf{z}}, 0), \mathbf{z}_\gamma - \bar{\mathbf{z}} \big\rangle. \end{aligned}$$

Recall (5.6a), (5.6f) and (5.6g), therefore the first two terms on the right-hand side converge to $2\langle \bar{\mu}, \bar{\theta} \rangle$, and the third term converges to zero. Finally, the last term also converges to zero due to (5.13), therefore (5.7j) follows. □

We have proved our main result Theorem 5.0.1 under the restriction towards one time step only. For the case $M > 1$, we can identify the major limiting factor to be (5.8), where we rely on a γ-independent norm bound for the adjoint state $\mathbf{z}_\gamma = (z_\gamma, \psi_\gamma)$ in the space V. To extend our result towards the multi time step model, it is necessary to also obtain a bound

$$\|\mathbf{z}_{\gamma,\mathbb{I}}\|_{V^M} \leq c \|\mathbf{u}_{\gamma,\mathbb{I}} - \mathbf{u}_{d,\mathbb{I}}\|_{(V^u)^M}, \tag{5.15}$$

for a $c > 0$ independently of γ. For this, it is necessary to revisit Corollary 3.4.3, and therefore ultimately Lemma 3.2.3, utilizing different techniques. Without going into too much detail, let us recall that the constraint violation estimate (5.2) for λ_γ, which we recall to depict the operator R, was an essential cornerstone in the γ-independent bound for the solution $\mathbf{u}_\gamma$ of (EL$^\gamma$). Let us put on record that similarly, a bound like (5.15) seems to be closely connected to γ-independent bounds of the (adjoint linearized penalization) operator $R_{l,*}$, or due to Remark 3.1.2, of the (linearized penalization) operator R_l.

Let us close this chapter by emphasizing that uniform bounds in the penalization parameter γ and the behavior and interconnection of all involved (physically and numerically motivated) parameters for the linearized and adjoint equations, as well as the operators R_l and R_{l*}, would be of further interest. This is the case e.g. in the context of stability not only of first-order necessary conditions in the multi time step setting, but also of second-order conditions. In a future stability analysis of the SQP method w.r.t. the penalization limit, both the linearized penalization operator R_l and its adjoint R_{l*} e.g. emerge in the subproblems of the SQP method, see the following Chapter 6. Similarly, norm estimates of R_l and their dependence on the penalization parameter γ would be of interest for [84, Section 4.3] and [128, Theorem 2 in Section 3.2 and Corollary 2 in Section 3.3], where error estimates for the finite element approximation of an associated quadratic subproblem were investigated. These error estimates involve constants that in particular depend on R_l.

6. Convergence analysis of the Sequential Quadratic Programming method

This chapter is concerned with the second main result of this thesis, a convergence result for the sequential quadratic programming (SQP) method for the optimal control problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$). In particular, we prove local quadratic convergence of the SQP method for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) with a classical L^∞-closeness condition for the controls in Theorem 6.3.15, and with L^2-closeness in Theorem 6.4.10. For $M = 1$, i.e. the one time step model, these results are published as joint work [85] of the author and I. Neitzel. Note that for the L^∞-convergence result, we adapt the ideas of [152] to our settings. While [152] proves convergence of the SQP method for optimal control problems constrained by (semilinear) partial differential equations with control constraints, we recall that our problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) involves a quasilinear partial differential equation setting as well as control-constraints. For the L^2-convergence result, we additionally use ideas from [96], which, to the best of the authors' knowledge, is the first publication to establish such an L^2-closeness result in the context of (parabolic) optimal control problems.

Let us start with some general remarks. The SQP method is a well-known and popular class of algorithms that can be used to numerically solve nonlinear optimal control problems in a fast and efficient way. We do not give an in-depth overview of the general concept of the SQP method, but instead refer the interested reader to [94]. In short the SQP method reads: Instead of directly solving a nonlinear optimization problem, a sequence of linear quadratic subproblems is iteratively solved. For optimal control problems, this is comparable to a Lagrange-Newton method, and the SQP method also shares the local convergence properties. In particular, if the initial value is close to the local optimal solution, then quadratic convergence towards the local optimal solution can be showed. Note that there exists a meanwhile generally acknowledged procedure to prove convergence of (general) SQP methods, that can be found in e.g. [6]. To the best of the authors' knowledge, first convergence analyses of SQP methods in the context of PDE constrained optimal control problems are conducted in [155] (in the semilinear elliptic case) and in [70, 152] (in the semilinear parabolic case).

One important question is in which sense the closeness has to be chosen. A second aspect is which assumptions have to be made to ensure that the quadratic subproblems are uniquely solvable and that the generated sequence converges towards the local optimal solution of the original nonlinear problem. We have already stated at the beginning of Chapter 4 that SSCs are an important tool for the convergence analysis of many numerical algorithms, and in particular also for the SQP method. In fact, we have also already asserted that the σ-strongly active SSCs for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) proved in Section 4.3 are suitable assumptions for the analysis of the SQP method of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$).

In the first three sections of this chapter, we follow the approach of [152]. This means that the starting point for the convergence proof of the SQP method for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) is to reformulate the first-order necessary conditions from Lemma 4.1.3. Since they involve control constraints, we rewrite them into a generalized equation. Compare this to the case not involving control constraints, where the first-order necessary conditions can be expressed in the form of an "ordinary", i.e. a standard equation. Subsequently, Newton's method is applied and by showing that a property called strong regularity is fulfilled, it is possible to ensure the convergence of Newton's method for the generalized equation. Let us therefore put the focus on this property next, in particular on its connection to second-order sufficient conditions. Broadly speaking, the strong regularity concept can be seen as a generalization of the implicit function theorem towards generalized equations. It is a local property, that demands the existence of a unique solution, as well as a Lipschitz continuity condition of a perturbation of the problem, in a neighborhood of a given function. Strong regularity is introduced by [140], and subsequently used in [58] to prove convergence of Newton's method for an optimal control problem in a Banach space setting. Now, when conducting the SQP method, we solve the corresponding quadratic subproblem and generate a direction in every step. To ensure the required solvability, usually a second-order sufficient condition is assumed. However, if (too) weak SSCs, as e.g. in Theorem 4.2.4, are chosen, the quadratic subproblem generates directions which do not necessarily satisfy this weaker SSC for the succeeding step. The reason is that the directions might not belong to the cone of critical directions of the (too) weak SSC, i.e. this cone could be too small. As elaborated in Chapter 4, strong(er) second-order sufficient conditions can eliminate such issues, and therefore simplify the analysis of numerical methods like the SQP method. For example, choosing the critical cone to be the entire control space Q^M trivially ensures feasibility of all directions that are generated within the SQP method. For $M = 1$, i.e. the one time step setting, such a setting is presented in [84, Lemma 4.1]: There, a preliminary analysis of the SQP subproblems is done under a rather strong local coercivity condition assumption, cf. [84, Equation (4.2) and Proposition 4.3], that immediately ensures convexity and unique solvability of the quadratic subproblems. However, in the opinion of the author and many others[1], such SSCs on the entire control space are too strong. Instead, we use the idea of [152] and utilize the σ-strongly active second-order sufficient conditions

[1] see again the quote cited from [153, page 247] immediately below (4.10) on page 96

given in Assumption 4.3.1. We recall that these SSCs are close to the (weakest possible) SSCs given in Assumption 4.2.3, and only slightly stronger. Then following [70, 152], cf. also [156], strong regularity and therefore convergence of the SQP method for an auxiliary quadratic subproblem can be established under Assumption 4.3.1. We rely on the fact that the slightly stronger SSCs involving the cone of σ-critical directions allow for small perturbations in both L^∞ and L^2, which we need in the perturbed problems which are involved in the strong regularity property. In particular, this ensures that all in the SQP method (for an auxiliary problem) generated directions again stay feasible, i.e. again belong to the same cone of critical directions. Only in a second step, this convergence result can be transferred to the SQP method for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), if it is restricted to a local neighborhood of the optimal solution.

Let us conclude this introduction by giving an overview of the course of action and the main results of this chapter. We start by giving a precise formulation of the SQP algorithm and the involved quadratic subproblems, as well as the associated Newton's method for generalized equations, in the upcoming Section 6.1. Here, it is important to recognize that the associated first-order necessary optimality conditions of ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) from Section 4.1 can indeed be expressed as a generalized equation. Applying Newton's method, one has to solve a (linearized) generalized equation in every step, and it is demonstrated that this corresponds to the solution of the to the SQP method associated quadratic subproblem. Similarly to [74], we then prove a convergence theorem, cf. Theorem 6.2.10, which correlates to the well-known Newton-Kantorovich theorem used for finite dimensional problems. Applying the convergence theorem, we show local quadratic convergence of Newton's method, and therefore also of the SQP method for an auxiliary subproblem in Section 6.2. As prerequisites, we have to ensure the strong regularity property, as well as further technical results. The latter contain e.g. Lipschitz continuity of the reduced functional of the corresponding auxiliary optimal control problem, which involves a nontrivial analysis. Here, we can also utilize the preliminary results of the operators A and R as well as the Lagrangian $\mathcal{L}$, cf. Section 3.1 and 3.5. In Section 6.3, we then transfer this result to the SQP method with L^∞-closeness condition of the controls, following [152], which is our first convergence Theorem 6.3.15. Note that we incorporate (a.e.) pointwise arguments here, i.e. we need to restrict ourselves to the L^∞-localization setting, although the second-order sufficient condition does not, as a matter of fact, involve a two-norm discrepancy, as is proved in Chapter 4. Subsequently in Section 6.4, we establish our second convergence result Theorem 6.4.10, weakening the L^∞-closeness towards an L^2-localization, i.e. we effectively allow L^2-neighborhoods for the localization in the optimal control problems. Here we use ideas from [96], and apply techniques originally stemming from [40] from the context of two-norm discrepancy. Finally, in Section 6.5, the theoretical results are substantiated by some (simplified) numerical examples, which indicate that the proved convergence orders also occur in numerical examples.

6.1 The SQP method, quadratic subproblem and Newton's method

Before we start to state the SQP method for $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$ in detail, let us make an additional assumption and notational convention, that shall hold throughout the remainder of this chapter.

Assumption 6.1.1 (Fixed function triple $\bar{y}_{\mathbb{I}}$). *Assume that $\bar{q}_{\mathbb{I}}$ is a fixed local minimizer of $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$. The associated $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}}) \in Y_\infty^M \subset Y^M$ denotes a fixed function triple that satisfies the second-order sufficient conditions from Assumption 4.3.1, i.e. in particular also the first-order necessary condition from Lemma 4.1.3.*

We can now look at the SQP method for $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$. In the introduction of this chapter, it was outlined that the SQP method is given through iteratively solving a sequence of quadratic subproblems. Evidently, a thorough description of these subproblems is of interest: We start by introducing a quadratic subproblem (QP_k) via:

Let $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k) \in Y^M$ be given, find a pair of functions $\mathbf{d}_{\mathbb{I}}^k = (dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k) = (q_{\mathbb{I}} - q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k) \in Q^M \times W^M$ that solves

$$\left.\begin{aligned} &\min_{\mathbf{d}_{\mathbb{I}}^k} && J_{\mathbb{I},k}(\mathbf{d}_{\mathbb{I}}^k) := J_{\mathbb{I}}'(q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k)\mathbf{d}_{\mathbb{I}}^k + \frac{1}{2}\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}}^k)[(\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k), (\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k)],\\ &\text{subject to:} && \mathbf{du}_{\mathbb{I}}^k \text{ satisfies } (\mathrm{EL}_k) \text{ for data } dq_{\mathbb{I}}^k,\\ &\text{and:} && dq_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^k. \end{aligned}\right\} \tag{QP_k}$$

In this context, analogously to [85, Section 4], we define

$$\begin{aligned} Q_{\mathrm{ad},\mathbb{I}}^k := \{dq_{\mathbb{I}} \in Q^M \mid\ & q_a^i - q^{i,k} \le dq^i \le q_b^i - q^{i,k} \text{ a.e. on } \Gamma \\ & \text{for all } i = 1, \dots, M\}, \end{aligned}$$

and the linear partial differential equation (EL_k) is given by

$$\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}^{i,k}, d\varphi^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi^{i,k}, d\varphi^{i-1,k})\\ &\quad = B dq^{i,k} + B q^{i,k} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma), \end{aligned} \tag{EL_k}$$

for all $i = 1, \dots, M$.

Note that we use a new naming convention from here on, in contrast to the previous sections: The control function $dq_{\mathbb{I}}$ is used to emphasize its use as a direction for the SQP method, and a similar notation is used below for associated states $\mathbf{du}_{\mathbb{I}} = (du_{\mathbb{I}}, d\varphi_{\mathbb{I}})$ as well.

Under the assumption that (QP_k) is solvable, the iteration point is updated via $\mathbf{u}_{\mathbb{I}}^{k+1} = \mathbf{u}_{\mathbb{I}}^k + \mathbf{du}_{\mathbb{I}}^k \in W^M$ and $q_{\mathbb{I}}^{k+1} = q_{\mathbb{I}}^k + dq_{\mathbb{I}}^k \in Q_{\mathrm{ad},\mathbb{I}}$, with associated adjoint $\mathbf{z}_{\mathbb{I}}^{k+1}$ to be introduced below. In summary, the SQP algorithm for the model problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$), similarly to the case of the one time step model of [85, Algorithm 4.2] and [84], is given by:

Algorithm 6.1.2 (SQP algorithm for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$))**.**

(0) Choose a starting triple $y_{\mathbb{I}}^0 = (\mathbf{u}_{\mathbb{I}}^0, q_{\mathbb{I}}^0, \mathbf{z}_{\mathbb{I}}^0) \in Y^M$ *and set* $k = 0$.

(1) Terminate the algorithm with solution $y_{\mathbb{I}}^k$*, if* $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k)$ *satisfies the first-order necessary conditions of* ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) *from Lemma 4.1.3.*

(2) Solve (QP_k) *to obtain* $\mathbf{d}_{\mathbb{I}}^k$ *with associated adjoint* $\mathbf{z}_{\mathbb{I}}^{k+1}$.

(3) Set $(q_{\mathbb{I}}^{k+1}, \mathbf{u}_{\mathbb{I}}^{k+1}) = (q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k) + \mathbf{d}_{\mathbb{I}}^k$*, with associated adjoint* $\mathbf{z}_{\mathbb{I}}^{k+1}$*, set* $k = k+1$ *and go to step (1).*

The first task of the analysis of Algorithm 6.1.2 is the investigation of the underlying quadratic subproblem. Naturally, the questions arise whether the quadratic subproblems (QP_k) are (uniquely) solvable in every step k, which assumptions, e.g. on $y_{\mathbb{I}}^k$ are required, and if (QP_k) can be used in an iterative method, i.e. if solutions suffice to the assumptions that are required for the succeeding step. Subsequently, convergence of Algorithm 6.1.2 is of interest, and so is the order of convergence in case of convergence.

Before we continue, let us collect the following facts concerning the subproblem (QP_k) to be utilized in the remainder of this chapter. We omit the proofs, since they are straightforward.

Corollary 6.1.3.

- *For the control constraints* $dq_{\mathbb{I}} \in Q_{ad,\mathbb{I}}^k$*, due to* $q_{\mathbb{I}} := q_{\mathbb{I}}^k + dq_{\mathbb{I}}^k$*, we can equivalently demand* $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$*, if* ($\mathrm{QP}_k$) *is solvable.*

- $(dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k)$ *satisfying* (EL_k) *is equivalent to* $(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}}) \in Q^M \times W^M$ *solving*

$$\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{u}^i, \varphi^{i-1}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^i, \varphi^{i-1}) \\ &\quad = Bq^i - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \\ &\qquad + A_l(\mathbf{u}^{i,k})(\mathbf{u}^{i,k}, \varphi^{i-1,k}) \\ &\qquad + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^{i,k}, \varphi^{i-1,k}) \quad \forall i = 1, ..., M. \end{aligned} \tag{6.1}$$

In fact (6.1) *is independent of the control iterate* $q_{\mathbb{I}}^k$*, since it cancels out due to the linearity of the operator* B*.*

We frequently use the linear partial differential equations (EL_k) and (6.1) in its equivalent formulations without further mention, cf. the equivalent formulations for linearized equations from (3.72)-(3.74).

For theoretical reasons and to facilitate the notation, let us further introduce the equivalent reduced formulation for (QP_k), which is given via

$$\min f_{\mathbb{I},k}(q_{\mathbb{I}}) := J_{\mathbb{I},k}(q_{\mathbb{I}} - q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k), \quad \text{such that } q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}, \qquad (\mathrm{QP}_k^{\mathrm{red}})$$

where $\mathbf{u}_{\mathbb{I}}$ satisfies (6.1) for right-hand side data $q_{\mathbb{I}}$. We frequently use the reduced formulation in the analysis of our theoretical results. Note that analogously to the differentiability results of Section 3.4, it immediately holds:

Corollary 6.1.4.

- *The first derivative of $f_{\mathbb{I},k}$ can be determined to be*

$$f'_{\mathbb{I},k}(q_{\mathbb{I}})dq_{\mathbb{I}} = \sum_{i=1}^{M} \alpha\big(q^i, dq^i\big)_Q + \big(B^*\mathbf{z}_q^i, dq^i\big)_Q, \tag{6.2}$$

for an adjoint state $\mathbf{z}_{\mathbb{I},q} = (\mathbf{z}_q^i)_{i=1,...,M}$ that satisfies

$$\begin{aligned} &A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}_q^i, \psi_q^{i+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\psi_q^i, \psi_q^{i+1}) \\ &\quad = u^i - u_d^i - A_{b*}(\mathbf{u}^{i,k}, \mathbf{u}^i - \mathbf{u}^{i,k})\mathbf{z}^{i,k} \\ &\qquad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \varphi^i - \varphi^{i,k}, \varphi^{i-1} - \varphi^{i-1,k}, \varphi^{i+1} - \varphi^{k+1,k}; \gamma) \\ &\qquad\quad \cdot (\psi^{i,k}, \psi^{i+1,k}) \qquad \forall\, i = 1, ..., M. \end{aligned} \tag{6.3}$$

If we look at $\mathbf{z}_{\mathbb{I},q}$ for the optimal $q_{\mathbb{I}} = q_{\mathbb{I}}^{k+1}$, it holds that $\mathbf{z}_{\mathbb{I},q} = \mathbf{z}_{\mathbb{I}}^{k+1}$, and $\mathbf{z}_{\mathbb{I},q}$ is in fact the associated adjoint state, see Lemma 6.1.6 below.

- *For the second derivative, it holds*

$$f''_{\mathbb{I},k}(q_{\mathbb{I}})[dq_{\mathbb{I},1}, dq_{\mathbb{I},2}] = \mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}}^k)[(\tilde{\mathbf{u}}_{\mathbb{I},1}^k, dq_{\mathbb{I},1}), (\tilde{\mathbf{u}}_{\mathbb{I},2}^k, dq_{\mathbb{I},2})], \tag{6.4}$$

where $\tilde{\mathbf{u}}_{\mathbb{I},j}^k$, $j = 1, 2$ satisfies the linearized state equation in $\mathbf{u}_{\mathbb{I}}^k$, i.e.

$$A_l(\mathbf{u}^{i,k}, \varphi^{i-1,k})(\tilde{\mathbf{u}}_j^{i,k}, \tilde{\varphi}_j^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\tilde{\varphi}^{i,k}, \tilde{\varphi}^{i-1,k}) = B dq_j^i,$$

for all $i = 1, ..., M$ and for any $q_{\mathbb{I}}, dq_{\mathbb{I},1}, dq_{\mathbb{I},1} \in Q^M$. This immediately follows from the fact that $J'_{\mathbb{I}}(q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k)(\mathbf{d}_{\mathbb{I}}^k, \mathbf{d}_{\mathbb{I}}^k)$ is linear in the pair $(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}})$, and $\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}})[\mathbf{d}_{\mathbb{I}}^k, \mathbf{d}_{\mathbb{I}}^k]$ is bilinear in both derivative directions, i.e. quadratic for the chosen directions.

Some more properties of both $f'_{\mathbb{I},k}$ and $f''_{\mathbb{I},k}$, which follow analogously to the results for the reduced functional $f_{\mathbb{I}}$ from Section 3.4 are postponed to Lemma 6.4.1. We come back to them below, when we use them for our second main result in Section 6.4. Let us, at this point already, emphasize the following two properties:

Remark 6.1.5. *Both the remarks in the second bullet point in Corollary 6.1.3 and the second bullet point in Corollary 6.1.4 are important properties in the analysis of L^2-localization of the SQP method, cf. Section 6.4. We rely on the independence of $q_{\mathbb{I}}^k$ of* (6.1)*, as well as the fact that $f''_{\mathbb{I},k}$ is constant in the sense that it is independent of $q_{\mathbb{I}}$. The latter follows from the structure of $f_{\mathbb{I},k}$, and can immediately be seen from* (6.4)*.*

As explained earlier, the convergence of the SQP method is closely related to (suitable) SSCs, which are involved in the analysis of the (unique) solvability of the quadratic subproblem. However, we have to put on record that under Assumption 4.3.1, the objective functional $J_k(\mathbf{d}_{\mathbb{I}}^k)$ of (QP_k) is not necessarily convex for every given $y_{\mathbb{I}}^k \in Y^M$. Therefore at this point, an existence and uniqueness result is not established. Yet, if we assume that $\mathbf{d}_{\mathbb{I}}^k = (dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k)$ is a solution to (QP_k), then first-order necessary conditions are a standard result, that can e.g be proved similarly to Lemma 4.1.3 or [85, Lemma 4.1], or be adapted from [84, Section 4.2].

Lemma 6.1.6. *Let $y_{\mathbb{I}}^k \in Y^M$ be given and $q_{\mathbb{I}}^{k+1} \in Q^M$ be a minimizer of* (QP_k)*. Then, there exists an adjoint state $\mathbf{z}_{\mathbb{I}}^{k+1} = (z_{\mathbb{I}}^{k+1}, \psi_{\mathbb{I}}^{k+1}) \in W^M$ such that,*

$$\left.\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}^{i,k}, d\varphi^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi^{i,k}, d\varphi^{i-1,k}) \\ &\quad = Bq^{i,k+1} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \qquad \forall i = 1, ..., M, \end{aligned}\right\} \tag{6.5a}$$

$$\left.\begin{aligned} &A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}^{i.k+1}, \psi^{i+1,k+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma)(\psi^{i,k+1}, \psi^{i+1,k+1}) \\ &\quad = u^{i,k+1} - u_d^i - A_{b*}(\mathbf{u}^{i,k}, \mathbf{du}^{i,k})\mathbf{z}^{i,k} \\ &\qquad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, d\varphi^{i,k}, d\varphi^{i-1,k}, d\varphi^{i+1,k}; \gamma)(\psi^{i,k}, \psi^{i+1,k}) \\ &\qquad\quad \forall i = 1, ..., M, \end{aligned}\right\} \tag{6.5b}$$

$$\left.\left(B^*\mathbf{z}^{i,k+1} + \alpha q^{i,k+1}, q^i - q^{i,k+1}\right)_Q \geq 0 \quad \forall i = 1, ..., M \text{ and } \forall q_{\mathbb{I}} \in Q_{ad,\mathbb{I}} \right\} \tag{6.5c}$$

holds, where $\mathbf{du}_{\mathbb{I}}^k = \mathbf{u}_{\mathbb{I}}^{k+1} - \mathbf{u}_{\mathbb{I}}^k$.

Remark 6.1.7. *Note that in Lemma 6.1.6 we use the update directions $\mathbf{du}_{\mathbb{I}}^k$ in a short notation in both* (6.5a) *and* (6.5b)*, while the optimal control update directions $dq_{\mathbb{I}}^k$ do not appear in* (6.5c)*. Similarly as in* (6.1)*, the linearity of the operator B is used here. Of course, also* (6.5c) *can be given in terms of $dq_{\mathbb{I}}$ and $q_{\mathbb{I}}^k$, both in $Q_{ad,\mathbb{I}}^k$. In slight abuse of notation, both notations are frequently used where applicable and useful to ease readability, and we also call $q_{\mathbb{I}}^{k+1}$ and $\mathbf{u}_{\mathbb{I}}^{k+1}$ with associated $\mathbf{z}_{\mathbb{I}}^{k+1}$ a solution of both the nonreduced subproblem* (QP_k) *and the reduced subproblem* $(\mathrm{QP}_k^{\mathrm{red}})$*. Analogously, we say that a triple $y_{\mathbb{I}}^{k+1} = (\mathbf{u}_{\mathbb{I}}^{k+1}, q_{\mathbb{I}}^{k+1}, \mathbf{z}_{\mathbb{I}}^{k+1})$ satisfies the first-order necessary conditions of both* (QP_k) *and* $(\mathrm{QP}_k^{\mathrm{red}})$ *if it satisfies* (6.5a)-(6.5c).

We again want to point out that convexity of (QP_k), or equivalently $(\mathrm{QP}_k^{\mathrm{red}})$ is an open question at this point. The reason is that we involve control constraints and also only demand that $dq_{\mathbb{I}} \in C_\sigma(\bar{q}_{\mathbb{I}})$, i.e. we use only the (weaker) Assumption 4.3.1. In contrast to the setting of e.g. [84], as explained in the introduction, we therefore cannot use a direct approach to establish solvability of the quadratic subproblems, cf. e.g. also the references in [153, Section 4.11.3]. Instead, we need to use an indirect route through several auxiliary subproblems and results following the course of action of [43]. Let us start the analysis by stating Newton's method for a generalized equation, that emerges from equivalently rewriting the first-order optimality conditions of $(\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta})$ from Lemma 4.1.3. It is then possible to investigate convergence of Newton's method for auxiliary subproblems. Following the ideas of [5, 152], inspired by the first-order necessary conditions $(\mathrm{EL}^{\gamma,\eta})$, $(\mathrm{AE}^{\gamma,\eta})$ and $(\mathrm{VE}^{\gamma,\eta})$, we state the generalized equation

$$0 \in F_{\mathbb{I}}(y_{\mathbb{I}}) + N_{\mathbb{I}}(y_{\mathbb{I}}). \tag{GE}$$

In this context, the mapping $F_{\mathbb{I}}\colon Y^M \to Z^M$ and the set valued map $N_{\mathbb{I}}\colon Y^M \rightrightarrows Z^M$, as well as (GE), is understood via

$$0 \in F^i(y^i, y^{i-1}, y^{i+1}) + N^i(y^i) \qquad \text{for all } i = 1, ..., M. \tag{GE^i}$$

Here, the mappings $F^i\colon Y \times Y \times Y \to Z$ and the set valued map $N^i\colon Y \rightrightarrows Z$ are defined via

$$F^i(y^i, y^{i-1}, y^{i+1}) := \begin{pmatrix} A(\mathbf{u}^i, \varphi^{i-1}) + R(\varphi^i, \varphi^{i-1}; \gamma) - Bq^i \\ A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) - u^i + u_d^i \\ B^*\mathbf{z}^i + \alpha q^i \end{pmatrix}, \tag{6.6}$$

and

$$N^i(y^i) := \left(0,\, 0,\, N_{\mathrm{nc}}(q^i)\right)^T, \tag{6.7}$$

where $N_{\mathrm{nc}}(q^i)$ denotes the normal cone of $(Q_{\mathrm{ad},\mathbb{I}})_{|i}$ at a fixed $q^i \in Q$. In this context,

$$N_{\mathrm{nc}}(q^i) = \{dq^i \in Q \,|\, (dq^i, \tilde{q}^i - q^i)_Q \leq 0 \quad \text{for all} \quad \tilde{q}^i \in (Q_{\mathrm{ad},\mathbb{I}})_{|i}\},$$

slightly abusing notation, meaning that $(Q_{\mathrm{ad},\mathbb{I}})_{|i}$ is the i-th entry of $(Q_{\mathrm{ad},\mathbb{I}})$ in the sense that for a fixed i, it holds

$$(Q_{\mathrm{ad},\mathbb{I}})_{|i} = \{q^i \in Q \quad | \quad q_a^i \leq q^i \leq q_b^i \quad \text{a.e. on } \Gamma\}. \tag{6.8}$$

The mapping $F_{\mathbb{I}}$ is nonlinear in the state variable $\mathbf{u}_{\mathbb{I}}$, since the operators A and A_l are nonlinear in $\mathbf{u}_{\mathbb{I}}$. It is Fréchet differentiable from Y^M into Z^M, a result established below in Corollary 6.1.8, where also explicit representations of the derivatives $(F^i)'$ are stated. For better readability, this result and further properties of $F_{\mathbb{I}}$ that are essential for the convergence analysis of Algorithm 6.1.2 are postponed to Section 6.1.1. In any case, Newton's method can be applied to (GE): Given the function triple $y_{\mathbb{I}}^k \in Y^M$, the next iterate $y_{\mathbb{I}}^{k+1}$ is determined by solving

$$0 \in F_{\mathbb{I}}(y_{\mathbb{I}}^k) + F'_{\mathbb{I}}(y_{\mathbb{I}}^k)(y_{\mathbb{I}}^{k+1} - y_{\mathbb{I}}^k) + N_{\mathbb{I}}(y_{\mathbb{I}}^{k+1}) \tag{NM}$$

which is again a generalized equation. Now, simply inserting the definitions of F^i, N^i, cf. (6.6)-(6.7), and $(F^i)'$, cf. (6.9), into (NM), we can conclude, after some rearranging:

$$\begin{aligned} A(\mathbf{u}^{i,k},\varphi^{i-1,k}) + R(\varphi^{i,k},\varphi^{i-1,k};\gamma) - Bq^{i,k+1} \\ +A_l(\mathbf{u}^{i,k})(\mathbf{u}^{i,k+1}-\mathbf{u}^{i,k},\varphi^{i-1,k+1}-\varphi^{i-1,k}) \\ +R_l(\varphi^{i,k},\varphi^{i-1,k};\gamma)(\varphi^{i,k+1}-\varphi^{i,k},\varphi^{i-1,k+1}-\varphi^{i-1,k}) &= 0, \\ A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}^{i,k+1},\psi^{i+1,k+1}) \\ +R_{l*}(\varphi^{i,k},\varphi^{i-1,k},\varphi^{i+1,k};\gamma)(\psi^{i,k+1},\psi^{i+1,k+1}) \\ -u^{i,k+1} + u_d^i + A_{b*}(\mathbf{u}^{i,k},\mathbf{u}^{i,k+1}-\mathbf{u}^{i,k})\mathbf{z}^{i,k} \\ +R_{b*}(\varphi^{i,k},\varphi^{i-1,k},\varphi^{i+1,k},\varphi^{i,k+1}-\varphi^{i,k}, \\ \varphi^{i-1,k+1}-\varphi^{i-1,k},\varphi^{i+1,k+1}-\varphi^{i+1,k};\gamma)(\psi^{i,k},\psi^{i+1,k}) &= 0, \\ \left(B^*\mathbf{z}^{i,k+1}+\alpha q^{i,k+1}, q^i - q^{i,k+1}\right)_Q &\geq 0 \quad \forall q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}, \end{aligned}$$

for all $i = 1,...,M$. It is easy to see that these are precisely the first-order necessary conditions (6.5a), (6.5b) and (6.5c) from Lemma 6.1.6, setting $\mathbf{du}_{\mathbb{I}}^k = \mathbf{u}_{\mathbb{I}}^{k+1} - \mathbf{u}_{\mathbb{I}}^k$ and $dq_{\mathbb{I}}^k = q_{\mathbb{I}}^{k+1} - q_{\mathbb{I}}^k$. This means, that it is possible to investigate convergence of Newton's method given through iteratively solving (NM), and to obtain an equivalent result for the convergence of the SQP method for ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$). Note that again the main difficulty is to ensure that the iterates generated by Newton's method (NM) fulfill the assumptions needed to continue Newton's method for the next iterate, which means they have to stay once more within a neighborhood, where a local coercivity condition holds true. This is ensured by investigating convergence of an auxiliary subproblem in the next Section 6.2.

6.1.1 Auxiliary results for the operator $F_{\mathbb{I}}$

In this subsection, we establish some auxiliary results for the operator F from (GE), the operator F^i from (6.6) and its derivatives. They follow along the lines of [74, Lemma 6.2], and are e.g. required for the application of Dontchev's implicit function theorem [58, Theorem 2.4], that is used in Theorem 6.2.10. The key point is again to ensure the differentiability and Lipschitz properties in suitable Banach spaces, which can be inherited from the operators A and R, cf. Chapter 3.

Corollary 6.1.8. *The mapping F^i from* (6.6) *is Fréchet differentiable from $Y \times Y \times Y$ into Z. The derivative $(F^i)'$ is given by:*

$$(F^i)'(y^i,y^{i-1},y^{i+1})(\tilde{y}^i,\tilde{y}^{i-1},\tilde{y}^{i+1}) = \left((F^i)_1', (F^i)_2', (F^i)_3'\right)^T, \tag{6.9}$$

where

$$(F^i)_1' := A_l(\mathbf{u}^i)(\tilde{\mathbf{u}}^i,\tilde{\varphi}^{i-1}) + R_l(\varphi^i,\varphi^{i-1};\gamma)(\tilde{\varphi}^i,\tilde{\varphi}^{i-1}) - B\tilde{q}^i,$$

$$
\begin{aligned}
(F^i)'_2 :=& A_{b*}(\mathbf{u}^i, \tilde{\mathbf{u}}^i)\mathbf{z}^i + A_{l*}(\mathbf{u}^i)(\tilde{\mathbf{z}}^i, \tilde{\psi}^{i+1}) \\
&+ R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}, \tilde{\varphi}^i, \tilde{\varphi}^{i-1}, \tilde{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&+ R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\tilde{\psi}^i, \tilde{\psi}^{i+1}) - \tilde{u}^i, \\
(F^i)'_3 :=& B^*\tilde{\mathbf{z}}^i + \alpha\tilde{q}^i.
\end{aligned}
$$

This in turn means that the operator $F_{\mathbb{I}}$ is Fréchet differentiable from Y^M into Z^M.

Proof. For the case $M = 1$, this result has been given in [85, Section 5.1] by I. Neitzel and the author. It follows directly from Fréchet differentiability of A, A_l, R and R_l, cf. Lemma 3.1.4 and Lemma 3.1.7, and the linearity of the operator B, see Definition 2.3.8. □

Lemma 6.1.9. *Let $\bar{y}_{\mathbb{I}} \in Y^M$ be given. For any $0 < \tilde{\omega}_1, \tilde{\omega}_2 \in \mathbb{R}$, there exists a constant $0 < L(\tilde{\omega}_1, \tilde{\omega}_2) \in R$ such that for all $y_{\mathbb{I},j} = (\mathbf{u}_{\mathbb{I},j}, q_{\mathbb{I},j}, \mathbf{z}_{\mathbb{I},j}) \in Y^M$ with $\|\mathbf{u}_{\mathbb{I},j} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I},j} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \tilde{\omega}_1$, $j = 1, 2$, and for all $y_{\mathbb{I}} \in Y^M$ with $\|\mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \tilde{\omega}_2$, the following Lipschitz condition holds:*

$$
\begin{aligned}
&\|F_{\mathbb{I}}(y_{\mathbb{I},1}) + F'_{\mathbb{I}}(y_{\mathbb{I},1})(y_{\mathbb{I}} - y_{\mathbb{I},1}) - F_{\mathbb{I}}(y_{\mathbb{I},2}) - F'_{\mathbb{I}}(y_{\mathbb{I},2})(y_{\mathbb{I}} - y_{\mathbb{I},2})\|_{Z^M} \\
&\quad \leq L(\tilde{\omega}_1, \tilde{\omega}_2)(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}).
\end{aligned}
$$

Proof. For the case $M = 1$, this result has been proved in [85, Lemma A.1]. Let $y_{\mathbb{I}}, y_{\mathbb{I},j}$ be as assumed in the lemma. We establish the following result:

$$
\begin{aligned}
&\|F^i(y_1^i, y_1^{i-1}, y_1^{i+1}) + (F^i)'(y_1^i, y_1^{i-1}, y_1^{i+1})(y^i - y_1^i, y^{i-1} - y_1^{i-1}, y^{i+1} - y_1^{i+1}) \\
&\quad - F^i(y_2^i, y_2^{i-1}, y_2^{i+1}) - (F^i)'(y_2^i, y_2^{i-1}, y_2^{i+1})(y^i - y_2^i, y^{i-1} - y_2^{i-1}, y^{i+1} - y_2^{i+1})\|_Z \\
&\qquad \leq c(\tilde{\omega}_1, \tilde{\omega}_2)(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}),
\end{aligned}
$$

for all $i = 1, ..., M$. The statement of the lemma then immediately follows from the definition of the norm of Z^M. A quick calculation verifies

$$
\begin{aligned}
&F^i(y_1^i, y_1^{i-1}, y_1^{i+1}) + (F^i)'(y_1^i, y_1^{i-1}, y_1^{i+1})(y^i - y_1^i, y^{i-1} - y_1^{i-1}, y^{i+1} - y_1^{i+1}) \\
&- F^i(y_2^i, y_2^{i-1}, y_2^{i+1}) - (F^i)'(y_2^i, y_2^{i-1}, y_2^{i+1})(y^i - y_2^i, y^{i-1} - y_2^{i-1}, y^{i+1} - y_2^{i+1}) \\
&= \begin{pmatrix} f_1(\mathbf{u}_1^i, \varphi_1^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1}) \\ f_2(\mathbf{u}_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \mathbf{z}_1^i, \psi_1^{i+1}) - f_2(\mathbf{u}_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \mathbf{z}_2^i, \psi_2^{i+1}) \\ 0 \end{pmatrix},
\end{aligned}
$$

with

$$
\begin{aligned}
&f_1(\mathbf{u}_j^i, \varphi_j^{i-1}) \\
&\quad := A(\mathbf{u}_j^i, \varphi_j^{i-1}) + R(\varphi_j^i, \varphi_j^{i-1}; \gamma) + A_l(\mathbf{u}_j^i)(\mathbf{u}^i - \mathbf{u}_j^i, \varphi^{i-1} - \varphi_j^{i-1}) \\
&\qquad + R_l(\varphi_j^i, \varphi_j^{i-1}; \gamma)(\varphi^i - \varphi_j^i, \varphi^{i-1} - \varphi_j^{i-1}), \\
&f_2(\mathbf{u}_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}, \mathbf{z}_j^i, \psi_j^{i+1})
\end{aligned}
$$

$$
\begin{aligned}
&:= A_{l*}(\mathbf{u}_j^i)(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\varphi_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\quad + A_{b*}(\mathbf{u}_j^i, \mathbf{u}^i - \mathbf{u}_j^i)\mathbf{z}_j^i \\
&\quad + R_{b*}(\varphi_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}, \varphi^i - \varphi_j^i, \varphi^{i-1} - \varphi_j^{i-1}, \varphi^{i+1} - \varphi_j^{i+1}; \gamma)(\psi_j^i, \psi_j^{i+1}),
\end{aligned}
$$

We want to point out that neither f_1 nor f_2 depend on any of the controls q, q_1, q_2.

