ADAPTIVE MULTILEVEL INEXACT SQP–METHODS FOR PDE–CONSTRAINED OPTIMIZATION

J. CARSTEN ZIEMS∗ AND STEFAN ULBRICH†

Abstract. We present a class of inexact adaptive multilevel trust-region SQP-methods for the efficient solution of optimization problems governed by nonlinear partial differential equations. The algorithm starts with a coarse discretization of the underlying optimization problem and provides during the optimization process 1) implementable criteria for an adaptive refinement strategy of the current discretization based on local error estimators and 2) implementable accuracy requirements for iterative solvers of the linearized PDE and adjoint PDE on the current grid. We prove global convergence to a stationary point of the infinite-dimensional problem. Moreover, we illustrate how the adaptive refinement strategy of the algorithm can be implemented by using existing reliable a posteriori error estimators for the state and the adjoint equation. Numerical results are presented.

Key words. Optimal control, adaptive mesh adaptation, PDE constraints, finite elements, a posteriori error estimator, trust-region methods, inexact linear system solvers.

1. Introduction. In this paper we introduce and analyze a class of adaptive multilevel inexact sequential quadratic programming (SQP) methods for the solution of nonlinear PDE-constrained optimization problems. Nowadays, adaptive discretization techniques for partial differential equations based on a posteriori error estimators are well established to obtain accurate solutions with considerably less grid points than in the case of uniform meshes. In the context of optimization adaptive mesh refinement offers the potential to perform most of the optimization iterations on coarse meshes and to approach the infinite-dimensional problem during optimization in an efficient way.

We consider PDE–constrained optimization problems of the form

\[
\min_{y \in Y, u \in U} f(y, u) \quad \text{subject to} \quad C(y, u) = 0,
\]

where \(U\) is the control space, \(Y\) is the state space, \(f : Y \times U \to \mathbb{R}\) is the objective function. The state equation \(C : Y \times U \to V^*, C(y, u) = 0\) comprises a (system of) partial differential equation(s) with appropriate initial and/or boundary conditions in a variational formulation with \(V\) as the set of test functions. Here \(V^*\) denotes as usual the dual space of \(V\).

It would be possible to include constraints on the control \(u\) in our approach without significant changes. We leave this issue to a forthcoming paper.

We assume that \(Y\) and \(U\) are Hilbert spaces and that \(V\) is a reflexive Banach space. Moreover, let \(f\) and \(C\) be twice continuously Fréchet differentiable.

Often, the PDE constraint is given by a variational formulation of the form

\[ a(y; v) = b(u; v) \quad \forall v \in V. \]

In this case, \(C(y, u)\) is given by

\[ C : Y \times U \to V^*, \quad C(y, u) = a(y; \cdot) - b(u; \cdot) \in V^*. \]

∗TU Darmstadt, Department of Mathematics, Nonlinear Optimization, Schlossgartenstr. 7, D-64289 Darmstadt, Germany (ziems@mathematik.tu-darmstadt.de).

†TU Darmstadt, Department of Mathematics, Nonlinear Optimization, Schlossgartenstr. 7, D-64289 Darmstadt, Germany (ulbrich@mathematik.tu-darmstadt.de). The author was supported by the DFG priority program 1253 and in parts by SFB 666.
The proposed multilevel SQP-algorithm for (1.1) generates a hierarchy of finite-dimensional approximations

\[
\min_{y^h \in Y_h, u^h \in U_h} f(y^h, u^h) \quad \text{subject to} \quad C^h(y^h, u^h) = 0,
\]

which result from conformal discretizations, e.g. by the finite element method, of (1.1) on adaptively refined meshes. Our assumptions on the conformal discretization will be made precise in section 2.

In this paper we develop an implementable adaptive refinement strategy based on error estimators and combine it with an efficient inexact composite-step trust-region SQP method inspired by [18, 28]. The resulting adaptive multilevel SQP-method generates a hierarchy of adaptive discretizations (1.2), controls the inexactness of iterative solvers on the current grid and refines the grid – if necessary – adaptively in an appropriate way based on local error estimators, e.g. [1, 8, 9, 11, 30, 32], to ensure convergence to the solution of the original problem (1.1). We will prove global convergence under standard assumptions to a first–order optimality point of the infinite–dimensional problem (1.1).

The major advantages of the multilevel approach are that most optimization iterations are carried out on coarse meshes while the accuracy of the optimization result is controlled, since the mesh adaptation is tailored to the needs of the optimization method. This offers the possibility to obtain optimization results of high accuracy by an effort of a few simulation runs.

In recent years, multilevel techniques in optimization have received considerable attention [6, 7, 14, 15, 16, 23, 29]. These approaches focus on the efficient use of a hierarchy of discretizations to solve an optimization problem on the finest grid. [6, 7] consider multigrid solvers for the optimality system of PDE-constrained problems without globalization, [7] studies such methods with control constraints and [6] with state constraints. [15, 16, 23, 29] apply multigrid ideas in a recursive fashion for optimization problems, the coupling with adaptive mesh refinement is not considered.

The rigorous combination of adaptive error control techniques and modern globally convergent optimization techniques, which is the topic of this paper, was so far to the best of our knowledge not considered. On the other hand, a posteriori error estimators in the context of PDE-constrained optimization are an active research area [2, 3, 4, 20, 19, 24]. The rigorous imbedding of error estimators in multilevel optimization methods was to the best of our knowledge not considered so far. Truncated Newton methods in the presence of inexact function and gradient evaluations were studied in [22], but the combination with error estimators was not considered. [26] proposes a general algorithmic framework based on consistent approximations for optimal control problems which deals with approximate function and gradient evaluations in steepest descent algorithms. The accuracy control mechanism requires an error estimator for the function and gradient value depending on a scalar mesh parameter and is very different from the approach in this paper.

The purpose of this paper is to provide a rigorous framework for the combination of efficient and robust inexact SQP-methods with appropriate a posteriori error estimators. For the solution of the auxiliary trust-region problems, our method offers the possibility to use any kind of iterative solver, in particular the above mentioned multilevel solvers.

The paper is organized as follows. In section 2 we describe the optimality conditions and introduce our notations for the discretized problems. In section 3 we start with basic notations and requirements for inexact SQP methods followed by
a description of the basic components of our multilevel composite–step trust–region SQP algorithm before we state the refinement criteria and the algorithm itself. The convergence analysis can be found in section 4. In section 5 we show how the inexactness in linear equation solves and how the decrease conditions can be satisfied in an implementation. Averaging and residual based error estimators for a general semilinear elliptic PDE with inexact states can be found in section 6. Numerical results are presented in section 7.

We will often use the following notation: \( X := Y \times U, x = (y, u) \in X \).

2. Optimality conditions and discretization.

2.1. Optimality conditions. Let \( G_w \) denote the Fréchet derivative of an operator \( G \) w.r.t. a variable \( w \), e.g. \( C_y \) denotes the Fréchet derivative of the PDE-constraint operator \( C \) with respect to the state \( y \). Throughout the paper we assume that \( C_y(y, u) \in \mathcal{L}(Y, V^*) \) has an bounded inverse. Let

\[
 l : Y \times U \times V \to \mathbb{R}, \quad l(y, u, \lambda) = f(y, u) + \langle \lambda, C(y, u) \rangle_{V', V}.
\]

denote the Lagrangian function, where \( \langle \lambda, C(y, u) \rangle_{V', V} \) denotes the dual pairing. Note that \( V'^* = V \) and thus \( \lambda \in V'^* = V \).

Let \((\bar{y}, \bar{u})\) be an optimal solution of problem (1.1). Then the following first–order necessary optimality conditions hold: There exists an adjoint state (Lagrange multiplier) \( \bar{\lambda} \in V \) such that

\[
\begin{align*}
 l_y(\bar{y}, \bar{u}, \bar{\lambda}) &= f_y(\bar{y}, \bar{u}) + C_y(\bar{y}, \bar{u})^* \bar{\lambda} = 0, \\
 l_u(\bar{y}, \bar{u}, \bar{\lambda}) &= f_u(\bar{y}, \bar{u}) + C_u(\bar{y}, \bar{u})^* \bar{\lambda} = 0, \\
 C(\bar{y}, \bar{u}) &= 0.
\end{align*}
\]

Thus, the adjoint state \( \bar{\lambda} \) is uniquely determined by \( \bar{\lambda} = -C_y(\bar{y}, \bar{u})^{-1} f_y(\bar{y}, \bar{u}) \), since \( C_y(\bar{y}, \bar{u}) \) has a bounded inverse.

2.2. Discretized problem. For simplicity we assume that problem (1.1) is approximated by a conformal finite element discretization. More precisely, let \( Y_h \subset Y \), \( V_h \subset V \) be finite element subspaces on a triangulation \( \mathcal{T}_h \) of the computational domain \( \Omega \) consisting of closed cells \( T \). The mesh parameter \( h \) is defined as a cell-wise constant function by setting \( h_T = h_T \) and \( h_T \) is the diameter of \( T \). The mesh \( \mathcal{T}_h \) is assumed to be shape regular. Moreover, we introduce a finite dimensional subspace \( U_h \subset U \) of the control space. Depending on the concrete situation there are different possibilities to choose the space \( U_h \). It is reasonable to set \( U_h = U \) if \( U \) is finite dimensional. We set

\[
 X_h := Y_h \times U_h.
\]

We assume that the discretized PDE-constraint \( C^h : Y_h \times U_h \to V_h^* \) is given by the conformal finite element discretization

\[
 (C^h(y^h, u^h), v^h)_{V_h^*, V_h} := \langle C(y^h, u^h), v^h \rangle_{V', V} \quad \forall v^h \in V_h.
\]

The discretized optimization problem is then given by

\[
\min_{y^h \in Y_h, u^h \in U_h} f(y^h, u^h) \quad \text{subject to} \quad C^h(y^h, u^h) = 0,
\]

and the Lagrangian function of the discretized problem by

\[
 l^h : Y_h \times U_h \times V_h \to \mathbb{R}, \\
l^h(y^h, u^h, \lambda^h) = f(y^h, u^h) + \langle \lambda^h, C^h(y^h, u^h) \rangle_{V_h'^*, V_h} = l(y^h, u^h, \lambda^h),
\]
where the last identity follows from (2.3).

Similar to (2.2) the optimality conditions at a local solution \((\tilde{y}^h, \tilde{u}^h)\) of the discretized problem (1.2) read with an appropriate Lagrange multiplier \(\tilde{\lambda}^h \in V_h\)

\[
\begin{align*}
\langle l_y(\tilde{y}^h, \tilde{u}^h, \tilde{\lambda}^h), w_y^h \rangle_{Y^*, Y} &= 0 \quad \forall w_y^h \in Y_h, \\
\langle l_u(\tilde{y}^h, \tilde{u}^h, \tilde{\lambda}^h), w_u^h \rangle_{U^*, U} &= 0 \quad \forall w_u^h \in U_h, \\
(C(\tilde{y}^h, \tilde{u}^h), w_U^h)_{V^*, V} &= 0 \quad \forall w_U^h \in V_h.
\end{align*}
\]

(2.4)

For given \((x^h, \lambda^h) \in X_h \times V_h\) the residuals in the original optimality system (2.2) are given by

\[
\begin{align*}
\|l_y(x^h, \lambda^h)\|_{Y^*} &= \sup_{w_y \in Y, \|w_y\|_Y = 1} \langle l_y(x^h, \lambda^h), w_y \rangle_{Y^*, Y}, \\
\|l_u(x^h, \lambda^h)\|_{U^*} &= \sup_{w_u \in U, \|w_u\|_U = 1} \langle l_u(x^h, \lambda^h), w_u \rangle_{U^*, U}, \\
\|C(x^h)\|_{V^*} &= \sup_{v \in V, \|v\|_V = 1} \langle C(x^h), v \rangle_{V^*, V},
\end{align*}
\]

and the residuals of the discrete optimality system (2.4) by

\[
\begin{align*}
\|l_y(x^h, \lambda^h)\|_{Y^*_h} &= \sup_{w_y \in Y_h, \|w_y\|_Y = 1} \langle l_y(x^h, \lambda^h), w_y \rangle_{Y^*, Y}, \\
\|l_u(x^h, \lambda^h)\|_{U^*_h} &= \sup_{w_u \in U_h, \|w_u\|_U = 1} \langle l_u(x^h, \lambda^h), w_u \rangle_{U^*, U}, \\
\|C(x^h)\|_{V^*_h} &= \sup_{v \in V_h, \|v\|_V = 1} \langle C(x^h), v \rangle_{V^*, V}.
\end{align*}
\]

Note that the inequality \(\|C(x^h)\|_{V^*} \geq \|C(x^h)\|_{V^*_h}\) always holds. We assume that we are able to calculate norms in \(V^*_h\).

By refining the meshes we can generate a hierarchy of approximations.

Derivatives of functions from the discrete problem will also be denoted by subset variables, since by inserting the discrete values they can be defined via dual pairings in infinite dimensions which can be calculated as a vector vector product, e.g.

\[
\langle (C^h(x^h))^* \lambda^h, w_U^h \rangle_{V^*_h, Y_h} = \langle (C(y^h))^* \lambda^h, w_U^h \rangle_{Y^*, Y}.
\]

**Example 2.1.** Consider the problem (Problem 7.1 in section 7.1)

\[
\begin{align*}
\min_{y \in H^1_0(\Omega), u \in L^2(\Omega)} f(y, u) := \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2 \\
\text{s.t.} \quad -\Delta y + y^3 = u \quad \text{in } \Omega, \\
\quad y = 0 \quad \text{on } \partial \Omega,
\end{align*}
\]

where \(\Omega \subset \mathbb{R}^2\) is a polygonal domain, \(y_d \in H^1_0(\Omega)\) and \(\alpha > 0\). Here, the state equation has to be understood in the weak sense, more precisely, the state equation is given by the variational equation

\[
\int_{\Omega} (\nabla y \cdot \nabla v + y^3 v - uv) \, dx = 0 \quad \forall v \in H^1_0(\Omega).
\]

Therefore, we set \(Y = V := H^1_0(\Omega), \ U := L^2(\Omega), \ V = Y^*\) and define

\[
\begin{align*}
\begin{split}
C : (y, u) \in Y \times U &\mapsto (C(y, u) \in V^* = Y^*), \\
\langle C(y, u), v \rangle_{V^*, V} &:= a(y; v) - b(u; v), \quad v \in V,
\end{split}
\end{align*}
\]

\[
\frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2
\]
with
\[ a(y; v) = \int_\Omega (\nabla y \cdot \nabla v + y^3 v) \, dx, \quad b(u; v) = \int_\Omega uv \, dx. \]

The Lagrangian function is thus given by
\[ l(y, u, \lambda) = f(y, u) + (C(y, u), \lambda)_{V^*, V} = f(y, u) + a(y; \lambda) - b(u; \lambda). \]

Now let \( Y_h = V_h \subset Y \) and \( U_h \subset U \) be finite dimensional subspaces. Then the conformal discretization is given by
\[ \min_{y^h \in Y_h, u^h \in U_h} f(y^h, u^h) := \frac{1}{2} \| y^h - y_d \|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \| u^h \|_{L^2(\Omega)}^2 \]
subject to \( C^h(y^h, u^h) = 0 \), where
\[ C^h : (y^h, u^h) \in Y_h \times U_h \mapsto C^h(y^h, u^h) \in V_h^* = Y_h^*, \]
\[ \langle C^h(y^h, u^h), v^h \rangle_{V^*_h, V_h} := a(y^h; v^h) - b(y^h; v^h) = \langle C(y^h, u^h), v^h \rangle_{V^*, V}, \quad v^h \in V_h = Y_h. \]

The discrete Lagrangian function \( l^h \) is just the restriction of \( l \)
\[ l^h(y^h, u^h, \lambda^h) = f(y^h, u^h) + a(y^h; \lambda^h) - b(u^h; \lambda^h) = l(y^h, u^h, \lambda^h). \]


3.1. Main components of our multilevel trust–region SQP algorithm.
In this section we give a brief introduction to trust–region SQP methods and introduce the main components of our multilevel trust–region SQP algorithm. For further information on trust–region techniques we refer to [12] and for inexact trust–region techniques to [18].