- For the difference in the f_1 terms, it holds

$$
\begin{aligned}
&f_1(\mathbf{u}_1^i, \varphi_1^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1}) \\
&\quad = A(\mathbf{u}_1^i, \varphi_1^{i-1}) - A(\mathbf{u}_2^i, \varphi_2^{i-1}) + R(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R(\varphi_2^i, \varphi_2^{i-1}; \gamma) \\
&\qquad + \big(A_l(\mathbf{u}_1^i) - A_l(\mathbf{u}_2^i)\big)(\mathbf{u}^i - \mathbf{u}_1^i, \varphi^{i-1} - \varphi_1^{i-1}) \\
&\qquad + A_l(\mathbf{u}_2^i)(\mathbf{u}_2^i - \mathbf{u}_1^i, \varphi_2^{i-1} - \varphi_1^{i-1}) \\
&\qquad + \big(R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)(\varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}) \\
&\qquad + R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\varphi_2^i - \varphi_1^i, \varphi_2^{i-1} - \varphi_1^{i-1}).
\end{aligned}
$$

  Estimating the terms in the $W^\times$ and L^q norm, respectively, using Lemma 3.1.5 and Lemma 3.1.8, leads to

$$
\begin{aligned}
&\|A(\mathbf{u}_1^i, \varphi_1^{i-1}) - A(\mathbf{u}_2^i, \varphi_2^{i-1})\|_{W^\times} \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \\
&\|R(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R(\varphi_2^i, \varphi_2^{i-1}; \gamma)\|_{L^q(\Omega)} \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \\
&\|\big(A_l(\mathbf{u}_1^i) - A_l(\mathbf{u}_2^i)\big)(\mathbf{u}^i - \mathbf{u}_1^i, \varphi^{i-1} - \varphi_1^{i-1})\|_{W^\times} \\
&\quad \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}, \\
&\|\big(R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)(\varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1})\|_{L^q(\Omega)} \\
&\quad \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}.
\end{aligned}
$$

  Note that the constants $0 < c(\tilde{\omega}_1) \in \mathbb{R}$ stem from the constants in (3.36), (3.56), (3.38) and (3.57), and are bounded depending on $\tilde{\omega}_1$ (and on $\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}$), but not on $\mathbf{u}_{\mathbb{I}}, \mathbf{u}_{\mathbb{I},j}$, $j = 1, 2$, due to the triangle inequalities

$$
\|\mathbf{u}_{\mathbb{I},j}\|_{W^M} \le \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},j} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \le \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \tilde{\omega}_1,
$$

  for $j = 1, 2$, as well as our assumptions.

  Finally, by Lemma 3.1.3 and Lemma 3.1.6

$$
\begin{aligned}
\|A_l(\mathbf{u}_2^i)(\mathbf{u}_2^i - \mathbf{u}_1^i, \varphi_2^{i-1} - \varphi_1^{i-1})\|_{W^\times} &\le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \\
\|R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\varphi_2^i - \varphi_1^i, \varphi_2^{i-1} - \varphi_1^{i-1})\|_{L^q(\Omega)} &\le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},
\end{aligned}
$$

  where the constants $0 < c(\tilde{\omega}_1) \in \mathbb{R}$ stem from (3.15) and (3.52), and the analogous remark to above holds.

  Combining all estimates, and recognizing that $\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},j}\|_{W^M} \le \|\mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},j}\|_{W^M} \le \tilde{\omega}_1 + \tilde{\omega}_2$, for $j = 1, 2$, we conclude

$$
\|f_1(\mathbf{u}_1^i, \varphi_1^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1})\|_{W^\times} \le c(\tilde{\omega}_1, \tilde{\omega}_2)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}. \quad (6.10)
$$

- For the difference in the f_2-terms it holds:

$$
\begin{aligned}
&f_2(\mathbf{u}_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \mathbf{z}_1^i, \psi_1^{i+1}) - f_2(\mathbf{u}_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \mathbf{z}_2^i, \psi_2^{i+1}) \\
&\quad = (A_{l*}(\mathbf{u}_1^i) - A_{l*}(\mathbf{u}_2^i))(\mathbf{z}^i, \psi^{i+1}) + A_{b*}(\mathbf{u}_1^i - \mathbf{u}_2^i, \mathbf{u}^i - \mathbf{u}_1^i)\mathbf{z}_1^i \\
&\qquad + A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i - \mathbf{u}_1^i)(\mathbf{z}_1^i - \mathbf{z}_2^i) + A_{b*}(\mathbf{u}_2^i, \mathbf{u}_2^i - \mathbf{u}_1^i)\mathbf{z}_2^i \\
&\qquad + (R_{l*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}; \gamma) - R_{l*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \gamma))(\psi^i, \psi^{i+1}) \\
&\qquad + R_{b*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma) \\
&\qquad\quad \cdot (\psi_1^i, \psi_1^{i+1}) \\
&\qquad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma) \\
&\qquad\quad \cdot (\psi_1^i, \psi_1^{i+1}) \\
&\qquad + R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma) \\
&\qquad\quad \cdot (\psi_1^i - \psi_2^i, \psi_1^{i+1} - \psi_2^{i+1}) \\
&\qquad + R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi_2^i - \varphi_1^i, \varphi_2^{i-1} - \varphi_1^{i-1}, \varphi_2^{i+1} - \varphi_1^{i+1}, \gamma) \\
&\qquad\quad \cdot (\psi_2^i, \psi_2^{i+1}).
\end{aligned}
$$

Again, estimating the terms in the $W^\times$, using Lemma 3.1.5 and Lemma 3.1.3, yields

$$
\|(A_{l*}(\mathbf{u}_1^i) - A_{l*}(\mathbf{u}_2^i))(\mathbf{z}^i, \psi^{i+1})\|_{W^\times} \le c(\tilde{\omega}_1, \tilde{\omega}_2)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},
$$

as well as

$$
\begin{aligned}
\|A_{b*}(\mathbf{u}_1^i - \mathbf{u}_2^i, \mathbf{u}^i - \mathbf{u}_1^i)\mathbf{z}_1^i\|_{W^\times} &\le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}, \\
\|A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i - \mathbf{u}_1^i)(\mathbf{z}_1^i - \mathbf{z}_2^i)\|_{W^\times} &\le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}\|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}, \\
\|A_{b*}(\mathbf{u}_2^i, \mathbf{u}_2^i - \mathbf{u}_1^i)\mathbf{z}_2^i\|_{W^\times} &\le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M},
\end{aligned}
$$

where the constants $0 < c(\tilde{\omega}_1, \tilde{\omega}_2) \in \mathbb{R}$ stem from (3.41), and are bounded depending on $\tilde{\omega}_1$ (and $\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}$), but not on $\mathbf{u}_{\mathbb{I}}, \mathbf{u}_{\mathbb{I},j}, \mathbf{u}_{\mathbb{I}}, \mathbf{z}_{\mathbb{I},j}$, again due to the triangle inequality and our assumptions. Similarly, using Lemma 3.1.8 and Lemma 3.1.6, we estimate

$$
\begin{aligned}
&\|(R_{l*}(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_{l*}(\varphi_2^i, \varphi_2^{i-1}; \gamma))(\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
&\quad \le c(\tilde{\omega}_1, \tilde{\omega}_2)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}, \\
&\|R_{b*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma)(\psi_1^i, \psi_1^{i+1}) \\
&\quad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma) \\
&\qquad\quad \cdot (\psi_1^i, \psi_1^{i+1})\|_{L^q(\Omega)} \\
&\quad \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}, \\
&\|R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i - \varphi_1^i, \varphi^{i-1} - \varphi_1^{i-1}, \varphi^{i+1} - \varphi_1^{i+1}; \gamma) \\
&\qquad \cdot (\psi_1^i - \psi_2^i, \psi_1^{i+1} - \psi_2^{i+1})\|_{L^q(\Omega)} \\
&\quad \le c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},1}\|_{W^M}\|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M},
\end{aligned}
$$

$$\|R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi_2^i - \varphi_1^i, \varphi_2^{i-1} - \varphi_1^{i-1}, \varphi_2^{i+1} - \varphi_1^{i+1}, \gamma)$$
$$\cdot (\psi_2^i, \psi_2^{i+1})\|_{L^q(\Omega)}$$
$$\leq c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}.$$

Combining all estimates and again using $\|\mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},j}\|_{W^M} \leq \|\mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},j}\|_{W^M} \leq \tilde{\omega}_1 + \tilde{\omega}_2$, as well as $\|\mathbf{z}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I},j}\|_{W^M} \leq \|\mathbf{z}_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{z}}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I},j}\|_{W^M} \leq \tilde{\omega}_1 + \tilde{\omega}_2$, for $j = 1, 2$, we conclude

$$\|f_2(\mathbf{u}_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \mathbf{z}_1^i, \psi_1^{i+1}) - f_2(\mathbf{u}_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \mathbf{z}_2^i, \psi_2^{i+1})\|_{W^\times}$$
$$\leq c(\tilde{\omega}_1, \tilde{\omega}_2)\big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}\big). \tag{6.11}$$

The statement for all $i = 1, ..., M$ now follows from (6.10) and (6.11), and the definition of the operators $F_{\mathbb{I}}$, $F'_{\mathbb{I}}$ respectively, as well as the definition of the norm Z^M. □

Lemma 6.1.10. *The operator $F'_{\mathbb{I}}$, given implicitly through $(F^i)'$, cf.* (6.9) *for all $i = 1, ..., M$, is locally Lipschitz continuous w.r.t. $y_{\mathbb{I}}$ as a mapping from Y^M into Z^M, i.e. for any $0 < \tilde{\omega}_1 \in \mathbb{R}$ there exists a constant $0 < L(\tilde{\omega}_1) \in \mathbb{R}$, such that for all $y_{\mathbb{I},j} = (\mathbf{u}_{\mathbb{I},j}, q_{\mathbb{I},j}, \mathbf{z}_{\mathbb{I},j}) \in Y^M$, with $\|\mathbf{u}_{\mathbb{I},j} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I},j} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \tilde{\omega}_1$, $i = 1, 2$ and all $y_{\mathbb{I}} \in Y^M$, it holds*

$$\|\big(F'_{\mathbb{I}}(y_{\mathbb{I},1}) - F'_{\mathbb{I}}(y_{\mathbb{I},2})\big)y_{\mathbb{I}}\|_{Z^M}$$
$$\leq L\big(\tilde{\omega}_1\big)\big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}\big)\big(\|\mathbf{u}_{\mathbb{I}}\|_W + \|\mathbf{z}_{\mathbb{I}}\|_{W^M}\big).$$

Proof. For the case $M = 1$, this result has been proved in [85, Lemma A.2] of the author and I. Neitzel. As above, we again establish a Lipschitz condition for the operator $(F^i)'$, for $i = 1, .., M$ arbitrary, i.p.

$$\Big\|\big((F^i)'(y_1^i, y_1^{i-1}, y_1^{i+1}) - (F^i)'(y_2^i, y_2^{i-1}, y_2^{i+1})\big)(y^i, y^{i-1}, y^{i+1})\Big\|_Z$$
$$\leq c\big(\tilde{\omega}_1, \tilde{\omega}_2\big)\big(\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M} + \|\mathbf{z}_{\mathbb{I},1} - \mathbf{z}_{\mathbb{I},2}\|_{W^M}\big)\big(\|\mathbf{u}_{\mathbb{I}}\|_W + \|\mathbf{z}_{\mathbb{I}}\|_{W^M}\big).$$

A quick calculation verifies

$$\big((F^i)'(y_1^i, y_1^{i-1}, y_1^{i+1}) - (F^i)'(y_2^i, y_2^{i-1}, y_2^{i+1})\big)(y^i, y^{i-1}, y^{i+1})$$
$$= \begin{pmatrix} f_1(\mathbf{u}_1^i, \varphi_j^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1}) \\ f_2(\mathbf{u}_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \mathbf{z}_1^i, \psi_1^{i+1}) - f_2(\mathbf{u}_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \mathbf{z}_2^i, \psi_2^{i+1}) \\ 0 \end{pmatrix},$$

with

$$f_1(\mathbf{u}_j^i, \varphi_j^{i-1}) := A_l(\mathbf{u}_j^i)(\mathbf{u}^i, \varphi^{i-1}) + R_l(\varphi_j^i, \varphi_j^{i-1}; \gamma)(\varphi^i, \varphi^{i-1}).$$
$$f_2(\mathbf{u}_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}, \mathbf{z}_j^i, \psi_j^{i+1}) := A_{b*}(\mathbf{u}_j^i, \mathbf{u}^i)\mathbf{z}_j^i + A_{l*}(\mathbf{u}_j^i)(\mathbf{z}^i, \psi^{i+1})$$
$$+ R_{b*}(\varphi_j^i, \varphi_j^{i-1}, \varphi_j^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_j^i, \psi_j^{i+1})$$
$$+ R_{l*}(\varphi_j^i, \varphi_j^{i-1}; \gamma)(\psi^i, \psi^{i+1}),$$

where we again point out that both f_1 and f_2 are independent of any control $q_{\mathbb{I}}, q_{\mathbb{I},1}, q_{\mathbb{I},2}$.

- For the difference in the f_1-terms, it holds:

$$\begin{aligned}
&f_1(\mathbf{u}_1^i, \varphi_1^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1}) \\
&\quad = \big(A_l(\mathbf{u}_1^i) - A_l(\mathbf{u}_2^i)\big)(\mathbf{u}^i, \varphi^{i-1}) \\
&\qquad + \big(R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)(\varphi^i, \varphi^{i-1}).
\end{aligned}$$

By term-wise estimations, using Lemma 3.1.5 and Lemma 3.1.8, it follows:

$$\begin{aligned}
&\|\big(A_l(\mathbf{u}_1^i) - A_l(\mathbf{u}_2^i)\big)(\mathbf{u}^i, \varphi^{i-1})\|_{W^\times} \\
&\quad \leq c\big(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M} + \|\mathbf{u}_{\mathbb{I},2}\|_{W^M}\big)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}, \\
&\|\big(R_l(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_l(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)(\varphi^i, \varphi^{i-1})\|_{L^q(\Omega)} \\
&\quad \leq c(\|\mathbf{u}_{\mathbb{I},1}\|_{W^M}, \|\mathbf{u}_{\mathbb{I},2}\|_{W^M})\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}.
\end{aligned}$$

Note that as in the proof of Lemma 6.1.9, the constants on the right-hand side can again be bounded only depending on $\tilde{\omega}_1$ (and on $\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}$), due to our assumptions and the triangle inequality. We thus conclude

$$\|f_1(\mathbf{u}_1^i, \varphi_1^{i-1}) - f_1(\mathbf{u}_2^i, \varphi_2^{i-1})\|_{W^\times} \leq c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}. \tag{6.12}$$

- For the difference in the f_2-terms it holds:

$$\begin{aligned}
&f_2(\mathbf{u}_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \mathbf{z}_1^i, \psi_1^{i+1}) - f_2(\mathbf{u}_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \mathbf{z}_2^i, \psi_2^{i+1}) \\
&\quad = A_{b*}(\mathbf{u}_1^i, \mathbf{u}^i)\mathbf{z}_1^i + A_{l*}(\mathbf{u}_1^i)(\mathbf{z}^i, \psi^{i+1}) \\
&\qquad + R_b(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_1^i, \psi_1^{i+1}) \\
&\qquad + R_{l*}(\varphi_1^i, \varphi_1^{i-1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i)\mathbf{z}_2^i - A_{l*}(\mathbf{u}_2^i)(\mathbf{z}^i, \psi^{i+1}) \\
&\qquad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}; \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_2^i, \psi_2^{i+1}) \\
&\qquad - R_{l*}(\varphi_2^i, \varphi_2^{i-1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\quad = \big(A_{b*}(\mathbf{u}_1^i, \mathbf{u}^i) - A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i)\big)\mathbf{z}_1^i + A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i)(\mathbf{z}_1^i - \mathbf{z}_2^i) \\
&\qquad + \big(R_{b*}(\varphi_1^i, \varphi_1^{i-1}, \varphi_1^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_1^i, \psi_1^{i+1}) \\
&\qquad - R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_1^i, \psi_1^{i+1})\big) \\
&\qquad + R_{b*}(\varphi_2^i, \varphi_2^{i-1}, \varphi_2^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi_1^i - \psi_2^i, \psi_1^{i+1} - \psi_2^{i+1}) \\
&\qquad + \big(A_{l*}(\mathbf{u}_1^i) - A_{l*}(\mathbf{u}_2^i)\big)(\mathbf{z}^i, \psi^{i+1}) \\
&\qquad + \big(R_{l*}(\varphi_1^i, \varphi_1^{i-1}; \gamma) - R_{l*}(\varphi_2^i, \varphi_2^{i-1}; \gamma)\big)(\psi^i, \psi^{i+1}).
\end{aligned}$$

Again, term-wise estimations, utilizing Lemma 3.1.5 and Lemma 3.1.8, it follows

$$\begin{aligned}
&\|\big(A_{b*}(\mathbf{u}_1^i, \mathbf{u}^i) - A_{b*}(\mathbf{u}_2^i, \mathbf{u}^i)\big)\mathbf{z}_1^i\|_{W^\times} \\
&\quad \leq c(\tilde{\omega}_1)\|\mathbf{u}_{\mathbb{I},1} - \mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M},
\end{aligned}$$

$$
\begin{aligned}
&\|\big(R_{b*}(\varphi_1^i,\varphi_1^{i-1},\varphi_1^{i+1},\varphi^i,\varphi^{i-1},\varphi^{i+1};\gamma)(\psi_1^i,\psi_1^{i+1})\\
&\qquad - R_{b*}(\varphi_2^i,\varphi_2^{i-1},\varphi_2^{i+1},\varphi^i,\varphi^{i-1},\varphi^{i+1};\gamma)(\psi_1^i,\psi_1^{i+1})\big)\|_{L^q(\Omega)}\\
&\quad \le c(\tilde\omega)\|\mathbf{u}_{\mathbb{I},1}-\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M},\\
&\|\big(A_{l*}(\mathbf{u}_1^i)-A_{l*}(\mathbf{u}_2^i)\big)(\mathbf{z}^i,\psi^{i+1})\|_{W^\times}\\
&\quad \le c(\tilde\omega_1)\|\mathbf{u}_{\mathbb{I},1}-\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M},\\
&\|\big(R_{l*}(\varphi_1^i,\varphi_1^{i-1};\gamma)-R_{l*}(\varphi_2^i,\varphi_2^{i-1};\gamma)\big)(\psi^i,\psi^{i+1})\|_{L^q(\Omega)}\\
&\quad \le c(\tilde\omega_1)\|\mathbf{u}_{\mathbb{I},1}-\mathbf{u}_{\mathbb{I},2}\|_{W^M}\|\mathbf{z}_{\mathbb{I}}\|_{W^M},
\end{aligned}
$$

From Lemma 3.1.3 and Lemma 3.1.6, it immediately follows

$$
\begin{aligned}
&\|A_{b*}(\mathbf{u}_2^i,\mathbf{u}^i)(\mathbf{z}_1^i-\mathbf{z}_2^i)\|_{W^\times}\\
&\quad \le c(\tilde\omega_1)\|\mathbf{u}_{\mathbb{I}}]\|_{W^M}\|\mathbf{z}_{\mathbb{I},1}-\mathbf{z}_{\mathbb{I},2}\|_{W^M},\\
&\|R_{b*}(\varphi_2^i,\varphi_2^{i-1},\varphi_2^{i+1},\varphi^i,\varphi^{i-1},\varphi^{i+1};\gamma)(\psi_1^i-\psi_2^i,\psi_1^{i+1}-\psi_2^{i+1})\|_{L^q(\Omega)}\\
&\quad \le c(\tilde\omega_1)\|\mathbf{u}_{\mathbb{I}}]\|_{W^M}\|\mathbf{z}_{\mathbb{I},1}-\mathbf{z}_{\mathbb{I},2}\|_{W^M}.
\end{aligned}
$$

In all above estimates, as in the proof of Lemma 6.1.9, the constants $c(\tilde\omega_1)$ on the right-hand side can again be bounded only depending on $\tilde\omega_1$ (and on $\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}$ and $\|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}$), due to our assumptions and the triangle inequality.

Combining all estimates, analogously to the proof of Lemma 6.1.9, it is now possible to conclude

$$
\begin{aligned}
&\|f_2(\mathbf{u}_1^i,\varphi_1^{i-1},\varphi_1^{i-1},\mathbf{z}_1^i,\psi^{i+1})-f_2(\mathbf{u}_2^i,\varphi_2^{i-1},\varphi_2^{i+1},\mathbf{z}_2^i,\psi_2^{i+1})\|_{W^\times}\\
&\quad \le c(\tilde\omega_1)\big(\|\mathbf{u}_{\mathbb{I},1}-\mathbf{u}_{\mathbb{I},2}\|_{W^M}+\|\mathbf{z}_{\mathbb{I},1}-\mathbf{z}_{\mathbb{I},2}\|_{W^M}\big)\big(\|\mathbf{u}_{\mathbb{I}}\|_{W^M}+\|\mathbf{z}_{\mathbb{I}}\|_{W^M}\big). \qquad (6.13)
\end{aligned}
$$

Finally, combining (6.12) and (6.13) concludes the proof, analogously to the conclusion in the proof of Lemma 6.1.9. □

Let us finally show a quadratic bound for the second-order remainder of the derivative of $F_{\mathbb{I}}$, which is used for the quadratic convergence result in the proof of Theorem 6.2.10. In contrast to [73, Theorem 7.1], where such a quadratic bound follows immediately from the second-order Fréchet differentiability of $F_{\mathbb{I}}$, for the $F_{\mathbb{I}}$ of (GE) this requires some additional work, since the operator R is not three times differentiable, and hence $F_{\mathbb{I}}$ is not twice differentiable.

Lemma 6.1.11. *Let $\bar y_{\mathbb{I}} \in Y^M$ be given and $y_{\mathbb{I}} \in Y^M$ with $\|\mathbf{u}_{\mathbb{I}}-\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\bar{\mathbf{z}}_{\mathbb{I}}-\mathbf{u}_{\mathbb{I}}\|_{W^M} \le \tilde\omega_3$ for some $0<\tilde\omega_3\in\mathbb{R}$. There exists a constant $0<L(\tilde\omega_3)\in\mathbb{R}$ such that*

$$
\|F_{\mathbb{I}}(\bar y_{\mathbb{I}})-F_{\mathbb{I}}(y_{\mathbb{I}})-F_{\mathbb{I}}'(y_{\mathbb{I}})(\bar y_{\mathbb{I}}-y_{\mathbb{I}})\|_{Z^M} \le L(\tilde\omega_3)\big(\|\mathbf{u}_{\mathbb{I}}-\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}^2+\|\mathbf{z}_{\mathbb{I}}-\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}^2\big).
$$

Proof. For the case $M=1$, this result has been proved in [85, Lemma A.3] by the author and I. Neitzel. As already explained, the quadratic bound on the right-hand side cannot be deduced from twice Fréchet differentiability of $F_{\mathbb{I}}$, instead the structure of $F'_{\mathbb{I}}$ is taken advantage of. As in the previous lemma, a quick calculation shows, for all $i = 1, ..., M$,

$$\begin{aligned}
&F^i(\bar{y}^i, \bar{y}^{i-1}, \bar{y}^{i+1}) - F^i(y^i, y^{i-1}, y^{i+1}) \\
&\quad - (F^i)'(y^i, y^{i-1}, y^{i+1})((\bar{y}^i, \bar{y}^{i-1}, \bar{y}^{i+1}) - (y^i, y^{i-1}, y^{i+1})) \\
&\quad = \begin{pmatrix} f_1(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \mathbf{u}^i, \varphi^{i-1}) \\ f_2(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \bar{\mathbf{z}}^i, \bar{\psi}^{i+1}, \mathbf{u}^i, \varphi^{i-1}, \varphi^{i+1}, \mathbf{z}^i, \psi^{i+1}) \\ 0 \end{pmatrix},
\end{aligned}$$

with

$$\begin{aligned}
&f_1(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \mathbf{u}^i, \varphi^{i-1}) \\
&\quad := A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) + R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma) - A(\mathbf{u}^i, \varphi^{i-1}; \gamma) - R(\varphi^i, \varphi^{i-1}; \gamma) \\
&\qquad - A_l(\mathbf{u}^i)(\bar{\mathbf{u}}^i - \mathbf{u}^i, \bar{\varphi}^{i-1} - \varphi^{i-1}) \\
&\qquad - R_l(\varphi^i, \varphi^{i-1}; \gamma)(\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}), \qquad (6.14) \\
&f_2(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \bar{\mathbf{z}}^i, \bar{\psi}^{i+1}, \mathbf{u}^i, \varphi^{i-1}, \varphi^{i+1}, \mathbf{z}^i, \psi^{i+1}) \\
&\quad := A_{l*}(\bar{\mathbf{u}}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) + R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}; \gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) \\
&\qquad - A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) - R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\mathbf{z}^i - A_{l*}(\mathbf{u}^i)(\bar{\mathbf{z}}^i - \mathbf{z}^i, \bar{\psi}^{i+1} - \psi^{i+1}) \\
&\qquad - R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - R_{l*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\bar{\psi}^i - \psi^i, \bar{\psi}^{i+1} - \psi^{i+1}). \qquad (6.15)
\end{aligned}$$

We note again that the difference in the last component is zero, and that there is no dependence on any control $\bar{q}_{\mathbb{I}}, q_{\mathbb{I}}$.

- We start again with term-wise estimations of f_1: For the terms involving R in (6.14), introduce the auxiliary functional $T\colon [0,1] \to L^q(\Omega)$, $T(\theta) := R(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}); \gamma)$, due to Lemma 3.1.7. Using Taylor's expansion $T(1) = T(0) + T'(0) + \frac{1}{2}T''(\theta)$, for $\theta \in (0,1)$, this means

  $$\begin{aligned}
  &R(\bar{\varphi}^{i-1}, \bar{\varphi}^{i-1}; \gamma) - R(\varphi^i, \varphi^{i-1}; \gamma) - R'(\varphi^i, \varphi^{i-1}; \gamma)(\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}) \\
  &\quad = \frac{1}{2} R''(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}); \gamma) \\
  &\qquad \cdot [(\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}), (\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1})],
  \end{aligned}$$

  thus estimating in the L^q-norm, using Lemma 3.1.6, we obtain for all terms involving R:

  $$\begin{aligned}
  &\|R(\bar{\varphi}^{i-1}, \bar{\varphi}^{i-1}; \gamma) - R(\varphi^i, \varphi^{i-1}; \gamma) \qquad (6.16) \\
  &\qquad - R'(\varphi^i, \varphi^{i-1}; \gamma)(\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1})\|_{L^q(\Omega)} \\
  &\quad = c\|R''(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}); \gamma) \\
  &\qquad \cdot [(\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}), (\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1})]\|_{L^q(\Omega)}
  \end{aligned}$$

$$\leq c(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|^2_{W^M}. \tag{6.17}$$

Analogously, for the terms involving A in (6.14), we obtain using Lemma 3.1.4 and then Lemma 3.1.3:

$$\begin{aligned}
&\|A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) - A(\mathbf{u}^i, \varphi^{i-1};\gamma) - A_l(\mathbf{u}^i)(\bar{\mathbf{u}}^i - \mathbf{u}^i, \bar{\varphi}^{i-1} - \varphi^{i-1})\|_{W^\times} \\
&\quad = c\|A_b(\mathbf{u}^i + \theta(\bar{\mathbf{u}}^i - \mathbf{u}^i))[(\bar{\mathbf{u}}^i - \mathbf{u}^i), (\bar{\mathbf{u}}^i - \mathbf{u}^i)]\|_{W^\times} \\
&\quad \leq c(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|^2_{W^M}.
\end{aligned} \tag{6.18}$$

Combining (6.17) and (6.18) yields

$$\|f_1(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \mathbf{u}^i, \varphi^{i-1})\|_{W^\times} \leq c(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|^2_{W^M}. \tag{6.19}$$

- For term-wise estimations of f_2, we introduce the auxiliary functional $T\colon [0,1] \to L^q(\Omega)$, $T(\theta) := R_{l*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1});\gamma)(\bar{\psi}^i, \bar{\psi}^{i+1})$, due to Lemma 3.1.7. Using Taylor's expansion $T(1) = T(0) + T'(\theta)$, for $\theta \in (0,1)$ this means

  $$\begin{aligned}
  &R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1};\gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) - R(\varphi^i, \varphi^{i-1}, \varphi^{i+1};\gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) \\
  &\quad = R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}), \\
  &\qquad\qquad \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}).
  \end{aligned}$$

  Thus, the terms involving R in (6.15) can be directly estimated in the L^q-norm,

  $$\begin{aligned}
  &\|R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}), \\
  &\qquad \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) \\
  &\quad - R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma) \\
  &\qquad (\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
  &\leq \|R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}), \\
  &\qquad \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma) \\
  &\qquad (\bar{\psi}^i - \psi^i, \bar{\psi}^{i+1} - \psi^{i+1})\|_{L^q(\Omega)} \\
  &\quad + \|R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}), \\
  &\qquad \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma)(\psi^i, \psi^{i+1}) \\
  &\qquad - R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1};\gamma) \\
  &\qquad (\psi^i, \psi^{i+1})\|_{L^q(\Omega)}.
  \end{aligned}$$

  Using the definition of the operators R_{b*} from (3.12), using Lemma 3.1.6, we continue to estimate

  $$\|R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}),$$

$$
\begin{aligned}
&\bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1}; \gamma) \\
&(\bar{\psi}^i - \psi^i, \bar{\psi}^{i+1} - \psi^{i+1})\|_{L^q(\Omega)} \\
\leq\, & c(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M}\|\bar{\mathbf{z}}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I}}\|_{W^M},
\end{aligned}
\tag{6.20}
$$

as well as, by Lemma 3.1.8:

$$
\begin{aligned}
&\|R_{b*}(\varphi^i + \theta(\bar{\varphi}^i - \varphi^i), \varphi^{i-1} + \theta(\bar{\varphi}^{i-1} - \varphi^{i-1}), \varphi^{i+1} + \theta(\bar{\varphi}^{i+1} - \varphi^{i+1}), \\
&\qquad \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\
&\qquad - R_{b*}(\varphi^i, \varphi^{i-1}, \varphi^{i+1}; \bar{\varphi}^i - \varphi^i, \bar{\varphi}^{i-1} - \varphi^{i-1}, \bar{\varphi}^{i+1} - \varphi^{i+1}; \gamma) \\
&\qquad\qquad (\psi^i, \psi^{i+1})\|_{L^q(\Omega)} \\
&\leq c(\tilde{\omega}_3)\|\mathbf{u}_{\mathbb{I}} + \theta(\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}) - \mathbf{u}_{\mathbb{I}}\|_{W^M}\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M} \\
&\leq c(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M}^2.
\end{aligned}
\tag{6.21}
$$

Analogously, for the terms involving A in (6.15), we obtain using Taylor's expansion due to Lemma 3.1.4,

$$
\begin{aligned}
&A_{l*}(\bar{\mathbf{u}}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) - A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) \\
&\quad - A_{l*}(\mathbf{u}^i)(\bar{\mathbf{z}}^i - \mathbf{z}^i, \bar{\psi}^{i+1} - \psi^{i+1}) - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\mathbf{z}^i \\
&= A_{l*}(\bar{\mathbf{u}}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) - A_{l*}(\mathbf{u}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\mathbf{z}^i \\
&= A_{b*}(\mathbf{u}^i + \theta(\bar{\mathbf{u}}^i - \mathbf{u}^i), \bar{\mathbf{u}}^i - \mathbf{u}^i)\bar{\mathbf{z}}^i - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\mathbf{z}^i \\
&= \big(A_{b*}(\mathbf{u}^i + \theta(\bar{\mathbf{u}}^i - \mathbf{u}^i), \bar{\mathbf{u}}^i - \mathbf{u}^i) - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\big)\bar{\mathbf{z}}^i \\
&\quad + A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)(\bar{\mathbf{z}}^i - \mathbf{z}^i),
\end{aligned}
$$

which can be estimated using Lemma 3.1.5 and Lemma 3.1.3 to be

$$
\begin{aligned}
&\|A_{l*}(\bar{\mathbf{u}}^i)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) - A_{l*}(\mathbf{u}^i)(\mathbf{z}^i, \psi^{i+1}) \\
&\quad - A_{l*}(\mathbf{u}^i)(\bar{\mathbf{z}}^i - \mathbf{z}^i, \bar{\psi}^{i+1} - \psi^{i+1}) - A_{b*}(\mathbf{u}^i, \bar{\mathbf{u}}^i - \mathbf{u}^i)\mathbf{z}^i\|_{W^\times} \\
&\leq c(\tilde{\omega}_3)\|\mathbf{u}_{\mathbb{I}} + \theta(\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M}\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M} \\
&\quad + c)(\tilde{\omega}_3)\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M}\|\bar{\mathbf{z}}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I}}\|_{W^M}.
\end{aligned}
\tag{6.22}
$$

Combining (6.20), (6.21) and (6.22), and using Young's inequality, yields

$$
\begin{aligned}
&\|f_2(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \bar{\mathbf{z}}^i, \bar{\psi}^{i+1}, \mathbf{u}^i, \varphi^{i-1}, \varphi^{i+1}, \mathbf{z}^i, \psi^{i+1})\|_{W^\times} \\
&\quad \leq c(\tilde{\omega}_3)\big(\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}\|_{W^M}^2 + \|\bar{\mathbf{z}}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I}}\|_{W^M}^2\big).
\end{aligned}
\tag{6.23}
$$

Note that again all constants $0 < c(\tilde{\omega}_3) \in \mathbb{R}$ only depend on $\tilde{\omega}_3$ (and on $\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}$ and $\|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}$), cf. the proof of Lemma 6.1.9 and Lemma 6.1.11. The statement for all $i = 1, .., M$ now follows from (6.19) and (6.23), and the definition of the operators $F_{\mathbb{I}}, F'_{\mathbb{I}}$ as well as the definition of the norm of Z^M. □

We have already stated in Lemma 6.1.9, Lemma 6.1.10 and Lemma 6.1.11, that all results are independently of any controls and control directions $q_{\mathbb{I}}, q_{\mathbb{I},j}$, $j = 1, 2$. In particular, the locality assumptions for the controls are never incorporated into the results. It is therefore immediately possible to replace all spaces Y^M and Z^M by the spaces Y^M_∞ and Z^M_∞, and we can conclude:

Corollary 6.1.12. *The results of Lemma 6.1.9, 6.1.10 and 6.1.11 hold true in the $Y^M_\infty - Z^M_\infty$ setting. In particular, we can simply replace all involved spaces Y^M and Z^M by the spaces Y^M_∞ and Z^M_∞.*

6.2 Convergence analysis for an auxiliary sequence

In the previous section, the SQP method was equivalently expressed in the form of a Newton method. Yet, the lack of convexity of $(\mathrm{NLP}^{\gamma,\eta}_{\mathbb{I}})$ under Assumption 4.3.1 is still an impediment, and it is still not clear whether the generated directions again lie in the cone of critical directions from Assumption 4.3.1, regardless of whether the SQP method or Newton's method is used. In a first step, we alter the setting towards an auxiliary subproblem, that involves not the admissible set $Q_{\mathrm{ad},\mathbb{I}}$, but a slightly different admissible set that fits the critical cone involving σ-active constraints from Assumption 4.3.1. This idea stems from [152], and suggests to split the analysis into several steps. In a first step, an auxiliary problem, called $(\widehat{\mathrm{QP}}_k)$, is introduced and analyzed, and the strong regularity property is proved for this problem. Based on this, a convergence result can then be utilized to ensure quadratic convergence of the generated iterates towards $\bar{q}_{\mathbb{I}}$. In two further steps in Section 6.3 and Section 6.4, introducing yet two other auxiliary, localized subproblems, we transfer the convergence results towards localized versions of Algorithm 6.1.2, first with L^∞-localization as in [152], and then with L^2-localization, using the ideas of [96]. For the setting $M = 1$, i.e. the one time-step setting, these results are proved in [85, Section 5, 6 and 7] by I. Neitzel and the author.