In a classical local SQP method one minimizes a quadratic approximation of the Lagrangian function \( l \) in the current iterate \((x^k_h, \lambda^k_h)\) subject to the linearized constraint. That is, one computes the next iterate \( x^k_{h+1} = x^k + s_k \) where \( s_k \) solves the SQP-problem at \((x^k_h, \lambda^k_h)\)
\[ \min_{s \in X_h} q_k(s) := l_k + \langle (l_x)_k, s \rangle_{X^*, X} + \frac{1}{2} \langle s, H_k s \rangle_{X^*, X} \]
subject to \( C^h_k + (C^h_x) k s = 0 \)
with \( x^k = (y^k_h, u^k_h) \), \( l_k = l(x^k_h, \lambda^k_h) \), \( (l_x)_k = l_x(x^k_h, \lambda^k_h) \), \( H_k \approx l_{xx}(x^k_h, \lambda^k_h) \), \( C^h_k = C^h(x^k_h) \), \((C^h_x)_k = C^h_x(x^k_h)\) and accordingly all other abbreviations throughout the paper.

Note that by the conformity of the discretization, see in particular (2.3), \( C^h_k + (C^h_x) k s = 0 \) is equivalent to \( \| C^h_k + (C^h_x) k s \|_{V^*_h} = 0 \) and \( q_k(s) \) can also be written in terms of \( l^h \), more precisely,
\[ q_k(s) := l^h + \langle (l^h_x)_k, s \rangle_{X^*_h, X_h} + \frac{1}{2} \langle s, H_k s \rangle_{X^*_h, X^*_h}. \]

Since it is helpful to view our algorithm as a method for (1.1) that works with a hierarchy of adaptive discretizations, we will sometimes prefer to use \( l \) instead of \( l^h \), since \( l^h \) is only the restriction of \( l \) to the current subspaces.
One way to globalize a local SQP-method is using trust-region techniques. The idea is to trust the quadratic approximation of the Lagrangian function and the linearized constraint only in a trust-region which is adjusted during the algorithm to the quality of the approximations. Since the local SQP problem may become infeasible when joining an additional trust-region constraint \( \|s\| \leq \Delta_k \) for a trust-region radius \( \Delta_k > 0 \) one uses a step decomposition as suggested for example by Byrd, Omojokun [10, 25] and Dennis, El Alem, Maciel [13]. Here the step \( s_k \) is split into a sum of two steps, the quasi-normal step \( s^n = (s^n_y, 0) \) to improve feasibility and the tangential step \( s^t = (s^t_y, s_u) \) to improve optimality.

### 3.1.1. Quasi-normal step towards feasibility.

First, we compute a quasi-normal step \( s^n_k \), which is responsible for moving towards feasibility. Since we assume that \( C^h_y(x^k) \) is invertible, we perform the quasi-normal step only in the state variables. The \( y \)-component of \( s^n_k \) is an approximate solution of

\[
\begin{align*}
\min_{s^n_y \in Y_h} & \quad \|(C^h_y)_{k} s^n_y + C^h_k\|_{V^*_h} \\
\text{s.t.} & \quad \|s^n_y\|_Y \leq \Delta_k,
\end{align*}
\]

and the \( u \)-component is given by \( s^n_{u,k} = 0 \). Subproblem (3.1) is not solved exactly. A rather coarse solution is sufficient to ensure basic global convergence. The quasi-normal component is required to satisfy a Fraction of Cauchy Decrease condition

\[
C^h_k \|s^n_y\|_{V^*_h} - \|(C^h_y)_{k} s^n_y + C^h_k\|_{V^*_h} \geq \kappa_1 \|C^h_k\|_{V^*_h} \min \{\kappa_2 \|C^h_k\|_{V^*_h}, \Delta_k\}
\]

for all \( k \in \mathbb{N} \), where \( \kappa_1, \kappa_2 \in (0,1) \) are fixed constants independent of \( k \) and the grid. It is well known, that for example the Steihaug-CG method or a truncated Newton step, which is scaled back into the trust region if necessary, satisfies (3.2).

**Remark 3.1.** Usually, there exists already an efficient iterative solver for the linearized state equation \((C^h_y)_{k} s^n_y + C^h_k = 0\). Then \( s^n_k \) can be computed as an inexact solution, which is scaled back into the trust region. See section 5.2 for more details.

### 3.1.2. Tangential step towards optimality.

In a second step, the trust-region SQP-algorithm computes a tangential step \( s^t_k \) which is responsible for moving towards optimality but has to maintain linearized feasible, i.e. has to be in the nullspace of the linearized constraints. Let \( q_k \) be the quadratic approximation of the Lagrangian function in \((x^k_h, \lambda^k_h)\)

\[
q_k(s) := l_k + \langle (l_x)_k, s \rangle_{x^*,x} + \frac{1}{2} \langle s, H_k s \rangle_{x^*,x^*},
\]

where \( H_k \) is a symmetric approximation to the Hessian of the Lagrangian function in \((x^k_h, \lambda^k_h)\). We will assume that the sequence of approximated Hessians is bounded.

The tangential step is then an approximate solution of

\[
\begin{align*}
\min_{s^t \in X_h} & \quad q_k(s^n_k + s^t) \\
\text{s.t.} & \quad (C^h_y)_{k} s^n_y + (C^h_u)_{k} s_u = 0, \\
& \quad \|s_u\|_U \leq \Delta_k
\end{align*}
\]

Note that the tangential equation in the constraint is a variational equation for test functions from the finite element space \( V_h \). Consequently, the residual in the tangential equation must be orthogonal on a basis of \( V_h \). We can reduce \( q_k(s^n_k + s^t) \) to the control-component \( s_u \) of the tangential step \( s^t \) by solving the tangential equation

\[
(C^h_y)_{k} s^n_y + (C^h_u)_{k} s_u = 0,
\]
Thus, we can write the tangential problem entirely in
\[ q^L \] 
we obtain
\[ W_k = \left( -(C^h_y)_{k}^{-1} C^h_u \right)_k \in \mathcal{L}(U_h, Y_h \times U_h) \]
we obtain \( s^t = W_k s_u \) and we arrive at the reduced quadratic approximation of the Lagrangian
\[ \hat{q}_k(s_u) := q_k(s^u) + W^*_k (H_k s^u_k + (l_x)_k), s_u) + \frac{1}{2} s_u, W^*_k H_k W_k s_u \].
Thus, we can write the tangential problem entirely in \( s_u \)
\[ \min_{s_u \in U_h} \hat{q}_k(s_u) \]
\[ \text{s.t.} \quad \| s_u \|_U \leq \Delta_k, \]
but have afterwords to compute \( s^t_y \) by using (3.5).

Now we allow inexactness in the derivatives and the solutions of linear systems. Instead of computing the reduced gradient by \( W^*_k (H_k s^u_k + (l_x)_k) \) we solve the adjoint equation after the quasi-normal step on the current grid
\[ l_y(x^h_k, \lambda^h_k + \Delta \lambda^h_k) + (H_k s^u_k)_y(y) = 0 \quad \text{in } Y_h^* \]
in the variable \( \Delta \lambda^h_k \) sufficiently well (index \( y \) denotes the \( y \)-component) such that the following accuracy condition is satisfied
\[ \| l_y(x^h_k, \lambda^h_k + \Delta \lambda^h_k) + (H_k s^u_k)_y(y) \|_{Y_h^*} \leq \kappa_\lambda \min \{ \| l_u(x^h_k, \lambda^h_k + \Delta \lambda^h_k) + (H_k s^u_k)_y(y) \|_{U^*_h, \Delta_k} \}, \]
where \( \Delta_k \) denotes the trust-region radius and \( \kappa_\lambda > 0 \). A similar criterion was proposed in [18]. We define the inexact reduced gradient \( \hat{g}^h_k \) as approximation to the reduced gradient of \( \hat{q}_k \) by
\[ \hat{g}^h_k := l_u(x^h_k, \lambda^h_k + \Delta \lambda^h_k) + (H_k s^u_k)_y(y). \]
Any suitable iterative solver can be applied to the adjoint equation (3.8) until the stopping criterion (3.9) is satisfied. It is then easy to show that there exists \( \xi_1 > 0 \) such that
\[ \| \hat{g}^h_k - W^*_k (H_k s^u_k + l_x(x^h_k, \lambda^h_k)) \|_{U^*_h} \leq \xi_1 \min \{ \| \hat{g}^h_k \|_{U^*_h, \Delta_k} \}. \]
Moreover, let \( \hat{H} \) be an approximation to the reduced Hessian \( W^*_k H_k W_k \) satisfying
\[ \langle s_{u,k}, \hat{H} s_{u,k} \rangle \leq \xi_2 \| s_{u,k} \|_U^2 \]
for all steps \( s_{u,k} \in U_h \) computed by the algorithm and some fixed \( \xi_2 > 0 \). Then we define our approximate reduced quadratic approximation of the Lagrangian as
\[ \hat{m}_k(s_u) := q_k(s^u) + \langle \hat{g}^h_k, s_u \rangle + \frac{1}{2} s_u, \hat{H}_k s_u \],
where \( s^h_n \) denotes the quasi-normal step. And we compute \( s_u \) as an approximate solution of the inexact reduced tangential problem

\[
\begin{align*}
\min_{s_u \in U_h} & \quad \hat{m}_k(s_u) \\
\text{s.t.} & \quad \|s_u\|_U \leq \Delta_k.
\end{align*}
\]

The approximate solution of (3.13) must provide a fraction of the Cauchy decrease in the approximate model \( \hat{m}_k \), i.e.

\[
\hat{m}_k(0) - \hat{m}_k(s_u,k) \geq \kappa_4 \| \hat{g}_h \|_{U_h} \min \left\{ \kappa_5 \| \hat{g}_h \|_{U_h}, \kappa_6 \Delta_k \right\} \quad \forall k \in \mathbb{N},
\]

where \( \kappa_4, \kappa_5, \kappa_6 \) are positive constants independent of \( k \) and the grid.

The \( y \)-component of the tangential step is then given by

\[
s^t_{y,k} = -(C_{y}^h)_{k}^{-1}(C_{u}^h)_{k} s_{u,k}.
\]

Since we allow linear system solutions to be inexact, solving this equation approximately creates the residual

\[
r^t_k := (C_{y}^h)_{k} s^t_{y,k} + (C_{u}^h)_{k} s_{u,k}.
\]

Accuracy conditions on the residual in this tangential equation are presented in the next section.

### 3.1.3. Derivation of the predicted decrease.

To decide about the acceptance of the step we use the augmented Lagrangian merit function

\[
L_h(x^h_k, \lambda^h_k; \rho_k) := f(x^h_k) + \langle \lambda^h_k, C^h_k \rangle + \rho_k \| C^h_k \|^2_{V_k^*}.
\]

The decision about the acceptance of the step and update of the trust-region radius \( \Delta_k \) is then based on the ratio of actual reduction \( \text{ared}_h(s_k, \rho_k) \), given by

\[
\text{ared}_h(s_k, \rho_k) := L_h(x^h_k, \lambda^h_k; \rho_k) - L_h(x^h_k + s_k, \lambda^h_{k+1}; \rho_k)
\]

and predicted reduction based on the quadratic models in the quasi-normal and tangential step

\[
\text{pred}(s_k; \rho_k) = L_h(x^h_k, \lambda^h_k; \rho_k) - q_k(s_k) - \langle \Delta \lambda^h_k, C^h_k \rangle s_k + \rho_k \| C^h_k s_k \|^2_{V_k^*} + \rho_k \| C^h_k s_k \|^2_{V_k^*},
\]

where \( \Delta \lambda^h_k = \lambda^h_{k+1} - \lambda^h_k \). Since we solve the linear system for the \( y \)-component of the tangential step (3.15) inexact with residual \( r^t_k = (C_{y}^h)_{k} s^t_{y,k} + (C_{u}^h)_{k} s_{u,k} \), we obtain for \( s_k = s^n_k + s^t_k \), \( s^n_k = (s^n_{y,k})_{k} + (s^n_{u,k})_{k} \),

\[
\text{pred}(s_k; \rho_k) = L_h(x^h_k, \lambda^h_k; \rho_k) - q_k(s_k) - \langle \Delta \lambda^h_k, C^h_k \rangle s^n_k + \langle (C_{y}^h)_{k} s^n_{y,k}, V^*_k \rangle - \langle (C_{u}^h)_{k} s^n_{u,k}, V^*_k \rangle - \rho_k \| C^h_k + (C_{y}^h)_{k} s^n_{y,k} + r^t_k \|^2_{V_k^*}.
\]

Since \( V \) is not necessarily a Hilbert space we use the triangle inequality in the last summand reducing the predicted reduction

\[
\text{pred}(s_k; \rho_k) \geq L_h(x^h_k, \lambda^h_k; \rho_k) - q_k(s_k) - \langle \Delta \lambda^h_k, C^h_k + (C_{y}^h)_{k} s^n_{y,k}, V^*_k \rangle - \langle (C_{y}^h)_{k} r^t_k, V^*_k \rangle
\]

\[
- \rho_k \left( \| C^h_k + (C_{y}^h)_{k} s^n_{y,k}, V^*_k \|^2_{V_k^*} + \| r^t_k \|^2_{V_k^*} \right)^2
\]

\[
= L_h(x^h_k, \lambda^h_k; \rho_k) - q_k(s_k) - \langle \Delta \lambda^h_k, C^h_k + (C_{y}^h)_{k} s^n_{y,k}, V^*_k \rangle - \langle (C_{y}^h)_{k} r^t_k, V^*_k \rangle
\]

\[
- \rho_k \left( \| C^h_k + (C_{y}^h)_{k} s^n_{y,k}, V^*_k \|^2_{V_k^*} + 2 \| C^h_k + (C_{y}^h)_{k} s^n_{y,k}, V^*_k \|_{V^*_k} \| r^t_k \|_{V^*_k} \right).
\]
Certainly the right hand side is not the same model of the actual reduction as before (only if $r^s_k = 0$). But since we reduced $\text{pred}(s_k; \rho_k)$ this will only lead to a stronger requirement on the residual $r^t_k$.

Note that

$$L_h(x^h_k, \lambda^h_k; \rho_k) = q_k(0) + \hat{q}_k(0) - q_k(s^n_k) + \rho_k\|C_h^h\|_{V^*_h}^2.$$ 

Now, the quadratic model $q_k(s_k)$ of the Lagrangian is replaced by the approximate reduced quadratic model $\tilde{m}_k(s_{u,k})$ and we define

$$\text{pred}_h(s^n_k, s_{u,k}; \rho_k) := \tilde{m}_k(0) - \tilde{m}_k(s_{u,k}) + q_k(0) - q_k(s^n_k)$$

$$(3.17)$$

$$- \langle \Delta \lambda^h_h, C_h^h + (C^h_h)_k s^n_{y,k} \rangle_{V,V^*} + \rho_k \left( \|C_h^h\|_{V^*_h}^2 - \|C_h^h + (C^h_h)_k s^n_{y,k}\|_{V^*_h}^2 \right),$$

and

$$\text{rpred}_h(r^t_k; \rho_k) := - \langle \Delta \lambda^h_h, r^t_k \rangle_{V,V^*} - \rho_k\|r^t_k\|_{V^*_h}^2 - 2\rho_k\|r^t_k\|_{V^*_h} \|((C^h_y)_k s^n_{y,k} + C^h_h)\|_{V^*_h}.$$ 

We now view

$$\text{pred}_h(s^n_k, s_{u,k}; \rho_k) + \text{rpred}_h(r^t_k; \rho_k)$$

as the (approximate) quadratic model of the actual reduction in the augmented Lagrangian.

**Remark 3.2.** If $V$ is a Hilbert space, then we obtain

$$\|C_h^h + (C^h_h)_k s^n_{y,k}\|_{V}^2 = \|C_h^h + (C^h_y)_k s^n_{y,k} + r^t_k, C_h^h + (C^h_y)_k s^n_{y,k} + r^t_k \rangle_{V}$$

$$= \|C_h^h + (C^h_y)_k s^n_{y,k}\|_{V}^2 + \|r^t_k\|_{V}^2 + 2 \big(r^t_k, C_h^h + (C^h_y)_k s^n_{y,k} \big)_{V}$$

and we can define $\text{rpred}_h(r^t_k; \rho_k)$ more exactly as

$$\text{rpred}_h(r^t_k; \rho_k) := - \langle \Delta \lambda^h_h, r^t_k \rangle_{V,V^*} - \rho_k\|r^t_k\|_{V^*_h}^2 - 2 \big(r^t_k, C_h^h + (C^h_y)_k s^n_{y,k} \big)_{V},$$

which is larger than the above defined $\text{rpred}_h(r^t_k; \rho_k)$.

Nevertheless, step evaluations are performed based on $\text{pred}_h(s^n_k, s_{u,k}; \rho_k)$ only: If

$$\frac{\text{ared}_h(s_k; \rho_k)}{\text{pred}_h(s^n_k, s_{u,k}; \rho_k)} \geq \eta_1,$$

where $\eta_1 \in (0, 1)$ is a given constant, then $s_k$ is accepted, otherwise $s_k$ is rejected and the trust–region is reduced. As in [18], the conditions

$$(3.18)$$

$$|\text{rpred}_h(r^t_k; \rho_k)| \leq \eta_0 \text{pred}_h(s^n_k, s_{u,k}; \rho_k),$$

where $\eta_0 \in (0, 1 - \eta_1)$ is a given constant, and

$$(3.19)$$

$$\|r^t_k\|_{V^*_h} \leq \xi_3 \Delta^1 + p,$$

for some constant $\xi_3 > 0$ independent of $k$ and given $p \in (0, 1]$ ensure that the inexactness in the tangential step $s^t_k$ does not dominate the quadratic model. Inequality (3.18) is implied by

$$(3.20)$$

$$\|r^t_k\|_{V^*_h} \leq -\sigma + \sqrt{\sigma^2 + \eta_0 \text{pred}_h(s^n_k, s_{u,k}; \rho_k)/\rho_k},$$
where \( \sigma = \|(C^h_y)^n_{y,k} + C^h_y\|_{V^*_k} + \|\Delta \lambda^b_k\|_V/(2\rho_k) \).

**Remark 3.3.** Since only the size of \( \|\text{pred}_h(r^h_k; \rho_k)\| \) is of interest as seen in the estimates (3.18) and (3.19), where this size depends on the residual accuracy of an inexact solution of the tangential equation (3.15) the difference in the definitions of estimates (3.18) and (3.19), where this size depends on the residual accuracy of an acceptation of a trial-step depends on the ratio \( \rho_{\text{ared}} \). As suggested above we require the following convergence condition on \( Y \) during optimization we refine the discrete state equation using error estimators. Note that for Galerkin discretizations the constraint is of no importance for that decision.

### 3.1.4. Update of the penalty parameter.

We choose the penalty parameter \( \rho_k \) so large such that for a given \( \kappa \in (0, 1) \) the inequality

\[
\text{pred}_h(s^n_{u,k}; \rho_k) \geq \kappa (\hat{m}_k(0) - \hat{m}_k(s_{u,k})) + \frac{\rho_k}{2} \left( \|C^h_y\|^2_{V^*_k} - \|(C^h_y)^n_{y,k} + C^h_k\|^2_{V^*_k} \right)
\]

holds. Let \( 0 < \nu \ll 1 \) and \( \kappa \in (0, 1) \). If (3.21) is satisfied with \( \rho_k = \rho_{k-1} \), then we set \( \rho_k := \rho_{k-1} \). Otherwise, we choose the smallest \( \rho_k \geq (1 + \nu)\rho_{k-1} \) that satisfies (3.21).

### 3.1.5. Update of the trust–region radius.

Let \( 0 < \alpha_0 \leq \alpha_1 < \alpha_2 \), let \( 0 < \eta_1 < \eta_2 < 1 \) and let \( 0 < \Delta_{\text{min}} \leq \Delta_{\text{max}} \). We choose the trust–region radius as follows:

\[
\Delta_{k+1} = \begin{cases} 
\alpha_0 \Delta_k, \alpha_1 \Delta_k & \text{if } \text{ared}_{\text{pred}} < \eta_1, \\
\max\{\Delta_{\text{min}}, \alpha_1 \Delta_k\}, \max\{\Delta_{\text{min}}, \Delta_k\} & \text{if } \text{ared}_{\text{pred}} \in [\eta_1, \eta_2), \\
\max\{\Delta_{\text{min}}, \Delta_k\}, \min\{\max\{\Delta_{\text{min}}, \alpha_2 \Delta_k\}, \Delta_{\text{max}}\} & \text{if } \text{ared}_{\text{pred}} \geq \eta_2.
\end{cases}
\]

### 3.1.6. Refinement of the grids.

The main idea for refinement is to control the infinite dimensional norms of the residuals in the infinite dimensional optimality system by using the corresponding finite dimensional norms and the (discrete) norm of the reduced gradient and the constraint. Thus, if the norm of the reduced gradient or the constraint is large enough compared to the infinite dimensional counterparts, the current discretization will be good enough to compute sufficient descent. On the other hand, if the discrete norm of the reduced gradient and/or the constraint on the current grid are small compared to the continuous norms, one has to ensure by mesh refinement that the infinite dimensional problem and, in particular, the infinite dimensional reduced gradient are well represented in the current discretization such that reasonable steps can be computed. Observe that the inexact reduced gradient \( \hat{g}^h_k \) depends on the (inexact) state \( y^h_k \) and the (inexact) adjoint \( \lambda^h + \Delta \lambda_k \). Therefore, the residual norms of the infinite dimensional state- and adjoint equation must be controlled. Since these residual norms cannot be computed directly, we will use reliable error estimators instead.

We will give brief motivations for the different refinement criteria before we state implementable versions using error estimators. Note that for Galerkin discretizations \( V_k \) is the test function space corresponding to the discrete state space \( Y_k \) and therefore a refinement of \( Y_k \) implies a refinement of \( V_k \) and vice versa.

**Error control for the discrete state equation.** To control the accuracy of the discrete state equation during optimization we refine the \( Y \) and \( V \)-grid adaptively if necessary. As suggested above we require the following convergence condition on the constraint

\[
\|C(x^h_k)\|_{V^*} \leq c_1\|C^h_k\|_{V^*_k} + c_2\|\hat{g}^h_k\|_{V^*_k} \quad \forall k \in \mathbb{N}, x^h_k \in X_k,
\]

(3.22)
with fixed arbitrary constants $c_1 > 1$ and $c_2 > 0$.

**Remark 3.4.** Note that this convergence condition for the constraint can only be applied after the computation of the approximate reduced gradient (3.10) and, thus, after the computation of the quasi-normal step. Since the discretized norms in $Y^*_h$ and $V^*_h$ change due to refinement, condition (3.2) needs to be checked for the prolonged $s^*_h$ after a refinement of the grids. Moreover, the dimension of $V_h$ affects the computation of the adjoint state and, thus, also the approximate reduced gradient. Consequently, condition (3.11) has to be reviewed. Hence, if the prolonged $s^*_h$ does not meet (3.2), then $s^*_h$ and $\hat{g}^*_h$ are recomputed on the refined grids, since the computation of $\hat{g}^*_h$ depends also on $s^*_h$. Otherwise, if the prolonged $s^*_h$ meets (3.2), then $\hat{g}^*_h$ only needs to be recomputed if (3.11) does not hold for the prolonged $\hat{g}^*_h$.

After the computation of a successful step on the current grid we need to verify that the next iterate is also well represented on the current grid. That is, the difference of the discrete norm and the infinite dimensional norm of the constraint in the next iterate may not become much larger. Otherwise we may have no decrease in the constraint.

After a successful step if the current discretization was suitable to compute sufficient descent. And, hence, this criterion guarantees suitable (adaptive) refinements. Note that this convergence condition for the constraint can only be estimated by an estimator $\beta(x^h_k, s_k) > 0$ such that

\[
\alpha(x^h_k) := \|C(x^h_k)\|_{V^*} - \|C^{(h)}(x^h_k)\|_{V^{(h)(k)}} \to 0
\]

\[
\alpha(x^h_k + s_k) := \|C(x^h_k + s_k)\|_{V^*} - \|C^{(h)}(x^h_k + s_k)\|_{V^{(h)(k)}} \to 0
\]

for $h(k) \searrow 0$ as $k \to \infty$, condition (3.23) can be formulated in a weaker version, which is easier to implement. If the last term on the right hand side in (3.23) can be estimated by an estimator $\beta(x^h_k, s_k) > 0$ such that

\[
\alpha(x^h_k + s_k) - \alpha(x^h_k) = K(h, k)\beta(x^h_k, s_k)
\]

with unknown constants satisfying $1/K \leq K(h, k) \leq K$, $k \in \mathbb{N}$, for some fixed $K > 0$, then it suffices to verify the following criterion

\[
\text{ared}_h(s_k; \rho_k) \geq \xi \rho_k \beta(x^h_k, s_k)^\omega
\]
for fixed $\omega \in (0, 1)$ and $\xi > 0$. In fact, assumption (3.24) guarantees with (3.25) and the uniform boundedness of $K(h, k)$ from below and above that $\beta(x_h^k, s_k) \leq ((1 + \delta)K/\xi)^{-1/(1-\omega)}$ for $k$ large enough which implies

$$(1+\delta)(\alpha(x_h^k + s_k) - \alpha(x_h^k)) = (1+\delta)K(h, k)\beta(x_h^k, s_k) \leq (1+\delta)K\beta(x_h^k, s_k) \leq \xi \beta(x_h^k, s_k)^\omega$$

and consequently (3.23). This way one does not need to know the constants $K(h, k)$. If the algorithm does not terminate after finitely many iterations and if the problem is well conditioned in such a way that (3.24) holds, then after finitely many iterations and refinements (3.26) implies (3.23) which suffices for the convergence proof.

An alternative criterion to (3.23) is the following condition

$$(3.27) \quad \sum_{k=0}^{\infty} \|C(x_h^{(k+1)})\|_{V^*} - \|C_h^{(k)}(x_h^{(k)})\|_{V_{h(k)}^*} < \infty.$$ 

that originates from the jumps in the differences of the norms of the constraint due to refinement of the meshes which shall be summable. Nevertheless the convergence proof is given for criterion (3.23). A convergence proof using condition (3.27) instead of (3.23) in the algorithm is very similar. Only a few details in the proof of theorem 4.14 need to be adapted.

**Error control for the reduced gradient and the discrete adjoint equation.** To control the quality of the discrete adjoint equation and the discrete reduced gradient during the optimization iteration we have to refine the $U$–grid and the $Y$– and $V$–grid, respectively, if necessary. To control the error in the first optimality condition $D_y l(x_h^k, \lambda_h^k) = 0$, i.e. the adjoint equation, we apply a similar criterion as for the state equation constraint. We use $\lambda_h^{k+1} = \lambda_h^k + \Delta \lambda_h^k$ as inexact solution of the discrete adjoint equation $l_h^k(x_h^k, \lambda_h^{k+1}) = 0$ with $\Delta \lambda_h^k$ from (3.8) and (3.9). Note that using the computation rule of $\Delta \lambda_h^k$ and Lemma 4.1 together with our assumptions on the boundedness it is easy to show that

$$(3.28) \quad \|l_y(x_h^k, \lambda_h^{k+1})\|_{V_h^*} \leq \xi_3 \|\hat{g}_h^k\|_{V_h^*} + \xi_4 \|C_h^k\|_{V_h^*}$$

for some $\xi_3, \xi_4 > 0$. This justifies the choice of $\lambda_h^{k+1}$ as inexact discrete adjoint state since $\|\hat{g}_h^k\|_{U_h^*}$ and $\|C_h^k\|_{V_h^*}$ tend to zero during the optimization. Thus, we require the following convergence condition on the adjoint equation

$$(3.29) \quad \|l_y(x_h^k, \lambda_h^{k+1})\|_{V^*} \leq c_1 \|l_y(x_h^k, \lambda_h^{k+1})\|_{V^*}^* + c_2 (\|\hat{g}_h^k\|_{U_h^*} + \|C_h^k\|_{V_h^*})$$

with fixed arbitrary constants $c_1 > 1$ and $c_2 > 0$.