6.2.1 The auxiliary subproblem $(\widehat{\mathrm{QP}}_k)$

Let us straightaway introduce the following adjusted admissible set

$$\widehat{Q_{\mathrm{ad},\mathbb{I}}} := \{q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}} \mid q_{\mathbb{I}} = \bar{q}_{\mathbb{I}} \text{ on } \mathcal{I}(\sigma)\},$$

where we recall from (4.20) that $\mathcal{I}(\sigma) = \{x \in \Gamma \mid |B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i| \geq \sigma \ \forall i = 1, ..., M\}$, and that $\bar{q}_{\mathbb{I}}$ is a local optimal control for $(\mathrm{NLP}^{\gamma,\eta}_{\mathbb{I}})$, cf. Assumption 6.1.1. The auxiliary subproblem $(\widehat{\mathrm{QP}}_k)$ of this section can then be stated via:

Let $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k) \in Y^M$ be given, find a pair of functions $\mathbf{d}_{\mathbb{I}}^k = (dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k) = (q_{\mathbb{I}} - q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k) \in Q^M \times W^M$ that solves

$$\left.\begin{aligned} &\min_{\mathbf{d}_{\mathbb{I}}^k} \quad J_{\mathbb{I},k}(\mathbf{d}_{\mathbb{I}}^k) := J'_{\mathbb{I}}(q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k)\mathbf{d}_{\mathbb{I}}^k + \frac{1}{2}\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}}^k)[(\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k), (\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k)], \\ &\text{subject to:} \quad \mathbf{du}_{\mathbb{I}}^k \text{ satisfies } (\mathrm{EL}_k) \text{ for data } dq_{\mathbb{I}}^k, \\ &\text{and} \qquad\quad q_{\mathbb{I}} \in \widehat{Q_{\mathrm{ad},\mathbb{I}}}, \end{aligned}\right\} \tag{$\widehat{\mathrm{QP}}_k$}$$

where we recall (EL_k) from the definition of the problem (QP_k) to be

$$\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}^{i,k}, d\varphi^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi^{i,k}, d\varphi^{i-1,k}) \\ &\quad = Bdq^{i,k} + Bq^{i,k} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \quad \forall i = 1, ..., M, \end{aligned}$$

cf. the equivalent formulations for linearized equations from (3.72)-(3.74), as well as Corollary 6.1.3 and Remark 6.1.7.

Similarly to $(\mathrm{QP}_k^{\mathrm{red}})$, the reduced version is introduced. For the same $f_{\mathbb{I},k}$ as in $(\mathrm{QP}_k^{\mathrm{red}})$, it reads

$$\min f_{\mathbb{I},k}(q_{\mathbb{I}}), \qquad \text{such that} \quad q_{\mathbb{I}} \in \widehat{Q_{\mathrm{ad},\mathbb{I}}}. \tag{$\widehat{\mathrm{QP}}_k^{\mathrm{red}}$}$$

Using the same ideas as in [152, Lemma 6.2], we investigate existence and uniqueness of a solution of $(\widehat{\mathrm{QP}}_k)$, which we denote by $\hat{\mathbf{d}}_{\mathbb{I}}^k = (\widehat{dq_{\mathbb{I}}^k}, \widehat{\mathbf{du}_{\mathbb{I}}^k}) = (\hat{q}_{\mathbb{I}}^{k+1} - q_{\mathbb{I}}^k, \hat{\mathbf{u}}^{k+1} - \mathbf{u}_{\mathbb{I}}^k) \in Q^M \times W^M$. For this purpose, in [85, Lemma 5.1] of the author and I. Neitzel, for the case $M = 1$ a coercivity condition is proved, and for $(\widehat{\mathrm{QP}}_k)$, we can analogously show the following coercivity condition:

Lemma 6.2.1. *Let Assumption 4.3.1 hold and $c_{SSC} > 0$ be as in Assumption 4.3.1. There exists a constant $\omega_1 > 0$ such that for all $y_{\mathbb{I}}^k \in Y^M$ with $\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \leq \omega_1$, the coercivity condition*

$$\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}}^k)[(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}})] \geq \frac{c_{SSC}}{2}\|\tilde{q}_{\mathbb{I}}\|_{Q^M}^2$$

holds for all $\tilde{q}_{\mathbb{I}}$ which satisfy $\tilde{q}_{\mathbb{I}} = 0$ on $\mathcal{I}(\sigma)$, and $(\tilde{q}_{\mathbb{I}}, \tilde{\mathbf{u}}_{\mathbb{I},k}) \in Q_{ad,\mathbb{I}} \times W^M$ satisfying

$$A_l(\mathbf{u}^{i,k})(\tilde{\mathbf{u}}_k^i, \tilde{\varphi}_k^{i-1}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\tilde{\varphi}_k^i, \tilde{\varphi}_k^{i-1}) = B\tilde{q}^i, \tag{6.24}$$

for all $i = 1, ..., M$.

Proof. The proof of the one time step problem is recapitulated for the multi time step setting: First, assume that $y_{\mathbb{I}}^k \in Y^M$ is fixed but arbitrary, and fulfills

$$\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega_1, \tag{6.25}$$

for an $0 < \omega_1 \in \mathbb{R}$ to be determined below. Let $\tilde{q}_{\mathbb{I}}$ and $\tilde{\mathbf{u}}_{\mathbb{I},k}$ be as assumed, and let further $\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}$ be the solution to

$$A_l(\bar{\mathbf{u}}^i)(\tilde{\mathbf{u}}^i_{\text{-}}, \tilde{\varphi}^{i-1}_{\text{-}}) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\tilde{\varphi}^i_{\text{-}}, \tilde{\varphi}^{i-1}_{\text{-}}) = B\tilde{q}^i \quad \forall i = 1, ..., M. \tag{6.26}$$

Note that by Lemma 3.2.3, we obtain

$$\|\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}\|_{W^M} \leq c\|\tilde{q}_{\mathbb{I}}\|_{Q^M} \quad \text{and} \quad \|\tilde{\mathbf{u}}_{\mathbb{I},k}\|_{W^M} \leq \big(c + c_1(\omega_1)\big)\|\tilde{q}_{\mathbb{I}}\|_{Q^M}, \tag{6.27}$$

for a constant $0 < c \in \mathbb{R}$ that depends on $\bar{y}_{\mathbb{I}}$, but not on $y^k_{\mathbb{I}}$, and a $0 < c_1(\omega_1) = \mathcal{O}(\omega_1)$, also independently of $y^k_{\mathbb{I}}$. The latter holds true due to the dependencies of the constant involved in (3.77) on the norm of the linearization point, here $\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M}$, in combination with (6.25) and the triangle inequality

$$\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M} \leq \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \leq c + \omega_1. \tag{6.28}$$

For later use, we point out that completely analogously it also holds

$$\|\mathbf{z}^k_{\mathbb{I}}\|_{W^M} \leq \|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{z}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq c + \omega_1. \tag{6.29}$$

An easy calculation ensures that the difference $\tilde{\mathbf{u}}_{\mathbb{I},k} - \tilde{\mathbf{u}}_{\mathbb{I},\text{-}}$ is the solution of

$$\begin{aligned} &A_l(\bar{\mathbf{u}}^i)(\tilde{\mathbf{u}}^i_k - \tilde{\mathbf{u}}^i_{\text{-}}, \tilde{\varphi}^{i-1}_k - \tilde{\varphi}^{i-1}_{\text{-}}) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\tilde{\varphi}^i_k - \tilde{\varphi}^i_{\text{-}}, \tilde{\varphi}^{i-1}_k - \tilde{\varphi}^{i-1}_{\text{-}}) \\ &\quad = \big[A_l(\bar{\mathbf{u}}^i) - A_l(\mathbf{u}^{k,i})\big](\tilde{\mathbf{u}}^i_k, \tilde{\varphi}^{i-1}_k) \\ &\qquad + \big[R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma) - R_l(\varphi^{k,i}, \varphi^{k,i-1}; \gamma)\big](\tilde{\varphi}^i_k, \tilde{\varphi}^{i-1}_k). \end{aligned} \tag{6.30}$$

The right-hand side can be estimated, using Lemma 3.1.5 and Lemma 3.1.8,

$$\begin{aligned} &\|A_l(\bar{\mathbf{u}}^i)(\tilde{\mathbf{u}}^i_k, \tilde{\varphi}^{i-1}_k) - A_l(\mathbf{u}^{k,i})(\tilde{\mathbf{u}}^i_k, \tilde{\varphi}^{i-1}_k)\|_{W^\times} \\ &\quad + \|R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\tilde{\varphi}^i_k, \tilde{\varphi}^{i-1}_k) - R_l(\varphi^{k,i}, \varphi^{k,i-1}; \gamma)(\tilde{\varphi}^i_k, \tilde{\varphi}^{i-1}_k)\|_{L^q(\Omega)} \\ &\quad \leq 2c(\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{u}^k_{\mathbb{I}}\|_{W^M})\|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I},k}\|_{W^M}\|\tilde{\mathbf{u}}_{\mathbb{I},k}\|_{W^M} \\ &\quad \leq c_2(\omega_1)\|\tilde{\mathbf{u}}_{\mathbb{I},k}\|_{W^M}, \end{aligned}$$

again with a constant $0 < c_2(\omega_1) = \mathcal{O}(\omega_1)$, independent of $y^k_{\mathbb{I}}$ due to the dependencies of the constants from (3.37) and (3.57), and the triangle inequality (6.28), as well as (6.25). Therefore, from Lemma 3.2.3 it follows

$$\|\tilde{\mathbf{u}}_{\mathbb{I},k} - \tilde{\mathbf{u}}_{\mathbb{I},\text{-}}\|_{W^M} \leq c_2(\omega_1)\|\tilde{\mathbf{u}}_{\mathbb{I},k}\|_{W^M}. \tag{6.31}$$

A short calculation now leads to

$$\begin{aligned} &\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}})] \\ &\quad = \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})] + \Big[\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}}) - \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})\Big][(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})] \\ &\qquad + \Big[\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}})] - \mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})]\Big]. \end{aligned} \tag{6.32}$$

The aim is to bound all terms of the right-hand side of (6.32) from below. Recognizing that $\tilde{q}_{\mathbb{I}}$ lies in the cone of ($\sigma-$)critical directions $C_\sigma(\bar{q}_{\mathbb{I}})$ from (4.21), by Assumption 4.3.1 it holds

$$\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})] \geq c_{SSC} \|\tilde{q}_{\mathbb{I}}\|^2_{Q^M}. \tag{6.33}$$

The Lipschitz results Lemma 3.5.3, yields, for a $0 < c \in \mathbb{R}$ not depending on $y^k_{\mathbb{I}}$, that

$$\begin{aligned}
&\Big[\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}}) - \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})\Big][(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})] \\
&\quad \geq -c\|\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}\|^2_{W^M} \big(\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{z}^k_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}\big) \\
&\qquad \cdot \big(\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{z}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}\big).
\end{aligned}$$

Continuing, using (6.27)-(6.29), as well as (6.25), leads to

$$\begin{aligned}
\Big[\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}}) - \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})\Big][(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})] &\geq -c\omega_1(c+\omega_1)\|\tilde{q}_{\mathbb{I}}\|^2_{Q^M} \\
&\geq -c_3(\omega_1)\|\tilde{q}_{\mathbb{I}}\|^2_{Q^M},
\end{aligned} \tag{6.34}$$

for an $0 < c_3(\omega_1) = \mathcal{O}(\omega_1)$.

Similarly, by Lemma 3.5.4, for a $0 < c \in \mathbb{R}$ not depending on $y^k_{\mathbb{I}}$,

$$\begin{aligned}
&\Big[\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}})] - \mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}, \tilde{q}_{\mathbb{I}})]\Big] \\
&\quad \geq -c\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M}\|\mathbf{z}^k_{\mathbb{I}}\|_{W^M}\big(\|\tilde{\mathbf{u}}_{\mathbb{I},k}\|_{W^M} + \|\tilde{\mathbf{u}}_{\mathbb{I},\text{-}}\|_{W^M}\big)\|\tilde{\mathbf{u}}_{\mathbb{I},k} - \tilde{\mathbf{u}}_{\mathbb{I},\text{-}}\|_{W^M} \\
&\quad \geq -c(c+\omega_1)^2\big(c + c_1(\omega_1)\big)c_2(\omega_1)\|\tilde{q}_{\mathbb{I}}\|^2_{W^M},
\end{aligned} \tag{6.35}$$

where (6.28)-(6.29), and (6.27) as well as (6.31) were used to obtain the last inequality.

Finally, collecting all estimates from (6.33), (6.34) and (6.35) we conclude from (6.32) that

$$\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}}), (\tilde{\mathbf{u}}_{\mathbb{I},k}, \tilde{q}_{\mathbb{I}})] \geq \big(c_{SSC} - c(\omega_1)\big)\|\tilde{q}_{\mathbb{I}}\|^2_{Q^M},$$

for a $0 < c(\omega_1) = \mathcal{O}(\omega_1)$. Thus, choosing ω_1 sufficiently small, it holds $\big(c_{SSC} - c(\omega_1)\big) = \frac{c_{SSC}}{2}$, which concludes the proof. □

Existence and uniqueness of a solution to $(\widehat{\text{QP}}_k)$ now follow by standard arguments, cf. the one time step case $M = 1$ in [86, Corollary 5.2] of the author and I. Neitzel.

Corollary 6.2.2. *Let $y^k_{\mathbb{I}} \in Y^M$ fulfill $\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega_1$, for an $\omega_1 > 0$ sufficiently small as in Lemma 6.2.1. Then $(\widehat{\text{QP}}_k)$ has a unique solution $\hat{q}^{k+1}_{\mathbb{I}} \in \widehat{Q_{ad,\mathbb{I}}}$ with associated $\hat{\mathbf{u}}^{k+1}_{\mathbb{I}} \in W^M$.*

Proof. The proof is standard, see e.g. [152, Corollary 6.3]: The auxiliary subproblem $(\widehat{\mathrm{QP}}_k)$ is of linear quadratic nature, where the quadratic part is given by the (constant) second derivative $f''_{\mathbb{I},k} = \mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})$, cf. (6.4). Coercivity thus immediately follows from Lemma 6.2.1, under the assumed smallness condition for $\mathbf{u}^k_{\mathbb{I}}$ and $\mathbf{z}^k_{\mathbb{I}}$, and hence $(\widehat{\mathrm{QP}}_k)$ is a strict convex optimal control problem on the feasible region of $(\widehat{\mathrm{QP}}_k)$. The remainder now follows by standard theory, cf. e.g. [153, Theorem 2.14], and is omitted.

□

First-order necessary conditions for the one time step model are given in [85, Corollary 5.3] of the author and I. Neitzel, and once more immediately follow in a standard way both for the case $M = 1$ and $M > 1$. Therefore, the proof is omitted. Note that under the same locality condition for $y^k_{\mathbb{I}}$ as in Lemma 6.2.1 and Corollary 6.2.2, the first-order necessary conditions are also sufficient.

Corollary 6.2.3. *Let $y^k_{\mathbb{I}} \in Y^M$ be given, such that $\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega_1$, with ω_1 sufficiently small as in Lemma 6.2.1. A control $\hat{q}^{k+1}_{\mathbb{I}} = \widehat{dq}^k_{\mathbb{I}} + q^k_{\mathbb{I}}$ with $\hat{q}^{k+1}_{\mathbb{I}} \in \widehat{Q_{ad,\mathbb{I}}}$, with associated optimal state $\hat{\mathbf{u}}^{k+1}_{\mathbb{I}} = \widehat{\mathbf{du}}^k_{\mathbb{I}} + \mathbf{u}^k_{\mathbb{I}}$ is a minimizer for the subproblem $(\widehat{\mathrm{QP}}^{\mathrm{red}}_k)$ if and only if there exists an adjoint state $\hat{\mathbf{z}}^{k+1}_{\mathbb{I}} = (\hat{z}^{k+1}_{\mathbb{I}}, \hat{\psi}^{k+1}_{\mathbb{I}})$, such that the optimality system*

$$\left.\begin{aligned} &A_l(\mathbf{u}^{i,k})(\widehat{\mathbf{du}}^{i,k}, \widehat{d\varphi}^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\widehat{d\varphi}^{i,k}, \widehat{d\varphi}^{i-1,k}) \\ &\quad = B\hat{q}^{i,k+1} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \qquad \forall i = 1, ..., M, \end{aligned}\right\} \tag{6.36a}$$

$$\left.\begin{aligned} &A_{l*}(\mathbf{u}^{i,k})(\hat{\mathbf{z}}^{i,k+1}, \hat{\psi}^{i+1,k+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\hat{\psi}^{i,k+1}, \hat{\psi}^{i+1,k+1}) \\ &\quad = \hat{u}^{i,k+1} - u^i_d - A_{b*}(\mathbf{u}^{i,k}, \widehat{\mathbf{du}}^{i,k})\mathbf{z}^{i,k} \\ &\qquad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \widehat{d\varphi}^{i,k}, \widehat{d\varphi}^{i-1,k}, \widehat{d\varphi}^{i+1,k}; \gamma)(\psi^{i,k}, \psi^{i+1,k}) \\ &\qquad \forall i = 1, ..., M, \end{aligned}\right\} \tag{6.36b}$$

$$\left.\left(B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q^i - \hat{q}^{i,k+1}\right)_Q \geq 0 \qquad \forall i = 1, ..., M \text{ and } \forall q_{\mathbb{I}} \in \widehat{Q_{ad,\mathbb{I}}},\right\} \tag{6.36c}$$

is satisfied.

Again, as it is the case for (QP_k), the auxiliary problem $(\widehat{\mathrm{QP}}_k)$ is linked to a generalized equation and subsequently an associated Newton method. In particular, we state the generalized equation, in a given triple $y_{\mathbb{I}} = (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}})$, by

$$0 \in F_{\mathbb{I}}(y_{\mathbb{I}}) + \hat{N}_{\mathbb{I}}(y_{\mathbb{I}}), \tag{$\widehat{\mathrm{GE}}$}$$

where we again understand the generalized equation analogously to (GE) and (GE^i), and use the mappings $F_{\mathbb{I}}, F^i$ respectively, as in (6.6), as well as $\hat{N}^i$ defined by

$$\hat{N}^i(y^i) := \Big(0,\, 0,\, \hat{N}_{\mathrm{nc}}(q^i)\Big)\,, \tag{6.37}$$

where

$$\hat{N}_{\mathrm{nc}}(q^i) = \{dq^i \in Q \,|\, (dq^i, \tilde{q}^i - q^i)_Q \leq 0 \quad \text{for all} \quad \tilde{q}^i \in (\widehat{Q_{\mathrm{ad},\mathbb{I}}})_{|i}\},$$

again, slightly abusing notation for the i-th entry of $\widehat{Q_{\mathrm{ad},\mathbb{I}}}$ by using $(\widehat{Q_{\mathrm{ad},\mathbb{I}}})_{|i}$, which is understood analogously to (6.8).

This is again inspired by the simple fact that from the system given through (6.36a), (6.36b) and (6.36c), one easily sees that these first-order optimality conditions of $(\widehat{\mathrm{QP}}_k)$ are precisely given by the generalized equation

$$0 \in F_{\mathbb{I}}(y_{\mathbb{I}}^k) + F_{\mathbb{I}}'(y_{\mathbb{I}}^k)(\hat{y}_{\mathbb{I}}^{k+1} - y_{\mathbb{I}}^k) + \hat{N}_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^{k+1}), \tag{$\widehat{\mathrm{NM}}$}$$

for given $y_{\mathbb{I}}^k$ as in Corollary 6.2.3, and where ($\widehat{\mathrm{NM}}$) is understood in the sense of (NM). We can therefore investigate convergence of the sequence of solutions generated by ($\widehat{\mathrm{NM}}$). This is done using the concept of strong regularity, and the topic of the next subsection.

6.2.2 Strong regularity

To prove convergence of the sequence generated by ($\widehat{\mathrm{NM}}$), and thus equivalently $(\widehat{\mathrm{QP}}_k)$, a convergence theorem similar to Newton-Kantorovich is utilized, cf. [74, 152], which is based on ideas from [4]. The key idea is to use a property called strong regularity (of the generalized equation ($\widehat{\mathrm{GE}}$)), which, in short, demands local unique solvability and a Lipschitz condition of a perturbed version of (the to ($\widehat{\mathrm{GE}}$) associated generalized equation) ($\widehat{\mathrm{NM}}$). Then, the generated sequence $\{\hat{q}^k\}_{k\in\mathbb{N}}$ of global solutions of $(\widehat{\mathrm{QP}}_k)$ is well-defined, stays within the convergence radius of Newton's method, and converges quadratically towards $\bar{q}_{\mathbb{I}}$, if started from a good initial guess.

Before we can start, it is necessary to introduce some new notation, and also recall some essential notation from previous sections, especially Remark 2.3.10. Let $\delta_{\mathbb{I}} = (\delta_{1,\mathbb{I}}, \delta_{2,\mathbb{I}}, \delta_{\mathbb{I},3})$ and $\tilde{\delta}_{\mathbb{I}} = (\tilde{\delta}_{1,\mathbb{I}}, \tilde{\delta}_{2,\mathbb{I}}, \tilde{\delta}_{\mathbb{I},3})$ be triples of perturbations that lie in the space Z^M or Z_∞^M, for which Z and Z_∞ shall be recalled from Definition 2.3.3 as

$$Z = W^\times \times Q \times W^\times \quad \text{and} \quad Z_\infty = W^\times \times L^\infty(\Gamma) \times W^\times.$$

Function triples that are dependent on $\delta_{\mathbb{I}}$ and $\tilde{\delta}_{\mathbb{I}}$ shall be denoted by $y_{\mathbb{I},\delta} = (\mathbf{u}_{\mathbb{I},\delta}, q_{\mathbb{I},\delta}, \mathbf{z}_{\mathbb{I},\delta})$ and $y_{\mathbb{I},\tilde{\delta}} = (\mathbf{u}_{\mathbb{I},\tilde{\delta}}, q_{\mathbb{I},\tilde{\delta}}, \mathbf{z}_{\mathbb{I},\tilde{\delta}})$ respectively, for which we recall the function spaces

$$Y = W \times Q \times W \quad \text{and} \quad Y_\infty = W \times L^\infty(\Gamma) \times W.$$

Finally, for radii $\rho > 0$ and $r > 0$, we introduce the open balls

$$\begin{aligned}
B_r^{Z^M}(\tilde{\delta}_{\mathbb{I}}) &:= \{\delta_{\mathbb{I}} \in Z^M \quad | \quad \|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M} \leq r\},\\
B_r^{Z_\infty^M}(\tilde{\delta}_{\mathbb{I}}) &:= \{\delta_{\mathbb{I}} \in Z_\infty^M \quad | \quad \|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z_\infty^M} \leq r\},\\
B_\rho^{Y^M}(\tilde{y}_{\mathbb{I}}) &:= \{y_{\mathbb{I}} \in Y^M \quad | \quad \|y_{\mathbb{I}} - \tilde{y}_{\mathbb{I}}\|_{Y^M} \leq \rho\},\\
B_\rho^{Y_\infty^M}(\tilde{y}_{\mathbb{I}}) &:= \{y_{\mathbb{I}} \in Y_\infty^M \quad | \quad \|y_{\mathbb{I}} - \tilde{y}_{\mathbb{I}}\|_{Y_\infty^M} \leq \rho\}.
\end{aligned}$$

We are now in a position to first state the perturbed generalized equation, and then the strong regularity property. The perturbation of the generalized equation ($\widehat{\text{GE}}$) shall be given, for the fixed function triple $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$, cf. Assumption 6.1.1, via

$$\delta_{\mathbb{I}} \in F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) + \hat{N}_{\mathbb{I}}(\bar{y}_{\mathbb{I}}), \tag{$\widehat{\text{GE}_\delta}$}$$

and the perturbation of ($\widehat{\text{NM}}$) via

$$\delta_{\mathbb{I}} \in F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) + F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(y_{\mathbb{I},\delta} - \bar{y}_{\mathbb{I}}) + \hat{N}_{\mathbb{I}}(y_{\mathbb{I},\delta}), \tag{$\widehat{\text{NM}_\delta}$}$$

which is understood, analogously to (GE^i), in the sense that for all $i = 1, ..., M$

$$\begin{aligned}
(\delta_1^i, \delta_2^i, \delta_3^i) \in\, & F^i(\bar{y}^i; \bar{y}^{i-1}, \bar{y}^{i+1})\\
& + (F^i)'(\bar{y}^i, \bar{y}^{i-1}, \bar{y}^{i+1})(y_\delta^i - \bar{y}^i, y_\delta^{i-1} - \bar{y}^{i-1}, y_\delta^{i+1} - \bar{y}^{i+1})\\
& + \hat{N}^i(\bar{y}_{\mathbb{I},\delta}).
\end{aligned}$$

Now, we can define strong regularity property, cf. [58, 140].

Definition 6.2.4 (The strong regularity property)**.**

- *The generalized equation ($\widehat{\text{GE}}$) has the strong regularity property in the space Y^M at $\bar{y}_{\mathbb{I}}$, if there exist radii $\rho, r > 0$ and a constant $L_2 > 0$ such that for all perturbations $\delta \in B_r^{Z^M}(0)$, ($\widehat{\text{NM}_\delta}$) suffices to the following properties:*
  1. *($\widehat{\text{NM}_\delta}$) has a solution $y_{\mathbb{I},\delta} \in B_\rho^{Y^M}(\bar{y}_{\mathbb{I}})$.*
  2. *$y_{\mathbb{I},\delta}$ is the only solution of ($\widehat{\text{NM}_\delta}$) in $B_\rho^{Y^M}(\bar{y}_{\mathbb{I}})$.*
  3. *Let $y_{\mathbb{I},\delta}, y_{\mathbb{I},\tilde{\delta}}$ be the unique solutions to ($\widehat{\text{NM}_\delta}$) in $B_\rho^{Y^M}(\bar{y}_{\mathbb{I}})$ for $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}} \in B_r^{Z^M}(0)$. Then the Lipschitz condition*

     $$\|y_{\mathbb{I},\delta} - y_{\mathbb{I},\tilde{\delta}}\|_{Y^M} \leq L_2 \|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}$$

     holds.
- *The strong regularity property in the space Y_∞^M is defined analogously, with the spaces Y^M and Z^M replaced by Y_∞^M and Z_∞^M, and for a constant $L_\infty > 0$, respectively.*

As a first remark, let the following immediate properties be put on record.

Remark 6.2.5.

- $(\widehat{\text{NM}_\delta})$ *is linear in* δ.
- *The fixed triple* $\bar{y}$ *is a solution to both* $(\widehat{\text{GE}})$ *and* $(\widehat{\text{NM}_\delta})$ *for* $\delta = 0$.
- $(\widehat{\text{NM}_\delta})$ *is the perturbation of* $(\widehat{\text{NM}})$ *in* $\bar{y}$*, in particular it is therefore the perturbation of the linearization of* $(\widehat{\text{GE}})$ *in* $\bar{y}$.

Inspired by the relations between $(\widehat{\text{NM}})$ and $(\widehat{\text{QP}_k})$, let another auxiliary problem be tacitly introduced: Again, it is clear that $(\widehat{\text{NM}_\delta})$ is the first-order necessary condition to the following quadratic optimization problem $(\widehat{\text{QP}_\delta})$:

Let $\delta_{\mathbb{I}} = (\delta_{\mathbb{I},1}, \delta_{\mathbb{I},2}, \delta_{\mathbb{I},3}) \in Z^M$ be given, and $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$ be as in Assumption 6.1.1. Find a pair $(q_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}})$, respectively a direction $\mathbf{d}_{\mathbb{I}} = (dq_{\mathbb{I}}, \mathbf{du}_{\mathbb{I}}) := (q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}) \in Q^M \times W^M$, that solves

$$\left.\begin{aligned} &\min_{\mathbf{d}_{\mathbb{I}}} J_{\mathbb{I},\delta}(\mathbf{d}_{\mathbb{I}}) = J'_{\mathbb{I}}(\bar{q}_{\mathbb{I}}, \bar{\mathbf{u}}_{\mathbb{I}})\mathbf{d}_{\mathbb{I}} + \frac{1}{2}\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\mathbf{du}_{\mathbb{I}}, dq_{\mathbb{I}}), (\mathbf{du}_{\mathbb{I}}, dq_{\mathbb{I}})] \\ &\qquad\qquad - \langle \delta_{\mathbb{I},1}, \mathbf{du}_{\mathbb{I}} \rangle_{((W^{1,p'} \times L^{q'})^*)^M, (W^{1,p} \times L^q)^M} - (\delta_{\mathbb{I},2}, dq_{\mathbb{I}})_{Q^M}, \\ &\text{subject to:} \quad \mathbf{du}_{\mathbb{I}} \text{ satisfies } (\text{EL}_\delta) \text{ for data } dq_{\mathbb{I}}, \\ &\text{and:} \qquad\quad q_{\mathbb{I}} \in \widehat{Q_{\text{ad},\mathbb{I}}}, \end{aligned}\right\} \qquad (\widehat{\text{QP}_\delta})$$

where (EL_δ) is given by

$$\begin{aligned} &A_l(\bar{\mathbf{u}}^i)(\mathbf{du}^i, d\varphi^{i-1}) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(d\varphi^i, d\varphi^{i-1}) \\ &\quad = B dq^i + B\bar{q}^i + \delta_3^i - A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) - R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma) \quad \forall i = 1, ..., M, \end{aligned} \qquad (\text{EL}_\delta)$$

cf. the equivalent formulations for linearized equations from (3.72)-(3.74), as well as Corollary 6.1.3 and Remark 6.1.7.

As before, the reduced version can again be immediately introduced via

$$\min f_{\mathbb{I},\delta}(q_{\mathbb{I}}) := J_{\mathbb{I},\delta}(q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}, \mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}), \quad \text{such that } q_{\mathbb{I}} \in \widehat{Q_{\text{ad},\mathbb{I}}}, \qquad (\widehat{\text{QP}_\delta^{\text{red}}})$$

where $\mathbf{u}_{\mathbb{I}}$ satisfies (EL_δ) for right-hand side data $q_{\mathbb{I}} = \bar{q}_{\mathbb{I}} + dq_{\mathbb{I}}$.

Following the usual course of action, the consequential next step is to investigate existence and uniqueness of the optimal control problem. For the setting $M = 1$, this is showed in [85, Lemma 5.5] of I. Neitzel and the author, and for $(\widehat{\text{QP}_\delta})$ we can show the following result.

Lemma 6.2.6. *For each* $\delta_{\mathbb{I}} = (\delta_{\mathbb{I},1}, \delta_{\mathbb{I},2}, \delta_{\mathbb{I},3}) \in Z^M$, $(\widehat{\text{QP}_\delta})$ *has a unique solution* $(\widehat{dq}_{\mathbb{I},\delta}, \widehat{\mathbf{du}}_{\mathbb{I},\delta}) \in Q_{ad,\mathbb{I}} \times W^\times$ *with* $\hat{q}_{\mathbb{I},\delta} = \widehat{dq}_{\mathbb{I},\delta} + \bar{q}_{\mathbb{I}} \in \widehat{Q_{ad,\mathbb{I}}}$*, that depends on* δ.

Proof. The proof follows in the same way as in [151, Lemma 4.1], and is only outlined: By assumption, it holds $\widehat{dq}_{\mathbb{I},\delta} \in \widehat{Q_{\text{ad},\mathbb{I}}}$, i.e. it holds $\hat{q}_{\mathbb{I},\delta} = \bar{q}_{\mathbb{I}}$ on $\mathcal{I}(\sigma)$, and therefore $\widehat{dq_{\mathbb{I},\delta}} = 0$ on $\mathcal{I}(\sigma)$. Let further $\mathbf{u}_{\mathbb{I},\wedge}$ and $\mathbf{u}_{\mathbb{I},c}$ satisfy, for all $i = 1, ..., M$,

$$
\begin{aligned}
&A_l(\bar{\mathbf{u}}^i)(\mathbf{u}^i_\wedge, \varphi^{i-1}_\wedge) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\varphi^i_\wedge, \varphi^{i-1}_\wedge) = B\widehat{dq^i_\delta} \\
&A_l(\bar{\mathbf{u}}^i)(\mathbf{u}^i_c, \varphi^{i-1}_c) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\varphi^i_c, \varphi^{i-1}_c) \\
&\quad = B\bar{q}^i + \delta^i_3 - A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) - R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma).
\end{aligned}
$$

Note that $\mathbf{u}_{\mathbb{I},c}$ is constant, i.e. does not depend on the control $\widehat{dq_{\mathbb{I},\delta}}$, and by definition of $\mathbf{u}_{\mathbb{I},\wedge}$ and $\mathbf{u}_{\mathbb{I},c}$ it holds $\widehat{\mathbf{du}_{\mathbb{I},\delta}} = \mathbf{u}_{\mathbb{I},\wedge} + \mathbf{u}_{\mathbb{I},c}$. The objective functional $J_{\mathbb{I},k}$ of $(\widehat{\text{QP}}_\delta)$ now decomposes into a quadratic part in $(\mathbf{u}_{\mathbb{I},\wedge}, \widehat{dq_{\mathbb{I},\delta}})$, on which Assumption 4.3.1 holds, a linear part in $(\mathbf{u}_{\mathbb{I},\wedge}, \widehat{dq_{\mathbb{I},\delta}})$ and a constant not depending on $(\mathbf{u}_{\mathbb{I},\wedge}, \widehat{dq_{\mathbb{I},\delta}})$. Thus $J_{\mathbb{I},\delta}$ is coercive and $(\widehat{\text{QP}}_\delta)$ is a strictly convex optimal control problem on the closed, convex and bounded set $\widehat{Q_{\text{ad},\mathbb{I}}}$. Existence of a unique solution now follows again by standard theory. □

Again, similarly to above and to [85, Corollary 5.6] of the author and I. Neitzel, where the one time step model is investigated, first-order necessary conditions for $(\widehat{\text{QP}}_\delta)$ follow immediately, thus the proof is omitted. Due to the strict convexity of $J_{\mathbb{I},\delta}(\hat{\mathbf{d}}_\delta)$, they are also sufficient.

Lemma 6.2.7. *Let $\delta_{\mathbb{I}} \in Z^M$ be given. A control direction $\widehat{dq}_{\mathbb{I},\delta} \in \widehat{Q_{ad,\mathbb{I}}}$, with control $\hat{q}_{\mathbb{I},\delta} = \widehat{dq}_{\mathbb{I},\delta} + \bar{q}_{\mathbb{I}}$ and associated optimal state $\hat{\mathbf{u}}_{\mathbb{I},\delta} = \widehat{\mathbf{du}}_{\mathbb{I},\delta} + \bar{\mathbf{u}}_{\mathbb{I}}$ and adjoint state $\hat{\mathbf{z}}_{\mathbb{I},\delta} = (\hat{z}_{\mathbb{I},\delta}, \hat{\psi}_{\mathbb{I},\delta})$, is optimal for the subproblem $(\widehat{\text{QP}}_\delta)$ if and only if the optimality system*

$$
\left.
\begin{aligned}
&A_l(\bar{\mathbf{u}}^i)(\widehat{\mathbf{du}}^i_\delta, \widehat{d\varphi}^{i-1}_\delta) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\widehat{d\varphi}^i_\delta, \widehat{d\varphi}^{i-1}_\delta) \\
&\quad = B\hat{q}^i_\delta - A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) - R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma) + \delta^i_3 \qquad \forall i = 1, .., M,
\end{aligned}
\right\} \tag{6.38a}
$$

$$
\left.
\begin{aligned}
&A_{l*}(\bar{\mathbf{u}}^i)(\hat{\mathbf{z}}^i_\delta, \hat{\psi}^{i+1}_\delta) + R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}; \gamma)(\hat{\psi}^i_\delta, \hat{\psi}^{i+1}_\delta) \\
&\quad = \hat{u}^i_\delta - u^i_d - A_{b*}(\bar{\mathbf{u}}^i, \widehat{\mathbf{du}}^i_\delta)\bar{\mathbf{z}}^i \\
&\qquad - R_{b*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \widehat{d\varphi}^i_\delta, \widehat{d\varphi}^{i-1}_\delta, \widehat{d\varphi}^{i+1}_\delta; \gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}) - \delta^i_1 \\
&\qquad\quad \forall i = 1, ..., M,
\end{aligned}
\right\} \tag{6.38b}
$$

$$
\left.
\Big(B^*\hat{\mathbf{z}}^i_\delta + \alpha\hat{q}^i_\delta - \delta^i_2, q^i - \hat{q}^i_\delta\Big) \geq 0 \quad \forall i = 1, ..., M \text{ and } q_{\mathbb{I}} \in \widehat{Q_{ad,\mathbb{I}}},
\right\} \tag{6.38c}
$$

is satisfied.