For given $Y_h$ and $V_h$ it is often easily possible to choose $U_h \subset U$ in such a way that

$$(3.30) \quad \|l_u(x_h^k, \lambda_h^k)\|_{U^*} = \|l_u(x_h^k, \lambda_h^k)\|_{U_h^*}.$$ 

In this case the refinement of $V_h$ implies the refinement of $U_h$ and there is no additional criterion necessary for refining the control space.

**Example 3.5.** Consider again the problem (Problem 7.1 in section 7.1)

$$\min_{y \in H^1_0(\Omega), u \in L^2(\Omega)} f(y, u) := \frac{1}{2} \| y - y_d \|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \| u \|_{L^2(\Omega)}^2$$

s.t. $\begin{align*}
-\Delta y + y^3 &= u & \text{in } \Omega, \\
y &= 0 & \text{on } \partial \Omega.
\end{align*}$
where \( \Omega \subset \mathbb{R}^2 \) is a polygonal domain, \( \alpha > 0 \). Then

\[
\langle l_u(x_k^h, \lambda_k^h), w_u \rangle_{U^*, U} = \alpha(u_h, w_u)_{L^2(\Omega)} - (\lambda^h, w_u)_{L^2(\Omega)} \quad \forall w_u \in U.
\]

Therefore, if we choose \( U_h = V_h \subset V \subset U \) then \( \alpha u_h - \lambda^h \in U_h \subset U \) is the Riesz representation of \( l_u(x_k^h, \lambda_k^h) \) in \( U \) as well as in \( U_h \) and therefore

\[
\| l_u(x_k^h, \lambda_k^h) \|_{U^*} = \| \alpha u_h - \lambda^h \|_{L^2(\Omega)} = \| l_u(x_k^h, \lambda_k^h) \|_{U^*_h}.
\]

On the other hand, if (3.30) does not hold then we require that the discretization of the control space meets the following accuracy condition

\[
(3.31) \quad \| l_u(x_k^h, \lambda_k^h) \|_{U^*} \leq c_1 \| l_u(x_k^h, \lambda_k^h) \|_{U^*_h} + c_2 (\| \hat{g}_k^h \|_{U^*_h} + \| C_k^h \|_{V^*_h}),
\]

with fixed arbitrary constants \( c_1 > 1 \) and \( c_2 > 0 \). Note that using Lemma 4.1 together with our assumptions on the boundedness it is easy to show that

\[
(3.32) \quad \| l_u(x_k^h, \lambda_{k+1}^h) \|_{U^*_h} \leq \xi_5 \| g_k^h \|_{U^*_h} + \xi_6 \| C_k^h \|_{V^*_h}
\]

for some \( \xi_5, \xi_6 > 0 \).

Remark 3.6. Note that after a refinement of the \( Y \)– and \( V \)-grid for the adjoint the discretized norms in \( Y_h^* \) and \( V_h^* \) change. Thus, condition (3.2) is not necessarily satisfied for the prolongated \( s^h \) that was computed on a coarser grid. Hence, possibly, the quasi–normal step needs to be recomputed. In any case, the inexact reduced gradient \( \hat{g}_k^h \) is recomputed.

Implementation of the refinement criteria with error estimators. As derived above we need to implement the following refinement criteria with fixed arbitrary constants \( c_{1i} > 1, k_i > 0, i = 1, 2, 3 \):

\[
\| C(x_k^h) \|_{V^*} \leq c_1 \| C_k^h \|_{V^*_h} + k_1 \| \hat{g}_k^h \|_{U^*_h},
\]

\[
\| l_y(x_k^h, \lambda_{k+1}^h) \|_{Y^*} \leq c_2 \| l_y(x_k^h, \lambda_{k+1}^h) \|_{Y^*_h} + k_2 (\| C_k^h \|_{V^*_h} + \| \hat{g}_k^h \|_{U^*_h}),
\]

\[
\| l_u(x_k^h, \lambda_{k+1}^h) \|_{U^*} \leq c_3 \| l_u(x_k^h, \lambda_{k+1}^h) \|_{U^*_h} + k_3 (\| C_k^h \|_{V^*_h} + \| \hat{g}_k^h \|_{U^*_h}).
\]

In general, infinite dimensional norms cannot be computed. Therefore, we assume that we have reliable error estimators \( \eta_{C,h}, \eta_{u,h}, \eta_{y,h} \) with

\[
(3.33a) \quad \| C(y^h, u^h) \|_{V^*} \leq C_1 \eta_{C,h}(y^h, u^h) + C_2 \| C_h^h(y^h, u^h) \|_{V^*_h},
\]

\[
(3.33b) \quad \| l_y(y^h, u^h, \lambda^h) \|_{Y^*} \leq C_3 \eta_{y,h}(y^h, u^h, \lambda^h) + C_4 \| l_y(y^h, u^h, \lambda^h) \|_{Y^*_h},
\]

\[
(3.33c) \quad \| l_u(y^h, u^h, \lambda^h) \|_{U^*} \leq C_5 \eta_{u,h}(y^h, u^h, \lambda^h) + C_6 \| l_u(y^h, u^h, \lambda^h) \|_{U^*_h}
\]

with unknown, bounded constants \( C_i > 0, i = 1, \ldots, 6 \), in such a way that \( \eta_h \to 0 \) as \( h \to 0 \) for fixed \( y_h, u_h, \lambda_h \). Such error estimators can be developed using the same techniques as for well known error estimators in the presence of exact discrete states. Examples for suitable residual based and averaging error estimators as well as their derivation will be shown in section 7.

Remark 3.7. For all error estimators in section 7 one can show that \( \eta_h \to 0 \) as \( h \to 0 \), i.e. if the maximal mesh size tends to zero. Therefore, the convergence conditions (3.34) can always be satisfied by sufficient refinement.
Now we insert these error estimator inequalities (3.33) in the above given criteria. Moreover, an algorithm will truncate for a given stop-tolerance \( \varepsilon_{\text{tol}} > 0 \). Since the norms of the reduced gradient and the constraint may become much smaller than the prescribed stop-tolerance in one (last) iteration we also include \( \varepsilon_{\text{tol}} \) in the refinement formulas. Thus, we obtain the following implementable sufficient refinement criteria:

Check for arbitrary fixed constants \( \tilde{c}_1 > 0 \), \( i = 1, \ldots, 9 \), if

$$
\eta_{C,h}(x^h_{k}) \leq \max \left\{ \tilde{c}_1 \| C^h_{k} \|_{V^*_h} + \tilde{c}_2 \| g^h_{k} \|_{U^*_h}, \tilde{c}_3 \varepsilon_{\text{tol}} \right\}
$$

$$
\eta_{v,h}(x^h_{k}, \lambda^h_{k+1}) \leq \max \left\{ \tilde{c}_4 \| I^h_y(x^h_{k}, \lambda^h_{k+1}) \|_{V^*_h} + \tilde{c}_5 \| C^h_{k} \|_{V^*_h} + \| \hat{g}^h_{k} \|_{U^*_h}, \tilde{c}_6 \varepsilon_{\text{tol}} \right\}
$$

$$
\eta_{u,h}(x^h_{k}, \lambda^h_{k+1}) \leq \max \left\{ \tilde{c}_7 \| U^h_{k+1} \|_{U^*_h} + \tilde{c}_8 \| C^h_{k} \|_{U^*_h} + \| \hat{g}^h_{k} \|_{U^*_h}, \tilde{c}_9 \varepsilon_{\text{tol}} \right\}
$$

(3.34b)

Otherwise refine the grids for \( Y_{h(k)}, V_{h(k)}, U_{h(k)} \), prolongate the functions and recompute the affected data.

Remark 3.8. With the choice of \( \tilde{c}_3, \tilde{c}_6, \tilde{c}_9 \) a different quality for the state and the adjoint state than for the norms of the reduced gradient and the constraint can be achieved in the stop-criterion of the algorithm. This is in particular of interest when dependent on PDEs or domains an approximate size of the error estimators on fine meshes (larger than \( \varepsilon_{\text{tol}} \)) is known. Note that \( \tilde{c}_1 \) and \( \tilde{c}_2 \) affect directly how soon meshes are refined.

Criterion (3.23) can be implemented in the form of (3.26) the following way. We assume that we have an error estimator as in (3.33a)

$$
\| C(y^h, u^h) \|_{V^*} \leq C_1 \eta_{C,h} + C_2 \| C^h(y^h, u^h) \|_{V^*_h}
$$

with \( C_2 = C_2(h) \rightarrow 1 \) as \( h \rightarrow 0 \) where \( \eta_{C,h} \) is an efficient and reliable error estimator in the presence of exact discrete states. Then \( C_1 \eta_{C,h}(C_1 \eta_{C,h} + 2\| C^h(y^h, u^h) \|_{V^*_h}) \) may be seen as good numerical approximation of

$$
\| C(x^h_{k}) \|_{V^*_h}^2 \leq \| C^h(x^h_{k}) \|_{V^*_h}^2
$$

for some bounded constant \( C_1 \). Therefore, we can consider

$$
\| C(x^h_{k}) \|_{V^*_h}^2 - \| C^h(x^h_{k}) \|_{V^*_h}^2 = K(h,k) \eta_{C,h}(x^h_{k+1})(C_1 \eta_{C,h}(x^h_{k+1}) + 2\| C^h(x^h_{k}) \|_{V^*_h})
$$

$$
\| C(x^h_{k+1}) \|_{V^*_h}^2 - \| C^h(x^h_{k+1}) \|_{V^*_h}^2 = K(h,k) \eta_{C,h}(x^h_{k+1})(C_1 \eta_{C,h}(x^h_{k+1}) + 2\| C^h(x^h_{k+1}) \|_{V^*_h})
$$

as residual estimator in the norm differences of the constraint with bounded constants \( 1/K \leq K(h,k) \leq K \) for some \( K > 0 \). Then \( \beta(x^h_{k}, s^h_{k}) \) in (3.25) can be computed as

$$
\beta(x^h_{k}, s^h_{k}) = \eta_{C,h}(x^h_{k+1})(C_1 \eta_{C,h}(x^h_{k+1}) + 2\| C^h(x^h_{k+1}) \|_{V^*_h})
$$

$$
\eta_{C,h}(x^h_{k})(C_1 \eta_{C,h}(x^h_{k}) + 2\| C^h(x^h_{k}) \|_{V^*_h})
$$

(3.35)

with appropriate choice of \( C_1 \). Thus, condition (3.26) is implementable in a heuristical version.

Note that using a residual based or averaging error estimator \( \eta_{C,h} \) condition (3.26) with \( \beta(x^h_{k}, s^h_{k}) \) as in (3.35) still contains the important geometrical meaning that the current grid must be good enough to represent the next iterate.
Local refinement strategy. The local refinement strategy is based on element-wise contributions to the error estimators

\[ \eta_{C,h}(\cdot) = \left( \sum_{T \in T_h} \eta_{C,h,T}^2(\cdot) \right)^{1/2} \]
\[ \eta_{g,h}(\cdot) = \left( \sum_{T \in T_h} \eta_{g,h,T}^2(\cdot) \right)^{1/2}. \]

Examples for suitable error estimators will be discussed in section 6. There exist many local refinement strategies to select elements for refinement. Typical examples for refinement strategies are refining the \( p \% \) elements with largest local errors \( \eta_{C,h,T}(\cdot) \) or \( \eta_{g,h,T}(\cdot) \) respectively, or refining where the local contribution to the error estimator is larger than \( p \% \) of the largest local error.

3.2. Multilevel trust–region composite–step SQP algorithm. In this section we state the common assumptions which are necessary for the convergence theory and our multilevel algorithm.

3.2.1. Assumptions. Our convergence theory requires the set of assumptions given below. For all iterations \( k \) we assume that \( x_k^h, x_k^h + s_k \in D \), where \( D \) is an open, convex subset of \( X \).

A.1. The functionals \( f, C \) are twice continuously Fréchet differentiable in \( D \).
A.2. The partial Jacobians \( (C^h_y)_k \) and \( C_y(x^h) \) have an inverse for all \( x^h \in D \).
A.3. The functionals and operators \( f, f_x, f_{xx}, C, (C^h_x), C^h_{xx} \) are bounded in \( D \).

The operators \( (C^h_y)_k^{-1} \) are uniformly bounded in \( D \).
A.4. The sequences \( \{H_k\} \), \( \{W_k\} \) and \( \{\lambda_k^h\} \) are bounded.

We will use the notation \( B_A \) in the convergence theory as a bound for the norm \( \|A\| \) for any quantity \( A \) that is bounded by the assumptions.

3.2.2. Multilevel trust–region composite–step SQP algorithm. We are now in the position to state the complete algorithm.

Algorithm 3.9 (Multilevel trust–region composite–step SQP algorithm).

\begin{align*}
S.0. \text{Initialization:} & \quad \text{Choose } \kappa \in (0, 1), 0 < \nu < 1, p \in (0, 1], \rho_{-1} \geq 1, \varepsilon_{tol} > 0, \\
& \quad 0 < \alpha_0 \leq \alpha_1 < 1 < \alpha_2, 0 < \eta_1 < \eta_2 < 1, 0 < \Delta_{\min} \leq \Delta_{\max}, 0 < \eta_0 < 1 - \eta_1, \\
& \quad \hat{c}_1 \geq 1, \hat{c}_2, \hat{c}_3 > 0, \text{a starting grid denoted by index } h, x_0^h \in X_h, \lambda_0^h \in V_h \text{ and } \\
& \quad \Delta_0 \in [\Delta_{\min}, \Delta_{\max}].
\end{align*}

For \( k = 0, 1, 2, \ldots \).

\begin{align*}
S.1. & \quad \text{Compute a quasi–normal step } s^n_k \text{ as inexact solution of (3.1) satisfying (3.2)}.
\end{align*}
\begin{align*}
S.2. & \quad \text{ Compute an inexact adjoint state } \lambda_{k+1}^h + \Delta \lambda_k \text{ by (3.8) satisfying (3.9) and the inexact reduced gradient } \hat{g}_k^h \text{ by (3.10)}.
\end{align*}
\begin{align*}
S.3. & \quad \text{ If the refinement conditions (3.34b) and (3.34c) for the adjoint equation and the control-gradient hold then goto S.4.. Otherwise refine the } U–\text{grid and the } Y–\text{ and } V–\text{grid (adaptively) and, if (3.2) is satisfied for the prolongated } s^n_k, \\
& \quad \text{ then go to S.2., otherwise go to S.1.}
\end{align*}
\begin{align*}
S.4. & \quad \text{ If the refinement condition (3.34a) for the state equation holds, then go to S.5.. Otherwise refine the } Y–\text{ and } V–\text{grid (adaptively) until (3.34a) is satisfied. If (3.2) and (3.11) hold for the prolongated } s^n_k \text{ and } \hat{g}_k^h, \\
& \quad \text{ then go to S.5.. If (3.11) is not satisfied for the prolongated } \hat{g}_k^h, \text{ then go to S.2.. But if (3.2) is also not satisfied for the prolongated } s^n_k, \text{ then go to S.1.}
\end{align*}
S.5. If \( \| C_h^k \|_{V^*_h} \leq \varepsilon_{tol} \) and \( \| \hat{q}_k \|_{U^*_h} \leq \varepsilon_{tol} \), then stop and return \( x_k^h = (y_k^h, u_k^h) \) as an approximate solution for problem (1.1).

S.6. Compute \( s_{u,k} \) as inexact solution of (3.13) satisfying (3.14).

S.7. Update the penalty parameter according to subsection 3.1.4.

S.8. Compute \( s_{u,k} \) as inexact solution of (3.13) satisfying (3.14).

S.9. Compute \( \text{pred}_h(s_{n,k}, s_{u,k}; \rho_k) \) using (3.17). Update the trust–region radius according to subsection 3.1.5.

If \( \text{ared}_h(s_k; \rho_k) / \text{pred}_h(s_{n,k}, s_{u,k}; \rho_k) < \eta_1 \), then reject \( s_k \) and go back to S.1.

With \( x_k^h \) and \( \lambda_k^h \), else go to S.10.

S.10. If (3.23) is satisfied, then accept \( s_k \) and go to S.1 with \( x_{k+1}^h = x_k^h + s_k \) and \( \lambda_{k+1}^h = \lambda_k^h \). Otherwise reject \( s_k \), refine the \( Y \)- and \( V \)-grid properly and go back to S.1. with \( x_k^h \) and \( \lambda_k^h \).

Remark 3.10.

1. For the convergence theory we need the Lagrange multipliers to be bounded. As stated in the algorithm above we use the adjoint states \( \lambda_k \) as Lagrange multipliers in the Lagrangian function \( l \). If the sequence of adjoint states is not bounded one can distinguish between adjoint states and (different) bounded Lagrange multipliers.

2. Generally, if one refines reasonably, criterion (3.23) is always satisfied and, therefore, S.10. does not need to be implemented.


4.1. Auxiliary estimates. We start with several technical lemmas.

Lemma 4.1. There exists \( \kappa_3 > 0 \) such that for all steps \( s_k^h \) generated by the algorithm the inequality

\[
\| s_k^h \|_X \leq \kappa_3 \| C_h^k \|_{V^*_h}
\]

holds.

Proof. This is an immediate consequence of \( \| (C_h^h)_{y^h} s_{y,k}^h + C_h^h \|_{V^*_h} \leq \| C_h^h \|_{V^*_h} \) and the boundedness of \( (C_h^h)_{y^h}^{-1} \).

Lemma 4.2. There exists \( B_\Delta > 0 \) such that for all steps \( s_k \) generated by the algorithm the inequality \( \| s_k \| \leq B_\Delta \Delta_k \) holds.

Proof. Using \( \| s_k^h \|_Y \leq \Delta_k, \| s_{u,k} \|_U \leq \Delta_k, \) and \( \Delta_k \leq \Delta_{\max} \) together with the definition (3.16) of \( r_k^h \), (3.19) and the boundedness of \( (C_h^h)^{-1}(C_h^u) \), we obtain the desired result.

Lemma 4.3. There exists \( c > 0 \) independent of the grid such that

\[
| -l(x_{k+1}^h, \lambda_k^h) + q_k(s_k) | \leq c \Delta_k^2.
\]

Proof. By the definition (3.3) of \( q_k \) a Taylor expansion of \( l(x_{k+1}^h, \lambda_k^h) \) and Lemma 4.2 yields the desired result.

Lemma 4.4. There exists \( c > 0 \) independent of the grid such that

\[
| -q_k(s_k) + \hat{q}_k(s_{u,k}) | \leq c \Delta_k^{1+r}.
\]

for \( q_k \) and \( \hat{q}_k \) in (3.3), (3.6).
Proof. Recall that, by the definition (3.16) of $r^t_k$,

$$s^t_k = \left( (C^h_y)_k^{-1} r^t_k \right) + W_k s_{u,k}. $$

Using the definitions of $q_k$ and $\hat{q}_k$ in (3.3), (3.6) along with the above equality, we find that

\[-q_k(s_k) + \hat{q}_k(s_{u,k}) = \]

\[= (H_k s^t_k + \ell_r(x^h_k, \lambda^h_k), W_k s_{u,k}) - \langle \ell_r(x^h_k, \lambda^h_k), s^t_k \rangle \]

\[-\frac{1}{2} \langle s^t_k, H_k s^t_k \rangle + \frac{1}{2} \langle W_k s_{u,k}, H_k W_k s_{u,k} \rangle \]

\[= (H_k s^t_k + \ell_r(x^h_k, \lambda^h_k), W_k s_{u,k} - s^t_k) \]

\[-\frac{1}{2} \langle s^t_k, H_k s^t_k \rangle + \frac{1}{2} \langle W_k s_{u,k}, H_k W_k s_{u,k} \rangle \]

\[\leq (B_H \|s^t_k\|_X + B_{V^1})\|W_k s_{u,k} - s^t_k\|_X + \frac{1}{2} B_H \|s^t_k\|_X^2 + \frac{1}{2} B_H B_W^2 \|s_{u,k}\|_U^2. \]

Note that

\[\|s^t_k\|_X \leq \|s^t_k - W_k s_{u,k}\|_X + \|W_k s_{u,k}\|_X \]

\[\leq \|(C^h_y)_k^{-1} c(V^1, s_{u,k})\|_{V^1} + B_W \|s_{u,k}\|_U \]

\[\leq B_{C^{-1}_p} \xi_3 \Delta^1_k + B_W \|s_{u,k}\|_U, \]

where we have used (3.19). Hence, we obtain by using $\Delta_k \leq \Delta_{\text{max}}$

\[\left| -q_k(s_k) + \hat{q}_k(s_{u,k}) \right| \leq \]

\[\leq (B_H \|s^t_k\|_X + B_{V^1})\|(C^h_y)_k^{-1} r^t_k\|_X + \frac{1}{2} B_H \|s^t_k\|_X^2 + \frac{1}{2} B_H B_W^2 \|s_{u,k}\|_U^2 \]

\[\leq (B_H \|s^t_k\|_X + B_{V^1})B_{C^{-1}_p} \xi_3 \Delta^1_k + \frac{1}{2} B_H \left( B_{C^{-1}_p} \xi_3 \Delta^1_k + B_W \|s_{u,k}\|_U \right)^2 \]

\[+ \frac{1}{2} B_H B_W^2 \|s_{u,k}\|_U^2 \]

\[\leq C \Delta^1_k \]

with some constant $C$. The proof is complete. \[\square\]

**Lemma 4.5.** There exists $c > 0$ independent of the grid such that

\[\left| \langle \hat{q}_k^h - W^*_k(q_k), s^t_k \rangle + \frac{1}{2} \langle s_{u,k}, H_k s_{u,k} \rangle - \frac{1}{2} \langle s_{u,k}, W^*_k H_k W_k s_{u,k} \rangle \right| \leq c \Delta^1_k. \]

**Proof.** This is an immediate consequence of (3.11), (3.12), $\Delta_k \leq \Delta_{\text{max}}$ and the assumptions on the boundedness. \[\square\]

**Lemma 4.6.** There exists $c > 0$ independent of the grid such that

\[\langle \Delta^h_{k+1}, -C_{2}^{h,k+1} + (C^h_y)_k s_k + C^h_y \rangle \leq c \Delta^2_k. \]

**Proof.** A Taylor expansion for the constraint together with the boundedness of the Lagrange multipliers yield the desired result. \[\square\]

**Remark 4.7.** For any norm $\| \cdot \|$ on a vectorspace $Z$ and $a, b, c \in Z$ the following inequality holds

\[\|a\|^2 - (\|b\| + \|c\|)^2 = \|a\| - \|b\| - \|c\| \cdot \|a\| + \|b\| + \|c\| \]

\[\leq \left( \|a - b\| + \|c\| \right) \left( \|a\| + \|b\| + \|c\| \right).\]

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Lemma 4.8. There exist \( c_1, c_2 > 0 \) independent of the grid such that

\[
\left| \rho_k \left( \left| C_k^{h+1} \right|^2 - (\left| C_k^h \right| + (C_y^h)_{k} s_{y,k}^n) \left| V^*_k \right| + \left| r^*_k \right| \right)^2 \right| \leq \rho_k c_1 \Delta_k^{1+p} C_k^{h+1} \left| V^*_k \right| + \rho_k c_2 \Delta_k^{2+p}.
\]

Proof. In view of Remark 4.7 we estimate as follows

\[
\left| \left| C_{k+1}^h \right|^2 - \left( \left| C_k^h \right| + (C_y^h)_{k} s_{y,k}^n \left| V^*_k \right| + \left| r^*_k \right| \right)^2 \right| \leq \left( \left| C_{k+1}^h - C_k^h \right| \left| s_{y,k}^n \right| \left| V^*_k \right| + \left| r^*_k \right| \right) \cdot \left( \left| C_{k+1}^h \right| + \left| C_k^h \right| + (C_y^h)_{k} s_{y,k}^n \left| V^*_k \right| + \left| r^*_k \right| \right)
\]

=: \([A] \cdot [B]\).

First, we estimate \([A]\) by using Taylor expansion, \( t \in [0,1], \) and \( (3.19) \). This yields with \( \Delta_k \leq \Delta_{\text{max}} \)

\[
[A] = \left| C_k^h + (C_y^h)_{k} s_{y,k}^n \right| \left| V^*_k \right| - \left| C_k^h \right| \left| s_{y,k}^n \right| \left| V^*_k \right| + \left| r^*_k \right| \left| V^*_k \right|
\]

\[
\leq \left| (C_y^h)_{k} s_{y,k} \left| V^*_k \right| + \left| C_k^h \right| \left| s_{y,k}^n \right| \left| V^*_k \right| + \left| r^*_k \right| \left| V^*_k \right|
\]

\[
\leq \left| C_k^h \right| \left| s_{y,k}^n \right| \left| V^*_k \right| + \left| C_k^h \right| \left| s_{y,k} \right| \left| V^*_k \right| + \left| r^*_k \right| \left| V^*_k \right|
\]

\[
\leq C \Delta_k^{1+p},
\]

for some \( C > 0 \). Now, we estimate \([B]\)

\[
\left| C_k^h + (C_y^h)_{k} s_{y,k}^n \right| \left| V^*_k \right| \leq \left| C_k^h \right| \left| V^*_k \right| + B \left| s_{y,k}^n \right| Y \leq \left| C_k^h \right| \left| V^*_k \right| + C \Delta_k,
\]

for some \( c > 0 \) and by using Lemma 4.2

\[
\left| C_k^h \right| \left| V^*_k \right| = \left| C_k^h \right| + (C_y^h)_{k} \left| s_{y,k} \right| \left| V^*_k \right|
\]

\[
\leq \left| C_k^h \right| \left| V^*_k \right| + B \left| s_{y,k} \right| X \leq \left| C_k^h \right| \left| V^*_k \right| + B \Delta \Delta_k,
\]

for some \( \tau \in [0,1] \). Thus, we obtain \([B] \leq \left| C_k^h \right| \left| V^*_k \right| + C \Delta_k \) for some \( c > 0 \). The estimates on \([A]\) and \([B]\) together imply

\[
[A] \cdot [B] \leq c_1 \Delta_k^{1+p} \left| C_k^h \right| \left| V^*_k \right| + c_2 \Delta_k^{2+p},
\]

for some \( c_1, c_2 > 0 \), which yields the desired result. \( \Box \)

Lemma 4.9. There exist \( K_0, K_1, K_2 > 0 \) independent of the grid such that

\[
(4.1) \quad | \text{pred}_h(x_t^k; \rho_k) - \text{pred}_h(x_t^k; \rho_k^*; s_{u,k}) - \text{pred}_h(x_t^k; \rho_k^*; \rho_k) | \leq K_0 \Delta_k^{1+p} + \rho_k K_1 \Delta_k^{1+p} \left| C_k^h \right| \left| V^*_k \right| + \rho_k K_2 \Delta_k^{2+p}.
\]
\textbf{Proof.} Using the definitions of \textit{ared}_h, \textit{pred}_h, \textit{rpred}_h, q_k, \tilde{q}_k and \hat{m}_h and some simple transformations we obtain

\begin{equation}
|\text{ared}_h(s_k; \rho_k) - \text{pred}_h(s^n_k, s_{u,k}; \rho_k) - \text{rpred}_h(r^*_k; \rho_k)| = \\
= -l(x^h_{k+1}, \lambda^h_k) + q_k(s_k) - q_k(s_k) + \tilde{q}_k(s_{u,k}) \\
+ \langle \hat{g}^h_k - W^*_k(q_k)_y(s^n_k), s_{u,k} \rangle \\
+ \frac{1}{2}(s_{u,k}, H_k s_{u,k}) - \frac{1}{2}(s_{u,k}, W^*_k H_k W_k s_{u,k}) \\
+ (\Delta \lambda^h_k, -C^h_{k+1} + (C^h_x)_k s_k + C^h_k) \\
- \rho_k \left( ||C^h_{k+1}||_{V^*_h}^2 - (||C^h_k||_{V^*_h} + \|r^*_k\|_{V^*_h})^2 \right)
\end{equation}

(4.2)

The asserted estimate follows now from the triangle inequality together with Lemmas 4.3, 4.4, 4.5, 4.6 and \(\Delta_k \leq \Delta_{\max}\). \(\Box\)

\textbf{4.2. Acceptance of steps.} We show now that there will always be a successful step on a fixed grid after finitely many iterations. Together with Remark 3.7, which states that the refinement conditions (3.34) can always be satisfied by sufficient refinement, this shows that the algorithm is well defined. We start with an auxiliary lemma.