It is clear that Lemma 6.2.6 and Lemma 6.2.7 remain valid for perturbations $\delta_{\mathbb{I}} \in Z^M_\infty$, since $Z^M_\infty \subset Z^M$. Next, the focus is put on establishing the Lipschitz conditions required in the third item of Definition 6.2.4, both in the L^2- and L^∞-setting. Here, the proof of [151, Theorem 4.2 and Theorem 5.2] is closely followed, on which also the proof for the one time step setting cf. [86, Lemma 5.7] of the author and I. Neitzel is based.

Proposition 6.2.8. *Let $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}} \in Z$, and $\hat{q}_{\mathbb{I},\delta}, \hat{q}_{\mathbb{I},\tilde{\delta}}$ be the unique associated solutions of $(\widehat{\mathrm{QP}}_\delta)$. Let $\hat{y}_{\mathbb{I},\delta} = (\hat{\mathbf{u}}_{\mathbb{I},\delta}, \hat{q}_{\mathbb{I},\delta}, \hat{\mathbf{z}}_{\mathbb{I},\delta})$ and $\hat{y}_{\mathbb{I},\tilde{\delta}} = (\hat{\mathbf{u}}_{\mathbb{I},\tilde{\delta}}, \hat{q}_{\mathbb{I},\tilde{\delta}}, \hat{\mathbf{z}}_{\mathbb{I},\tilde{\delta}})$, where $\hat{\mathbf{u}}_{\mathbb{I},\delta}, \hat{\mathbf{u}}_{\mathbb{I},\tilde{\delta}}$ and $\hat{\mathbf{z}}_{\mathbb{I},\delta}, \hat{\mathbf{z}}_{\mathbb{I},\tilde{\delta}}$ satisfy* (6.38a) *and* (6.38b)*, respectively. Then there exists a constant $0 < L_2 \in \mathbb{R}$, such that*

$$\|\hat{y}_{\mathbb{I},\delta} - \hat{y}_{\mathbb{I},\tilde{\delta}}\|_{Y^M} \leq L_2 \|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}. \tag{6.39}$$

If further $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}} \in Z^M_\infty$, then there exists a constant $0 < L_\infty \in \mathbb{R}$ such that

$$\|\hat{y}_{\mathbb{I},\delta} - \hat{y}_{\mathbb{I},\tilde{\delta}}\|_{Y^M_\infty} \leq L_\infty \|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M_\infty}. \tag{6.40}$$

Proof. Let us start with the first statement, i.e. the Y^M-Z^M-setting, for perturbations $\delta_{\mathbb{I}}, \delta'_{\mathbb{I}} \in Z^M$. Let

$$\mathbf{u}_{\mathbb{I}} := \hat{\mathbf{u}}_{\mathbb{I},\delta} - \hat{\mathbf{u}}_{\mathbb{I},\tilde{\delta}}, \qquad q_{\mathbb{I}} := \hat{q}_{\mathbb{I},\delta} - \hat{q}_{\mathbb{I},\tilde{\delta}}, \qquad \mathbf{z}_{\mathbb{I}} := \hat{\mathbf{z}}_{\mathbb{I},\delta} - \hat{\mathbf{z}}_{\mathbb{I},\tilde{\delta}},$$

which by (6.38a) and (6.38b) satisfy, for all $i = 1, ..., M$,

$$A_l(\bar{\mathbf{u}}^i)(\mathbf{u}^i, \varphi^{i-1}) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\varphi^i, \varphi^{i-1}) = Bq^i + (\delta^i_3 - \tilde{\delta}^i_3), \tag{6.41}$$

and

$$\begin{aligned} &A_{l*}(\bar{\mathbf{u}}^i)(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}; \gamma)(\psi^i, \psi^{i+1}) \\ &\quad = u^i - (\delta^i_1 - \tilde{\delta}_1) - A_{b*}(\bar{\mathbf{u}}^i, \mathbf{u}^i)\bar{\mathbf{z}}^i \\ &\qquad - R_{b*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\bar{\psi}^i, \bar{\psi}^{i+1}). \end{aligned} \tag{6.42}$$

It holds $q_{\mathbb{I}} \in Q^M$ and $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}} \in Z^M$, thus the terms on both right-hand sides can be estimated, using Lemma 3.1.3 and Lemma 3.1.6 in the $W^\times$-norm, respectively in the $L^q(\Omega)$-norm, for all $i = 1, ..., M$. Subsequently, utilizing Lemma 3.2.3 yields

$$\|\mathbf{u}_{\mathbb{I}}\|_{W^M} \leq c\|q_{\mathbb{I}}\|_{Q^M} + c\|\delta_{\mathbb{I},3} - \tilde{\delta}_{\mathbb{I},3}\|_{(W^\times)^M} \leq c\|q_{\mathbb{I}}\|_{Q^M} + c\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}, \tag{6.43}$$

$$\begin{aligned} \|\mathbf{z}_{\mathbb{I}}\|_{W^M} &\leq 2c\|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}\|\mathbf{u}_{\mathbb{I}}\|_{W^M}\|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} + c\|\delta_{\mathbb{I},1} - \tilde{\delta}_{\mathbb{I},1}\|_{(W^\times)^M} \\ &\leq c\|\mathbf{u}_{\mathbb{I}}\|_{W^M} + c\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M} \leq c\|q_{\mathbb{I}}\|_{Q^M} + c\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}, \end{aligned} \tag{6.44}$$

where the constant $0 < c \in \mathbb{R}$ is depending only on $\bar{y}_{\mathbb{I}}$, but not on $\mathbf{u}_{\mathbb{I}}$ (and thus also not on $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}}$). We can thus test (6.41) with $\mathbf{z}^i \in W$ and (6.42) with $\mathbf{u}^i \in W$, which leads after summing up both equations, and then also using the sum over all $i = 1, ..., M$, to

$$\begin{aligned} &\sum_{i=1}^M (q^i, B^*\mathbf{z}^i)_Q + \sum_{i=1}^M \langle \delta^i_3 - \tilde{\delta}^i_3, \mathbf{z}^i \rangle \\ &\quad = \sum_{i=1}^M \Big[(u^i, u^i) - \langle \delta^i_1 - \tilde{\delta}^i_1, \mathbf{u}^i \rangle - \big\langle A_b(\bar{\mathbf{u}}^i)[\mathbf{u}^i, \mathbf{u}^i], \bar{\mathbf{z}}^i \big\rangle \\ &\qquad\qquad - \big\langle R_b(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)[(\varphi^i, \varphi^{i-1}), (\varphi^i, \varphi^{i-1})], \bar{\psi}^i \big\rangle \Big]. \end{aligned} \tag{6.45}$$

Note that here the definitions of A_{l*}, A_{b*}, R_{l*} and R_{b*} were used, cf. in particular also (3.7), (3.8), (3.11) and (3.13). Next, we test (6.38c) once in $(\hat{\mathbf{z}}^i_\delta, \hat{q}^i_\delta)$ with $\hat{q}^i_{\tilde{\delta}}$ and once in $(\hat{\mathbf{z}}^i_{\tilde{\delta}}, \hat{q}^i_{\tilde{\delta}})$ with $\hat{q}^i_\delta$. Again, after summing both equations and also taking the sum over all $i = 1, ..., M$, this leads to

$$\sum_{i=1}^{M} (\delta_2^i - \tilde{\delta}_2^i, q^i)_Q - \sum_{i=1}^{M} \alpha(q^i, q^i)_Q \geq \sum_{i=1}^{M} (B^* \mathbf{z}^i, q^i)_Q. \tag{6.46}$$

Now, recalling the second derivative $\mathcal{L}''_{\mathbb{I}}$ of the Lagrangian function, cf. Corollary 3.5.2, and inserting (6.45) and (6.46), one obtains

$$\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}), (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})] \leq \sum_{i=1}^{M} \Big[\langle \delta_1^i - \tilde{\delta}_1^i, \mathbf{u}^i \rangle + (\delta_2^i - \tilde{\delta}_2^i, q^i)_Q + \langle \delta_3^i - \tilde{\delta}_3^i, \mathbf{z}^i \rangle \Big]. \tag{6.47}$$

Furthermore, let $\mathbf{u}_{\mathbb{I}}$ be split such that $\mathbf{u}_{\mathbb{I}} = \hat{\mathbf{u}}_{\mathbb{I}} + \mathbf{u}_{\mathbb{I},\delta}$, where

$$\begin{aligned} A_l(\bar{\mathbf{u}}^i)(\hat{\mathbf{u}}^i, \hat{\varphi}^{i-1}) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\hat{\varphi}^i, \hat{\varphi}^{i-1}) &= Bq^i, \\ A_l(\bar{\mathbf{u}}^i)(\mathbf{u}^i_\delta, \varphi^{i-1}_\delta) + R_l(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)(\varphi^i_\delta, \varphi^{i-1}_\delta) &= (\delta_3^i - \tilde{\delta}_3^i), \end{aligned}$$

for all $i = 1, ..., M$, i.e. there is a part $\hat{\mathbf{u}}_{\mathbb{I}}$ that depends on the control $q_{\mathbb{I}}$ and a part $\mathbf{u}_{\mathbb{I},\delta}$ that depends on the perturbations $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}}$. Using again Lemma 3.2.3, it immediately holds

$$\|\hat{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \leq c \|q_{\mathbb{I}}\|_{Q^M}, \qquad \|\mathbf{u}_{\mathbb{I},\delta}\|_{W^M} \leq c \|\delta_{\mathbb{I},3} - \tilde{\delta}_{\mathbb{I},3}\|_{(W^\times)^M}, \tag{6.48}$$

where again the constant $0 < c \in \mathbb{R}$ is a constant that depends on the functions $\bar{\mathbf{u}}_{\mathbb{I}}$ and $\bar{\mathbf{z}}_{\mathbb{I}}$.

Similarly to the calculations performed in the proof of Lemma 6.2.1, again from the definition of $\mathcal{L}''_{\mathbb{I}}$ from (3.5.2) one obtains

$$\begin{aligned} &\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}), (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})] \\ &\quad = \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\hat{\mathbf{u}}_{\mathbb{I}} + \mathbf{u}_{\mathbb{I},\delta}, q_{\mathbb{I}}), (\hat{\mathbf{u}}_{\mathbb{I}} + \mathbf{u}_{\mathbb{I},\delta}, q_{\mathbb{I}})] \\ &\quad = \mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\hat{\mathbf{u}}_{\mathbb{I}}, q_{\mathbb{I}}), (\hat{\mathbf{u}}_{\mathbb{I}}, q_{\mathbb{I}})] \\ &\qquad + \sum_{i=1}^{M} \Big[2(\hat{u}^i, u^i_\delta) + \|u^i_\delta\|^2 - 2\big\langle A_b(\bar{\mathbf{u}}^i)[\mathbf{u}^i_\delta, \hat{\mathbf{u}}^i], \bar{\mathbf{z}}^i \big\rangle - \big\langle A_b(\bar{\mathbf{u}}^i)[\mathbf{u}^i_\delta, \mathbf{u}^i_\delta], \bar{\mathbf{z}}^i \big\rangle \\ &\qquad\qquad - 2\big\langle R_b(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)[(\varphi^i_\delta, \varphi^{i-1}_\delta), (\hat{\varphi}^i, \hat{\varphi}^{i-1})], \bar{\psi}^i \big\rangle \\ &\qquad\qquad - \big\langle R_b(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)[(\varphi^i_\delta, \varphi^{i-1}_\delta), (\varphi^i_\delta, \varphi^{i-1}_\delta)], \bar{\psi}^i \big\rangle \Big]. \end{aligned} \tag{6.49}$$

Note that for the first term of the right-hand side, by construction of $(\bar{u}, q)$, from Assumption 6.3.6 it follows

$$\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\hat{\mathbf{u}}_{\mathbb{I}}, q_{\mathbb{I}}), (\hat{\mathbf{u}}_{\mathbb{I}}, q_{\mathbb{I}})] \geq c_{\mathrm{SSC}} \|q_{\mathbb{I}}\|^2_{Q^M},$$

and that from the definition of the norm, cf. also Remark 2.3.6, in combination with (6.48), it follows

$$\sum_{i=1}^{M}\Big[2(\hat{u}^i, u_\delta^i) + \|u_\delta^i\|^2\Big] \geq -2cM\|q_{\mathbb{I}}\|_{Q^M}\|\delta_{\mathbb{I},3} - \delta_{\mathbb{I},3}\|_{(W^\times)^M} - cM\|\delta_{\mathbb{I},3} - \tilde{\delta}_{\mathbb{I},3}\|^2_{(W^\times)^M}.$$

The remaining terms are estimated, using Lemma 3.1.3 and Lemma 3.1.6, in combination with (6.48). Overall, we can conclude from (6.49)

$$\begin{aligned}\mathcal{L}''_{\mathbb{I}}(\bar{y}_{\mathbb{I}})[(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}), (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})] \geq{}& c_{SSC}\|q_{\mathbb{I}}\|^2_{Q^M} - c(M)\|q_{\mathbb{I}}\|_{Q^M}\|\delta_{\mathbb{I},3} - \delta_{\mathbb{I},3}\|_{(W^\times)^M} \\ & - c(M)\|\delta_{\mathbb{I},3} - \tilde{\delta}_{\mathbb{I},3}\|^2_{(W^\times)^M}.\end{aligned} \tag{6.50}$$

Combining (6.47) and (6.50) then yields

$$\begin{aligned}c_{SSC}\|q_{\mathbb{I}}\|^2_{Q^M} \leq{}& c(M)\|q_{\mathbb{I}}\|_{Q^M}\|\delta_{\mathbb{I},3} - \delta_{\mathbb{I},3}\|_{(W^\times)^M} - c(M)\|\delta_{\mathbb{I},3} - \tilde{\delta}_{\mathbb{I},3}\|^2_{(W^\times)^M} \\ & + \sum_{i=1}^{M}\Big[\langle \delta_1^i - \tilde{\delta}_1^i, \mathbf{u}^i\rangle + (\delta_2^i - \tilde{\delta}_2^i, q^i)_Q + \langle \delta_3^i - \tilde{\delta}_3^i, \mathbf{z}^i\rangle\Big] \\ \leq{}& c(M)\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}\big(\|q_{\mathbb{I}}\|_{Q^M} + \|\mathbf{u}_{\mathbb{I}}\|_{W^M} + \|\mathbf{z}_{\mathbb{I}}\|_{W^M}\big) \\ & + c(M)\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|^2_{Z^M},\end{aligned}$$

which, after inserting (6.43) and (6.44) for $\|\mathbf{u}_{\mathbb{I}}\|_{W^M}$ and $\|\mathbf{z}_{\mathbb{I}}\|_{W^M}$, and utilizing Young's inequality, finally yields

$$c_{SSC}\|q_{\mathbb{I}}\|_{Q^M} \leq c(M)\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M},$$

for a $c(M)$ independently of $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}}$. Together with (6.43) and (6.44), this shows (6.39), and therefore concludes the proof of the first statement.

Let us now look at the second statement, i.e. the $Y_\infty^M - Z_\infty^M$-setting, and thus let $\delta_{\mathbb{I}}, \tilde{\delta}_{\mathbb{I}} \in Z_\infty^M$. Due to $Z_\infty \hookrightarrow Z$, $W_u \hookrightarrow L^\infty(\Omega;\mathbb{R}^2)$ and $W_\varphi \hookrightarrow L^\infty(\Omega)$, cf. Remark 2.3.6, it is clear that from (6.39) it follows

$$\begin{aligned}\|\mathbf{u}_{\mathbb{I}}\|_{(L^\infty(\Omega;\mathbb{R}^2))^M} &\leq c\|\mathbf{u}_{\mathbb{I}}\|_{W^M} \leq L_2\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}, \\ \|\mathbf{z}_{\mathbb{I}}\|_{(L^\infty(\Omega;\mathbb{R}^2))^M} &\leq c\|\mathbf{z}_{\mathbb{I}}\|_{W^M} \leq L_2\|\delta_{\mathbb{I}} - \tilde{\delta}_{\mathbb{I}}\|_{Z^M}.\end{aligned} \tag{6.51}$$

Further, by assumption $\hat{q}_{\mathbb{I},\delta} = \hat{q}_{\mathbb{I},\tilde{\delta}} = \bar{q}_{\mathbb{I}}$ on $\mathcal{I}(\sigma)$. Thus the variational inequalities (6.38c) of $(\widehat{\text{QP}}_\delta)$ imply

$$q_\delta^i = \frac{1}{\alpha}\text{Proj}_{\left(\widehat{Q_{\text{ad},\mathbb{I}}}\right)_{|i}}\Big(B^*\mathbf{z}_\delta^i - \delta_2^i\Big), \quad q_{\tilde{\delta}}^i = \frac{1}{\alpha}\text{Proj}_{\left(\widehat{Q_{\text{ad},\mathbb{I}}}\right)_{|i}}\Big(B^*\mathbf{z}_{\tilde{\delta}}^i - \tilde{\delta}_2^i\Big)$$

on $\Gamma\backslash\mathcal{I}(\sigma)$ and for all $i = 1, ..., M$. In this context, $\text{Proj}_{\left(\widehat{Q_{\text{ad},\mathbb{I}}}\right)_{|i}}$ is the pointwise projection on the given set, noting that once more the same slight abuse of notation for the set $\left(\widehat{Q_{\text{ad},\mathbb{I}}}\right)_{|i}$ is used for the $i-th$ dimensional box constraint, cf.

(6.37) and (6.8), and that $B^*\mathbf{z}_\delta^i, B^*\mathbf{z}_{\tilde\delta}^i \in L^\infty(\Gamma)$. By Lipschitz continuity of the pointwise projection, and the space embeddings from Remark 2.3.6, this means

$$\begin{aligned}\|q^i\|_{L^\infty(\Gamma)} &\le c\|B^*\mathbf{z}^i\|_{L^\infty(\Gamma)} + c\|\delta_2^i - \tilde\delta_2^i\|_{L^\infty(\Gamma)}\\ &\le c\|\mathbf{z}^i\|_W + c\|\delta_2^i - \tilde\delta_2^i\|_{L^\infty(\Gamma)}\\ &\le c\|\mathbf{z}_{\mathbb{I}}\|_W + c\|\delta_{\mathbb{I},2} - \tilde\delta_{\mathbb{I},2}\|_{(L^\infty(\Gamma))^M}.\end{aligned}$$

The claim now follows by the last estimate in combination with (6.51) for an $L_\infty = c(M, L_2)$. □

By Lemma 6.2.6 and Proposition 6.2.8, all requirements of the strong regularity property from Definition 6.2.4 have been showed, overall it holds:

Theorem 6.2.9. *The generalized equation* $(\widehat{\text{GE}})$ *is strongly regular in both* Y^M *and* Y_∞^M *at* $\bar y_{\mathbb{I}}$*, where the latter suffices to Assumption 6.1.1.*

6.2.3 Convergence of $(\widehat{\text{NM}})$

The previous section establishes strong regularity of $(\widehat{\text{GE}})$. We also already asserted that if the strong regularity property is fulfilled, a generalization of the well-known implicit function theorem can be used to ensure convergence of the sequence $\{\hat q_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ that is generated by $(\widehat{\text{NM}})$, and therefore also by $(\widehat{\text{QP}_k})$. Although the proof of the convergence theorem relies on standard arguments, cf. [6, 73, 74, 152], for completeness the proof of [73, Theorem 7.1] is adapted to the setting of (the one time step equivalent of) $(\widehat{\text{GE}})$ in [85, Theorem 5.9] by I. Neitzel and the author. This is also the proof which we recapitulate below for the multi time step setting. Note that several technical result concerning the operator F are used, which are established in Section 6.1.1. Let us point out that most convergence results prove convergence if the initial guess for the control, state and adjoint triple is taken sufficiently close to the local minimizer $\bar q_{\mathbb{I}}$ with associated optimal state $\bar{\mathbf{u}}_{\mathbb{I}}$ and adjoint $\bar{\mathbf{z}}_{\mathbb{I}}$ in the norm implied from the strong regularity property, i.e. in Y^M or Y_∞^M. In [96], it is observed that the control iterate $\hat q_{\mathbb{I}}^k$ from the previous iteration in fact cancels out in the update directions, thus the first iterate $y_{\mathbb{I}}^1$ is already independent of the initial control $q_{\mathbb{I}}^0$. This is also the case for $(\widehat{\text{QP}_k})$, cf. Corollary 6.2.3, and also Remark 6.1.5. Note that the closeness condition for $\mathbf{u}_{\mathbb{I}}^0$ and $\mathbf{z}_{\mathbb{I}}^0$ in the W^M-norm can be deduced in the following way: For the choice $q_{\mathbb{I}}^0$ such that $\|q_{\mathbb{I}}^0 - \bar q_{\mathbb{I}}\|_{Q^M}$ small enough, due to the Lipschitz results of the control-to-state operator, cf. Lemma 3.3.3, the state $\mathbf{u}_{\mathbb{I}}^0 = G_{\mathbb{I}}(q_{\mathbb{I}}^0)$ automatically fulfills a closeness property in the space W^M. By Corollary 3.4.5, the same holds true for the associated adjoint state $\mathbf{z}_{\mathbb{I}}^0$.

Theorem 6.2.10. *There exists a radius* $0 < \omega_{2,2} \in \mathbb{R}$ *and a constant* $0 < C_{N,2} \in \mathbb{R}$*, such that for each starting point* $y_{\mathbb{I}}^0 \in Y^M$ *with* $\|\mathbf{u}_{\mathbb{I}}^0 - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^0 - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \le \omega_{2,2}$ *and* $q_{\mathbb{I}}^0 \in Q_{ad,\mathbb{I}}$*, the auxiliary subproblem* $(\widehat{\text{QP}_k})$ *generates a unique sequence of iterates* $\{\hat y_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ *with* $\|\hat y_{\mathbb{I}}^k - \bar y_{\mathbb{I}}\|_{Y^M} \le \omega_{2,2}$ *and* $\hat q_{\mathbb{I}}^k \in \widehat{Q_{ad,\mathbb{I}}}$*, which satisfies*

$$\|\hat y_{\mathbb{I}}^{k+1} - \bar y_{\mathbb{I}}\|_{Y^M} \le C_{N,2}\|\hat y_{\mathbb{I}}^k - \bar y_{\mathbb{I}}\|_{Y^M}^2 \qquad \textit{for all } k \in \mathbb{N}. \tag{6.52}$$

In particular, the choice $q_{\mathbb{I}}^0 \in Q_{ad,\mathbb{I}}$ and $\|q_{\mathbb{I}}^0 - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq \epsilon$, for $0 < \epsilon \in \mathbb{R}$ sufficiently small, and $\mathbf{u}_{\mathbb{I}}^0 = G_{\mathbb{I}}(q_{\mathbb{I}}^0)$, and $\mathbf{z}_{\mathbb{I}}^0 = (z_{\mathbb{I}}^0, \psi_{\mathbb{I}}^0)$ satisfying

$$A_{l*}(\mathbf{u}^{i,0})(\mathbf{z}^{i,0}, \psi^{i+1,0}) + R_{l*}(\varphi^{i,0}, \varphi^{i-1,0}, \varphi^{i+1,0}; \gamma)(\psi^{i,0}, \psi^{i+1,0}) = u^{i,0} - u_d^i,$$

is possible.

An analogous convergence result holds for a radius $0 < \omega_{2,\infty} \in \mathbb{R}$ and a constant $0 < C_{N,\infty} \in \mathbb{R}$, if we replace Y^M with Y_∞^M and Z^M with Z_∞^M,

Proof. We start with the convergence proof in the $Y^M - Z^M$-setting. By Theorem 6.2.9, $(\widehat{\text{GE}})$ is strongly regular in Y^M at $\bar{y}_{\mathbb{I}}$. Further, a Lipschitz condition for $F_{\mathbb{I}}$ holds, as proved in Lemma 6.1.9. As a result, Dontchev's implicit function theorem for generalized equations, cf. [58, Theorem 2.4], is applicable: It proves existence of radii $0 < \rho_1, \rho_2 \in \mathbb{R}$ such that for any $y_{\mathbb{I}}^k = \hat{y}_{\mathbb{I}}^k \in B_{\rho_1}^{Y^M}(\bar{y}_{\mathbb{I}})$, there exists a solution $\hat{y}_{\mathbb{I}}^{k+1} \in B_{\rho_2}^{Y^M}(\bar{y}_{\mathbb{I}})$ to $(\widehat{\text{NM}})$. Note that the update direction produced from $(\widehat{\text{QP}}_k)$ is independent of $q_{\mathbb{I}}^k = \hat{q}_{\mathbb{I}}^k$, as argued in [96, Theorem 6.2 (3)], due to the structure of the problem and the Lipschitz properties showed in Lemma 3.3.3 and Corollary 3.4.5. Let $\omega_{2,2}$ be chosen such that $0 < \omega_{2,2} \leq \rho_1$, it then holds

$$0 \in F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) + F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(\bar{y}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}) + N_{\mathbb{I}}(\bar{y}_{\mathbb{I}}), \tag{6.53}$$

$$0 \in F_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^k) + F_{\mathbb{I}}'(\hat{y}_{\mathbb{I}}^k)(\hat{y}_{\mathbb{I}}^{k+1} - \hat{y}_{\mathbb{I}}^k) + N_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^{k+1}). \tag{6.54}$$

Adding and subtracting $F_{\mathbb{I}}(\bar{y}_{\mathbb{I}})$ and $F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(\hat{y}_{\mathbb{I}}^{k+1} - \bar{y}_{\mathbb{I}})$ to (6.54), one obtains

$$\delta_{\mathbb{I}}^{k+1} \in F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) + F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(\hat{y}_{\mathbb{I}}^{k+1} - \bar{y}_{\mathbb{I}}) + N_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^{k+1}), \tag{6.55}$$

where $\delta_{\mathbb{I}}^{k+1}$ is defined as

$$\delta_{\mathbb{I}}^{k+1} := F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) - F_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^k) + F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(\hat{y}_{\mathbb{I}}^{k+1} - \bar{y}_{\mathbb{I}}) - F_{\mathbb{I}}'(\hat{y}_{\mathbb{I}}^k)(\hat{y}_{\mathbb{I}}^{k+1} - \hat{y}_{\mathbb{I}}^k). \tag{6.56}$$

Utilizing again the Lipschitz condition from Lemma 6.1.9, from (6.55) one obtains for a constant $0 < L \in \mathbb{R}$, only depending on ρ_1 and ρ_2, that

$$\|\delta_{\mathbb{I}}^{k+1}\|_{Z^M} \leq L\big(\|\hat{\mathbf{u}}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\hat{\mathbf{z}}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}\big) \leq L\,\omega_{2,2}. \tag{6.57}$$

Since (6.53) is equivalent to the first-order necessary conditions of $(\widehat{\text{QP}}_\delta)$ for $\delta_{\mathbb{I}} = 0$, and (6.55) is equivalent to the first-order necessary conditions of $(\widehat{\text{QP}}_\delta)$ for $\delta_{\mathbb{I}} = \delta_{\mathbb{I}}^{k+1}$, by Proposition 6.2.8 it immediately follows that

$$\|\hat{y}_{\mathbb{I}}^{k+1} - \bar{y}_{\mathbb{I}}\|_{Y^M} \leq L_2 \|\delta_{\mathbb{I}}^{k+1} - 0\|_{Z^M} = L_2 \|\delta_{\mathbb{I}}^{k+1}\|_{Z^M} \leq L_2 L \omega_{2,2}, \tag{6.58}$$

where (6.57) is used to obtain the last inequality. For a quadratic convergence result, further estimations of $\|\delta_{\mathbb{I}}^{k+1}\|_{Z^M}$ are required: Estimating $\delta_{\mathbb{I}}^{k+1}$ as given in (6.56) in the Z^M-norm yields

$$\|\delta_{\mathbb{I}}^{k+1}\|_{Z^M} \leq \|F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) - F_{\mathbb{I}}(\hat{y}_{\mathbb{I}}^k) - F_{\mathbb{I}}'(\hat{y}_{\mathbb{I}}^k)(\bar{y}_{\mathbb{I}} - \hat{y}_{\mathbb{I}}^k)\|_{Z^M}$$

$$+ \|(F'_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) - F'_{\mathbb{I}}(\hat{y}^k_{\mathbb{I}}))(\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}})\|_{Z^M}.$$

We estimate the right-hand side further: Due to $\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M} \leq \rho_1$, Lemma 6.1.11 and Lemma 6.1.10 are applicable, and for constants $0 < c_1, c_2 \in \mathbb{R}$, only depending on ρ_1, we obtain

$$\begin{aligned}
\|\delta^{k+1}_{\mathbb{I}}\|_{Z^M} \leq & c_1\big(\|\hat{\mathbf{u}}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|^2_{W^M} + \|\hat{\mathbf{z}}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|^2_{W^M}\big) \\
& + c_2\big(\|\hat{\mathbf{u}}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + |\hat{\mathbf{z}}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}\big) \\
& \cdot \big(\|\hat{\mathbf{u}}^{k+1}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\hat{\mathbf{z}}^{k+1}_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M}\big) \\
\leq & c_1\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|^2_{Y^M} + c_2\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M}\|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M}.
\end{aligned} \tag{6.59}$$

Now, combining the first part of (6.58) with (6.59) yields

$$\|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M} \leq L_2 c_1\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|^2_{Y^M} + L_2 c_2\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M}\|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M}. \tag{6.60}$$

Additionally to the demands above, now let $\omega_{2,2}$ suffice to $\omega_{2,2} \leq \frac{1}{L_2\, c_1 + L_2^2 c_2\, L}$. Then, recalling that by assumption, it holds $\hat{y}^k_{\mathbb{I}} \in B^{Y^M}_{\omega_{2,2}}(\bar{y}_{\mathbb{I}})$, thus from (6.60), and also using (6.58), one obtains

$$\begin{aligned}
\|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M} & \leq L_2\, c_1 \omega^2_{2,2} + L_2\, c_2 \omega_{2,2}\, L_2\, L\, \omega_{2,2} \\
& \leq \omega^2_{2,2}\Big[L_2 c_1 + L_2^2 c_2\, L\Big] \leq \omega_{2,2},
\end{aligned}$$

i.e. we have proved $\hat{y}^{k+1}_{\mathbb{I}} \in B^{Y^M}_{\omega_{2,2}}(\bar{y}_{\mathbb{I}})$. Now, let finally furthermore $\omega_{2,2} \leq \frac{1}{2L_2 c_2}$, then again from (6.59) and (6.60),

$$\begin{aligned}
\|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M} & \leq L_2 c_1\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|^2_{Y^M} + L_2\, c_2\, \omega_{2,2}\, \|\hat{y}^{k+1}_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M} \\
& \leq C_{N,2}\|\hat{y}^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|^2_{Y^M},
\end{aligned}$$

for a constant $C_{N,2} = \frac{L_2 c_1}{1 - \omega_{2,2} c_2 L_2} > 0$. Note that overall, $\omega_{2,2}$ is chosen such that $\omega_{2,2} =: \min\left(\rho_1, \frac{1}{L_2\, c_1 + L_2^2 c_2\, L}, \frac{1}{2L_2\, c_2}\right) > 0$, and this concludes the proof.

The convergence result for the $Y^M_\infty - Z^M_\infty$-setting follows in the same way. Note the independence of the control update directions debated above, thus due to Corollary 6.1.12 the results from Lemma 6.1.9, Lemma 6.1.10 and Lemma 6.1.11 hold true in this setting as well, and that $(\widehat{\text{GE}})$ is strongly regular in Y^M_∞ by Theorem 6.2.9. Choosing $0 < \omega_{2,\infty} =: \min\left(\rho_1, \frac{1}{L_\infty\, c_1 + L_\infty^2 c_2\, L}, \frac{1}{2L_\infty\, c_2}\right) \in \mathbb{R}$ and $0 < C_{N,\infty} = \frac{L_\infty c_1}{1 - \omega_{2,\infty} c_2 L_\infty} \in \mathbb{R}$ concludes the proof. □

Let us conclude this section with a summary of the current progress: Under Assumption 4.3.1, the auxiliary subproblem $(\widehat{\text{QP}}_k)$ is well-defined, and existence and uniqueness of solutions can be positively answered, cf. Corollary 6.2.2. The unique solution suffices to first-order optimality conditions, that are also sufficient, cf. Corollary 6.2.3. Furthermore, iteratively solving $(\widehat{\text{QP}}_k)$ generates a sequence that converges quadratically towards $\bar{q}$ from Assumption 6.1.1, cf. Theorem 6.2.10. However, up until now this is only true for problems that are restricted to the admissible set $\widehat{Q_{\mathrm{ad},\mathbb{I}}}$. In the introduction of this chapter, it was already hinted that it is possible to transfer the convergence result to Algorithm 6.1.2 for a localized problem formulation, which is the topic of the next section.

6.3 Convergence of the SQP algorithm with L^∞-localization

In this section, a first main result of this chapter is showed: Local quadratic convergence of the sequence $\{q_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ of iterates produced by Algorithm 6.1.2 towards a local minimizer $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$, under a closeness condition for the controls in L^∞. This is done by transferring the Y_∞^M-convergence result of the iterative solution of $(\widehat{\mathrm{QP}_k})$ over to (QP_k). For this, again following the course of action of [152], we introduce another auxiliary intermediate subproblem, and show equivalence results of this intermediate subproblem and $(\widehat{\mathrm{QP}_k})$. This course of action relies on L^∞-techniques. For an analysis of the one time step analogous SQP method w.r.t. L^∞-localization, we refer to [85, Section 6.1] of the author and I. Neitzel.

Let us continue with the following assumption, which holds throughout the entire Section 6.3:

Assumption 6.3.1. *Let $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k) \in Y_\infty^M$ with $q_{\mathbb{I}}^k \in Q_{ad,\mathbb{I}}$ always denote a fixed function triple that lies in a neighborhood of $\bar{y}_{\mathbb{I}}$ from Assumption 6.1.1. The size of the neighborhood is specified in Assumption 6.3.6 below.*

6.3.1 The intermediate subproblem $(\mathrm{QP}_k^{\omega,\infty})$

As in [152], an intermediate subproblem is utilized to transfer the strong regularity property, and therefore the convergence result locally to Algorithm 6.1.2. This intermediate subproblem is called $(\mathrm{QP}_k^{\omega,\infty})$, and a localized version of (QP_k), in the sense that the admissible control set $Q_{\mathrm{ad},\mathbb{I}}$ is restricted to an L^∞-neighborhood of $\bar{q}_{\mathbb{I}}$.

We define an admissible set $Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty}$ with L^∞-closeness of $\bar{q}_{\mathbb{I}}$, for any $0 < \omega \in \mathbb{R}$ via

$$Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty} := \{q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}} \mid \|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{(L^\infty(\Gamma))^M} \leq \omega\}.$$

The intermediate subproblem $(\mathrm{QP}_k^{\omega,\infty})$ is then introduced as:

Let $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k) \in Y_\infty^M$ be given, find a pair of functions $\mathbf{d}_{\mathbb{I}}^k = (dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k) = (q_{\mathbb{I}} - q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k) \in Q^M \times W^M$ that solves

$$\left.\begin{aligned} &\min_{\mathbf{d}_{\mathbb{I}}^k} && J_{k,\mathbb{I}}(\mathbf{d}_{\mathbb{I}}^k) := J'_{\mathbb{I}}(q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k)\mathbf{d}_{\mathbb{I}}^k + \frac{1}{2}\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}}^k)[(\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k), (\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k)], \\ &\text{subject to:} && \mathbf{du}_{\mathbb{I}}^k \text{ satisfies } (\mathrm{EL}_k) \text{ for data } dq_{\mathbb{I}}^k, \\ &\text{and:} && q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty}, \end{aligned}\right\} \tag{$\mathrm{QP}_k^{\omega,\infty}$}$$

where we recall (EL_k) from the definition of the problem (QP_k) to be

$$\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}^{i,k}, d\varphi^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi^{i,k}, d\varphi^{i-1,k}) \\ &\quad = B dq^{i,k} + Bq^{i,k} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \quad \forall i = 1, ..., M, \end{aligned}$$

cf. again the equivalent formulations for linearized equations from (3.72)-(3.74), as well as Corollary 6.1.3 and Remark 6.1.7.

Similarly to $(\mathrm{QP}_k^{\mathrm{red}})$ and $(\widehat{\mathrm{QP}}_k^{\mathrm{red}})$, the reduced version is introduced, which is given by

$$\min f_{\mathbb{I},k}(q_{\mathbb{I}}), \qquad \text{such that} \quad q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty}. \tag{$\mathrm{QP}_k^{\omega,\infty,\mathrm{red}}$}$$

As also done for the previous optimal control problems, the first task is the investigation of the existence of (at least one) solution, similarly to [85, Lemma 6.2] of the author and I. Neitzel for the one time step setting.

Lemma 6.3.2. *Let $\omega > 0$ be sufficiently small and $y_{\mathbb{I}}^k \in Y_\infty^M$ be given such that $\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_W, \|\mathbf{z}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_W \leq \omega$. The intermediate subproblem $(\mathrm{QP}_k^{\omega,\infty})$ has at least one solution $q_{\mathbb{I},\omega}^{k+1} \in Q_{ad,\mathbb{I}}^{\omega,\infty}$ with $\mathbf{u}_{\mathbb{I},\omega}^{k+1} \in W^M$, satisfying (6.61a) immediately below, and control and state directions $dq_{\mathbb{I},\omega}^k = q_{\mathbb{I},\omega}^{k+1} - q_{\mathbb{I}}^k$ and $\mathbf{du}_{\mathbb{I},\omega}^k = \mathbf{u}_{\mathbb{I},\omega}^{k+1} - \mathbf{u}_{\mathbb{I}}^k$.*

Proof. The proof follows standard arguments, noting that the admissible set $Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty}$ is closed, convex and bounded. The remainder of the proof is omitted. □

Once more, first-order necessary optimality conditions for $(\mathrm{QP}_k^{\omega,\infty})$ also follow by standard theory, cf. [85, Corollary 6.2] of the author and I. Neitzel for the setting $M = 1$.

Corollary 6.3.3. *Let $y_{\mathbb{I}}^k \in Y_\infty^M$ be given and $q_{\mathbb{I},\omega}^{k+1}$ with state $\mathbf{u}_{\mathbb{I},\omega}^{k+1}$ be a solution to $(\mathrm{QP}_k^{\omega,\infty})$. Then, there exists an adjoint state pair $\mathbf{z}_{\mathbb{I},\omega}^{k+1} = (z_{\mathbb{I},\omega}^{k+1}, \psi_{\mathbb{I},\omega}^{k+1}) \in W^M$ such that*

$$\left.\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}_\omega^{i,k}, d\varphi_\omega^{i-1,k}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi_\omega^{i,k}, d\varphi_\omega^{i-1,k}) \\ &\quad = Bq_\omega^{i,k+1} - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \qquad \forall i = 1, ..., M, \end{aligned}\right\} \tag{6.61a}$$

$$\left.\begin{aligned}&A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}_\omega^{i,k+1},\psi^{i+1,k+1}) + R_{l*}(\varphi^{i,k},\varphi^{i-1,k},\varphi^{i+1,k};\gamma)(\psi_\omega^{i,k+1},\psi^{i+1,k+1})\\ &\quad = u_\omega^{i,k+1} - u_d^i - A_{b*}(\mathbf{u}^{i,k},\mathbf{du}_\omega^{i,k})\mathbf{z}^{i,k}\\ &\qquad - R_{b*}(\varphi^{i,k},\varphi^{i-1,k},\varphi^{i+1,k},d\varphi_\omega^{i,k},d\varphi_\omega^{i-1,k},d\varphi_\omega^{i+1,k};\gamma)(\psi^{i,k},\psi^{i+1,k})\\ &\qquad\quad \forall i=1,...,M,\end{aligned}\right\} \tag{6.61b}$$

$$\left(B^*\mathbf{z}_\omega^{i,k+1} + \alpha q_\omega^{i,k+1}, q^i - q_\omega^{i,k+1}\right)_Q \geq 0 \qquad \forall i=1,...,M \text{ and } q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}^{\omega,\infty}, \quad \Big\} \tag{6.61c}$$

where again the notation $\mathbf{du}_{\mathbb{I},\omega}^k = \mathbf{u}_{\mathbb{I},\omega}^{k+1} - \mathbf{u}_{\mathbb{I}}^k$ *is used to improve readability.*

At this point, we collect some remarks as well as some immediately obvious facts that are used in the equivalence considerations of the next Section 6.3.2.

Remark 6.3.4.

- *Lemma 6.3.2 only ensures existence of solutions of* $(\mathrm{QP}_k^{\omega,\infty})$*, uniqueness is showed in Lemma 6.3.11 below.*

- *It is clear that the first-order optimality conditions of* $(\widehat{\mathrm{QP}}_k)$ *from Corollary 6.2.3 and the first-order optimality conditions of* $(\mathrm{QP}_k^{\omega,\infty})$ *from Corollary 6.3.3 only differ in the admissible control spaces* $\widehat{Q_{ad,\mathbb{I}}}$, $Q_{ad,\mathbb{I}}^{\omega,\infty}$ *respectively, that appear in the respective variational inequalities. The same is true for the first-order necessary conditions of* (QP_k) *from Lemma 6.1.6.*

- *From the definition of the admissible set* $Q_{ad,\mathbb{I}}^{\omega,\infty}$ *and the definition of the* $(L^\infty(\Omega))^M$*-norm, it immediately follows that also all* q^i *are close to the* $\bar{q}^i$*, since for any* $i=1,...,M$ *it holds*

$$\|q^i - \bar{q}^i\|_{L^\infty(\Omega)} \leq \sum_{i=1}^M \|q^i - \bar{q}^i\|_{L^\infty(\Omega)} = \|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{(L^\infty(\Omega))^M} \leq \omega. \tag{6.62}$$

6.3.2 Equivalence of $(\widehat{\mathrm{QP}}_k)$ and $(\mathrm{QP}_k^{\omega,\infty})$

In this section, we show that the (unique) solution $\hat{y}_{\mathbb{I}}^{k+1}$ of $(\widehat{\mathrm{QP}}_k)$, together with the state $\hat{\mathbf{u}}_{\mathbb{I}}^{k+1}$ and adjoint $\hat{\mathbf{z}}_{\mathbb{I}}^{k+1}$ satisfying (6.36a) and (6.36b), respectively, also satisfies the optimality conditions of $(\mathrm{QP}_k^{\omega,\infty})$. It is then possible to prove uniqueness of solutions of $(\mathrm{QP}_k^{\omega,\infty})$, if $y_{\mathbb{I}}^k$ lies sufficiently close to $\bar{y}_{\mathbb{I}}$ in the L^∞-sense. The start is made with an auxiliary lemma, cf. [85, Lemma 6.3] of the author and I. Neitzel for the setting $M=1$, which closely follows ideas from [152, Lemma 6.5].

Lemma 6.3.5. *There exists an* $\omega_3 > 0$ *with the following properties: Suppose* $\omega \leq \omega_3$*, and* $y_{\mathbb{I}}^k \in Y_\infty^M$ *with* $\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega_3$*, and let* $y_{\mathbb{I}} =$

$(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}, \mathbf{z}_{\mathbb{I}})$ *satisfy*

$$\left.\begin{aligned} &A_l(\mathbf{u}^{i,k}(\mathbf{u}^i), \varphi^{i-1}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^i, \varphi^{i-1}) \\ &\quad = B(q^i) + A_l(\mathbf{u}^{i,k})\mathbf{u}^{i,k} + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^{i,k}, \varphi^{i-1,k}) \\ &\qquad - A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) \quad \forall i = 1, ..., M, \end{aligned}\right\}$$

$$\left.\begin{aligned} &A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma)(\psi^i, \psi^{i+1}) \\ &\quad = u^i - u_d^i - A_{b*}(\mathbf{u}^{i,k}, \mathbf{u}^i - \mathbf{u}^{i,k})\mathbf{z}^{i,k} \\ &\qquad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \varphi^i - \varphi^{i,k}, \varphi^{i-1} - \varphi^{i-1,k}, \varphi^{i+1} - \varphi^{i+1,k}; \gamma) \\ &\qquad\quad \cdot (\psi^{i,k}, \psi^{i+1,k}) \quad \forall i = 1, ..., M, \end{aligned}\right\}$$

and $q_{\mathbb{I}} \in Q^{\omega,\infty}_{ad,\mathbb{I}}$.

Then, it holds

$$\begin{aligned} sign(B^*\mathbf{z}^i + \alpha q^i)(x) &= sign(B^*\bar{\mathbf{z}}^i + \alpha \bar{q}^i)(x) \quad \forall i = 1, ..., M \quad a.e.\ on \quad \mathcal{I}(\sigma), \\ \left|(B^*\mathbf{z}^i + \alpha q^i)(x)\right| &\geq \frac{\sigma}{2} \quad \forall i = 1, ..., M \quad a.e.\ on \quad \mathcal{I}(\sigma). \end{aligned}$$

Proof. Let $\mathbf{du}_{\mathbb{I}} = (du_{\mathbb{I}}, d\varphi_{\mathbb{I}}) := \mathbf{u}_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}$, which satisfies for all $i = 1, ..., M$,

$$\begin{aligned} &A_l(\mathbf{u}^{i,k})(\mathbf{du}^i, d\varphi^{i-1}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(d\varphi^i, d\varphi^{i-1}) \\ &\quad = B(q^i - \bar{q}^i) + A_l(\mathbf{u}^{i,k})(\mathbf{u}^{i,k} - \bar{\mathbf{u}}^i, \varphi^{i-1,k} - \bar{\varphi}^{i-1}) \\ &\qquad + R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^{i,k} - \bar{\varphi}^i, \varphi^{i-1,k} - \bar{\varphi}^{i-1}) \\ &\qquad - \big(A(\mathbf{u}^{i,k}, \varphi^{i-1,k}) - A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1})\big) - \big(R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma) - R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma)\big). \end{aligned} \tag{6.63}$$

To estimate the right-hand side, we utilize Lemma 3.1.3 as well as Lemma 3.1.5 to obtain

$$\begin{aligned} \|A_l(\mathbf{u}^{i,k})(\mathbf{u}^{i,k} - \bar{\mathbf{u}}^i, \varphi^{i-1,k} - \bar{\varphi}^{i-1})\|_{W^\times} &\leq c(\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M})\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \\ &\leq c(\omega_3)\omega_3, \end{aligned} \tag{6.64}$$

$$\begin{aligned} \|A(\bar{\mathbf{u}}^i, \bar{\varphi}^{i-1}) - A(\mathbf{u}^{i,k}, \varphi^{i-1,k})\|_{W^\times} &\leq c(\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M}, \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M})\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \\ &\leq c(\omega_3)\omega_3, \end{aligned} \tag{6.65}$$

for constants $0 < c(\omega_3) \in \mathbb{R}$ independently of $y^k_{\mathbb{I}}$. To obtain (6.64) and (6.65), $\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \leq \omega_3$, and the triangle inequality $\|\mathbf{u}^k_{\mathbb{I}}\|_{W^M} \leq \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}$ is used, cf. (6.28). Analogously, utilizing Lemma 3.1.6 and Lemma 3.1.8 yield

$$\|R_l(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)(\varphi^{i,k} - \bar{\varphi}^i, \varphi^{i-1,k} - \bar{\varphi}^{i-1})\|_{L^q(\Omega)} \leq c(\omega_3)\omega_3, \tag{6.66}$$

$$\|R(\bar{\varphi}^i, \bar{\varphi}^{i-1}; \gamma) - R(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)\|_{L^q(\Omega)} \leq c(\omega_3)\omega_3. \tag{6.67}$$

Finally, using $q_{\mathbb{I}} \in Q^{\omega,\infty}_{\mathrm{ad},\mathbb{I}}$, in combination with the embedding $L^\infty(\Gamma) \hookrightarrow L^2(\Gamma) \hookrightarrow W^{-1,p}(\Omega)$, it holds

$$\|B(q^i - \bar{q}^i)\|_{W^\times} \leq c\|q^i - \bar{q}^i\|_Q \leq c\|q^i - \bar{q}^i\|_{L^\infty(\Gamma)} \leq \omega \leq \omega_3, \tag{6.68}$$

since $\omega \leq \omega_3$ by assumption, as well as (6.62). By (6.64)-(6.68), the right-hand side of (6.63) is in $W^\times$ for any $i = 1, ..., M$. Therefore using Lemma 3.2.3, it holds

$$\|\mathbf{u}_\mathbb{I} - \bar{\mathbf{u}}_\mathbb{I}\|_{W^M} = \|\mathbf{du}_\mathbb{I}\|_{W^M} \leq c(\omega_3)\omega_3,$$

which, using the embeddings $W_u \hookrightarrow L^\infty(\Omega; \mathbb{R}^2)$ and $W_\varphi \hookrightarrow L^\infty(\Omega)$, immediately leads to

$$\|\mathbf{u}_\mathbb{I} - \bar{\mathbf{u}}_\mathbb{I}\|_{L^\infty(\Omega;\mathbb{R}^2)^M} \leq c(\omega_3)\omega_3. \tag{6.69}$$

Next, let $\mathbf{dz}_\mathbb{I} := \mathbf{z}_\mathbb{I} - \bar{\mathbf{z}}_\mathbb{I}$. We calculate the difference to obtain

$$\begin{aligned}
A_{l*}&(\mathbf{u}^{i,k})(\mathbf{dz}^i, d\psi^{i+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma)(d\psi^i, d\psi^{i+1}) \\
&= u^i - \bar{u}^i - A_{b*}(\mathbf{u}^{i,k}, \mathbf{u}^i - \mathbf{u}^{i,k})\mathbf{z}^{i,k} \\
&\quad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \varphi^i - \varphi^{i,k}, \varphi^{i-1} - \varphi^{i-1,k}, \varphi^{i+1} - \varphi^{i+1,k}; \gamma) \\
&\qquad \cdot (\psi^{i,k}, \psi^{i+1,k}) \\
&\quad + \big(A_{l*}(\mathbf{u}^{i,k}) - A_{l*}(\bar{\mathbf{u}}^i)\big)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1}) \\
&\quad + \big(R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma) - R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}; \gamma)\big)(\bar{\psi}^i, \bar{\psi}^{i+1}).
\end{aligned} \tag{6.70}$$

We again estimate the right-hand side in the $W^\times$-norm. From Lemma 3.1.3, we conclude using the triangle inequality, cf. (6.28) and (6.29), as well as (6.69),

$$\begin{aligned}
\|A_{b*}(\mathbf{u}^{i,k}, \mathbf{u}^i - \mathbf{u}^{i,k})\mathbf{z}^{i,k}\|_{W^\times} &\leq c\|\mathbf{u}_\mathbb{I}^k\|_{W^M}\|\mathbf{u}_\mathbb{I} - \mathbf{u}_\mathbb{I}^k\|_{W^M}\|\mathbf{z}_\mathbb{I}^k\|_{W^M} \\
&\leq c(\omega_3)\|\mathbf{u}_\mathbb{I} - \bar{\mathbf{u}}_\mathbb{I}\|_{W^M} + c(\omega_3)\|\bar{\mathbf{u}}_\mathbb{I} - \mathbf{u}_\mathbb{I}^k\|_{W^M} \\
&\leq c(\omega_3)\omega_3.
\end{aligned}$$

Similarly, from Lemma 3.1.5, Lemma 3.1.6 and Lemma 3.1.8, it follows

$$\begin{aligned}
&\|\big(A_{l*}(\mathbf{u}^{i,k}) - A_{l*}(\bar{\mathbf{u}}^i)\big)(\bar{\mathbf{z}}^i, \bar{\psi}^{i+1})\|_{W^\times} \\
&\quad \leq c(\omega_3)\|\mathbf{u}_\mathbb{I}^k - \bar{\mathbf{u}}_\mathbb{I}^k\|_{W^M}\|\bar{\mathbf{z}}_\mathbb{I}\|_{W^M} \leq c(\omega_3)\omega_3, \\
&\|\big(R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma) - R_{l*}(\bar{\varphi}^i, \bar{\varphi}^{i-1}, \bar{\varphi}^{i+1}; \gamma)\big)(\bar{\psi}^i, \bar{\psi}^{i+1})\|_{L^q(\Omega)} \\
&\quad \leq c(\omega_3)\|\mathbf{u}_\mathbb{I}^k - \bar{\mathbf{u}}_\mathbb{I}\|_{W^M}\|\bar{\mathbf{z}}_\mathbb{I}\|_{W^M} \leq c(\omega_3)\omega_3, \\
&\|R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \varphi^i - \varphi^{i,k}, \varphi^{i-1} - \varphi^{i-1,k}, \varphi^{i+1} - \varphi^{i+1,k}; \gamma) \\
&\qquad \cdot (\psi^{i,k}, \psi^{i+1,k})\|_{L^q(\Omega)} \\
&\quad \leq c\|\mathbf{u}_\mathbb{I}^k\|_{W^M}\|\mathbf{u}_\mathbb{I} - \mathbf{u}_\mathbb{I}^k\|_{W^M}\|\mathbf{z}_\mathbb{I}^k\|_{W^M} \leq c(\omega_3)\omega_3.
\end{aligned}$$

Finally, from (6.69) it immediately follows

$$\|u^i - \bar{u}^i\|_{L^\infty(\Omega;\mathbb{R}^3)} \leq \|\mathbf{u}_\mathbb{I} - \bar{\mathbf{u}}_\mathbb{I}\|_{(L^\infty(\Omega;\mathbb{R}^2))^M} \leq c(\omega_3).$$

Therefore, the right-hand side of (6.70) is in $W^\times$ for all $i = 1, ..., M$, and from Corollary 3.4.3 and the L^∞-embedding it follows

$$\|\mathbf{z}_\mathbb{I} - \bar{\mathbf{z}}_\mathbb{I}\|_{L^\infty(\Omega;\mathbb{R}^2)} \leq c\|\mathbf{z}_\mathbb{I} - \bar{\mathbf{z}}_\mathbb{I}\|_{W^M} \leq c(\omega_3)\omega_3. \tag{6.71}$$

Now, from $q_{\mathbb{I}} \in Q^{\omega,\infty}_{\mathrm{ad},\mathbb{I}}$, and due to $\omega \leq \omega_3$ by assumption, one concludes

$$|B^*(\mathbf{z}^i - \bar{\mathbf{z}}^i) + \alpha(q^i - \bar{q}^i)| \leq c(\omega_3)(\omega_3 + \omega) \leq c(\omega_3)\omega_3. \tag{6.72}$$

Therefore, for all $i = 1, ..., M$, it holds

$$\begin{aligned} B^*\mathbf{z}^i + \alpha q^i &= B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i + B^*(\mathbf{z}^i - \bar{\mathbf{z}}^i) + \alpha(q^i - \bar{q}^i) \\ &\geq \sigma - c(\omega_3)\omega_3 \quad \text{a.e. on} \quad \mathcal{I}(\sigma), \end{aligned}$$

where (6.72) is used, and $|B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i| \geq \sigma$ holds due to Assumption 4.3.1. Note that we can look at every $i = 1, ..., M$ separately, due to the structure of the (σ-)active set $\mathcal{I}(\sigma)$. Choosing $\omega_3 > 0$ sufficiently small completes the proof. □

We wish to highlight that the prerequisites of Lemma 6.3.5 in particular demand that $y_{\mathbb{I}}$ suffices to both the state and adjoint equations of $(\mathrm{QP}^{\omega,\infty}_k)$, cf. (6.61a) and (6.61b), and that $q_{\mathbb{I}}$ is an admissible control. However, optimality of $y_{\mathbb{I}}$ for $(\mathrm{QP}^{\omega,\infty}_k)$ is not demanded, since satisfaction of the variational inequality (6.61c) is not assumed.

Summarizing all requirements on ω from the analysis up until now, all statements can tacitly be applied if the following assumption is satisfied. Without further mention, we suppose it to hold true in the remainder of the chapter.

Assumption 6.3.6. *The constant $\omega > 0$ is chosen, such that*

$$\omega := \min(\omega_1, \omega_{2,\infty}, \omega_3),$$

where $\omega_1, \omega_{2,\infty}$, and ω_3 are taken from Lemma 6.2.1, Theorem 6.2.10 and Lemma 6.3.5, respectively.

Remark 6.3.7. *Note that the constant ω depends on the physical parameters $\varepsilon, \kappa, \eta$. We recall that it describes the size of the local neighborhoods around the local minimizer $\bar{y}_{\mathbb{I}}$ of Assumption 6.1.1, in which the linearization point for every $(\mathrm{QP}^{\omega,\infty}_k)$, and subsequently the initial function $q^0_{\mathbb{I}}$ in the SQP method, has to lie. It further also depends on the penalization parameter γ. Note that for the entire analysis of Chapter 6, we consider all parameters to be fixed. A precise tracking of the involvement and scaling of ω on these parameters has not been conducted, and is beyond the scope of this thesis.*

Note that admissibility of $\hat{q}^{k+1}_{\mathbb{I}}$, which we recall to be the unique solution of $(\widehat{\mathrm{QP}}_k)$, for $(\mathrm{QP}^{\omega,\infty}_k)$ has already been proved above, in particular:

Corollary 6.3.8. *The unique solution $\hat{q}^{k+1}_{\mathbb{I}}$ of $(\widehat{\mathrm{QP}}_k)$ is an admissible function for $(\mathrm{QP}^{\omega,\infty}_k)$, i.e. $\hat{q}^{k+1}_{\mathbb{I}} \in Q^{\omega,\infty}_{ad,\mathbb{I}}$.*

Proof. This follows directly from Theorem 6.2.10. □

Next, we show feasibility of $q^{k+1}_{\mathbb{I},\omega}$ for $(\widehat{\mathrm{QP}}_k)$, which can be established similarly to [152, Corollary 6.6], cf. [85, Lemma 6.6] of the author and I. Neitzel for the setting $M = 1$.

Lemma 6.3.9. *Any locally optimal control* $q^{k+1}_{\mathbb{I},\omega} \in Q^{\omega,\infty}_{ad,\mathbb{I}}$ *of* $(\mathrm{QP}^{\omega,\infty}_k)$ *that satisfies the first-order optimality conditions of* $(\mathrm{QP}^{\omega,\infty}_k)$ *from Corollary 6.3.3, together with* $\mathbf{u}^{k+1}_{\mathbb{I},\omega}$ *and* $\mathbf{z}^{k+1}_{\mathbb{I},\omega}$ *satisfying* (6.61a) *and* (6.61b)*, respectively, fulfills*

$$q^{k+1}_{\mathbb{I},\omega}(x) = \bar{q}_{\mathbb{I}}(x) \quad a.e \quad on \quad \mathcal{I}(\sigma).$$

Proof. For all $x \in \mathcal{I}(x)$ and for all $i = 1, ..., M$, it holds either $\bar{q}^i(x) = q^i_b$ if $(B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i)(x) \leq -\sigma$, or $\bar{q}^i(x) = q^i_a$ if $(B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i)(x) \geq \sigma$. Thus for any $q_{\mathbb{I}} \in Q^{\omega,\infty}_{\mathrm{ad},\mathbb{I}}$, either $q^i(x) \in [q^i_b - \omega, q^i_b]$, or $q^i(x) \in [q^i_a, q^i_a + \omega]$, due to the structure of the admissible set in $i = 1, ..., M$ directions, cf. also Remark 6.3.4. Due to the assumptions on $q^{k+1}_{\mathbb{I},\omega}$, Lemma 6.3.13 is applicable. For all $i = 1, ..., M$, it thus holds either

$$B^*\mathbf{z}^{i,k+1}_\omega + \alpha q^{i,k+1}_\omega \geq \frac{\sigma}{2} \quad \text{or} \quad B^*\mathbf{z}^{i,k+1}_\omega + \alpha q^{i,k+1}_\omega \leq -\frac{\sigma}{2},$$

but this means that either $q^{i,k+1}_\omega = q^i_b$ or $q^{i,k+1}_\omega = q^i_a$, by (6.61c). However, this means that $q^{i,k+1}_\omega = \bar{q}^i$, therefore $q^{k+1}_{\mathbb{I}} = \bar{q}_{\mathbb{I}}$ on $\mathcal{I}(\sigma)$. ☐

At this point, it is important to emphasize the following important fact:

Remark 6.3.10. *In both Lemma 6.3.5 and Lemma 6.3.9, pointwise arguments involving the controls* q^i *are used. This is the reason, that in this section the localized admissible set* $Q^{\omega,\infty}_{ad,\mathbb{I}}$ *is a localization of* $Q_{ad,\mathbb{I}}$ *w.r.t. the* L^∞*-neighborhood around* $q_{\mathbb{I}}$*. As a consequence, we have to work with strong regularity in the* $Y^M_\infty - Z^M_\infty$*-setting. This might stand in contrast to a (possible) first intuition that may propose to work in the* $Y^M - Z^M$*-setting, inspired by the lack of the two-norm discrepancy in the second-order sufficient conditions proved in Chapter 4.*

Next, along the lines of [152, Theorem 6.12], uniqueness of solutions of the optimality conditions of $(\mathrm{QP}^{\omega,\infty}_k)$, cf. Corollary 6.3.3, under Assumption 4.3.1 and Assumption 6.3.6, is showed. Again, this result for the one time step setting is proved in [85, Lemma 6.7] by the author and I. Neitzel.

Lemma 6.3.11. *Let* $y^k_{\mathbb{I}} \in Y^M_\infty$ *satisfy* $\|\mathbf{u}^k_{\mathbb{I}} - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}^k_{\mathbb{I}} - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega$*. The first-order optimality conditions of* $(\mathrm{QP}^{\omega,\infty}_k)$ *from Corollary 6.3.3 admit a unique solution triple* $y^{k+1}_{\mathbb{I},\omega} \in Y^M_\infty$*.*

Proof. By Lemma 6.3.2, there exists at least one solution to $(\mathrm{QP}^{\omega,\infty}_k)$. The associated solution triple is denoted by $y^{k+1}_{\mathbb{I},\omega,1}$, and satisfies the first-order optimality conditions from Corollary 6.3.3. Assume that a second triple, denoted by $y^{k+1}_{\mathbb{I},\omega,2}$ also satisfies the first-order optimality conditions from Corollary 6.3.3. Since both $y^{k+1}_{\mathbb{I},\omega,1}$ and $y^{k+1}_{\mathbb{I},\omega,2}$ are admissible, it is possible to test the variational inequality (6.61c), once in $q^{k+1}_{\mathbb{I},\omega,1}$ with $q^{k+1}_{\mathbb{I},\omega,2}$, and once in $q^{k+1}_{\mathbb{I},\omega,2}$ with $q^{k+1}_{\mathbb{I},\omega,1}$. After summing up, this leads to

$$\begin{aligned} 0 \leq\, & (B^*\mathbf{z}^{i,k+1}_{\omega,1} + \alpha q^{i,k+1}_{\omega,1}, q^{i,k+1}_{\omega,2} - q^{i,k+1}_{\omega,1}) \\ & + (B^* z^{i,k+1}_{\omega,2} + \alpha q^{i,k+1}_{\omega,2}, q^{i,k+1}_{\omega,1} - q^{i,k+1}_{\omega,2}), \end{aligned}$$

for all $i = 1, ..., M$. This in turn can be simplified to

$$\left\langle \mathbf{z}^i, Bq^i \right\rangle - \alpha(q^i, q^i)_Q \geq 0 \quad \forall i = 1, ..., M, \tag{6.73}$$

after introducing

$$\mathbf{u}_{\mathbb{I}} := \mathbf{u}^{k+1}_{\mathbb{I},\omega,2} - \mathbf{u}^{k+1}_{\mathbb{I},\omega,1}, \quad q_{\mathbb{I}} := q^{k+1}_{\mathbb{I},\omega,2} - q^{k+1}_{\mathbb{I},\omega,1}, \quad \mathbf{z}_{\mathbb{I}} := \mathbf{z}^{k+1}_{\mathbb{I},\omega,2} - \mathbf{z}^{k+1}_{\mathbb{I},\omega,1}.$$

An easy calculation also shows that $\mathbf{u}_{\mathbb{I}}$ and $\mathbf{z}_{\mathbb{I}}$ suffice to

$$\begin{aligned}
&A_l(\mathbf{u}^{i,k})(\mathbf{u}^i, \varphi^{i+1}) + R_l(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma)(\varphi^i, \varphi^{i+1}) = Bq^i, \\
&A_{l*}(\mathbf{u}^{i,k})(\mathbf{z}^i, \psi^{i+1}) + R_{l*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}; \gamma)(\psi^i, \psi^{i+1}) \\
&\quad = - A_{b*}(\mathbf{u}^{i,k}, \mathbf{u}^i)(\mathbf{z}^{i,k}, \psi^{i+1,k}) \\
&\qquad - R_{b*}(\varphi^{i,k}, \varphi^{i-1,k}, \varphi^{i+1,k}, \varphi^i, \varphi^{i-1}, \varphi^{i+1}; \gamma)(\psi^{i,k}, \psi^{i+1,k}) + u^i,
\end{aligned}$$

again for all $i = 1, ..., M$. Testing the weak formulation of the first equation with $\mathbf{z}_{\mathbb{I}}$, and the weak formulation of the second equation with $\mathbf{u}_{\mathbb{I}}$ respectively, and again summing up and using the definition of A_{l*}, R_{l*} from (3.7) and (3.8), as well as the definition of A_{b*} and R_{b*} from (3.11) and (3.13), leads to

$$\begin{aligned}
\left\langle Bq^i, \mathbf{z}^i \right\rangle &= (u^i, u^i) - \left\langle A_b(\mathbf{u}^{i,k})[\mathbf{u}^i, \mathbf{u}^i], \mathbf{z}^{i,k} \right\rangle \\
&\quad - \left\langle R_b(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)[(\varphi^i, \varphi^{i-1}), (\varphi^i, \varphi^{i-1})], \psi^{i,k} \right\rangle. \qquad (6.74)
\end{aligned}$$

Now, using (6.73), (6.74), and summing up over all $i = 1, ...M$, from the definition of the second derivative $\mathcal{L}''_{\mathbb{I}}$ of the Lagrangian from (3.126), one easily obtains

$$\begin{aligned}
0 &\geq \sum_{i=1}^{M} \Big[(u^i, u^i) + \alpha(q^i, q^i)_Q - \left\langle A_b(\mathbf{u}^{i,k})[\mathbf{u}^i, \mathbf{u}^i], \mathbf{z}^{i,k} \right\rangle \\
&\qquad - \left\langle R_b(\varphi^{i,k}, \varphi^{i-1,k}; \gamma)[(\varphi^i, \varphi^{i-1}), (\varphi^i, \varphi^{i-1})], \psi^{i,k} \right\rangle \Big] \\
&= \mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}), (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})].
\end{aligned}$$

Due to Assumption 6.3.6, by Lemma 6.3.9 it holds $q_{\mathbb{I}} = 0$ on $\mathcal{I}(\sigma)$. Therefore, from Lemma 6.2.1 it follows that

$$\frac{c_{SSC}}{2} \|q_{\mathbb{I}}\|^2_{Q^M} \leq \mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})[(\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}}), (\mathbf{u}_{\mathbb{I}}, q_{\mathbb{I}})] \leq 0.$$

But this already ensures $q_{\mathbb{I}} = 0$, thus $q^{k+1}_{\mathbb{I},\omega,1} = q^{k+1}_{\mathbb{I},\omega,2}$. □

Note that existence of at least one solution of $(\mathrm{QP}^{\omega,\infty}_k)$ is established in Lemma 6.3.2, and uniqueness of solutions of the associated optimality system is proved in Lemma 6.3.11. In combination, this means:

Corollary 6.3.12. *The subproblem* $(\mathrm{QP}^{\omega,\infty}_k)$ *has a unique solution, denoted by* $q^{k+1}_{\mathbb{I},\omega} \in Q^{\omega,\infty}_{ad,\mathbb{I}}$.

The crucial step is now to show that $\hat{q}_{\mathbb{I}}^{k+1}$ is not only admissible, but in fact also satisfies the optimality conditions of $(\mathrm{QP}_k^{\omega,\infty})$, and is therefore the unique solution of Corollary 6.3.12. In the course of the proof, it is also be showed that $\hat{q}_{\mathbb{I}}^{k+1}$ in fact already satisfies the optimality conditions of (QP_k) from (6.1.6). The result is showed along the lines of [152, Corollary 6.9], and is conducted for the setting $M = 1$ in [85, Lemma 6.9] by the author and I. Neitzel. Note that a closeness assumption on q^k is included in addition to the closeness demanded for $\mathbf{u}^k, \mathbf{z}^k$ up until now.

Lemma 6.3.13. *Let $y_{\mathbb{I}}^k \in Y_\infty^M$, such that $\|y_{\mathbb{I}}^k - \bar{y}_{\mathbb{I}}\|_{Y_\infty^M} \leq \omega$, where $\omega > 0$ satisfies Assumption 6.3.6. The unique solution $\hat{q}_{\mathbb{I}}^{k+1}$ of $(\widehat{\mathrm{QP}}_k)$, with associated state $\hat{\mathbf{u}}_{\mathbb{I}}^{k+1}$ and adjoint state $\hat{\mathbf{z}}_{\mathbb{I}}^{k+1}$ satisfying* (6.36a) *and* (6.36b)*, respectively, satisfies the optimality conditions of* $(\mathrm{QP}_k^{\omega,\infty})$ *from Corollary 6.3.3 and the optimality conditions of* (QP_k) *from Lemma 6.1.6.*

Proof. Due to Remark 6.3.4 and Corollary 6.3.8, the only remaining task is to ensure that the functions $(\hat{q}_{\mathbb{I}}^{k+1}, \hat{\mathbf{z}}_{\mathbb{I}}^{k+1})$ satisfy the variational inequality (6.61c) for all $i = 1, ..., M$. The starting point is the fact that $(\hat{q}_{\mathbb{I}}^{k+1}, \hat{\mathbf{z}}_{\mathbb{I}}^{k+1})$ satisfies the variational inequality (6.36c) of $(\widehat{\mathrm{QP}}_k)$, cf. Corollary 6.2.3, i.e.

$$(B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q^i - \hat{q}^{i,k+1}) \geq 0 \qquad \forall i = 1, ..., M \text{ and } q_{\mathbb{I}} \in \widehat{Q_{\mathrm{ad},\mathbb{I}}}. \quad (6.75)$$

Since $\hat{q}_{\mathbb{I}}^{k+1} \in \widehat{Q_{\mathrm{ad},\mathbb{I}}}$, it holds $\hat{q}_{\mathbb{I}}^{k+1} = \bar{q}_{\mathbb{I}}$ on $\mathcal{I}(\sigma)$. Therefore, for all $i = 1, ..., M$ there are two cases on $\mathcal{I}(\sigma)$:

- $B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1} \geq \sigma$, then it follows from (6.75) $q_a^i = \bar{q}^i = \hat{q}^{i,k+1}$.
- $B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1} \leq -\sigma$, then it follows again from (6.75) $q_b^i = \bar{q}^i = \hat{q}^{i,k+1}$.

Further, since $\hat{q}_{\mathbb{I}}^{k+1}$, together with $\hat{\mathbf{u}}_{\mathbb{I}}^{k+1}$ and $\hat{\mathbf{z}}_{\mathbb{I}}^{k+1}$, is feasible for $(\mathrm{QP}_k^{\omega,\infty})$, thus by Lemma 6.3.5 one obtains that for all $i = 1, ..., M$ either

$$B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1} \geq \frac{\sigma}{2} \qquad \text{or} \qquad B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1} \leq -\frac{\sigma}{2}.$$

Thus, for all $q_{\mathbb{I}}$ with $q^i \in [q_a^i, q_b^i]$, for all $i = 1, ..., M$, on $\mathcal{I}(\sigma)$ it holds

$$\left(B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q^i - \hat{q}^{i,k+1}\right) \geq 0 \qquad \forall i = 1, ..., M.$$

On $Q \setminus \mathcal{I}(\sigma)$, the only requirement for the controls $q_{\mathbb{I}} \in \widehat{Q_{\mathrm{ad},\mathbb{I}}}$ is $q^i \in [q_a^i, q_b^i]$ for all $i = 1, ..., M$. Overall, it holds

$$\begin{aligned}
&(B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q^i - \hat{q}^{i,k+1})_Q \\
&\quad = (B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q^i - \hat{q}^{i,k+1})_{Q\setminus\mathcal{I}(\sigma)} \\
&\qquad + (B^*\hat{\mathbf{z}}^{i,k+1} + \alpha\hat{q}^{i,k+1}, q - \hat{q}^{i,k+1})_{\mathcal{I}(\sigma)} \geq 0 \quad \forall i = 1, ..., M \text{ and } q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}.
\end{aligned} \quad (6.76)$$

Recalling that $Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty} \subset Q_{\mathrm{ad},\mathbb{I}}$ concludes the proof. □

Since the unique solution $\hat{q}_{\mathbb{I}}^{k+1}$ of $(\widehat{\mathrm{QP}}_k)$, with associated triple $\hat{y}_{\mathbb{I}}^{k+1}$ satisfies the optimality conditions of $(\mathrm{QP}_k^{\omega,\infty})$ by Lemma 6.3.13, and Lemma 6.3.11 guarantees uniqueness thereof, it is immediately clear:

Corollary 6.3.14. *The unique solution $\hat{q}_{\mathbb{I}}^{k+1}$ of $(\widehat{\mathrm{QP}}_k)$ and the unique solution $q_{\mathbb{I},\omega}^{k+1}$ of $(\mathrm{QP}_k^{\omega,\infty})$ coincide.*

In particular, this means that $\hat{y}_{\mathbb{I}}^{k+1} = y_{\mathbb{I},\omega}^{k+1}$ and that $\hat{q}_{\mathbb{I}}^{k+1} = q_{\mathbb{I},\omega}^{k+1}$ is the unique (global) solution of both $(\widehat{\mathrm{QP}}_k)$ and $(\mathrm{QP}_k^{\omega,\infty})$ if $\|y_{\mathbb{I}}^k - \bar{y}_{\mathbb{I}}\|_{Y_\infty^M} \leq \omega$ for an ω sufficiently small, cf. Assumption 6.3.6.