\textbf{Lemma 4.10.} Let \(\Delta_k \leq \min \{ \delta, (\delta ||C^h_k||_{V^*_h})^{\frac{2}{p+2}} \} \) with \(0 < \delta < \min \{B^{-1}_C, 1 \} \).

Then the following inequalities hold:

(i) \(||C^h_k||_{V^*_h}^{\Delta_k + p} \leq ||C^h_k||_{V^*_h} \delta^p \min \{ \Delta_k, ||C^h_k||_{V^*_h} \} \),

(ii) \(\Delta_k^{p+2} \leq \delta \min \{ \Delta_k, ||C^h_k||_{V^*_h} \} \).

Proof. These estimates follow quite directly from the assumptions. \(\Box\)

\textbf{Lemma 4.11.} Let \(\varepsilon > 0\), then there exists a constant \(\delta > 0\) which depends on \(\varepsilon\) but not on \(||C^h_k||_{V^*_h}\) such that if

\[ ||C^h_k||_{V^*_h} + \|\hat{g}^h_k\|_{U^*_k} \geq \varepsilon, \]

then

\[ \frac{\text{ared}_h(s_k; \rho_k)}{\text{pred}_h(s^n_k, s_{u,k}; \rho_k)} \geq \eta \]

for \(\Delta_k \leq \min \{ \delta, \max \{ (\delta ||C^h_k||_{V^*_h})^{\frac{2}{p+2}}, (\delta \rho_k)^{\frac{2}{p}} \} \} \). In particular, the step \(s_k\) will be accepted and \(\Delta_{k+1} \geq \Delta_k\).

Proof. Using the triangle inequality and (3.18) we see that

\[ \left| \frac{\text{ared}_h(s_k; \rho_k)}{\text{pred}_h(s^n_k, s_{u,k}; \rho_k)} - 1 \right| \leq \frac{||\text{ared}_h(s_k; \rho_k) - \text{pred}_h(s^n_k, s_{u,k}; \rho_k) - \text{rpred}_h(r^*_k; \rho_k)||}{\text{pred}_h(s^n_k, s_{u,k}; \rho_k)} + \eta_0. \]

By the choice of the penalty parameter and by the decrease conditions (3.14) and (3.2), we obtain

\[ \text{pred}_h(s^n_k, s_{u,k}; \rho_k) \geq \kappa \kappa_4 \|\hat{g}^h_k\|_{U^*_k} \min \{ \kappa_5 ||\hat{g}^h_k||_{U^*_k}, \kappa_6 \Delta_k \} \]

\[ + \frac{\rho_k}{2} \|C^h_k||_{V^*_h} \min \{ \kappa_2 ||C^h_k||_{V^*_h}, \Delta_k \}. \]

Then there exists \(\tilde{K} > 0\) (depending on \(\rho_0\)) such that

\[ \text{pred}_h(s^n_k, s_{u,k}; \rho_k) \geq \tilde{K} \varepsilon \min \{ \varepsilon, \Delta_k \} + \tilde{K} \rho_k ||C^h_k||_{V^*_h} \min \{ ||C^h_k||_{V^*_h}, \Delta_k \}. \]
For the right hand side of inequality (4.1) from Lemma 4.9 we obtain
\[ K_0 \Delta_k^{1+p} + \rho_k K_1 \Delta_k^{1+p} \| C^h_k \|_{V^*_k} + \rho_k K_2 \Delta_k^{1+p} \leq \Delta_k^{1+p} \rho_k c, \]
for some \( c \geq 1 \). Now choose \( \delta_1 < \min \{ (1-\eta_1-\eta_0) \bar{K} \varepsilon, \varepsilon \} \) and let \( \Delta_k \leq \min \left\{ \left( \frac{\delta_1}{\rho_k c} \right)^{\frac{1}{p}}, \delta_1 \right\} \).

Then we obtain by using Lemma 4.9 and the previous inequalities
\[
\left| \frac{\text{ared}_k(s_k; \rho_k)}{\text{pred}_k(s^n_k, s_{u,k}; \rho_k)} - 1 \right| \leq \frac{\Delta_k^{1+p} \rho_k c}{K \varepsilon \Delta_k} + \eta_0 \leq 1 - \eta_1.
\]

Thus, the above chosen \( \Delta_k \) guarantees a successful step.

Now we consider the second part of the maximum in the lemma. Choose \( \delta_2 < \min \left\{ \left( \frac{1-\eta_1-\eta_0}{K} \right)^{\frac{1}{p}}, B_C^{-1}, 1 \right\} \) with \( \bar{K} = \frac{\max \{ K_0, 2K_1, 2K_2 \} }{\min \{ K, K\varepsilon \} } \) and let \( B_C \) be the bound on the norm of the constraint. Let \( \Delta_k \leq \min \left\{ (\delta_2 \| C^h_k \|_{V^*_k})^{\frac{p}{p+1}}, \delta_2 \right\} \), then we obtain by using Lemma 4.10 with \( \delta = \delta_2 \)
\[
\left| \frac{\text{ared}_k(s_k; \rho_k)}{\text{pred}_k(s^n_k, s_{u,k}; \rho_k)} - 1 \right| \leq \eta_0 + \frac{K_0 \Delta_k^{1+p} + \rho_k (K_1 \Delta_k^{1+p} \| C^h_k \|_{V^*_k} + K_2 \Delta_k^{2+p})}{K \varepsilon \Delta_k + \bar{K} \rho_k \| C^h_k \|_{V^*_k} \min \{ \Delta_k, \| C^h_k \|_{V^*_k} \} } \\
\leq \eta_0 + \frac{K_0 \Delta_k \delta_2^p + \rho_k \max \{ K_1, K_2 \} (\delta_2 + \delta_2^p) \| C^h_k \|_{V^*_k} \min \{ \Delta_k, \| C^h_k \|_{V^*_k} \} }{K \varepsilon \Delta_k + \bar{K} \rho_k \| C^h_k \|_{V^*_k} \min \{ \Delta_k, \| C^h_k \|_{V^*_k} \} } \\
\leq \eta_0 + \delta_2^p \bar{K} \frac{\Delta_k + \rho_k \| C^h_k \|_{V^*_k} \min \{ \Delta_k, \| C^h_k \|_{V^*_k} \} }{\Delta_k + \rho_k \| C^h_k \|_{V^*_k} \min \{ \Delta_k, \| C^h_k \|_{V^*_k} \} } \\
\leq \eta_0 + \bar{K} \frac{1 - \eta_1 - \eta_0}{K} = 1 - \eta_1.
\]

Thus, the step will be accepted. Now, we define \( \delta := \min \{ \delta_2, \delta_1/c \} \) and the proof is complete. \( \square \)

4.3. Penalty parameter. We study next the behaviour of the penalty parameter.

Lemma 4.12. Under the problem assumptions, there exists a constant \( K > 0 \) independent of the iterates such that
\[
q_k(0) - q_k(s^n_k) - \langle \Delta \lambda_k^h, (C^h_y)_k s^n_{y,k} + C^h_k \rangle \geq -K \| C^h_k \|_{V^*_k}.
\]

Proof. This result follows similarly as in [13, Lem. 7.3]. \( \square \)

Lemma 4.13. Let \( \varepsilon > 0 \) and assume that
\[
\| C^h_k \|_{V^*_k} + \| g^h_k \|_{V^*_k} \geq \varepsilon \quad \forall k \in \mathbb{N}.
\]

Then there exists \( \rho^* > 0 \) and \( K \in \mathbb{N} \) such that \( \rho_k = \rho^* \) for all \( k \geq K \).
Proof. Otherwise, we obtain \( \rho_k \to \infty \). Set \( \mathcal{M} := \{ k \in \mathbb{N} : \rho_k > \rho_{k-1} \} \) and consider \( k \in \mathcal{M} \). Then (3.21) is not valid. This implies

\[
q_k(0) - q_k(s^n_k) - (\Delta M_k, (C^h_k)_k s^n_{y,k} + C^h_k) \\
\leq (\kappa - 1) \left( m_k(0) - m_k(s_{u,k}) \right) \\
= -\frac{\rho_k-1}{2} \left( \|C^h_k\|_{V^*_h}^2 - \|(C^h_k)_k s^n_{y,k} + C^h_k\|_{V^*_h}^2 \right) \\
\leq 0.
\]

(4.3)

By Lemma 4.12, the left hand side of the above inequality is \( \geq -K\|C^h_k\|_{V^*_h} \). Thus, (4.3) and (3.2) imply

\[
-K\|C^h_k\|_{V^*_h} \leq -\frac{\rho_k-1}{2} \|C^h_k\|_{V^*_h} \min \{ \kappa_2, \|C^h_k\|_{V^*_h}, \Delta_k \}.
\]

If \( \|C^h_k\|_{V^*_h} = 0 \), then \( \min \{ \|C^h_k\|_{V^*_h}, \Delta_k \} = 0 \). Otherwise the previous inequality yields a constant \( C_\rho > 0 \) such that

\[
C_\rho \geq \rho_{k-1} \min \{ \|C^h_k\|_{V^*_h}, \Delta_k \}.
\]

Since \( \rho_k \to \infty \), this shows \( \min \{ \|C^h_k\|_{V^*_h}, \Delta_k \} \to 0 \). On the other hand, by Lemma 4.11 and the update rule for the trust–region radius, we obtain

\[
\Delta_k \geq \alpha_0 \min \left\{ \delta, \max \left\{ (\delta\|C^h_k\|_{V^*_h})^2, \left( \frac{1}{\rho_k} \right)^{\frac{1}{2}} \right\} \right\}.
\]

(4.4)

This yields \( \{ \|C^h_k\|_{V^*_h} \}_{k \in \mathcal{M}} \to 0 \). Consequently, for all \( k \in \mathcal{M} \) large enough, we get \( \|\hat{g}^h_k\|_{U^*_h} \geq \frac{\delta}{2} \). If (3.21) does not hold, then by (4.3) and (3.14) we obtain

\[
-K\|C^h_k\|_{V^*_h} \leq -(1 - \kappa) \|\hat{g}^h_k\|_{U^*_h} \min \{ \kappa_3, \|\hat{g}^h_k\|_{U^*_h}, \kappa_4 \Delta^p_k \}.
\]

Consequently, there exists \( c > 0 \) such that \( c\|C^h_k\|_{V^*_h} \geq \frac{\delta}{2} \min \{ \frac{\delta}{2}, \Delta^p_k \} \).

Since \( \{ \|C^h_k\|_{V^*_h} \}_{k \in \mathcal{M}} \to 0 \), this requires

\[
\Delta^p_k \leq \frac{2c}{\varepsilon}\|C^h_k\|_{V^*_h} \quad \forall k \in \mathcal{M}, \quad k \geq k_0 \in \mathbb{N}.
\]

Hence, by (4.4), we obtain

\[
\left( \frac{2c}{\varepsilon} \right)^{\frac{1}{2}} \|C^h_k\|_{V^*_h}^2 \geq \Delta_k \geq \alpha_0 \min \left\{ \delta, \max \left\{ (\delta\|C^h_k\|_{V^*_h})^2, \left( \frac{1}{\rho_k} \right)^{\frac{1}{2}} \right\} \right\}.
\]

If \( \|C^h_k\|_{V^*_h} = 0 \), this leads to the contradiction \( 0 \geq \min \{ \delta, (\delta/\rho_k)^{\frac{1}{2}} \} > 0 \). Thus, \( \|C^h_k\|_{V^*_h} > 0 \) holds, implying

\[
\left( \frac{2c}{\varepsilon} \right)^{\frac{1}{2}} \|C^h_k\|_{V^*_h}^2 \geq \alpha_0 \min \left\{ \delta, \delta \frac{2}{\rho_k} \|C^h_k\|_{V^*_h}^2 \right\},
\]

which contradicts \( \{ \|C^h_k\|_{V^*_h} \}_{k \in \mathcal{M}} \to 0 \). Consequently, the sequence of penalty parameters \( \{ \rho_k \} \) is bounded. Moreover, the update rule for the penalty parameter implies that there exists \( \rho^* > 0 \) and \( K \in \mathbb{N} \) such that \( \rho_k = \rho^* \) for all \( k \geq K \). \( \Box \)
4.4. Global convergence result. We show now global convergence to a stationary point of the infinite dimensional problem (1.1) if $\varepsilon_{\text{tol}} = 0$ or finite termination if $\varepsilon_{\text{tol}} > 0$ respectively. We start with the following result.

**Theorem 4.14.** Let the assumptions A.1., A.2., A.3. and A.4. hold. If $\varepsilon_{\text{tol}} = 0$ then the algorithm terminates finitely or the sequence of iterates generated by algorithm 3.9 satisfies

$$
\liminf_{k \to \infty} (\|C_k^h\|_{V_k^*} + \|g_k^h\|_{U_k^*}) = 0.
$$

For $\varepsilon_{\text{tol}} > 0$ the algorithm terminates finitely with $\|C_k^h\|_{V_k^*} \leq \varepsilon_{\text{tol}}$ and $\|g_k^h\|_{U_k^*} \leq \varepsilon_{\text{tol}}$.

**Proof.** Suppose not, then the algorithm runs infinitely and there exists $\varepsilon > 0$ such that

$$
\|C_k^h\|_{V_k^*} + \|g_k^h\|_{U_k^*} \geq \varepsilon \quad \forall k \in \mathbb{N}.
$$

Then, by Lemma 4.13, $\rho_k$ equals $\rho^*$ for all $k \geq K$ for some $K \in \mathbb{N}$. Let $S$ be the set of indices of accepted steps. By Lemma 4.11, there exists $\delta > 0$ such that for all accepted steps, $k \in S$, we obtain

$$
(4.5) \quad \Delta_k \geq \alpha_0 \min \left\{ \delta, \max \left\{ \left( \delta \|C_k^h\|_{V_k^*} \right)^{\frac{1}{\gamma_1}}, \left( \frac{\delta}{\rho^*} \right)^{\frac{1}{\gamma_2}} \right\} \right\} \geq \alpha_0 \min \left\{ \delta, \left( \frac{\delta}{\rho^*} \right)^{\frac{1}{\gamma_2}} \right\} =: \Delta_\ast.
$$

Moreover, for all $k \in S$ with $k \geq K$ we get by the decrease conditions (3.14) and (3.2)

$$
(4.6) \quad \text{ared}_h(s_k; \rho_k) \geq \eta_1 \text{pred}_h(s_k^a, s_{u,k}; \rho^*)
$$

$$
\geq \eta_1 \kappa_4 \|g_k^h\|_{U_k^*} \min \{ \kappa_5 \|g_k^h\|_{U_k^*}, \kappa_6 \Delta_\ast \}
$$

$$
+ \eta_2 \kappa_1 \|C_k^h\|_{V_k^*} \min \{ \kappa_2 \|C_k^h\|_{V_k^*}, \Delta_\ast \}.
$$

Let us define the infinite dimensional augmented Lagrangian function $L$ and the infinite dimensional actual reduction $\text{ared}^\infty$ by

$$
L(x, \lambda; \rho) := l(x, \lambda) + \rho \|C(x)\|_{V'}^2,
$$

$$
\text{ared}^\infty(s_k; \rho_k) := L(x_k^h, \lambda_k^h; \rho_k) - L(x_k^h + s_k, \lambda_{k+1}^h; \rho_k).
$$

The condition (3.23) for reasonable refinement yields

$$
\text{ared}_h(s_k; \rho_k) = \frac{\delta}{1+\delta} \text{ared}_h(s_k; \rho_k) + \frac{1}{1+\delta} \text{ared}_h(s_k; \rho_k)
$$

$$
\geq \frac{\delta}{1+\delta} \text{ared}_h(s_k; \rho_k) + \rho_k \left( \|C(x_{k+1}^h)\|_{V'}^2 - \|C_{h(k)}(x_{k+1}^h)\|_{V'_{h(k)}}^2 \right)
$$

$$
- \left( \|C(x_k^h)\|_{V'}^2 - \|C_{h(k)}(x_k^h)\|_{V'_{h(k)}}^2 \right) .
$$

Hence, using this inequality we obtain

$$
\text{ared}^\infty(s_k; \rho_k) \geq \frac{\delta}{1+\delta} \text{ared}_h(s_k; \rho_k) \geq \frac{\delta}{1+\delta} \eta_1 \text{pred}_h(s_k^a, s_{u,k}; \rho_k)
$$

since we assume conform discretizations and, thus, $l^h(x_k^h, \lambda_k^h) = l(x_k^h, \lambda_k^h)$ holds. Now, by assumption, $L$ is bounded from below. Summation of the infinite dimensional
actual reduction in the successive steps \( k \in S \) gives

\[
\sum_{k \in S} \text{ared}^{\infty}(s_k; \rho_k) = \sum_{k \in S} (L(x^h_k, \lambda^h_k; \rho_k) - L(x^h_{k+1}, \lambda^h_{k+1}; \rho_k))
\]

\[
= C + \sum_{S \ni k \geq K} (L(x^h_k, \lambda^h_k; \rho^*) - L(x^h_{k+1}, \lambda^h_{k+1}; \rho^*))
\]

\[
= C + L(x^h_K, \lambda^h_K; \rho^*) - \lim_{k \to \infty} L(x^h_{k+1}, \lambda^h_{k+1}; \rho^*) < \infty.
\]

Hence, by the summability, we obtain \( \text{ared}^{\infty}(s_k; \rho_k) \to 0 \) as \( S \ni k \to \infty \) which implies, by (4.5), (4.6), and (4.7) that \( \|C^h_k\|_{V^*_k} + \|\hat{g}^h_k\|_{U^*_k} \to 0 \). This contradicts our assumption from the beginning of the proof. \( \square \)

The following theorem states that there exists a subsequence of the iterates that satisfies the first–order necessary optimality conditions (cf. (2.2)) of the given problem (1.1) in the limit if \( \varepsilon_{tol} = 0 \).

**Theorem 4.15.** Let the assumptions A.1., A.2., A.3. and A.4. hold. Then for \( \varepsilon_{tol} > 0 \) the algorithm terminates finitely and for \( \varepsilon_{tol} = 0 \) the algorithm terminates finitely with a stationary point of problem (1.1) or the sequence of iterates \( (x^h_k, \lambda^h_{k+1}) \) generated by algorithm 3.9 satisfies

\[
\lim_{k \to \infty} (\|l_y(x^h_k, \lambda^h_{k+1})\|_{Y^*} + \|l_u(x^h_k, \lambda^h_{k+1})\|_{U^*} + \|C^h_k\|_{Y^*}) = 0.
\]

**Proof.** Using the convergence conditions (3.34) with \( \varepsilon_{tol} = 0 \) together with (3.28) for the adjoint equation and (3.32) for the \( u \)-gradient of the Lagrangian this is an immediate result of Theorem 4.14. \( \square \)

5. **Implementation.**

5.1. **Computation of norms.**

**Norms in the control space.** Let \( M = M_{U^h} \) denote the matrix (mass matrix if \( U = L^2 \) \( M = ((\psi_i, \psi_j)_U)_{i,j} \) for the basis \( \psi_i \) of \( U^h \) where \( (\cdot, \cdot)_U \) is the inner product in the Hilbert space \( U \). Then functions \( u^h \in U^h \) have the representation

\[
u^h = \sum u_i \psi_i =: \Psi^h u \quad \text{and we may identify} \quad U^h \text{ with the Hilbert space} \quad (\mathbb{R}^d, (\cdot, \cdot)_M),
\]

where the scalar product is given by \( (\bar{u}, \bar{v})_M = \bar{u}^T M \bar{v} \) and \( \|\bar{u}\|_M = \sqrt{\bar{u}^T M \bar{u}} \) is the induced norm. Then for any \( u^h = \Psi^h \bar{u} \in U^h \)

\[
\|u^h\|_U = \|u^h\|_{U^h} = \|\bar{u}\|_M.
\]

Furthermore, by the Riesz representation theorem the dual space \( U^*_h \) can be identified with \( U_h \), i.e., all functionals \( u^*_h \in U^*_h = U_h \) are given by

\[
\langle u^*_h, u^h \rangle_{U^*_h, U_h} = (u^*_h, u^h)_{U_h} = (u^*_h, u^h) = (\bar{u}^*, \bar{u})_M,
\]

\[
\|u^*_h\|_{U^*_h} = \|u^*_h\|_{U_h} = \|\bar{u}^*\|_M,
\]

where \( u^*_h = \Psi^h \bar{u}^* \). If, moreover, \( u^*_h \in U^*_h \) is given by \( u^h = \Psi^h \bar{u} \mapsto \bar{u}^T \bar{u} \) (which is e.g. the case for the euclidean representation of the reduced gradient) then \( u^*_h \) has the representation \( u^*_h = \Psi^h (M^{-T} \bar{u}) \in U_h \), since

\[
\langle u^*_h, u^h \rangle_{U^*_h, U_h} = \bar{u}^T \bar{u} = (M^{-T} \bar{u}, \bar{u})_M
\]

and one has

\[
\|u^*_h\|_{U^*_h} = \|\bar{u}^*\|_M = \|M^{-T} \bar{u}\|_M = \|\bar{u}\|_{M^{-T}}.
\]

In this way one can in particular compute a discrete representation and discrete norm of gradients in \( U^*_h = U_h \) that are appropriate in the function space setting.
Norms in state space and test function space. If \( Y \) and \( V \) are Hilbert spaces then the discrete norms \( \| \cdot \|_Y \), \( \| \cdot \|_V \), \( \| \cdot \|_V^* \) can be computed analogously as for the control space, where now \( M_Y = ((\psi_i, \psi_j)_Y)_{i,j} \) for the basis \( \{ \psi_i \} \) of \( Y_h \) and \( M_V = ((\psi_i, \psi_j)_V)_{i,j} \) for the basis \( \{ \psi_i \} \) of \( V_h \) have to be used instead of \( M_{U_h} \). In particular, the discrete norm of the residual in the constraint \( \| C_h \|_{V^*} \) can be computed. In the case \( Y = H^1_0(\Omega) \) the matrix \( M_Y \) is the sum of the usual stiffness and mass matrices. Often a spectrally equivalent (independent of the mesh size) matrix \( M_Y \) is used to reduce the costs for computing \( \| \cdot \|_Y \), \( \| \cdot \|_{V^*} \).

5.2. Computation of the quasi–normal component. The quasi–normal component \( s_h^k \) is an approximate solution of the trust–region subproblem (3.1) and it is required to satisfy (3.2).

One method to guarantee (3.2) is to use scaled approximate solutions which may be produced by the following simple procedure.

Apply an appropriate iterative solver for the linearized state equation \( (C_h^k)z^n = -C_h^k \) until with a fixed \( \nu \in (0,1) \) the stopping criterion holds

\[
\| (C_h^k)z^n + C^h_{k}\|_{V^*} \leq \nu \| C_h^k \|_{V^*}.
\]

Then scale this step back into the trust–region, i.e., set

\[
s_h^n = \left( \begin{array}{c} t_kz^n \\ 0 \end{array} \right), \quad \text{where} \quad t_k = \begin{cases} 1 & \text{if } \| z^n \|_Y \leq \Delta_k, \\ \Delta_k/\| z^n \|_Y & \text{otherwise}. \end{cases}
\]

The step \( s_h^n \) satisfies (3.2) (see Lemma 6.3.3 in [31]).

5.3. Computation of the tangential component.

5.3.1. Computation of the \( u \)–component of the tangential step. The \( u \)–component \( s_{u,k} \) of the tangential step \( s_h^k \) is an approximate solution of the trust–region subproblem (3.13) that is required to satisfy the fraction of Cauchy decrease condition (3.14).

As in section 5.1 denote by \( U_h \) the basis of \( U_h \) and by \( M = M_{U_h} \) the corresponding mass matrix. Since \( U_h \) is a Hilbert space, we may use the identification \( U^n_h = U_h \).

Then \( \tilde{g}^k_h \in U^n_h = U_h \) is given by \( \langle \tilde{g}^k_h, \cdot \rangle_{U_h} \), and \( -\tilde{g}^k_h \) is the steepest descent direction of \( \hat{m}_k \) in \( U_h \) at \( s_u = 0 \). It is well known that the decrease condition (3.14) can be ensured as long as \( s_{u,k} \) provides at least a fixed fraction of the decrease provided by the Cauchy point

\[
s_{u,k} = \arg\min \{ \hat{m}_k(s_u) : s_u = -t\tilde{g}_k, t \geq 0 \text{ and } \| s_u \|_{U_h} \leq \Delta_k \}.
\]

As described in section 5.1 \( U_h \) can be identified via the coordinate representation \( U_h \cong u^h = \Psi_h \bar{u} \) with the Hilbert space \((\mathbb{R}^l, (\cdot, \cdot)_M)\).

In practice, \( \hat{m}_k \) is given by its coordinate representation \( \hat{m}_k(\bar{s}_u) := \hat{m}_k(\Psi_h \bar{s}_u) \).

Then the correctly scaled steepest descent direction is given by \( -M^{-t} \nabla_{\bar{s}_u} \hat{m}_k(0) \) (not by the euclidean gradient representation \( -\nabla_{\bar{s}_u} \hat{m}_k(0) \)).

An approximate solution of (3.13) that satisfies (3.14) can be computed, e.g., by using the conjugate gradient (cg) method applied to \( \hat{m}_k(s_u) \) in the space \( U_h \) with scalar product \((\cdot, \cdot)_{U_h}\), or equivalently to \( \hat{m}_k(\bar{s}_u) \) in the space \((\mathbb{R}^l, (\cdot, \cdot)_M)\). Here the cg method with starting point \( s_u = 0 \) is applied to the minimization of \( \hat{m}_k \). The cg method is stopped if an approximate minimum of the quadratic model \( \hat{m}_k \) is reached, if negative curvature is detected, or if the iterates leave the trust–region bound. The
first iterate in the steihaug cg method is the Cauchy-step. Note that it is essential
to apply the cg-method with the scalar product \((\cdot,\cdot)_{V_h}\) in order to work with the
correct scaling and discrete norms. If \(\hat{H}_k\) can be applied exactly – which is usually
not realistic if the exact reduced Hessian \(\hat{H}_k = W_k^T H_k W_k\) is used –, then the cg
method ensures that \(\hat{m}_k\) decreases monotonically, and (3.14) remains satisfied for all
Steihaug cg iterates. If \(\hat{H}_k\) is applied inexactly, then one has to compare the function
values \(\hat{m}_k\) at the first Steihaug cg iterate and at the final Steihaug cg iterate.

Another possibility to compute steps is the application of suitable Krylov solvers
to the KKT system of the tangential problem (3.4). In that case the accuracy condi-
tions for the \(y\)-component of the tangential step (3.18) and (3.19) can be integrated in
the solver. If the exact Hessian is \(H_k\) available this method in combination with pre-
conditioners as suggested in [5] leads usually to very good steps after a few iterations
on the linear system.

5.3.2. Computation of the \(y\)–component of the tangential step. We
have already shown that (3.18) and (3.19) are satisfied if
\[ s_{y,k}^t \text{satisfies } \langle C(y)_{k} s_{y,k}^t \rangle_{V_h^*} = \langle C(y)_{k} s_{u,k} + r_{k}^t \rangle_{V_h^*} \]
with residual
\[ \|r_{k}^t\|_{V_h^*} \leq \min \left\{ \xi_3 \Delta_{k}^{1+p}, -\sigma + \sqrt{\sigma^2 + \eta_0 \text{pred}_h(s_{y,k}^n, s_{u,k}; \rho_k)}/\rho_k \right\}, \]
where \(\sigma = \| (C(y)_{k} s_{y,k}^n + C_{k}^* \|_{V_h^*} + \| \Delta \lambda_{k}^n \|_{V}/(2\rho_k) \). Note that all the quantities on
the right hand side of the above inequality are known by the time
\(s_{y,k}^t\) needs to be computed. Any iterative solver for the linearized state equation can be applied until
the stopping criterion ist satisfied.

6. A Posteriori Error Estimators for Inexact States and Adjoints. In
this section we show for a general semilinear elliptic PDE how the required estimates
(3.33) of the infinite dimensional residual norm in the weak formulation of the PDE
and adjoint PDE can be implemented by using well known a posteriori error estima-
tors.

We consider the following problem
\[ -\Delta y + s(y) = f \quad \text{in } \Omega \]
\[ \frac{\partial y}{\partial \nu} = g \quad \text{on } \Gamma_N \]
\[ y = 0 \quad \text{on } \Gamma_D \]
where \(\Omega \subset \mathbb{R}^2\) is an open polygonal domain with boundary \(\partial \Omega\) whose boundary
edges are partitioned into a Neumann part \(\Gamma_N\) and a disjoint Dirichlet part \(\Gamma_D\),
\(\partial \Omega = \Gamma_N \cup \Gamma_D\), \(s(y)\) denotes a (nonlinear) operator \(s : Y \to L^2(\Omega), f \in L^2(\Omega), \)
g \in \(L^2(\Gamma_N), \) and \(\frac{\partial y}{\partial \nu}\) denotes the normal derivative of \(y\) with the outer unit normal
vector field \(\nu\) of \(\partial \Omega\).