6.3.3 Local convergence of Algorithm 6.1.2 with L^∞-localization

As a consequence of Corollary 6.3.14 and Theorem 6.2.10 we can establish local quadratic convergence of Algorithm 6.1.2, if (QP_k) is replaced by $(\mathrm{QP}_k^{\omega,\infty})$, i.e. if a localization in a neighborhood of $\bar{q}_{\mathbb{I}}$ in the L^∞-sense is imposed. We again follow the course of action of [152, Theorem 6.13], and refer to [85, Theorem 6.11] of the author and I. Neitzel for the one time step analogon.

Theorem 6.3.15. *Let $\bar{y}_{\mathbb{I}}$ satisfy Assumption 6.1.1, and let Assumption 6.3.6 hold, i.e. ω be sufficiently small, i.p. let $0 < \epsilon_\infty \in \mathbb{R}$ be sufficiently small, such that for a $q_{\mathbb{I}}^0 \in Q_{ad,\mathbb{I}}$ it holds $\|q_{\mathbb{I}}^0 - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq \epsilon_\infty$. Set $\mathbf{u}_{\mathbb{I}}^0 = G_{\mathbb{I}}(q_{\mathbb{I}}^0)$ and $\mathbf{z}_{\mathbb{I}}^0 = (z_{\mathbb{I}}^0, \psi_{\mathbb{I}}^0)$ such that for all $i = 1, ..., M$,*

$$A_{l*}(\mathbf{u}^{i,0})(\mathbf{z}^{i,0}, \psi^{i+1,0}) + R_{l*}(\varphi^{i,0}, \varphi^{i-1,0}, \varphi^{i+1,0}; \gamma)(\psi^{i,0}, \psi^{i+1,0}) = u^{i,0} - u_d^i.$$

The sequence of iterates $\{y_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ generated by Algorithm 6.1.2 with quadratic sub-problem $(\mathrm{QP}_k^{\omega,\infty})$ converges quadratically in Y_∞^M to $\bar{y}_{\mathbb{I}}$.

Proof. As described in the paragraph before Theorem 6.2.10, for $\epsilon_\infty > 0$ sufficiently small, it holds $\|\mathbf{u}_{\mathbb{I}}^0 - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{u}_{\mathbb{I}}^0 - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} \leq \omega$, for the ω of Assumption 6.3.6, cf. Lemma 3.3.3 and Corollary 3.4.5. Theorem 6.2.10 ensures local quadratic convergences of $\{\hat{y}_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ to $\bar{y}_{\mathbb{I}}$ in Y_∞^M, and $\|y_{\mathbb{I}}^k - \bar{y}_{\mathbb{I}}\|_{Y_\infty^M} \leq \omega$ for all $k \geq 1$. By Corollary 6.3.14, the controls $\hat{q}_{\mathbb{I}}^{k+1}$ are the unique solutions of $(\mathrm{QP}_k^{\omega,\infty})$. This concludes the proof. □

6.4 Convergence of the SQP algorithm with L^2-localization

In this section, the second main result of this chapter is showed: Local quadratic convergence of the sequence $\{q_{\mathbb{I}}^k\}_{k\in\mathbb{N}}$ of iterates produced by Algorithm 6.1.2 towards a local minimizer $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, q_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$ under a closeness condition for the controls in L^2. This means that the difference to Section 6.3 is the use of L^2-closeness instead of the L^∞-closeness. The section closely follows the course of action of the joint work [85, Section 7] of the author and I. Neitzel, where the one time step setting is analyzed. It uses ideas of [96] which, to the best of knowledge of the author, is the first to relax the closeness condition from L^∞ to L^2 for an SQP convergence result for a tracking type optimal control problem in the setting of quasilinear parabolic partial differential equations, using techniques that are now well-established in the context of (two-norm discrepancy of) second-order sufficient conditions. At this point, we do not repeat the setting of [23, 96].

Recall from Section 4.2, that the second-order sufficient conditions for problem ($\mathrm{NLP}_{\mathbb{I}}^{\gamma,\eta}$) does not involve a two-norm discrepancy. The reason is that by Proposition 3.3.1 and Corollary 3.4.1 both the control-to-state operator $G_{\mathbb{I}}$ and the reduced functional $f_{\mathbb{I}}$ are twice Fréchet differentiable w.r.t. Q^M, i.e. in the L^2-norm. Nevertheless, the proofs presented in Section 6.3 involved L^∞-arguments that cannot be directly transferred to L^2-neighborhoods, cf. Remark 6.3.10. Using similar arguments as [96], the main idea is to show that the unique solution of ($\widehat{\mathrm{QP}}_k$) is not only a solution to (QP_k) with L^∞-localization, i.e. to ($\mathrm{QP}_k^{\omega,\infty}$) as showed in Section 6.3, but also a solution to (QP_k) with L^2-localization.

For the course of action, analogously to $Q_{\mathrm{ad},\mathbb{I}}^{\omega,\infty}$, let us define the admissible set $Q_{\mathrm{ad},\mathbb{I}}^{\omega,2}$ around $\bar{q}_{\mathbb{I}}$, for any $0 \leq \omega \in \mathbb{R}$, by

$$Q_{\mathrm{ad},\mathbb{I}}^{\omega,2} := \{q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}} \quad | \quad \|q_{\mathbb{I}} - \bar{q}_{\mathbb{I}}\|_{Q^M} \leq \omega\}.$$

The (L^2-) intermediate subproblem ($\mathrm{QP}_k^{\omega,2}$) is then introduced as:

Let $y_{\mathbb{I}}^k = (\mathbf{u}_{\mathbb{I}}^k, q_{\mathbb{I}}^k, \mathbf{z}_{\mathbb{I}}^k) \in Y_\infty^M$ be given, find a pair of functions $\mathbf{d}_{\mathbb{I}}^k = (dq_{\mathbb{I}}^k, \mathbf{du}_{\mathbb{I}}^k) = (q_{\mathbb{I}} - q_{\mathbb{I}}^k,\, \mathbf{u}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k) \in Q^M \times W^M$ that solves

$$\left.\begin{aligned} &\min_{\mathbf{d}_{\mathbb{I}}^k} && J_{\mathbb{I},k}(\mathbf{d}_{\mathbb{I}}^k) := J_{\mathbb{I}}'(q_{\mathbb{I}}^k, \mathbf{u}_{\mathbb{I}}^k)\mathbf{d}_{\mathbb{I}}^k + \frac{1}{2}\mathcal{L}_{\mathbb{I}}''(y_{\mathbb{I}}^k)[(\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k), (\mathbf{du}_{\mathbb{I}}^k, dq_{\mathbb{I}}^k)], \\ &\text{subject to} && \mathbf{du}_{\mathbb{I}}^k \text{ satisfies } (\mathrm{EL}_k) \text{ for data } dq_{\mathbb{I}}^k, \\ &\text{and} && q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^{\omega,2}, \end{aligned}\right\} \qquad (\mathrm{QP}_k^{\omega,2})$$

where, again, we refer to the definition of the problem (QP_k) on page 118 for the definition of the PDE (EL_k).

Similarly to $(\mathrm{QP}_k^{\mathrm{red}})$, $(\widehat{\mathrm{QP}}_k^{\mathrm{red}})$ and $(\mathrm{QP}_k^{\omega,\infty,\mathrm{red}})$, the reduced formulation is given by

$$\min f_{\mathbb{I},k}(q_{\mathbb{I}}), \qquad \text{such that} \quad q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^{\omega,2}, \tag{$\mathrm{QP}_k^{\omega,2,\mathrm{red}}$}$$

where $f_{\mathbb{I},k}$ is defined as in $(\mathrm{QP}_k^{\mathrm{red}})$.

Before we continue, we establish some additional bounds and Lipschitz conditions for the reduced functionals $f'_{\mathbb{I},k}$ and $f''_{\mathbb{I},k}$ from (6.2) and (6.4). In this context, let us also refer to the respective results for $f'_{\mathbb{I}}, f''_{\mathbb{I}}$, cf. Section 3.4. The main aspect is that the bounds are valid for all linearization points $y_{\mathbb{I}}^k$ that lie in a (small) neighborhood of a given $y_{\mathbb{I}}$. W.l.o.g. we choose the optimal triple $\bar{y}_{\mathbb{I}}$ from Assumption 6.1.1.

Lemma 6.4.1.

- *Let $y_{\mathbb{I}}^k \in Y^M$ (or Y_∞^M) such that $\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \tilde{\omega}$ for some $0 < \tilde{\omega} \in \mathbb{R}$. Then, there exist constants $0 < c_1(\tilde{\omega}), c_2(\tilde{\omega}) \in \mathbb{R}$ depending on $\bar{y}_{\mathbb{I}}$ and $\tilde{\omega}$, but not on $y_{\mathbb{I}}^k$, such that:*

$$|f'_{\mathbb{I},k}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}}| \leq c_1(\tilde{\omega})\|\tilde{q}_{\mathbb{I}}\|_{Q^M},$$
$$|f''_{\mathbb{I},k}(q_{\mathbb{I}})[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}] \leq c_2(\tilde{\omega})\|\tilde{q}_{\mathbb{I},1}\|_{Q^M}\|\tilde{q}_{\mathbb{I},2}\|_{Q^M},$$

  for all $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ and $\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2} \in Q^M$.

- *Let $y_{\mathbb{I}}^k \in Y^M$ (or Y_∞^M) such that $\|\mathbf{u}_{\mathbb{I}}^k - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^k - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \tilde{\omega}$ for some $0 < \tilde{\omega} \in \mathbb{R}$. Then, there exist constants $0 < c_3(\tilde{\omega}), c_4(\tilde{\omega}) \in \mathbb{R}$ depending on $\bar{y}_{\mathbb{I}}$ and $\tilde{\omega}$, but not on $y_{\mathbb{I}}^k$, such that:*

$$\left|\left(f'_{\mathbb{I},k}(q_{\mathbb{I},1}) - f'_{\mathbb{I},k}(q_{\mathbb{I},2})\right)\tilde{q}_{\mathbb{I}}\right| \leq c_3(\tilde{\omega})\|q_{\mathbb{I}}\|_{Q^M},$$
$$\left|\left(f''_{\mathbb{I},k}(q_{\mathbb{I},1}) - f''_{\mathbb{I},k}(q_{\mathbb{I},2})\right)[\tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2}]\right| \leq c_4(\tilde{\omega})\|q_{\mathbb{I},1}\|_{Q^M}\|q_{\mathbb{I},2}\|_{Q^M},$$

  for all $q_{\mathbb{I},1}, q_{\mathbb{I},1} \in Q_{ad,\mathbb{I}}$ and $\tilde{q}_{\mathbb{I}}, \tilde{q}_{\mathbb{I},1}, \tilde{q}_{\mathbb{I},2} \in Q^M$.

Proof.

- The first task is to estimate the adjoint state $\mathbf{z}_{\mathbb{I}}$, or equivalently $\mathbf{z}_{\mathbb{I},q}$, satisfying (6.3), which depends on $\mathbf{u}_{\mathbb{I}}$ satisfying (6.1), both for all $i = 1, ..., M$. Looking at the right-hand side of (6.1), and then subsequently of (6.3), using the triangle inequalities

$$\|\mathbf{u}_{\mathbb{I}}^k\|_{W^M} \leq \|\bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{u}}_{\mathbb{I}} - \mathbf{u}_{\mathbb{I}}^k\|_{W^M} \leq c + \tilde{\omega},$$
$$\|\mathbf{z}_{\mathbb{I}}^k\|_{W^M} \leq \|\bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} + \|\bar{\mathbf{z}}_{\mathbb{I}} - \mathbf{z}_{\mathbb{I}}^k\|_{W^M} \leq c + \tilde{\omega},$$

  in combination with the estimates from Lemma 3.1.3 and Lemma 3.1.6, it is clear that the right-hand sides can be bounded in $W^\times$ for every $i = 1, ..., M$. Note that this is the same approach also used in the proof of Lemma 6.2.1, cf. (6.28)-(6.31), and that the constant $0 < c \in \mathbb{R}$ depends on $\bar{y}_{\mathbb{I}}$, but not on $y_{\mathbb{I}}^k$. Applying Lemma 3.2.3, then leads to

$$\|\mathbf{u}_{\mathbb{I}}\|_{W^M} \leq c + c_3(\tilde{\omega}), \quad \|\mathbf{z}_{\mathbb{I}}\|_{W^M} \leq c + c_4(\tilde{\omega}), \tag{6.77}$$

for some $0 < c_3(\tilde{\omega}), c_4(\tilde{\omega}) \in \mathbb{R}$. From the definition (6.2) of $f_{\mathbb{I},k}$ it now follows

$$|f'_{\mathbb{I},k}(q_{\mathbb{I}})\tilde{q}_{\mathbb{I}}| \leq cM\big(\alpha + c + c_4(\tilde{\omega})\big)\|\tilde{q}_{\mathbb{I}}\|_{Q^M}.$$

The proof of the bound for $f''_{\mathbb{I},k}$ follows in the same way, using the equivalence (6.4) of $f''_{\mathbb{I},k}$ and the Lagrangian functional $\mathcal{L}''_{\mathbb{I}}(y^k_{\mathbb{I}})$, as well as the definition of the latter from Corollary 3.5.2.

- The proof follows analogously to the proof of the first part, but now using the estimations proved in Lemma 3.1.5 and Lemma 3.1.8 in combination with the triangle inequalities, as well as Lemma 3.2.3 and Corollary 3.4.5. The details are omitted.

□

Then we can show a first result, which already demonstrates some of the challenges and main techniques of this section:

Proposition 6.4.2. *Let $\bar{y}_{\mathbb{I}} = (\bar{\mathbf{u}}_{\mathbb{I}}, \bar{q}_{\mathbb{I}}, \bar{\mathbf{z}}_{\mathbb{I}})$ satisfy Assumption 6.1.1. There exist constants $0 < \omega_4 \in \mathbb{R}$ satisfying Assumption 6.3.6, and $0 < c_{k+1} \in \mathbb{R}$, $0 < \epsilon_{k+1} \in \mathbb{R}$ such that for all $y^k_{\mathbb{I}} \in Y^M_\infty$ with $\|y^k_{\mathbb{I}} - \bar{y}_{\mathbb{I}}\|_{Y^M_\infty} \leq \omega_4$, the unique solution $\hat{q}^{k+1}_{\mathbb{I}}$ of $(\widehat{\mathrm{QP}}_k)$ satisfies the quadratic growth condition*

$$f_{\mathbb{I},k}(q_{\mathbb{I}}) \geq f_{\mathbb{I},k}(\hat{q}^{k+1}_{\mathbb{I}}) + c_{k+1}\|q_{\mathbb{I}} - \hat{q}^{k+1}_{\mathbb{I}}\|^2_{Q^M}, \tag{6.78}$$

for every $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ with $\|q_{\mathbb{I}} - \hat{q}^{k+1}_{\mathbb{I}}\|_{Q^M} \leq \epsilon_{k+1}$. In particular $\hat{q}^{k+1}_{\mathbb{I}}$ is a strict L^2-local solution of (QP_k). Furthermore, the triple $\hat{y}^{k+1}_{\mathbb{I}}$ is the only stationary point of (QP_k) in $B^{Q^M}_{\epsilon_{k+1}}(\hat{q}^{k+1}_{\mathbb{I}})$.

Similarly as for the same result of the one time step model [85, Proposition 7.1] of the author and I. Neitzel, Proposition 6.4.2 is the analogue result to [96, Proposition 6.13]. It is important to recognize that there is one essential difference: Up until now it is not clear for Proposition 6.4.2 how the radius ϵ_{k+1} is determined, in particular, it can be dependent on $\hat{q}^{k+1}_{\mathbb{I}}$. We rectify this issue later at the end of this section. As in [85, Proposition 7.1], we do not adapt the proof of [96, Proposition 6.13], which itself is based on techniques from [40, Theorem 2.3 and Corollary 2.6] and [156, Theorem 3.22], using similar arguments as in [38]. Similarly as in Section 4.2, we directly verify the assumptions of [38, Theorem 2.5].

Proof. As already stated, the assumptions of [38, Theorem 2.5] are verified, similarly to the proof of Proposition 4.2.1 and Theorem 4.2.4. Again, setting $U_2 = U_\infty = Q^M$ and $\mathcal{K} = Q_{\mathrm{ad},\mathbb{I}}$. Note further that by (4.22), it holds $C(\bar{q}_{\mathbb{I}}) \subset C_\sigma(\bar{q}_{\mathbb{I}})$. We have also already seen that $\hat{q}^{k+1}_{\mathbb{I}}$ satisfies the first-order necessary conditions for both (QP_k) and $(\mathrm{QP}^{\omega,\infty}_k)$ by Lemma 6.3.13. In fact, the last argument of this proof can also be used for $Q^{\omega,2}_{\mathrm{ad},\mathbb{I}} \subset Q_{\mathrm{ad},\mathbb{I}}$, which means that $\hat{q}^{k+1}_{\mathbb{I}}$ satisfies also the first-order necessary conditions for $(\mathrm{QP}^{\omega,2}_k)$.

Furthermore, it is clear that the reduced functional $f_{\mathbb{I},k}$ is twice Fréchet differentiable, and by Lemma 6.4.1 its derivatives $f'_{\mathbb{I},k}$ and $f''_{\mathbb{I},k}$ are bounded and Lipschitz continuous.

Now finally, analogously to the proof of Proposition 4.2.1, we need to verify that the quadratic form $\tilde{q}_{\mathbb{I}} \mapsto f''_{\mathbb{I},k}(q_{\mathbb{I}})(\tilde{q}_{\mathbb{I}})^2$ is a Legendre form, cf. the fourth point of the properties given in Proposition 4.2.1. We again note that $\hat{\mathbf{u}}_{\mathbb{I}}^{k+1}$ and $\hat{\mathbf{z}}_{\mathbb{I}}^{k+1}$, being the solutions to (6.36a) and (6.36b), are in W^M, depending on $\bar{y}_{\mathbb{I}}$ and ω_4, but not on $y_{\mathbb{I}}^k$. This can be showed in the same way as (6.77) in the proof of Lemma 6.4.1. The weak lower semi-continuity *(1)* from the Legendre form definition of the properties given in Proposition 4.2.1 can then be showed as in Proposition 4.2.1. As for *(2)*, this also follows analogously to the proof of the aforementioned proposition: The only difference is that, due to $f''_{\mathbb{I},k}(\hat{q}_{\mathbb{I}})$ being identified via $\mathcal{L}''_{\mathbb{I}}(y_{\mathbb{I}}^k)$, we have to replace $y_{\mathbb{I}}$ with $y_{\mathbb{I}}^k$ in (4.14). This however does not have an effect on the course of action in the immediately following argument, and the remainder of the proof from (4.15) onwards can be conducted in the same way. Combining all arguments, [38, Theorem 2.5] is applicable. This concludes the proof. □

Our next task is to argue that the radius ϵ_{k+1} can indeed be chosen independently of $\hat{q}_{\mathbb{I}}^{k+1}$. Analogously to [96], some additional auxiliary subproblems need to be stated. Analogously to $(\widehat{\mathrm{QP}}_\delta)$, let

$$\min f_{\mathbb{I},\delta}(q_{\mathbb{I}}), \qquad \text{such that } q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}, \tag{$\mathrm{QP}_\delta^{\mathrm{red}}$}$$

where $f_{\mathbb{I},\delta}$ is defined as in $(\widehat{\mathrm{QP}}_\delta^{\mathrm{red}})$ on page 140. At the same time, let also

$$\min f_{\mathbb{I},\delta}(q_{\mathbb{I}}), \qquad \text{such that } q_{\mathbb{I}} \in Q_{\mathrm{ad},\mathbb{I}}^{\omega,2}. \tag{$\mathrm{QP}_\delta^{\omega,2,\mathrm{red}}$}$$

The key idea observed in [96] is that the problems $(\widehat{\mathrm{QP}}_\delta^{\mathrm{red}})$, $(\mathrm{QP}_\delta^{\mathrm{red}})$ and $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$ only differ in the admissible set, and that the linearization point in all subproblems is $\bar{y}_{\mathbb{I}}$, instead of the current iterate as in the problems $(\mathrm{QP}_k^{\mathrm{red}})$ and $(\mathrm{QP}_k^{\omega,2,\mathrm{red}})$. As a consequence, it is in fact possible to show that the unique solution $\hat{q}_{\mathbb{I},\delta}$ of $(\widehat{\mathrm{QP}}_\delta)$, or equivalently of $(\widehat{\mathrm{QP}}_\delta^{\mathrm{red}})$, is also a unique local solution of $(\mathrm{QP}_\delta^{\mathrm{red}})$ and the unique global solution of $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$, as long as the perturbations $\delta_{\mathbb{I}}$ are sufficiently small in Z_∞^M. Note that the smallness assumption of the perturbation $\delta_{\mathbb{I}}$ and the local neighborhood in which $\hat{q}_{\mathbb{I},\delta}$ is a global solution only depends on $\bar{y}_{\mathbb{I}}$, as is first observed in [96, Proposition 6.7].

Subsequently, we prove that the strong regularity property (in the space Y_∞^M) of $(\widehat{\mathrm{GE}})$ proved in Theorem 6.2.9 transfers to the generalized equation (GE), as well as to the generalized equation

$$0 \in F_{\mathbb{I}}(y_{\mathbb{I}}) + N_{\mathbb{I},2}(y_{\mathbb{I}}), \tag{$\mathrm{GE}^{\omega,2}$}$$

where analogously to (6.7), the set valued map $N_{\mathbb{I},2}\colon Y^M \rightrightarrows Z^M$ is defined via $N_2^i\colon Y \rightrightarrows Z, N_2^i(y^i) := \big(0, 0, N_{nc}^{\omega,2}(q^i)\big)^T$, and

$$N_{nc}^{\omega,2}(q^i) = \{dq^i \in Q \mid (dq^i, \tilde{q}^i - q^i)_Q \leq 0 \text{ for all } \tilde{q} \in (Q_{\mathrm{ad},\mathbb{I}}^{\omega,2})_{|i}\},$$

again using notation analogously to (6.8) and (6.37).

This in turn then means that within fixed neighborhoods of $\bar{y}_{\mathbb{I}}$, stationary points of $(\mathrm{QP}_k^{\mathrm{red}})$ and $(\mathrm{QP}_k^{\omega,2,\mathrm{red}})$ are in fact locally unique.

Similarly to Section 6.2.1, 6.2.2 and 6.3.1, it is again possible to show:

Corollary 6.4.3. *The (reduced) subproblem* $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$ *admits at least one solution for every perturbation vector* $\delta_{\mathbb{I}} \in Z_\infty^M$*. Further, first-order necessary conditions can be derived, which can equivalently be expressed by the generalized equation*

$$\delta_{\mathbb{I}} \in F_{\mathbb{I}}(\bar{y}_{\mathbb{I}}) + F_{\mathbb{I}}'(\bar{y}_{\mathbb{I}})(y_{\mathbb{I},\delta} - \bar{y}_{\mathbb{I}}) + N_{\mathbb{I},2}(y_{\mathbb{I},\delta}). \tag{NM$^{\omega,2}$}$$

Similarly to Proposition 6.4.2, the following result can then be proved. It is based on [96, Proposition 6.7], where the initial key idea of this approach is introduced. In [85, Proposition 7.2] of the author and I. Neitzel, the same result is proved for the one time step setting.

Proposition 6.4.4. *Let* $\bar{y}_{\mathbb{I}}$ *satisfy Assumption 6.1.1, and let* $0 < \sigma \in \mathbb{R}$ *and* $0 < L_\infty \in \mathbb{R}$ *be the constants from Assumption 6.1.1 and from Proposition 6.2.8, respectively. There exist constants* $\tilde{r} \in \left[0, \frac{\sigma}{2L_\infty}\right]$ *and* $0 < c \in 0$, $0 < \tilde{\epsilon} \in \mathbb{R}$ *such that the unique solution* $\hat{q}_{\mathbb{I},\delta}$ *of* $(\widehat{\mathrm{QP}}_\delta^{\mathrm{red}})$ *satisfies the quadratic growth condition*

$$f_{\mathbb{I},\delta}(q_{\mathbb{I}}) \geq f_{\mathbb{I},\delta}(\hat{q}_{\mathbb{I},\delta}) + c\|q_{\mathbb{I}} - \hat{q}_{\mathbb{I},\delta}\|_{Q^M}^2,$$

for every $q_{\mathbb{I}} \in Q_{ad,\mathbb{I}}$ *with* $\|q_{\mathbb{I}} - \hat{q}_{\mathbb{I},\delta}\|_{Q^M} \leq \tilde{\epsilon}$ *for all* $\|\delta_{\mathbb{I}}\|_{Z_\infty^M} \leq \tilde{r}$*. In particular,* $\hat{q}_{\mathbb{I},\delta}$ *is a strict* L^2*-local solution of* $(\mathrm{QP}_\delta^{\mathrm{red}})$*. Moreover,* $\hat{q}_{\mathbb{I},\delta} = (\hat{\mathbf{u}}_{\mathbb{I},\delta}, \hat{q}_{\mathbb{I},\delta}, \hat{\mathbf{z}}_{\mathbb{I},\delta})$ *is the only stationary point for* $(\mathrm{QP}_\delta^{\mathrm{red}})$ *in* $B_{\tilde{\epsilon}}^{Q^M}(\hat{q}_{\mathbb{I},\delta})$*.*

Proof. The proof is conducted in the same way as for Proposition 6.4.2, by utilizing again [38, Theorem 2.5]. The difference between $f_{\mathbb{I},k}$ and $f_{\mathbb{I},\delta}$ is the fact that the linearization point is $\bar{y}_{\mathbb{I}}$ instead of $y_{\mathbb{I}}^k$ and the added linear perturbations $\delta_{\mathbb{I}}$. The proof for the bounds, the Lipschitz conditions and the Legendre form properties for $f_{\mathbb{I},\delta}'$ and $f_{\mathbb{I},\delta}''$ can be established similarly to the respective properties of $f_{\mathbb{I}}$ in Section 3.4 or of $f_{\mathbb{I},k}$ in Lemma 6.4.1, and is omitted here. The choice of the involved spaces and cones is the same as in Proposition 6.4.2, note in particular again (4.22). It remains to show that $\hat{q}_{\mathbb{I},\delta}$ satisfies the first-order necessary conditions of $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$. As in [156], for perturbations $\delta_{\mathbb{I}}$ sufficiently small in the Z_∞^M norm, we can show this by adapting the proof of Lemma 6.3.13. The main idea is that the (σ-) strongly active set

$$\mathcal{I}_\delta(\sigma) := \left\{x \in \Gamma \;\middle|\; |B^*\bar{\mathbf{z}}^i + \alpha\bar{q}^i - \delta_2^i| > 0 \quad \text{for all } i = 1, ..., M\right\}$$

behaves sufficiently well for small perturbations $\delta_{\mathbb{I}} \in Z_\infty^M$, cf. also [96, Lemma 6.6] and [156, Corollary 5.3]. Note that the argument relies on the Z_∞^M regularity, especially on the L^∞-regularity of $\delta_{\mathbb{I},2}$. In particular, smallness of $\delta_{\mathbb{I}}$ w.r.t. Z^M, i.e. of $\delta_{\mathbb{I},2}$ w.r.t. L^2, is not sufficient. The reason is that we need to argue similarly to the proof of Lemma 6.3.5, cf. also Remark 6.3.10.

Overall, all assumptions of [38, Theorem 2.5] are satisfied, and the statement is concluded. ☐

At this point, let us again emphasize the importance of the smallness in Z_∞^M:

Remark 6.4.5. *Let us recall the course of action of Section 6.3. There, it was essential to use a localization w.r.t. L^∞ in the problem* $(\mathrm{QP}_k^{\omega,\infty})$*, as explained in Remark 6.3.10. For the same reason, we have seen in the last proof that perturbations have to be considered in the L^∞-sense. This is the reason that also in this section, we work with strong regularity in the $Y_\infty^M - Z_\infty^M$ setting. We see below in Theorem 6.4.8, that the problems* (GE) *and* $(\mathrm{GE}^{\omega,2})$ *are indeed strongly regular in this setting, but not in Y^M.*

Continuing with the same ideas as in [96, Corollary 6.8], it is now possible to show that $\hat{q}_{\mathbb{I},\delta}$ is in fact both the unique global solution of $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$ and a local solution of $(\mathrm{QP}_\delta^{\mathrm{red}})$.

Proposition 6.4.6. *Let $\bar{y}_\mathbb{I}$ satisfy Assumption 6.1.1. Then there exist a constant $0 < \omega_5 \in \mathbb{R}$ and a radius $0 < r \in \mathbb{R}$ such that the unique function triple $\hat{y}_{\mathbb{I},\delta} = (\hat{\mathbf{u}}_{\mathbb{I},\delta}, \hat{q}_{\mathbb{I},\delta}, \hat{\mathbf{z}}_{\mathbb{I},\delta})$ solving* $(\widehat{\mathrm{QP}}_\delta^{\mathrm{red}})$ *is also the unique solution of* $(\mathrm{QP}_\delta^{\omega,2,\mathrm{red}})$ *as well as the unique solution of* $(\mathrm{QP}_\delta^{\mathrm{red}})$ *which is contained in the set $Q_{ad,\mathbb{I}}^{\omega,2}$ for $\omega = \omega_5$, for all $\|\delta_\mathbb{I}\|_{Z_\infty^M} \le r$.*

Proof. The proof is the same as the proof of [85, Proposition 7.3] of the author and I. Neitzel, which in turn is the same as [96, Corollary 6.8]. For convenience of the reader, the main ideas are recapitulated. Set $\omega_5 = \frac{2\tilde{\epsilon}}{3}$ and choose $r < \min\left(\tilde{r}, \frac{\tilde{\epsilon}}{3c_e L_\infty}\right)$ with $\tilde{\epsilon}, \tilde{r}$ as in Proposition 6.4.4, $0 < c_e \in \mathbb{R}$ being a constant that stems from the $L^\infty \hookrightarrow L^2$-embedding, and L_∞ the Lipschitz-constant from Proposition 6.2.8. Due to Proposition 6.2.8, we can deduce

$$\|\hat{q}_{\mathbb{I},\delta} - \bar{q}_\mathbb{I}\|_{Q^M} \le c_e \|\hat{q}_{\mathbb{I},\delta} - \bar{q}_\mathbb{I}\|_{(L^\infty(\Gamma))^M} \le c_e L_\infty \|\delta_\mathbb{I}\|_{Z_\infty^M} \le \frac{\tilde{\epsilon}}{3}. \tag{6.79}$$

This then yields for all $q_\mathbb{I} \in B_{\omega_3}^{Q^M}(\bar{q}_\mathbb{I})$ that

$$\|q_\mathbb{I} - \hat{q}_{\mathbb{I},\delta}\|_{Q^M} \le \|q_\mathbb{I} - \bar{q}_\mathbb{I}\|_{Q^M} + \|\bar{q}_\mathbb{I} - \hat{q}_{\mathbb{I},\delta}\|_{Q^M} < \omega_5 + \frac{\tilde{\epsilon}}{3} \le \frac{2\tilde{\epsilon}}{3} + \frac{\tilde{\epsilon}}{3} = \tilde{\epsilon}. \tag{6.80}$$

Together, (6.79) and (6.80) mean that $\hat{q}_{\mathbb{I},\delta} \in \left(Q_{\mathrm{ad},\mathbb{I}} \cap \overline{B_{\omega_5}^{Q^M}(\bar{q}_\mathbb{I})}\right) \subset \left(Q_{\mathrm{ad},\mathbb{I}} \cap \overline{B_{\tilde{\epsilon}}^{Q^M}(\hat{q}_{\mathbb{I},\delta})}\right)$. In particular $\hat{q}_{\mathbb{I},\delta}$ satisfies a quadratic growth condition in the larger set by Proposition 6.4.4 and is contained in the smaller set. Further, again Proposition 6.4.4 ensures that there is no other stationary point inside the larger set. This concludes the proof. □

Remark 6.4.7. *Both Proposition 6.4.4 and Proposition 6.4.6 are based on the ideas and techniques of [96, Proposition 6.7 and Corollary 6.8]. Note that the authors of [96] distinguish between different neighborhoods for stationary points and solutions. As in the analogous results of the one time step setting from [85], the same radius can be, and in fact is, chosen in the two previous propositions without loss of generality.*

By combining Theorem 6.2.9 and Proposition 6.4.6, it is easy to conclude:

Theorem 6.4.8. *Let $\bar{y}_{\mathbb{I}}$ satisfy Assumption 6.1.1. The generalized equation* (GE) *is strongly regular at $\bar{y}_{\mathbb{I}}$ in Y_∞^M. Furthermore, there exists an $0 < \omega \in \mathbb{R}$ such that* (GE$^{\omega,2}$) *is strongly regular at $\bar{y}_{\mathbb{I}}$ in Y_∞^M.*

At this point, it is important to recall that while the auxiliary subproblem ($\widehat{\mathrm{QP}}_k$) is globally convex under Assumption 4.3.1 by Proposition 6.2.8, and therefore admits a unique solution, the quadratic subproblem (QP$_k$) can still have multiple solutions. This means that solving (QP$_k$) is not equivalent to solving the generalized equation (NM). Yet, for the localized version (NM$^{\omega,2}$) and (QP$_k^{\omega,2,\mathrm{red}}$), the equivalence is true. Analogously to the proof of Proposition 6.4.6 and as in [96, Proposition 6.14], we now obtain for the unperturbed subproblems:

Proposition 6.4.9. *Let $\bar{y}_{\mathbb{I}}$ satisfy Assumption 6.1.1. There exist a constant $0 < \omega_6 \in \mathbb{R}$ and a radius $0 < \epsilon \in R$ such that for all $y_{\mathbb{I}}^k \in Y_\infty^M$ with $\|y_{\mathbb{I}}^k - \bar{y}_{\mathbb{I}}\|_{Y_\infty^M} \leq \omega_6$, the unique function triple $\hat{y}_{\mathbb{I}}^{k+1} = (\hat{\mathbf{u}}_{\mathbb{I}}^{k+1}, \hat{q}_{\mathbb{I}}^{k+1}, \hat{\mathbf{z}}_{\mathbb{I}}^{k+1})$ solving ($\widehat{\mathrm{QP}}_k$) is also the unique solution of* (QP$_k^{\omega,2,\mathrm{red}}$)*, for $\omega = \epsilon$, as well as the unique solution of* (QP$_k^{\mathrm{red}}$) *which is contained in the set $Q_{ad,\mathbb{I}}^{\omega,2}$ for $\omega = \epsilon$.*

Proof. This works analogously to (6.80), using the results of Proposition 6.4.2 instead of Proposition 6.4.4. Note that the only important part is that due to the strong regularity property of (QP$_k$) from Theorem 6.4.8, we can in fact ensure the existence of a constant $0 < \omega_6 \in \mathbb{R}$ and a radius $0 < \epsilon \in \mathbb{R}$, now independent of $\hat{q}_{\mathbb{I}}^{k+1}$. Note that analogously to Remark 6.4.7, w.l.o.g. the same ω_6 is chosen for both problems. The remainder of the proof is omitted. □

Finally, it is possible to conclude the second main result of this chapter. The reasoning works analogously to [96, Theorem 6.15] and is also conducted for the setting $M = 1$ in [85, Theorem 7.5] of the author and I. Neitzel: Exploiting the strong regularity of (QP$_k$), as seen in Proposition 6.4.9, we have rectified the situation mentioned after Proposition 6.4.2, and the radius ϵ can now in fact be chosen uniformly. It immediately follows:

Theorem 6.4.10. *Let $\bar{y}_{\mathbb{I}}$ satisfy Assumption 6.1.1 and let initial data $\mathbf{u}_{\mathbb{I}}^0, \mathbf{z}_{\mathbb{I}}^0 \in W^M$ be given such that $\|\mathbf{u}_{\mathbb{I}}^0 - \bar{\mathbf{u}}_{\mathbb{I}}\|_{W^M}, \|\mathbf{z}_{\mathbb{I}}^0 - \bar{\mathbf{z}}_{\mathbb{I}}\|_{W^M} \leq \omega$ for an $0 < \omega \in \mathbb{R}$ sufficiently small. In particular, the choice $q_{\mathbb{I}}^0 \in Q_{ad,\mathbb{I}}$ with $\|q_{\mathbb{I}}^0 - \bar{q}_{\mathbb{I}}\|_{Q^M}$ sufficiently small, and $\mathbf{u}_{\mathbb{I}}^0 = G_{\mathbb{I}}(q_{\mathbb{I}})$ and $\mathbf{z}_{\mathbb{I}}^0$ such that for all $i = 1, ..., M$,*

$$A_{l*}(\mathbf{u}^{i,0})(\mathbf{z}^{i,0}, \psi^{i+1,0}) + R_{l*}(\varphi^{i,0}, \varphi^{i-1,0}, \varphi^{i+1,0}; \gamma)(\psi^{i,0}, \psi^{i+1,0}) = u^{i,0} - u_d^i,$$

is possible. Then the sequence generated by Algorithm 6.1.2 with quadratic subproblem (QP$_k^{\omega,2}$)*, or equivalently* (QP$_k^{\omega,2,\mathrm{red}}$)*, converges quadratically in Y_∞^M to $\bar{y}_{\mathbb{I}}$.*

Proof. The proof is now a simple consequence of Proposition 6.4.9 and Theorem 6.2.10. Concerning the choice of $q_{\mathbb{I}}^0$, and subsequently $\mathbf{u}_{\mathbb{I}}^0$ as well as $\mathbf{z}_{\mathbb{I}}^0$, we do not repeat the argumentation already given in the proof of Theorem 6.3.15. □

Let us close this section with three concluding remarks: First, comparing the results of Theorem 6.3.15 and Theorem 6.4.10, it is possible to replace the L^∞-localization by an L^2-localization, as in [96]. Secondly, note that again the size of the local neighborhood, in which the initial value is viable, depends on the physical parameters, cf. Remark 6.3.7. Finally, if we use the (rather weak, in comparison to e.g. [73, 74]) second-order sufficient conditions from Assumption 4.3.1, then some sort of localization, whether in L^∞ or in L^2, can unfortunately not be avoided. In particular, the local neighborhoods $Q^{\omega,\infty}_{\text{ad},\mathbb{I}}$ and $Q^{\omega,2}_{\text{ad},\mathbb{I}}$ chosen in this chapter involve the a-priori unknown function $\bar{q}_{\mathbb{I}}$ in its definition. In [152], it is stated that these sets can be replaced by certain convex, closed sets, and explained how the latter sets can be chosen in the L^∞-localization setting. The interested reader is referred to [152, page 311].

6.5 Numerical examples for the SQP method

We conclude this chapter with two numerical examples to substantiate the convergence results proved in the previous sections. These numerical results have not been published up until now. For the numerical examples, we use a simplified quasilinear phase-field optimal control problem, for which we can construct a so-called manufactured solution example. This means that the simplified problem in fact has an analytically known solution, which we state below. Furthermore, an explicit statement of the involved functions for both examples is given in Appendix B.

Let us directly introduce the simplified problem, which has the following differences in comparison to ($\text{NLP}^{\gamma,\eta}_{\mathbb{I}}$): Firstly, similarly as in Chapter 5, we restrict the model problem towards one time step, i.e. we set $M = 1$. Secondly, the displacement is simplified to only one direction, i.e. u lives on Ω, instead of Ω^2. In this context, instead of the operator $\mathbb{C}e(u)$, we now use the gradient ∇u, and the symmetric gradient $e(u)$ is likewise replaced by the gradient ∇u. The control $q = (q^u, q^\varphi)$ has both an entry corresponding to the displacement and to the phase-field, and an additional desired phase-field and desired controls are added in the objective functional. This means that we have a desired state (u_d, φ_d) and a desired control (q^u_d, q^φ_d) which we aim to steer towards in the optimization process. Finally, to avoid projection steps both in the implementation and for the manufactured solution, each of the entries of the control $q = (q^u, q^\varphi)$ lives on the domain Ω, instead of on the boundary Γ. For the latter reason, we also do not demand box-constraints as an admissible set for the controls.

Overall, we obtain the nonlinear phase-field optimal control problem

$$\left.\begin{aligned} \min_{q,\mathbf{u}} J_{ex}(q,\mathbf{u}) := \frac{1}{2}\|u - u_d\|^2 + \frac{1}{2}\|\varphi - \varphi_d\|^2 \\ + \frac{\alpha}{2}\|q^u - q^u_d\|^2 + \frac{\alpha}{2}\|q^\varphi - q^\varphi_d\|^2, \\ \text{subject to: } \mathbf{u} \text{ solves } (\text{EL}_{ex}) \text{ for data } q, \end{aligned}\right\} \qquad (\text{NLP}_{ex})$$

where (EL_{ex}) is given by:

$$\left.\begin{aligned}&\big(((1-\kappa)\varphi^2+\kappa)\nabla u,\nabla v^u\big)+\varepsilon\big(\nabla\varphi,\nabla v^\varphi\big)-\frac{1}{\varepsilon}\big(1-\varphi,v^\varphi\big)\\&+\eta\big(\varphi-\varphi^-,v^\varphi\big)+(1-\kappa)\big(\varphi\nabla u\colon\nabla u,v^\varphi\big)+\gamma\big([(\varphi-\varphi^-)^+]^3,v^\varphi\big)\\&=\Big(q^u,v^u\Big)+\Big(q^\varphi,v^\varphi\Big)\quad\forall(v^u,v^\varphi).\end{aligned}\right\}\quad(\mathrm{EL}_{ex})$$

The aim is to solve (NLP_{ex}) with the SQP method as described by Algorithm 6.1.2 in Section 6.1, thus we also introduce the associated quadratic subproblem: In the k-th step, let the current triple $((u^k,\varphi^k),(q^{k,u},q^{k,\varphi}),(z^k,\psi^k))$ be given. The quadratic subproblem then reads

$$\left.\begin{aligned}&\min_{q,\mathbf{u}} J_{ex,k}(q,\mathbf{u})\\&\qquad:=(u^k-u_d,u-u^k)+(\varphi^k-\varphi_d,\varphi-\varphi^k)\\&\qquad\quad+\alpha(q^{k,u}-q_d^u,q^u-q^{k,u})+\alpha(q^{k,\varphi}-q_d^\varphi,q^\varphi-q^{k,\varphi})\\&\qquad\quad+\frac{1}{2}\|u-u^k\|^2+\frac{1}{2}\|\varphi-\varphi^k\|^2\\&\qquad\quad+\frac{\alpha}{2}\|q^u-q^{k,u}\|^2+\frac{\alpha}{2}\|q^\varphi-q^{k,\varphi}\|^2\\&\qquad\quad-2(1-\kappa)\big(\varphi^k(\varphi-\varphi^k)\nabla(u-u^k),\nabla z^k\big)\\&\qquad\quad-(1-\kappa)\big((\varphi-\varphi^k)(\varphi-\varphi^k)\nabla u^k,\nabla z^k\big)\\&\qquad\quad-(1-\kappa)\big(\varphi^k\nabla(u-u^k)\colon\nabla(u-u^k),\psi^k\big)\\&\qquad\quad-2(1-\kappa)\big((\varphi-\varphi^k)\nabla(u-u^k)\colon\nabla u^k,\psi^k\big)\\&\qquad\quad-3\gamma((\varphi^k-\varphi^-)^+(\varphi-\varphi^k)(\varphi-\varphi^k),\psi^k),\\&\text{subject to: }\mathbf{u}\text{ solves }(\mathrm{EL}_{ex,k})\text{ for data }q,\end{aligned}\right\}\quad(\mathrm{QP}_{ex,k})$$

where ($\mathrm{EL}_{ex,k}$) is given by:

$$\left.\begin{aligned}&\big(((1-\kappa)(\varphi^k)^2+\kappa)\nabla u,\nabla v^u\big)+2(1-\kappa)\big(\varphi^k\nabla u\colon\nabla u^k,v^\varphi\big)\\&+2(1-\kappa)\big(\varphi^k\varphi\nabla u^k,\nabla v^u\big)+\varepsilon(\nabla\varphi,\nabla v^\varphi)+\frac{1}{\varepsilon}(\varphi,v^\varphi)+\eta(\varphi,v^\varphi)\\&+(1-\kappa)\big(\varphi\nabla u^k\colon\nabla u^k,v^\varphi\big)+3\gamma([(\varphi^k-\varphi^-)^+]^2\varphi,v^\varphi)\\&=(q^u,v^u)+(q^\varphi,v^\varphi)+\frac{1}{\varepsilon}(1,v^\varphi)+\eta(\varphi^-,v^\varphi)\\&\quad+2(1-\kappa)\big(\varphi^k\varphi^k\nabla u^k,\nabla v^u\big)+2(1-\kappa)\big(\varphi^k\nabla u^k\colon\nabla u^k,v^\varphi\big)\\&\quad-\gamma\big([(\varphi^k-\varphi^-)^+]^3,v^\varphi\big)+3\gamma([(\varphi^k-\varphi^-)^+]^2\varphi^k,v^\varphi)\quad\forall(v^u,v^\varphi).\end{aligned}\right\}\quad(\mathrm{EL}_{ex,k})$$

By using the update rule $(\mathbf{u}^{k+1},q^{k+1},\mathbf{z}^{k+1})=(\mathbf{u},q,\mathbf{z})$, we obtain the triple for the step $(k+1)$. In this context, $\mathbf{z}$ is the adjoint state associated to ($\mathrm{QP}_{ex,k}$), similarly to Lemma 6.1.6.

Note that the theoretical results from the previous sections hold true for (EL_{ex}), (NLP_{ex}), ($\mathrm{EL}_{ex,k}$) and ($\mathrm{QP}_{ex,k}$) by analogous arguments. In fact, due to the simplifications, i.p. the lack of control-box constraints, if anything, some of the arguments and proofs can be simplified. Let us therefore state the optimality conditions without further explanation: The to (NLP$_{ex}$) associated first-order necessary conditions can be given in implicit form via: If $(\bar{q^u}, \bar{q}^\varphi)$ is a local minimizer of (NLP$_{ex}$) with associated state $(\bar{u}, \bar{\varphi})$, there exists an adjoint state $(\bar{z}, \bar{\psi})$ such that

$$\left.\begin{aligned}&\big(((1-\kappa)\bar{\varphi}^2+\kappa)\nabla\bar{u},\nabla v^u\big)+\varepsilon\big(\nabla\bar{\varphi},\nabla v^\varphi\big)-\frac{1}{\varepsilon}\big(1-\bar{\varphi},v^\varphi\big)\\&+\eta\big(\bar{\varphi}-\varphi^-,v^\varphi\big)+(1-\kappa)\big(\bar{\varphi}\nabla\bar{u}\colon\nabla\bar{u},v^\varphi\big)+\gamma\big([(\bar{\varphi}-\varphi^-)^+]^3,v^\varphi\big)\\&=\Big(\bar{q}^u,v^u\Big)+\Big(\bar{q}^\varphi,v^\varphi\Big)\quad\forall(v^u,v^\varphi),\end{aligned}\right\}\quad(\mathrm{EL}_{ex})$$

$$\left.\begin{aligned}&\big(((1-\kappa)\bar{\varphi}^2+\kappa)\nabla\bar{z},\nabla v^u\big)+2(1-\kappa)\big(\bar{\varphi}\nabla\bar{u}\bar{\psi},\nabla v^u\big)\\&+\big(2(1-\kappa)\bar{\varphi}\nabla\bar{u}\colon\nabla\bar{z},v^\varphi\big)+\varepsilon(\nabla\bar{\psi},\nabla v^\varphi)+\frac{1}{\varepsilon}(\bar{\psi},v^\varphi)+\eta(\bar{\psi},v^\varphi)\\&+(1-\kappa)\Big(\bar{\psi}\nabla\bar{u}\colon\nabla\bar{u},v^\varphi\Big)+3\gamma\Big([(\bar{\varphi}-\varphi^-)^+]^2\bar{\psi},v^\varphi\Big)\\&=(\bar{u}-u_d,v^u)+(\bar{\varphi}-\varphi_d,v^\varphi)\quad\forall(v^u,v^\varphi),\end{aligned}\right\}\quad(\mathrm{AE}_{ex})$$

$$\big(\bar{z}+\alpha(\bar{q}^u-q_d^u),\tilde{q}^u\big)_Q+\big(\bar{\psi}+\alpha(\bar{q}^\varphi-q_d^\varphi),\tilde{q}^\varphi\big)_Q=0\quad\forall(\tilde{q}^u,\tilde{q}^\varphi).\quad\Big\}\quad(\mathrm{VE}_{ex})$$

The second-order sufficient conditions of (NLP$_{ex}$) can also be stated via: Let $(\bar{q^u}, \bar{q}^\varphi)$, with associated state $(\bar{u}, \bar{\varphi})$ and associated adjoint state $(\bar{z}, \bar{\psi})$ satisfy the first-order necessary conditions (EL$_{ex}$), (AE$_{ex}$) and (VE$_{ex}$), and assume that there exists a $c > 0$ such that

$$\left.\begin{aligned}&\|\tilde{u}\|^2+\|\tilde{\varphi}\|^2+\alpha\|\tilde{q}^u\|^2+\alpha\|\tilde{q}^\varphi\|^2\\&-4(1-\kappa)\big(\tilde{\varphi}\nabla\tilde{u}\bar{\varphi},\nabla\bar{z}\big)-2(1-\kappa)\big(\tilde{\varphi}^2\nabla\bar{u},\nabla\bar{z}\big)\\&-4(1-\kappa)\big(\tilde{\varphi}\nabla\tilde{u}\colon\nabla\bar{u},\bar{\psi}\big)-2(1-\kappa)\big(\bar{\varphi},\nabla\tilde{u}\colon\nabla\tilde{u},\bar{\psi}\big)\\&-6\gamma\big([(\bar{\psi}-\varphi^-)^+]\tilde{\varphi}^2,\bar{\psi}\big)\\&\geq c\|(\tilde{q}^u,\tilde{q}^\varphi)\|^2\quad\forall((\tilde{u},\tilde{\varphi}),(\tilde{q}^u,\tilde{q}^\varphi))\text{ that satisfy (6.81)},\end{aligned}\right\}\quad(\mathrm{SSC}_{ex})$$

where (6.81) is given by:

$$\left.\begin{aligned}&\big(((1-\kappa)\bar{\varphi}^2+\kappa)\nabla\tilde{u},\nabla v^u\big)+2(1-\kappa)\big(\bar{\varphi}\nabla\bar{u}\,\tilde{\varphi},\nabla v^u\big)\\&+\varepsilon\big(\nabla\tilde{\varphi}_1,\nabla v^\varphi\big)+\frac{1}{\varepsilon}\big(\tilde{\varphi},v^\varphi\big)+\eta\big(\tilde{\varphi},v^\varphi\big)+2(1-\kappa)\big(\bar{\varphi}\nabla\tilde{u}\colon\nabla\bar{u},v^\varphi\big)\\&+(1-\kappa)\Big(\tilde{\varphi}\nabla\bar{u}\colon\nabla\bar{u},v^\varphi\Big)+3\gamma([(\bar{\varphi}-\varphi^-)^+]^2\tilde{\varphi},v^\varphi)\\&=(\tilde{q}^u,v^u)+(\tilde{q}^\varphi,v^\varphi)\quad\forall(v^u,v^\varphi).\end{aligned}\right\}\quad(6.81)$$

A quadratic growth condition, and subsequently the local optimality of $\bar{q}$ of (NLP$_{ex}$) then holds analogously to the results of Chapter 4.

Now, manufactured solution examples can be constructed, using the approach explained in [153, Section 2.9]. We will not go into many details, and refer the reader to this publication for further information: In general, the starting point is fixing all data, e.g. φ^-, as well as a $\bar{\mathbf{u}}$ and a $\bar{\mathbf{z}}$, satisfying the required boundary conditions. For the given problem, these are zero Dirichlet boundary conditions. Then from (EL$_{ex}$), we can determine the optimal control $(\bar{q}^u, \bar{q}^\varphi)$, which in strong formulation is given by:

$$
\begin{aligned}
\bar{q}^u =& -\nabla\cdot\big(((1-\kappa)\bar{\varphi}^2+\kappa)\nabla\bar{u}\big)\\
=& -2(1-\kappa)\bar{\varphi}\nabla\varphi\cdot\nabla\bar{u} - \big((1-\kappa)-\kappa\big)\bar{\varphi}^2\triangle\bar{u}, \qquad (6.82)\\
\bar{q}^\varphi =& -\varepsilon\triangle\bar{\varphi} + \frac{1}{\varepsilon}\bar{\varphi} + \eta\bar{\varphi} - \frac{1}{\varepsilon} - \eta\varphi^- + (1-\kappa)\bar{\varphi}\nabla\bar{u}\colon\nabla\bar{u} + \gamma[(\bar{\varphi}-\varphi^-)^+]^3. \qquad (6.83)
\end{aligned}
$$

Similarly, from (AE$_{ex}$) we can determine the desired state (u_d, φ_d), which in strong formulation is given by:

$$
\begin{aligned}
u_d =& \bar{u} + 2(1-\kappa)\bar{\varphi}\nabla\bar{\varphi}\cdot\nabla\bar{z} + \big((1-\kappa)\bar{\varphi}^2+\kappa\big)\triangle\bar{z} + 2(1-\kappa)\nabla\bar{\varphi}\cdot\nabla\bar{u}\bar{\psi}\\
&+ 2(1-\kappa)\bar{\varphi}\triangle\bar{u}\bar{\psi} + 2(1-\kappa)\bar{\varphi}\nabla\bar{u}\cdot\nabla\bar{\psi}, \qquad (6.84)\\
\varphi_d :=& \bar{\varphi} - 2(1-\kappa)\bar{\varphi}\nabla\bar{z}\colon\nabla\bar{u} + \varepsilon\triangle\bar{\psi} - \frac{1}{\varepsilon}\bar{\psi} - \eta\bar{\psi}\\
&- (1-\kappa)\bar{\psi}\nabla\bar{u}\colon\nabla\bar{u} - 3\gamma[(\bar{\varphi}-\varphi^-)^+]^2\bar{\psi}. \qquad (6.85)
\end{aligned}
$$

Using (6.82)-(6.85), we can finally determine the desired controls (q_d^u, q_d^φ) from (VE$_{ex}$), which in strong formulation are given by:

$$
q_d^u := \bar{q}^u + \frac{1}{\alpha}\bar{z}, \qquad q_d^\varphi := \bar{q}^\varphi + \frac{1}{\alpha}\bar{\varphi}. \qquad (6.86)
$$

For convenience of the reader and better readability, we state all functions involved in the examples of Section 6.5.1 and 6.5.2 in explicit form in Appendix B.

Let us put on record that, if the SQP method is initialized with a suitable initial starting point, we also expect quadratic convergence in Y of the by Algorithm 6.1.2 with subproblem (QP$_{ex,k}$) generated sequence towards the optimal solution triple, which we call $\bar{y} := (\bar{\mathbf{u}}, \bar{q}, \bar{\mathbf{z}})$. Let us point out that in the SQP subproblems, we do not need the additional restrictions towards local neighborhoods in the quadratic sub-problems as in (QP$_k^{\omega,\infty}$) or (QP$_k^{\omega,2}$). As already mentioned in [70, 156], in the context of numerical examples restrictions towards local neighborhoods of the quadratic subproblems are only required for the analytical proofs of the SQP convergence results in function spaces, even for problems involving control box constraints, cf. also [95, 96].

Our examples are implemented in C++ using the DOpElib optimization library [72, 149], that is based on the deal.II finite element library [11, 12]. For the solution of the SQP subproblems, the "optproblem" class of DOpElib is used. This class provides a solver for optimal control problems constrained by partial differential equations, by utilizing the Newton algorithm. Let us point out that our focus is put on illustrating the order of convergence of our examples, and not on computational efficiency. In particular, this means that we do not optimize the interdependence of stopping criteria of (different solvers involved to solve) the subproblems. Further, choosing more efficient solvers (e.g. implementations involving sophisticated parallelization) can most certainly enhance the runtime of the implemented examples. For the domain, we choose $\Omega = [0,1]^2$, i.e. the unit square, with an initial mesh with four equidistant quadrilateral cells, i.e. an equidistant mesh with sidelength $h_0 = 0.5$. We uniformly refine this initial mesh five, six and seven times to obtain equidistant meshes with meshsizes $h_5 = 0.015625$, $h_6 = 0.0078125$ and $h_7 = 0.00390625$. Let us clarify that with meshsize we mean the sidelength of the quadrilaterals, i.e. $h_i = (\frac{1}{2})^{i+1}$ for the refinement levels $i = 5, 6, 7$, on which we run the SQP method. The control and state variables are discretized by piecewise linear finite elements on the respective meshes. Note that in contrast to h_i, we denote the SQP steps by k, where we let the SQP method run up to 6 steps, and functions indexed by $k = 0$ are from the initial step. Further implementation details including the desired states and controls, the initial values and all involved parameters, are given in the corresponding examples in Section 6.5.1 and 6.5.2 below. Let us point out, that for both our examples we choose a fixed penalization parameter $\gamma > 0$, and the behavior of the SQP method for the simplified problem w.r.t. the penalization limit is not subject of the examples presented. To conclude this overview of the implementation, note that the abstract exponents p and q from Assumption 2.3.1 have not been specified for a practical context in our theoretical results. We instead use both the L^2- and L^∞-norms for $q, \mathbf{u}, \mathbf{z}$, as well as the L^2-norm for q in combination with the $H^1(\Omega;\mathbb{R}^2) \times H^1(\Omega)$-norms for $\mathbf{u}, \mathbf{z}$ as the norms of the increments and of the error towards the known exact solutions.

Let us quickly outline the remainder of this section: For both examples in Section 6.5.1 and 6.5.2, we use the simplified optimal control problem (NLP_{ex}). For both examples, we state a manufactured solution example, including the details on the specific example setting involving all parameters and initial conditions, before presenting the convergence results of the SQP method as described above. In Section 6.5.1 we chose the given phase-field function φ^- such that the penalization term $\gamma[(\bar{\varphi} - \varphi^-)^+]^3$ is zero in the optimal condition, as well as very simple initial data. We also elaborate on the possible choice of initial data for phase-field optimal control problems. In Section 6.5.2, the data is chosen such that the penalization term in the model problem is positive, and the initial data is chosen more closely towards the manufactured solution. The numerical results indicate quadratic convergence for both examples.

6.5.1 Example 1

Let us construct the first manufactured solution example for (NLP_{ex}) as explained above. We choose the modelling parameters $\varepsilon, \kappa, \gamma, \eta$ and α as presented in Table 6.1, again pointing out that all parameters, including γ, remain fixed.

Parameter	Explanation	Value
ε	crack regularization	1.0e-3
κ	crack degradation	1.0e-5
γ	penalization	100.0
η	viscous approximation	10.0
α	Tikhonov parameter	1.0

Table 6.1: Parameters for Example 1.

Further, we also set

$$\mathbf{u}^- = (u^-, \varphi^-) = (0.0, 1.0),$$

and choose the desired functions u_d, φ_d, q_d^u and q_d^φ as defined in (B.3)-(B.6) in Appendix B. These functions are plotted in Figure 6.1, for the parameters stated in Table 6.1. For the chosen desired functions, we obtain the state $\bar{\mathbf{u}}$ with associated optimal adjoint $\bar{\mathbf{z}}$,

$$\begin{aligned}\bar{\mathbf{u}} &= (\bar{u}, \bar{\varphi}) := (\sin(\pi x)\sin(\pi y), (x-0.5)^2 + (y-0.5)^2 + 0.5),\\ \bar{\mathbf{z}} &= (\bar{z}, \bar{\psi}) := (4\sin(2\pi x)\sin(\pi y), (x-0.5)^2 + y^2),\end{aligned}$$

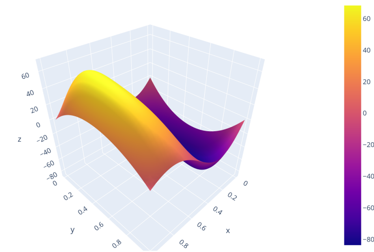
and then obtain from the first-order necessary conditions (EL$_{ex}$), (AE$_{ex}$) and (VE$_{ex}$), the control $\bar{q} = (\bar{q}^u, \bar{q}^\varphi)$, which is given in (B.1)-(B.2). The triple $((\bar{u}, \bar{\varphi}), (\bar{q}^u, \bar{q}^\varphi), (\bar{z}, \bar{\psi}))$ is plotted in Figure 6.2, again for the parameters stated in Table 6.1. Note that for this first example, we cannot easily verify whether the triple $((\bar{u}, \bar{\varphi}), (\bar{q}^u, \bar{q}^\varphi), (\bar{z}, \bar{\psi}))$ is indeed a (local) minimizer of (NLP$_{ex}$): In comparison to the second example from Section 6.5.2, the associated second-order conditions (SSC$_{ex}$) given on page 167 do not immediately ensure this property of the triple.

As an initial triple, with which we start in the first step of the SQP method, we finally choose

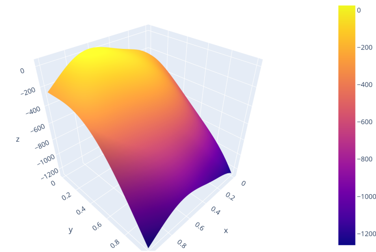
$$\mathbf{u}^0 = (0.0, 1.0), \quad q^0 = (0.0, 0.0), \quad \mathbf{z}^0 = (0.0, 0.0). \tag{6.87}$$

By construction we have $\bar{\varphi} \in [0,1]$ and $\varphi^- = 1$, which means that the penalization term $\gamma([(\bar{\varphi} - \varphi^-)^+]^3)$ is zero in the triple $(\bar{\mathbf{u}}, \bar{q}, \bar{\mathbf{z}})$. The same also holds true (at least) for the first SQP step, since $\varphi^k = 1$ for $k = 1$, and therefore $3\gamma([(\varphi^k - \varphi^-)^+]^2 \cdot) = 0$.

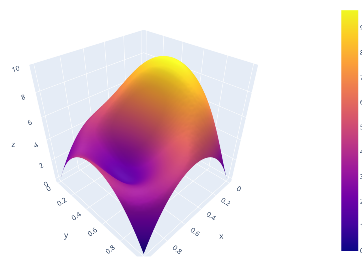
Note that we do not choose an initial triple were both the displacement variable u^0 and phase-field variable φ^0 are zero. In the fracture propagation setting this would suggest, that the entire domain already consists of a completely broken material, indicated through the phase-field variable $\varphi = 0$. In particular, further fracture propagation would not be possible, since adding a (traction) force as control then cannot put any strain on the already totally destroyed material. In this context, the interested reader is referred to the recent work [102]: For a (time and spatial continuous) phase-field fracture optimal control problem,



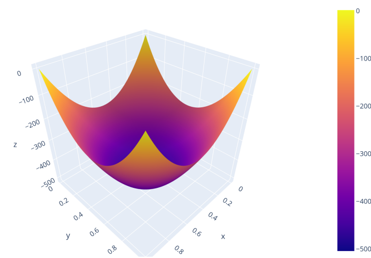
(a) u_d



(b) φ_d



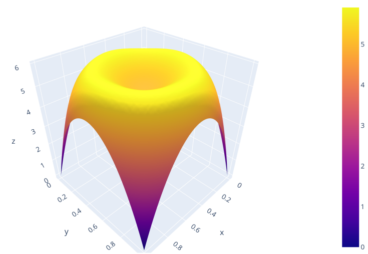
(c) q_d^u



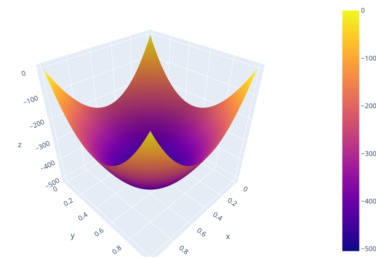
(d) q_d^φ

Figure 6.1: Example 1: Desired functions $\mathbf{u}_d, q_d$.

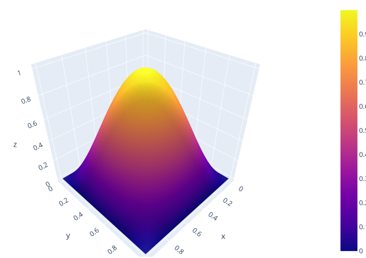
[102, Proposition 5.2] provides a sufficient condition for the characterization of regular points [102, Definion 2.1] (in the sense of Zowe and Kurcyusz [163]). These then imply KKT optimality conditions [102, Theorem 2.2]. Similarly to our case, [102, Remark 5.2] then summarizes that the in [102, Proposition 5.2] given condition cannot hold, if both $e(u)$ and φ are identically zero, and [102, page 19] states: "[...] we obtain trivial solutions, which are not of interest from the mechanical viewpoint". In particular, if one derives the to ($\mathrm{QP}_{ex,k}$) associated optimality conditions and starts with a zero initial triple, the associated optimality system would not only be uncoupled in the displacement and phase-field equations, but stay uncoupled throughout the SQP method. Note that the physical interpretation can also be seen in the numerical solution of optimal control fracture problems, where numerical instabilities occur (much) earlier than total failure, i.e. before the complete rupture throughout the entire domain is achieved and the phase-field variable φ is zero on a connected line segment or area along the traction force, cf. [103, 105].



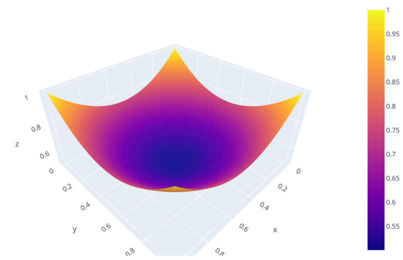
(a) $\bar{q}^u$



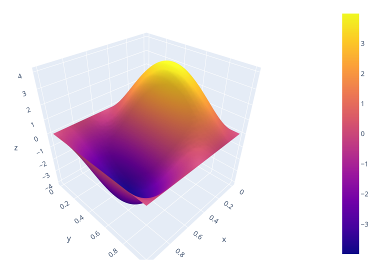
(b) $\bar{q}^\varphi$



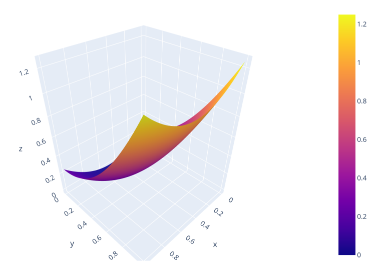
(c) $\bar{u}$



(d) $\bar{\varphi}$



(e) $\bar{z}$



(f) $\bar{\psi}$

Figure 6.2: Example 1: The triple $(\bar{\mathbf{u}}, \bar{q}, \bar{\mathbf{z}})$.

The norm of the increments and the absolute errors[2] against the interpolated exact solution are given in Table 6.2 and Table 6.3. Here, the interpolated exact solutions, denoted by $\bar{q}_{int}, \bar{\mathbf{u}}_{int}, \bar{\mathbf{z}}_{int}$, were calculated using the deal.ii

[2]for the L^2-norms of the control, the state and the adjoint, the L^2-norm of the control in combination with the H^1-norms of the state and the adjoint, and finally the L^∞-norms of the control, the state and the adjoint

function ”interpolate” from the class ”VectorTools” to (linearly) interpolate the respective exact functions at the support points to the finite element space of the current refinement level. Let us further recall that by $\| \cdot \|_2$ and $\| \cdot \|_\infty$ we denote the norm of the standard Lebesgue spaces $L^2(\Omega)$ and $L^\infty(\Omega)$, and by $\| \cdot \|_{1,2}$ we denote the norm of the standard Hilbert space $H^1(\Omega)$, cf. also Appendix A. For an illustration of our theoretical results from Section 6.3 and Section 6.4, we look at both the norm of the increments and the errors of the solutions towards the interpolated exact solutions for the three discretizations with meshsize h_5, h_6 and h_7 for $k = 1, ..., 6$ SQP steps. In Figure 6.3, we semi-log plot the corresponding graphs for the mesh with meshsize h_6. We omit plotting the other convergence graphs, since they look similar for the meshsizes h_5 and h_7. As a reference function for quadratic order of convergence in the semi-log graph of the absolute errors, we plot the function $f(k) = 2^{-2^k}, k = 1, ..., 6$ as a solid black line. The results indeed indicate a quadratic convergence, as can be deducted from the left three graphs of Figure 6.3. The rate of convergence involved in the numerical example is unknown, choosing a rate of convergence in the order of one, we can also approximately calculate orders of convergence from the erros presented in Table 6.3, which likewise indicates that the order of convergence is quadratic. The same convergence in function space is then indicated by the uniform behavior of the increments and errors w.r.t. the different refinements for the discretizations with meshsize h_5, h_6 and h_7. Note that until the convergence towards the (interpolated) exact solutions stops due to discretization (and possibly therewith connected interpolation) errors, the errors towards the exact solution also behaves uniformly w.r.t to the SQP steps.

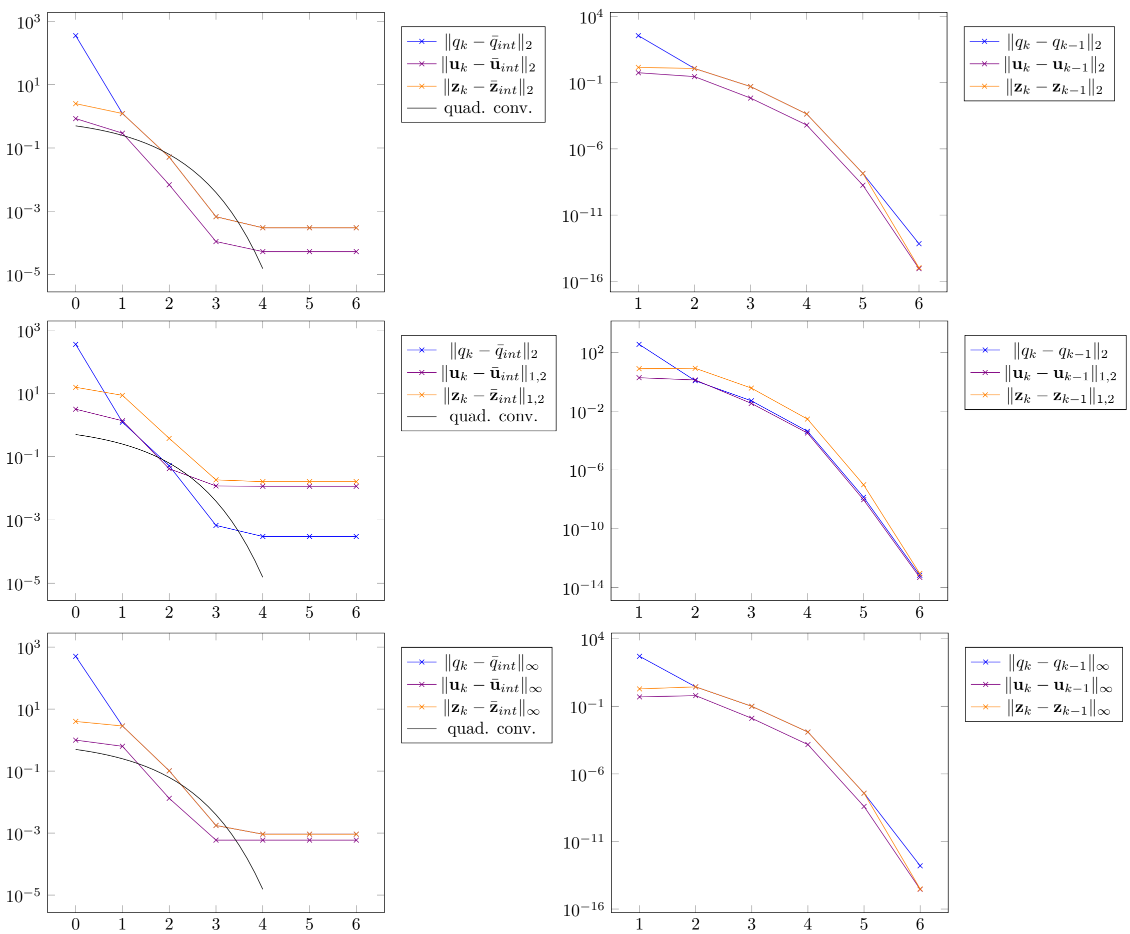


Figure 6.3: Absolute error against the interpolated exact solutions (left) and norm of the increments (right) for Example 1, on the mesh $h_6 = 0.0078125$.

	$\|q_{k-1} - q_k\|_2$			$\|\mathbf{u}_{k-1} - \mathbf{u}_k\|_2$			$\|\mathbf{z}_{k-1} - \mathbf{z}_k\|_2$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
1	3.55067e+02	3.55128e+02	3.55143e+02	5.60378e-01	5.60492e-01	5.60521e-01	1.42410e+00	1.42495e+00	1.42516e+00
2	1.17707e+00	1.17843e+00	1.17877e+00	2.87193e-01	2.87324e-01	2.87357e-01	1.17707e+00	1.17843e+00	1.17877e+00
3	5.06629e-02	5.07723e-02	5.07997e-02	6.80275e-03	6.81448e-03	6.81741e-03	5.06631e-02	5.07725e-02	5.07999e-02
4	4.27631e-04	4.29602e-04	4.30097e-04	6.23369e-05	6.26196e-05	6.26905e-05	4.27651e-04	4.29622e-04	4.30117e-04
5	1.37656e-08	1.39097e-08	1.39461e-08	1.77946e-09	1.79786e-09	1.80250e-09	1.38737e-08	1.40184e-08	1.40548e-08
6	6.87482e-14	6.88287e-14	6.90186e-14	8.98571e-16	8.99856e-16	8.86260e-16	1.05696e-15	1.04687e-15	1.15040e-15

	$\|\mathbf{u}_{k-1} - \mathbf{u}_k\|_{1,2}$			$\|\mathbf{z}_{k-1} - \mathbf{z}_k\|_{1,2}$		
k	h_5	h_6	h_7	h_5	h_6	h_7
1	1.89109e+00	1.89065e+00	1.88982e+00	7.76461e+00	7.76933e+00	7.76983e+00
2	1.33010e+00	1.33067e+00	1.33082e+00	8.33197e+00	8.34004e+00	8.34214e+00
3	3.38706e-02	3.39594e-02	3.39858e-02	3.72778e-01	3.73755e-01	3.74038e-01
4	3.23914e-04	3.25390e-04	3.25765e-04	2.89361e-03	2.90705e-03	2.91052e-03
5	9.21699e-09	9.31903e-09	9.34569e-09	9.63145e-08	9.76004e-08	9.79589e-08
6	2.90883e-14	4.92437e-14	7.71223e-14	4.59550e-14	9.03548e-14	1.87910e-13

	$\|q_{k-1} - q_k\|_\infty$			$\|\mathbf{u}_{k-1} - \mathbf{u}_k\|_\infty$			$\|\mathbf{z}_{k-1} - \mathbf{z}_k\|_\infty$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
1	5.04896e+02	5.04977e+02	5.04997e+02	4.99892e-01	4.99973e-01	4.99993e-01	1.95431e+00	1.95569e+00	1.95616e+00
2	2.76492e+00	2.76849e+00	2.76920e+00	6.21274e-01	6.21561e-01	6.21644e-01	2.76492e+00	2.76849e+00	2.76919e+00
3	1.00131e-01	1.00402e-01	1.00468e-01	1.30092e-02	1.30378e-02	1.30445e-02	1.00132e-01	1.00402e-01	1.00469e-01
4	1.25362e-03	1.25999e-03	1.26155e-03	1.47639e-04	1.48293e-04	1.48463e-04	1.25361e-03	1.25998e-03	1.26153e-03
5	3.68845e-08	3.73121e-08	3.74197e-08	3.87225e-09	3.91229e-09	3.92243e-09	3.68456e-08	3.72630e-08	3.73772e-08
6	1.62915e-13	1.58518e-13	1.84401e-13	2.84957e-15	2.88658e-15	2.99264e-15	2.66454e-15	3.09871e-15	3.45887e-15

Table 6.2: Norm of the increments during SQP method applied to Example 1.

	$\|\bar{q}_{int} - q_k\|_2$			$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_2$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_2$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
0	3.55177e+02	3.55237e+02	3.55252e+02	8.49325e-01	8.49533e-01	8.49586e-01	2.51580e+00	2.51726e+00	2.51762e+00
1	1.22654e+00	1.22721e+00	1.22738e+00	2.93696e-01	2.93802e-01	2.93829e-01	1.22654e+00	1.22721e+00	1.22738e+00
2	5.20936e-02	5.13904e-02	5.12150e-02	6.92056e-03	6.88591e-03	6.87747e-03	5.20936e-02	5.13904e-02	5.12150e-02
3	1.48284e-03	6.72732e-04	5.05607e-04	1.52731e-04	1.10397e-04	1.05753e-04	1.48267e-03	6.72530e-04	5.05415e-04
4	1.15018e-03	3.00236e-04	1.00905e-04	9.97690e-05	5.31295e-05	4.91604e-05	1.15004e-03	3.00051e-04	1.00700e-04
5	1.15017e-03	3.00228e-04	1.00898e-04	9.97677e-05	5.31285e-05	4.91610e-05	1.15003e-03	3.00044e-04	1.00693e-04
6	1.15017e-03	3.00228e-04	1.00898e-04	9.97677e-05	5.31285e-05	4.91610e-05	1.15003e-03	3.00044e-04	1.00693e-04

	$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_{1,2}$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_{1,2}$		
k	h_5	h_6	h_7	h_5	h_6	h_7
0	3.16439e+00	3.16501e+00	3.16516e+00	1.55727e+01	1.55798e+01	1.55816e+01
1	1.35838e+00	1.36174e+00	1.37103e+00	8.66068e+00	8.66417e+00	8.66617e+00
2	3.62294e-02	4.15915e-02	5.34154e-02	3.82882e-01	3.79281e-01	3.81866e-01
3	5.20464e-03	1.18587e-02	2.44144e-02	1.59877e-02	1.84812e-02	3.28028e-02
4	4.97277e-03	1.16260e-02	2.42390e-02	1.39337e-02	1.62053e-02	3.08667e-02
5	4.97277e-03	1.16260e-02	2.42390e-02	1.39336e-02	1.62052e-02	3.08667e-02
6	4.97277e-03	1.16260e-02	2.42390e-02	1.39336e-02	1.62052e-02	3.08667e-02

	$\|\bar{q}_{int} - q_k\|_\infty$			$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_\infty$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_\infty$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
0	5.04895e+02	5.04977e+02	5.04997e+02	9.99491e-01	9.99873e-01	9.99968e-01	3.99491e+00	3.99873e+00	3.99968e+00
1	2.85550e+00	2.85790e+00	2.85831e+00	6.31929e-01	6.32273e-01	6.32355e-01	2.85549e+00	2.85790e+00	2.85831e+00
2	1.03468e-01	1.02146e-01	1.01818e-01	1.32922e-02	1.32135e-02	1.31936e-02	1.03468e-01	1.02146e-01	1.01818e-01
3	3.38061e-03	6.72732e-04	1.51144e-03	3.07123e-04	5.92972e-04	1.00143e-03	3.38031e-03	1.75874e-03	1.51144e-03
4	2.13865e-03	3.00236e-04	1.51144e-03	3.07123e-04	5.92972e-04	1.00143e-03	2.13829e-03	9.21897e-04	1.51144e-03
5	2.13861e-03	3.00228e-04	1.51144e-03	3.07123e-04	5.92972e-04	1.00143e-03	2.13826e-03	9.21897e-04	1.51144e-03
6	2.13861e-03	3.00228e-04	1.51144e-03	3.07123e-04	5.92972e-04	1.00143e-03	2.13826e-03	9.21897e-04	1.51144e-03

Table 6.3: Errors of the iterates (against the interpolated exact solutions on the current grid) during the SQP method applied to Example 1.

6.5.2 Example 2

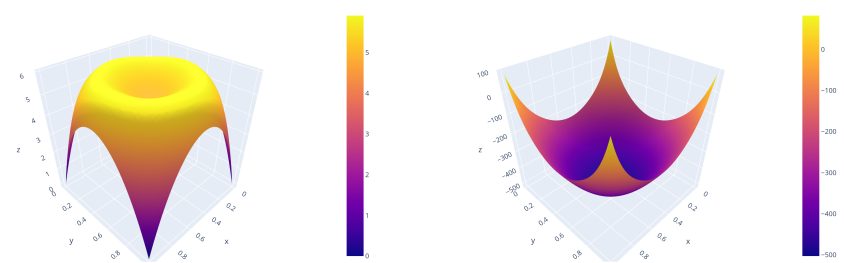
The second example is again constructed in Appendix B. For the parameters, we use the same as in Example 1, see Table 6.1, except for the penalization parameter, which shall be $\gamma = 10000.0$. We again want to point out that γ is a fixed parameter. Let further

$$\mathbf{u}^- = (u^-, \varphi^-) := (0.0, 0.8),$$

as well as the desired functions u_d, φ_d, q_d^u and q_d^φ be given as defined in (B.9)-(B.12). Subsequently, we obtain an optimal triple consisting of the functions $\bar{q}^u$ and $\bar{q}^\varphi$, as given in (B.7)-(B.8), together with

$$\begin{aligned}\bar{\mathbf{u}} &= (\bar{u}, \bar{\varphi}) := (\sin(\pi x)\sin(\pi y), (x-0.5)^2 + (y-0.5)^2 + 0.5),\\ \bar{\mathbf{z}} &= (\bar{z}, \bar{\psi}) := (0.0, 0.0).\end{aligned}$$

While the plot of $\bar{\mathbf{z}}$ is ommited, $\bar{\mathbf{u}}$ is the same as in Example 1, see Figure 6.2. The plot of $(\bar{q}^u, \bar{q}^\varphi)$ is given in Figure 6.4. Let us point out, that in contrast to Example 1, it is clear that the triple $(\bar{\mathbf{u}}, (\bar{q}^u, \bar{q}^\varphi), \bar{\mathbf{z}})$ for Example 2 is indeed a minimizer of (NLP$_{ex}$). This can easily be seen from (SSC$_{ex}$), stated on page 185, since all terms except for the squared norm terms vanish due to $\bar{\mathbf{z}} \equiv 0$. Note also that by construction, it holds $(u_d, \varphi_d) = (\bar{u}, \bar{\varphi})$ as well as $(q_d^u, q_d^\varphi) = (\bar{q}^u, \bar{q}^\varphi)$, and that the penalization term $\gamma([\bar{\varphi} - \varphi^-)^+]^3$ is now nonzero and positive for some points of the domain in the optimal state. As a consequence, we can see that the function $\bar{q}^\varphi$ has a shifted range, if we compare Figure 6.2 and Figure 6.4.



(a) $\bar{q}^u$ (b) $\bar{q}^\varphi$

Figure 6.4: Example 2: Optimal control $\bar{q}$.

As an initial triple for the SQP method, we choose

$$\mathbf{u}^0 = \frac{\bar{\mathbf{u}}}{2}, \quad q^0 = \frac{\bar{q}}{2}, \quad \mathbf{z}^0 = \frac{\bar{\mathbf{z}}}{2},$$

where we point out again that it is not reasonable to choose $\mathbf{u}^0 \equiv 0$ for the same reasons explained in the paragraph below (6.87). Note that due to the construction of the test example and the way we discretize the domain and interpolate the exact adjoint state, the norm in the adjoint increments for the initial step $k = 0$ in Table 6.5 is zero. The results after applying the SQP method are given in Table 6.4 and Table 6.5, cf. also Figure 6.5. We do not repeat the remarks given in the last paragraph of Section 6.5.1, which hold analogously. In particular, the results behave in a similar way as the ones for Example 1, indicating again quadratic convergence.

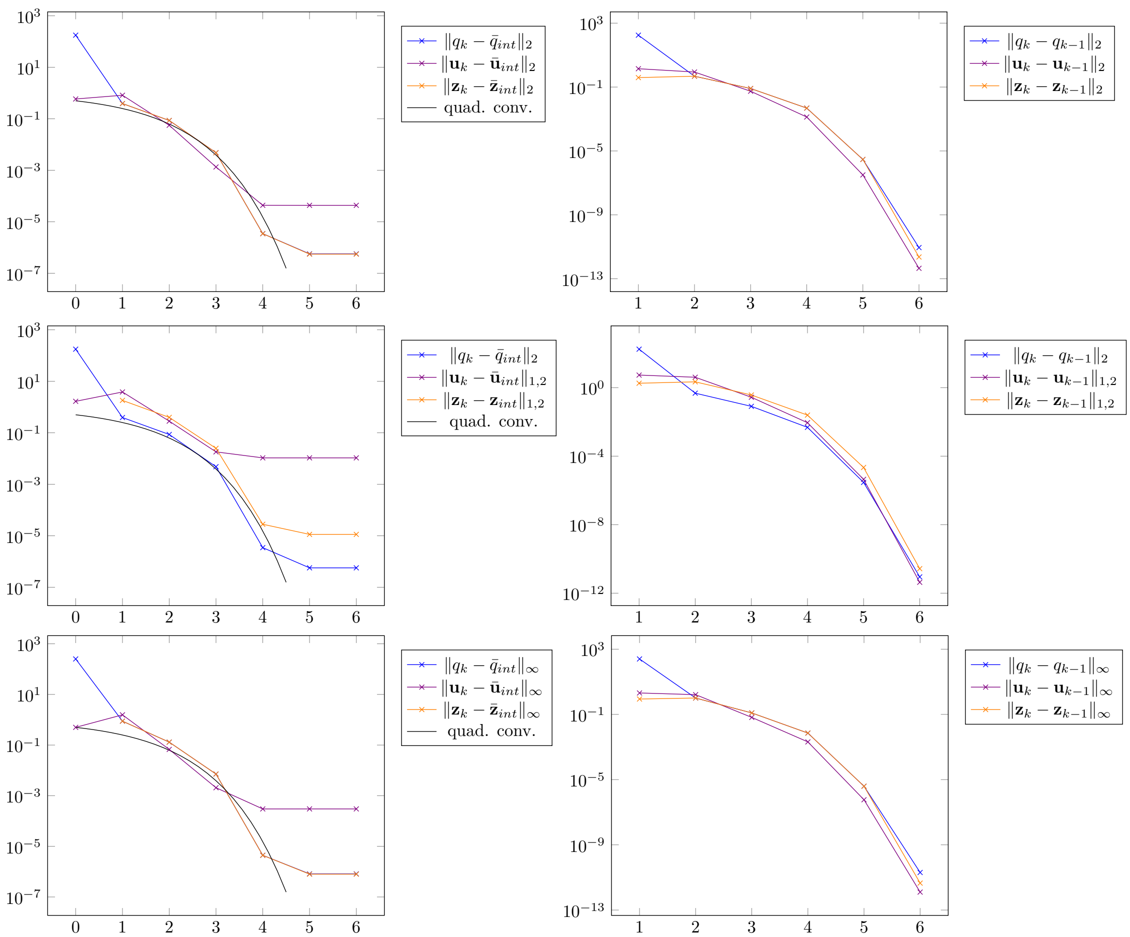


Figure 6.5: Absolute error against the interpolated exact solutions (left) and norm of the increments (right) for Example 2, on the mesh $h_6 = 0.0078125$.

	$\lVert q_{k-1} - q_k \rVert_2$			$\lVert \mathbf{u}_{k-1} - \mathbf{u}_k \rVert_2$			$\lVert \mathbf{z}_{k-1} - \mathbf{z}_k \rVert_2$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
1	1.76270e+02	1.76302e+02	1.76309e+02	1.40329e+00	1.40355e+00	1.40361e+00	3.90881e-01	3.91124e-01	3.91184e-01
2	4.76014e-01	4.76350e-01	4.76433e-01	8.73155e-01	8.73396e-01	8.73457e-01	4.76014e-01	4.76350e-01	4.76433e-01
3	8.10561e-02	8.11467e-02	8.11693e-02	5.46357e-02	5.46827e-02	5.46944e-02	8.10563e-02	8.11468e-02	8.11695e-02
4	4.80175e-03	4.81189e-03	4.81443e-03	1.32902e-03	1.33229e-03	1.33311e-03	4.80167e-03	4.81181e-03	4.81435e-03
5	2.91873e-06	2.93970e-06	2.94499e-06	3.11760e-07	3.15737e-07	3.16756e-07	2.91836e-06	2.93934e-06	2.94462e-06
6	8.85376e-12	8.94922e-12	8.97245e-12	4.43256e-13	4.50298e-13	4.52087e-13	2.23763e-12	2.30322e-12	2.32041e-12

	$\lVert \mathbf{u}_{k-1} - \mathbf{u}_k \rVert_{1,2}$			$\lVert \mathbf{z}_{k-1} - \mathbf{z}_k \rVert_{1,2}$		
k	h_5	h_6	h_7	h_5	h_6	h_7
1	5.42858e+00	5.42854e+00	5.42775e+00	1.81180e+00	1.81279e+00	1.81304e+00
2	4.05498e+00	4.05542e+00	4.05509e+00	2.18880e+00	2.19019e+00	2.19054e+00
3	2.74790e-01	2.75124e-01	2.75147e-01	3.72672e-01	3.73113e-01	3.73231e-01
4	8.94659e-03	8.98455e-03	8.97762e-03	2.48533e-02	2.49311e-02	2.49351e-02
5	4.30658e-06	4.43084e-06	4.44886e-06	2.16196e-05	2.18988e-05	2.19808e-05
6	3.90805e-12	4.31591e-12	4.31631e-12	2.55158e-11	2.70245e-11	2.75336e-11

	$\lVert q_{k-1} - q_k \rVert_\infty$			$\lVert \mathbf{u}_{k-1} - \mathbf{u}_k \rVert_\infty$			$\lVert \mathbf{z}_{k-1} - \mathbf{z}_k \rVert_\infty$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
1	2.51447e+02	2.51488e+02	2.51499e+02	2.06351e+00	2.06388e+00	2.06397e+00	8.78357e-01	8.79031e-01	8.79200e-01
2	1.00873e+00	1.00950e+00	1.00970e+00	1.62811e+00	1.62829e+00	1.62834e+00	1.00873e+00	1.00950e+00	1.00970e+00
3	1.23234e-01	1.23327e-01	1.23350e-01	6.55511e-02	6.55816e-02	6.55902e-02	1.23235e-01	1.23328e-01	1.23351e-01
4	7.15659e-03	7.16852e-03	7.17151e-03	2.04875e-03	2.05476e-03	2.05615e-03	7.15642e-03	7.16836e-03	7.17137e-03
5	3.90832e-06	3.93913e-06	3.94687e-06	5.74000e-07	5.81347e-07	5.83390e-07	3.90406e-06	3.93483e-06	3.94259e-06
6	2.00494e-11	2.02038e-11	2.02421e-11	1.24898e-12	1.26181e-12	1.26507e-12	4.35038e-12	4.49405e-12	4.52990e-12

Table 6.4: Norm of the increments during SQP method applied to Example 2.

	$\|\bar{q}_{int} - q_k\|_2$			$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_2$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_2$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
0	1.76576e+02	1.76607e+02	1.76615e+02	5.87414e-01	5.87459e-01	5.87471e-01	0.00000e+00	0.00000e+00	0.00000e+00
1	3.90881e-01	3.91124e-01	3.91184e-01	8.20582e-01	8.20774e-01	8.20822e-01	3.90881e-01	3.91124e-01	3.91184e-01
2	8.58213e-02	8.59184e-02	8.59427e-02	5.59739e-02	5.59868e-02	5.59901e-02	8.58213e-02	8.59184e-02	8.59427e-02
3	4.80842e-03	4.81528e-03	4.81699e-03	1.38387e-03	1.34285e-03	1.33737e-03	4.80832e-03	4.81518e-03	4.81690e-03
4	6.72049e-06	3.45868e-06	2.66825e-06	9.01919e-05	4.36785e-05	4.46278e-05	6.70739e-06	3.44646e-06	2.65684e-06
5	3.88474e-06	5.68002e-07	3.24142e-07	9.00179e-05	4.35328e-05	4.47928e-05	3.87161e-06	5.53075e-07	3.43469e-07
6	3.88474e-06	5.68003e-07	3.24141e-07	9.00179e-05	4.35328e-05	4.47928e-05	3.87161e-06	5.53075e-07	3.43471e-07

	$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_{1,2}$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_{1,2}$		
k	h_5	h_6	h_7	h_5	h_6	h_7
0	1.66782e+00	1.66809e+00	1.66816e+00	0.00000e+00	0.00000e+00	0.00000e+00
1	3.84416e+00	3.84383e+00	3.84423e+00	1.81180e+00	1.81279e+00	1.81304e+00
2	2.82465e-01	2.83130e-01	2.85876e-01	3.95804e-01	3.96271e-01	3.96392e-01
3	1.19410e-02	1.81389e-02	2.99712e-02	2.48866e-02	2.49495e-02	2.49498e-02
4	4.43211e-03	1.06149e-02	2.24624e-02	3.78871e-05	2.80285e-05	3.03608e-05
5	4.43104e-03	1.06149e-02	2.24630e-02	2.16206e-05	1.13290e-05	1.57991e-05
6	4.43104e-03	1.06149e-02	2.24630e-02	2.16206e-05	1.13290e-05	1.57991e-05

	$\|\bar{q}_{int} - q_k\|_\infty$			$\|\bar{\mathbf{u}}_{int} - \mathbf{u}_k\|_\infty$			$\|\bar{\mathbf{z}}_{int} - \mathbf{z}_k\|_\infty$		
k	h_5	h_6	h_7	h_5	h_6	h_7	h_5	h_6	h_7
0	2.51447e+02	2.51510e+02	2.51499e+02	4.99745e-01	5.00037e-01	4.99984e-01	0.00000e+00	0.00000e+00	0.00000e+00
1	8.78358e-01	8.79031e-01	8.79200e-01	1.56377e+00	1.56394e+00	1.56398e+00	8.78357e-01	8.79031e-01	8.79200e-01
2	1.30374e-01	1.30473e-01	1.30498e-01	6.72468e-02	6.72547e-02	6.72561e-02	1.30374e-01	1.30473e-01	1.30498e-01
3	7.16572e-03	7.17260e-03	7.17434e-03	2.10983e-03	2.06525e-03	2.05399e-03	7.16552e-03	7.17241e-03	7.17416e-03
4	9.22451e-06	4.42962e-06	3.73233e-06	2.54264e-04	2.99946e-04	5.07628e-04	9.18001e-06	4.42339e-06	3.72783e-06
5	6.03636e-06	8.16762e-07	6.39631e-07	2.54257e-04	3.00484e-04	5.08179e-04	5.97762e-06	7.95875e-07	7.36340e-07
6	6.03637e-06	8.16764e-07	6.39611e-07	2.54257e-04	3.00484e-04	5.08179e-04	5.97761e-06	7.95872e-07	7.36343e-07

Table 6.5: Errors for the iterates (against the interpolated exact solutions on the current grid) during the SQP method applied to Example 2.

7. Conclusion and outlook

In this thesis, the recent contributions of the author towards optimal control problems in the context of fracture propagation have been discussed. For one time step, these results have previously been published as joint works [85, 86] of the author and I. Neitzel and [84] of the author, M. Mohammadi, I. Neitzel and W. Wollner. For the results of [85, 86], this thesis also includes the case $M > 1$, i.e. the setting involving multiple time steps.

Second-order necessary and sufficient optimality conditions are derived in Chapter 4. Here, due to the nonlinear coupled structure (in the displacement and phase-field variable) of the underlying phase-field fracture partial differential equation, the involved improved regularity of the involved PDEs and solution operators, as well as the important preliminary (second-order) Lipschitz continuity results for the reduced functional, are essential in the analysis. Due to the extension towards the multi time step model, the coupling over consecutive time steps of the phase-field variable poses an additional working step that has to carefully be taken into consideration. This also leads to the substantial collection of technical results that are collected and established in Chapter 3. Nonetheless, second-order optimality results, not involving a two-norm discrepancy, and with only a minimal gap between necessary and sufficient conditions, can be established. Convergence of the dual variables and subsequently of the first-order necessary optimality conditions w.r.t. the fracture nonhealing property, modelled through a penalization for inequality conditions for the phase-field variables, are established in Chapter 5 for the one time step problem. Here, we rely on γ-independent norm bounds for the state in the W-setting and the adjoint state in the V-setting, respectively. The resulting system of (C-stationary) optimality conditions corresponds to a mathematical program involving complementarity constraints (MPCC). Finally in Chapter 6, a convergence analysis of the SQP method for the multi time step model is conducted. The aim is to base the convergence of the SQP method on weak second-order sufficient conditions, rather than stronger assumptions as e.g. in [84, Equation (4.2) and Proposition 4.3]. Thus, it is necessary to (initially) incorporate a pointwise analysis, cf. Remark 6.3.10, which subsequently involves techniques known from the analysis of sufficient optimality conditions involving the two-norm discrepancy, although originally an L^2-setting was satisfactory in the optimality conditions, cf. Remark 6.4.5. Here, quadratic convergence for localized subproblems in both L^∞- and L^2-neighborhoods is established. The SQP convergence result is substantiated by (up until now unpublished) numerical results.

Overall and in the context of the DFG Project 1962 *"Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization"* and the subproject *"Optimizing Fracture Propagation using a Phase-Field Approach"*, the results of this thesis can be seen as a continuation of the works [132, 133], complementing the analysis of optimality conditions for optimal control problems involving a phase-field fracture model, and includes aspects of nonlinear partial differential equations, optimal control theory as well as numerical methods such as the SQP method. As mentioned above, additionally some aspects are also related to the field of mathematical problems with complementarity constraints.

Let us conclude by gathering some open questions, which were beyond the scope of this thesis: Firstly, the model problem involved several physical and modelling parameters, which are involved in most of our results. We want to point out that, with the exception being the penalization parameter γ in Chapter 5, all parameters are assumed to be fixed. From the perspective of an applied reader, a more qualitative analysis of the exact dependence and behavior for each parameter is surely desirable, e.g. for the unique solvability of the state equation under the viscous approximation of Assumption 2.3.11. Additionally, a theoretical analysis of the behavior of e.g. the convergence radius when taking modelling parameters like ε or γ towards their limit might be of interest. The tracking of the penalization parameter and establishing further norm bounds independently of γ are of interest, e.g. also for the solutions of the linearized and adjoint equations for multiple time steps and in the improved W-setting. Such results can then be used as a foundation for a further stability analysis of the penalization limit of second-order optimality conditions and numerical methods like the SQP method, and are e.g. also of interest in the a-priori error analysis of solutions of associated model problems, like the quadratic subproblems of the SQP method. As for the limit in ε, this would e.g. be interesting in the context of a (potential future) analysis w.r.t. Γ-convergence of the Ambrosio/Tortorelli regularization, cf. Section 2.1. Secondly, further numerical results seem worthy of investigation: This aspect involves not only an experimental analysis of the behavior of different parameters in numerical tests. Certainly, also a full implementation of the SQP method of phase-field fracture optimal control, and a numerical convergence analysis which substantiates the theoretical convergence analysis from Section 6.3 and Section 6.4 for the exact same problem is worthy of further investigation. Both of these aspects are interesting for future research.

Appendix

A. Notation and abbreviations

Abbreviations:

a.e.	almost everywhere,
cf.	compare,
FMO	free material optimization,
FON	first-order necessary (conditions),
i.e.	id est, this means,
i.p.	in particular,
KKT	Karush-Kuhn-Tucker (conditions),
MPCC	mathematical program with complementarity constraints,
PDE	partial differential equation,
SNC	second-order necessary condition,
SQP	sequential quadratic programming,
SSC	second-order sufficient condition,
s.t.	such that or subject to, depending on the context,
w.l.o.g.	without loss of generality,
w.r.t.	with respect to.

Symbols and sets:

∇	Gradient,
$\triangle$	Laplace operator,
tr	the trace of anmatrix $A = (a_{ij}) \in \mathbb{R}^{n\times n}$, i.p. $tr(A) = \sum_{i=1}^{n} a_{ii}$,
$A\colon B := tr(B^T A)$	the inner product of two matrices $A = (a_{ij}), B = (b_{ij}) \in \mathbb{R}^{m\times d}$,

	i.p. $A : B = \sum_{j=1}^{m} \sum_{i=1}^{d} a_{ij} b_{ij} = tr(A^T B) = B : A$,
$\mathbb{R}$	real numbers,
$\mathbb{N}$	natural numbers,
I	identity matrix, dimension depending on context,
$(\cdot)^+ := \max(0, \cdot)$	see page: 28,
$a \ll b$	for $a, b \in \mathbb{R}$, a is significantly smaller than b,
$a \gg b$	for $a, b \in \mathbb{R}$, a is significantly greater than b,
$\mathbb{I} := \{1, ..., M\}$	set of natural numbers from 1 to M,
Ω	spatial domain, a subset of $\mathbb{R}^2$,
Γ	Neumann boundary part of the boundary $\partial\Omega$ of the spatial domain Ω, a subset of $\mathbb{R}$,
Γ_D	Dirichlet boundary part of the boundary $\partial\Omega$ of the spatial domain Ω, again a subset of $\mathbb{R}$.

Spaces:

$\mathbb{V}$	a generic Banach space,
$\mathbb{V}^*$	dual space of the space $\mathbb{V}$,
$B_r^{\mathbb{V}}(v)$	open ball of radius r centered at v w.r.t. $\mathbb{V}$ norm,
$L^p(\Omega)$	(Standard) Lebesgue space, see Definition 2.3.3,
$H^{1,2}(\Omega)$	(Standard) Hilbert (1,2) space, see Definition 2.3.3,
$C^{0,\alpha}(\Omega)$	(Standard) Hölder space of order zero and exponent $0 < \alpha \leq 1$,
$W^{s,p}(\Omega)$	Sobolev space of functions in L^p, whose weak partial derivatives of s-order lie in L^p,
$H^s(\Omega; \mathbb{R}^2)$	Hilbert space $W^{s,2}$,
$H^1_D(\Omega; \mathbb{R}^2)$	Hilbert space with zero Dirichlet data, i.p. $H^1_D(\Omega, \mathbb{R}^2) := \{v \in H^1(\Omega; \mathbb{R}^2) \mid v = 0 \text{ on } \Gamma_D\}$,
$W^{1,p}_D(\Omega; \mathbb{R}^2)$	Sobolev $W^{1,p}$ space with zero Dirichlet data, cf. the spaces $H^1_D(\Omega; \mathbb{R}^2)$ and $W^{s,p}(\Omega)$.

Finally, for a quick reference, where the operators $A, R, B, A_l, ...$ are rigorously introduced, the reader is referred to the beginning of Section 3.1, see page 40.

B. Manufactured solutions for the numerical examples from Section 6.5

In Section 6.5, we introduced the simplified optimal control problem (NLP_{ex}), together with its optimality conditions (EL_{ex}), (AE_{ex}), (VE_{ex}) and (SSC_{ex}). It was further explained how manufactured solutions can be constructed from these conditions. Here, we state the manufactured solutions used in Section 6.5.1 and Section 6.5.2 for reference in explicit form.

Manufactured solution for Example 1 from Section 6.5.1

We start by recalling the choice made in Section 6.5.1, i.p. let

$$\begin{aligned}
\mathbf{u}^- = (u^-, \varphi^-) &:= (0.0, 1.0),\\
\bar{\mathbf{u}} = (\bar{u}, \bar{\varphi}) &:= (\sin(\pi x)\sin(\pi y), (x-0.5)^2 + (y-0.5)^2 + 0.5),\\
\bar{\mathbf{z}} = (\bar{z}, \bar{\psi}) &:= (4\sin(2\pi x)\sin(\pi y), (x-0.5)^2 + y^2).
\end{aligned}$$

Then, we obtain from (6.82)-(6.86) the explicit representations

$$\begin{aligned}
\bar{q}^u :=& -2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&\quad \cdot \big((2x-1)\pi\cos(\pi x)\sin(\pi y) + (2y-1)\pi\sin(\pi x)\cos(\pi y)\big)\\
&+ 2(1-\kappa)\pi^2\sin(\pi x)\sin(\pi y)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)^2\\
&+ 2\kappa\pi^2\sin(\pi x)\sin(\pi y),
\end{aligned} \tag{B.1}$$

$$\begin{aligned}
\bar{q}^\varphi :=& -4\varepsilon + \frac{1}{\varepsilon}\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&+ \eta\Big((x-0.5)^2 + (y-0.5)^2 + 0.5\Big)\\
&+ (1-\kappa)\big((x-0.5)^2 + (y-0,5)^2 + 0.5\big)\\
&\quad \cdot \big(\pi^2\cos^2(\pi x)\sin^2(\pi y) + \pi^2\sin^2(\pi x)\cos^2(\pi y)\big)\\
&- \frac{1}{\varepsilon} - \eta,
\end{aligned} \tag{B.2}$$

$$\begin{aligned}
u_d =& \sin(\pi x)\sin(\pi y)\\
&+ 2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)
\end{aligned}$$

$$
\begin{aligned}
&\cdot \Big(16\pi(x-0.5)\cos(2\pi x)\sin(\pi y) + 8\pi(y-0.5)\sin(2\pi x)\cos(\pi y)\Big) \\
&- 20\pi^2\Big((1-\kappa)\big((x-0.5)^2 + (y-0,5)^2 + 0.5\big)^2 + \kappa\Big) \\
&\cdot \sin(2\pi x)\sin(\pi y) \\
&+ 2(1-\kappa)\Big((2x-1)\pi\cos(\pi x)\sin(\pi y) + (2y-1)\pi\sin(\pi x)\cos(\pi y)\Big) \\
&\cdot \Big((x-0.5)^2 + y^2\Big) \\
&- 4\pi^2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\sin(\pi x)\sin(\pi y) \\
&\cdot \Big((x-0.5)^2 + y^2\Big) \\
&+ 2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big) \\
&\cdot \Big((2x-1)\pi\cos(\pi x)\sin(\pi y) + 2y\pi\sin(\pi x)\cos(\pi y)\Big), \qquad \text{(B.3)}
\end{aligned}
$$

$$
\begin{aligned}
\varphi_d = &\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big) \\
&+ 2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big) \\
&\cdot \Big(8\pi^2\cos(2\pi x)\sin^2(\pi y)\cos(\pi x) + 4\pi^2\sin(2\pi x)\cos^2(\pi y)\sin(\pi x)\Big) \\
&+ 4\varepsilon - \frac{1}{\varepsilon}\Big((x-0.5)^2 + y^2\Big) - \eta\Big((x-0.5)^2 + y^2\Big) \\
&+ (1-\kappa)\Big((x-0.5)^2 + y^2\Big) \\
&\cdot \Big(\pi^2\cos^2(\pi x)\sin^2(\pi y) + \pi^2\sin^2(\pi x)\cos^2(\pi y)\Big), \qquad \text{(B.4)}
\end{aligned}
$$

$$
\begin{aligned}
q_d^u = &\frac{1}{\alpha}\Big(4\sin(2\pi x)\sin(\pi y)\Big) \\
&- 2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big) \\
&\cdot \big((2x-1)\pi\cos(\pi x)\sin(\pi y) + (2y-1)\pi\sin(\pi x)\cos(\pi y)\big) \\
&+ 2(1-\kappa)\pi^2\sin(\pi x)\sin(\pi y)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)^2 \\
&+ 2\kappa\pi^2\sin(\pi x)\sin(\pi y), \qquad \text{(B.5)}
\end{aligned}
$$

$$
\begin{aligned}
q_d^\varphi = &\frac{1}{\alpha}\Big((x-0.5)^2 + y^2\Big) \\
&- 4\varepsilon + \frac{1}{\varepsilon}\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big) \\
&+ \eta\Big((x-0.5)^2 + (y-0.5)^2 + 0.5\Big) \\
&+ (1-\kappa)\big((x-0.5)^2 + (y-0,5)^2 + 0.5\big) \\
&\cdot \big(\pi^2\cos^2(\pi x)\sin^2(\pi y) + \pi^2\sin^2(\pi x)\cos^2(\pi y)\big) \\
&- \frac{1}{\varepsilon} - \eta. \qquad \text{(B.6)}
\end{aligned}
$$

Manufactured solution for Example 2 from Section 6.5.2

We start by recalling the choice made in Section 6.5.2, i.p. let

$$
\begin{aligned}
\mathbf{u}^- &= (u^-, \varphi^-) := (0.0, 0.8),\\
\bar{\mathbf{u}} &= (\bar{u}, \bar{\varphi}) := (\sin(\pi x)\sin(\pi y), (x-0.5)^2 + (y-0.5)^2 + 0.5),\\
\bar{\mathbf{z}} &= (\bar{z}, \bar{\psi}) := (0.0, 0.0).
\end{aligned}
$$

Again, we obtain again from (6.82) - (6.86) the explicit representations

$$
\begin{aligned}
\bar{q}^u :=& -2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&\quad \cdot \big((2x-1)\pi\cos(\pi x)\sin(\pi y) + (2y-1)\pi\sin(\pi x)\cos(\pi y)\big)\\
&+ 2(1-\kappa)\pi^2\sin(\pi x)\sin(\pi y)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)^2\\
&+ 2\kappa\pi^2\sin(\pi x)\sin(\pi y), \qquad \text{(B.7)}\\
\bar{q}^\varphi :=& -4\varepsilon + \frac{1}{\varepsilon}\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&+ \eta\Big((x-0.5)^2 + (y-0.5)^2 + 0.5\Big)\\
&+ (1-\kappa)\big((x-0.5)^2 + (y-0,5)^2 + 0.5\big)\\
&\quad \cdot \big(\pi^2\cos^2(\pi x)\sin^2(\pi y) + \pi^2\sin^2(\pi x)\cos^2(\pi y)\big)\\
&- \frac{1}{\varepsilon} - \eta + \gamma\big(\max(0, (x-0.5)^2 + (y-0.5)^2 + 0.5 - 0.8)\big)^3, \qquad \text{(B.8)}\\
u_d =& \bar{u} = \sin(\pi x)\sin(\pi y), \qquad \text{(B.9)}\\
\varphi_d =& \bar{\varphi} = \Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big), \qquad \text{(B.10)}\\
q_d^u =& \bar{q}^u = \frac{1}{\alpha}\Big(4\sin(2\pi x)\sin(\pi y)\Big)\\
&- 2(1-\kappa)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&\quad \cdot \big((2x-1)\pi\cos(\pi x)\sin(\pi y) + (2y-1)\pi\sin(\pi x)\cos(\pi y)\big)\\
&+ 2(1-\kappa)\pi^2\sin(\pi x)\sin(\pi y)\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)^2\\
&+ 2\kappa\pi^2\sin(\pi x)\sin(\pi y), \qquad \text{(B.11)}\\
q_d^\varphi =& \bar{q}^\varphi = -4\varepsilon + \frac{1}{\varepsilon}\Big((x-0.5)^2 + (y-0,5)^2 + 0.5\Big)\\
&+ \eta\Big((x-0.5)^2 + (y-0.5)^2 + 0.5\Big)\\
&+ (1-\kappa)\big((x-0.5)^2 + (y-0,5)^2 + 0.5\big)\\
&\quad \cdot \big(\pi^2\cos^2(\pi x)\sin^2(\pi y) + \pi^2\sin^2(\pi x)\cos^2(\pi y)\big)\\
&- \frac{1}{\varepsilon} - \eta + \gamma\big(\max(0, (x-0.5)^2 + (y-0.5)^2 + 0.5 - 0.8)\big)^3. \qquad \text{(B.12)}
\end{aligned}
$$

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