Typical examples for the control action are distributed control, i.e., \(u = f\), and
Neumann boundary control, i.e., \(u = g\).

We use the notation \(C(y) = 0\) for the weak formulation of the PDE
\[ \langle C(y), v \rangle_{V^*,V} = \langle \nabla y, \nabla v \rangle_{L^2(\Omega)} + \langle s(y), v \rangle_{L^2(\Omega)} - \langle f, v \rangle_{L^2(\Omega)} - \langle g, v \rangle_{L^2(\Gamma_N)} \]
We set \(Y = V = H^1_D(\Omega) := \{ y \in H^1(\Omega) : y|_{\Gamma_D} = 0 \} \) and assume that the given PDE
has a unique solution. See [21, 27] for sufficient assumptions on \(s(y)\). For example
in the case \( s(y) = y^3 \), as occurring in the following examples, the theory of maximal monotone operators guarantees a unique solution operator \((f, g) \in L^2(\Omega) \times L^2(\Gamma_N) \mapsto y \in Y\) for this PDE that is locally bounded, see for example [21, 27].

We discretize the problem by using a finite element method on a regular triangulation \( T_h \) of \( \Omega \) consisting of closed triangles \( T \) and choose the standard finite element space

\[
Y_h = V_h := \{ y^h \in C(\Omega) : \ y^h|_T \in \mathcal{P}_k(T), \ \forall T \in T_h \},
\]

where \( \mathcal{P}_k(T) \) denotes the space of polynomials of degree \( \leq k \). Then the discretized constraint is given by

\[
\langle C^h(y^h), v^h \rangle_{V^*_h,V_h} = (\nabla y^h, \nabla v^h)_{L^2(\Omega)} + (s(y^h), v^h)_{L^2(\Omega)} - (f, v^h)_{L^2(\Gamma_N)} - (g, v^h)_{L^2(\Gamma_N)}.
\]

Now let \( y^h \in Y_h \) be a possibly inexact solution of the finite element discretization. We want to estimate the residual \( \| C(y^h) \|_{V^*} \). The desired estimate \((3.33a)\) is then

\[
\| C(y^h) \|_{V^*} \leq C_1 \eta(y^h) + C_2 \| C^h(y^h) \|_{V^*_h}
\]

for some bounded constants \( C_1, C_2 > 0 \). As we consider this general semilinear case the results can be applied not only to the state equation but also to the corresponding estimate \((3.33b)\) for the adjoint equation.

We consider both averaging and residual based error estimation techniques. As we will see these well known a posteriori error estimators can be used in our context.

**Triangulation and Notation.** We will use the following notation for the triangulation. Let as already introduced \( T_h \) denote a triangulation of the computational domain \( \Omega \subset \mathbb{R}^2 \) consisting of closed triangles \( T \). Let \( \mathcal{N} \) denote the set of nodes (i.e. the vertices of elements of the triangulation \( T_h \)) and let \( \mathcal{E} \) denote the edges in \( T_h \). Let \( \mathcal{E}_\Omega = \mathcal{E} \setminus \{ E \in \mathcal{E}, E \subset \partial \Omega \} \) denote the inner edges in \( \Omega \). We assume that the edges can be partitioned into the Neumann edges \( \mathcal{E}_\mathcal{N} = \{ E \in \mathcal{E}, E \subset \Gamma_N \} \) and the Dirichlet edges \( \mathcal{E}_D \). For any node \( z \in \mathcal{N} \) we define the patch around \( z \) as \( \omega_z := \text{int}(\cup \{ T \in T_h : z \in T \}) \). Moreover, let \( \omega_T \) denote the patch around a triangle \( T \in T_h \) and let \( \omega_E \) be the union of those two triangles that share the edge \( E \in \mathcal{E} \). Let \( h_T \) and \( h_E \) be \( h_T \)– and \( \mathcal{E} \)–piecewise constants on \( \Omega \) defined by \( h_T|_T := h_T := \text{diam}(T) \) and \( h_E|_E := h_E := \text{diam}(E) \) for \( T \in T_h \) and \( E \in \mathcal{E} \), respectively. Finally, let \( h_z = \text{diam}(\omega_z) \) for \( z \in \mathcal{N} \) and denote by \( \mathcal{K} := \mathcal{N} \setminus \Gamma_D \) the set of free nodes.

**6.1. Averaging Error Estimators for Inexact States.** Averaging techniques, also called (gradient) recovery estimators, estimate the energy error \( \| \nabla y - \nabla y^h \|_{L^2(\Omega)} \) by \( \| q^h - \nabla y^h \|_{L^2(\Omega)} \), where \( q^h \) is generated from postprocessing \( p^h := \nabla y^h \) such that it is a "higher order" approximation of \( \nabla y \) than \( p^h \). In global averaging techniques the procedure consists in approximating the piecewise smooth discontinuous function \( p^h = \nabla y^h \) by some globally continuous function \( q^h = A(p^h) \), which is piecewise a polynomial of higher degree. A well known example is the ZZ-estimator of Zienkiewicz and Zhu [32] that will be discussed below.

In local averaging techniques \( p^h = \nabla y^h \) is locally approximated on patches \( \omega \) by polynomials of higher order.

**6.1.1. Averaging Error Estimator for Linear Finite Elements.** Consider the linear finite element space

\[
Y_h = V_h = Q := \{ y^h \in C(\Omega) : \ y^h|_T \in \mathcal{P}_1(T), \ \forall T \in T_h, \ y^h|_{\Gamma_D} = 0 \}.
\]
Let \( y^h \in Y_h \) and \( p^h = \nabla y^h \) be its piecewise constant gradient. Define the average \( A_z p^h := \int_{\omega_z} p^h \, dx/|\omega_z| \in \mathbb{R}^2 \) of \( p^h \) on \( \omega_z \). With the nodal basis function \( \varphi \) (defined as \( \varphi \) continuous, piecewise linear, \( \varphi_z(z) = 1 \) and \( \varphi_z(x) = 0 \) for all \( x \in N \setminus \{ z \} \)) define

\[
A(p^h) := \sum_{z \in N} (A_z p^h) \varphi_z \in Q \times Q.
\]

Then the averaging estimator is defined by

\[
\eta_A(y^h) := \| \nabla y^h - A(y^h) \|_{L^2(\Omega)^2}.
\]

Notice that there is a minimal version

\[
\eta_M(y^h) := \min_{q \in Q} \| \nabla y^h - q \|_{L^2(\Omega)^2} \leq \eta_A(y^h).
\]

**Remark 6.1.**

1. \( \eta_A \) is a reliable and efficient error estimator for the energy norm of the difference of the smooth solution \( y \) of the weak formulation of the Poisson problem and its first order finite element approximation \( y^h, \| \nabla y - \nabla y^h \|_{L^2(\Omega)^2} \), (cf. [9, 5.5]).

2. Following Brenner and Carstensen in [9], \( \eta_A \) and \( \eta_M \) are very close and accurate estimators in many numerical examples.

3. Note that the averaging estimator \( \eta_A \) is locally computable. Indeed, we see that

\[
\eta_A(p^h) = \| p^h - \sum_{z \in N} (A_z p^h) \varphi_z \|_{L^2(\Omega)}
\]

\[= \left( \sum_{T \in T_h} \int_T \left| \frac{p^h}{|T|} - \sum_{z \in N} (A_z p^h) \varphi_z |_T \right|^2 \, dx \right)^{1/2}. \]

Let \( y^h \in Y_h \) be an inexact solution of the finite element discretization of the PDE on the given mesh \( T_h \). To evaluate the residual in the variational formulation

\[
\int_C(y^h) = a(y^h, \cdot) - (g, \cdot)_{L^2(\Gamma_N)} + (s(y), \cdot)_{L^2(\Omega)} - (f, \cdot)_{L^2(\Omega)} \in V^* = Y^*,
\]

where \( a(v, w) = (\nabla v, \nabla w)_{L^2(\Omega)} \), we consider

\[
\langle C(y^h), v \rangle_{V^*, V} = (\nabla y^h, \nabla v)_{L^2(\Omega)} - (g, v)_{L^2(\Gamma_N)} + (s(y), v)_{L^2(\Omega)} - (f, v)_{L^2(\Omega)}.
\]

with \( v \in V, \| v \|_V = 1 \). Then taking the supremum over all such \( v \) we obtain the norm \( \| C(y^h) \|_{V^*} \). Let \( \Pi \) denote the \( L^2 \)-projection onto the first–order finite element space \( V_h \) on \( \Omega \) and set \( v^h := \Pi v \) for \( v \in V \). By linearity we have

\[
\langle C(y^h), v \rangle_{V^*, V} = \langle C(y^h), v - v^h \rangle_{V^*, V} + \langle C(y^h), v^h \rangle_{V^*, V}.
\]

It remains to derive upper bounds for the last two summands to estimate the norm as desired.

We begin with the estimation of the first summand of the right hand side of equation (6.5). Here, we first consider the last two summands of (6.4) tested with \( v - v^h \). Since \( v - v^h \) is \( L^2 \)-orthogonal onto \( \Pi f \) we obtain

\[
\int_\Omega f(v - v^h) \, dx = \int_\Omega (f - \Pi f)(v - v^h) \, dx \leq h_T^{-1}(v - v^h) \| L^2(\Omega) \| h_T(f - \Pi f) \| L^2(\Omega),
\]

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Notice that \(\|h_T(f - \Pi f)\|_{L^2(\Omega)} = \text{h.o.t. is of higher order. We use h.o.t. to denote higher order terms. These are generically much smaller than an estimator } \eta, \text{ but this depends on the smoothness of the given data. In general, h.o.t. may be neglected, but in case if high oscillations they may even dominate } \eta.\)

The first-order approximation property of the \(L^2\) projection,

\[
\|h_T^{-1}(v - v^h)\|_{L^2(\Omega)} \leq C_{\text{approx}} \|\nabla v\|_{L^2(\Omega)},
\]

(cf. [9, 5.5]), yields

\[
\int_{\Omega} f(v - v^h) \, dx \leq C_{\text{approx}} \|\nabla v\|_{L^2(\Omega)} \|h_T(f - \Pi f)\|_{L^2(\Omega)} = \text{h.o.t.}(f)
\]

since \(\|\nabla v\|_{L^2(\Omega)} \leq \|v\|_V = 1\). Similarly we obtain

\[
\int_{\Omega} s(y)(v - v^h) \, dx \leq C_{\text{approx}} \|\nabla v\|_{L^2(\Omega)} \|h_T(s(y) - \Pi s(y))\|_{L^2(\Omega)} = \text{h.o.t.}(s(y)).
\]

Now we proceed to the first two summands in (6.4) tested with \(v - v^h\). We follow the analysis in [9]. Set \(p^h := \nabla y^h\) and let \(q\) be arbitrary in \(Q^n\). Then there holds

\[
(\nabla y^h, \nabla (v - v^h))_{L^2(\Omega)} - (g, v - v^h)_{L^2(\Gamma_N)}
= \int_{\Omega} (p^h - q) \nabla (v - v^h) \, dx + \int_{\Omega} q \nabla (v - v^h) \, dx - \int_{\Gamma_N} g(v - v^h) \, dS(x).
\]

The \(H^1\)-stability of the projection \(\Pi\) yields

\[
\|\nabla (v - \Pi v)\|_{L^2(\Omega)} \leq C_{\text{stab}} \|\nabla v\|_{L^2(\Omega)}
\]

for some \(C_{\text{stab}} > 0\). Thus, using the Cauchy–Schwarz inequality and (elementwise) integration by parts together with Gauss’ theorem we obtain

\[
(\nabla y^h, \nabla (v - v^h))_{L^2(\Omega)} - (g, v - v^h)_{L^2(\Gamma_N)} \leq \\
\leq C_{\text{stab}} \|\nabla v\|_{L^2(\Omega)} \|p^h - q\|_{L^2(\Omega)} - \int_{\Omega} (v - v^h) \text{div } T q \, dx + \int_{\partial \Omega} (v - v^h)(q \cdot n - g) \, dS(x)
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + \|h_T^{-1}(v - \Pi v)\|_{L^2(\Omega)} \|h_T \text{div } T q\|_{L^2(\Omega)}
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + \|h_T^{-1}(v - \Pi v)\|_{L^2(\Omega)} \|h_T^{1/2}(v - v^h)\|_{L^2(\Gamma_N)} \|h_T^{1/2}(q \cdot n - g)\|_{L^2(\Gamma_N)}.
\]

Note that \((\text{div } p^h)|_T = 0\) for all \(T \in \mathcal{T}\), since \(y^h\) is piecewise linear. Therefore, the inverse inequality

\[
\|h_T \text{div } q\|_{L^2(T)} = \|h_T \text{div } (q - p^h)\|_{L^2(T)} \leq C_{\text{inv}} \|q - p^h\|_{L^2(T)} \quad \forall T \in \mathcal{T}
\]

yields

\[
\|h_T \text{div } T q\|_{L^2(\Omega)} \leq C_{\text{inv}} \|q - p^h\|_{L^2(\Omega)}.
\]

Together with the approximation property of \(\Pi\) on the edges

\[
\|h_T^{-1/2}(v - v^h)\|_{L^2(\Gamma_N)} \leq C_{\text{approx}} \|\nabla v\|_{L^2(\Omega)},
\]

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(cf. [9, 5.5]), we obtain
\[

(\nabla y^h, \nabla (v - v^h))_{L^2(\Omega)} - (g, v - v^h)_{L^2(\Gamma_N)} \\
\leq (C_{\text{stab}} + C_{\text{approx}} C_{\text{inv}}) \|p^h - q\|_{L^2(\Omega)} + C_{\text{approx}} \|h_{\kappa}^{1/2}(q \cdot n - g)\|_{L^2(\Gamma_N)}.
\]

Hence, the estimates of the summands in (6.4) yield for \( v \in V \) with \( \|v\|_V = 1 \)
\[

\langle C(y^h), v - v^h \rangle \leq C_{\text{est}} \min_{q \in Q_n} \{ \|p^h - q\|_{L^2(\Omega)} + \|h_{\kappa}^{1/2}(q \cdot n - g)\|_{L^2(\Gamma_N)} \}
\]

(6.7)
\[

+ \text{h.o.t.}(f) + \text{h.o.t.}(s(y))
\]

\[

\eta(y^h, g) = C_{\text{est}} \eta(y^h, g) + \text{h.o.t.}(f) + \text{h.o.t.}(s(y))
\]

where \( \eta(y^h, g) \) denotes the desired estimator. Note that the higher order terms may be integrated in the estimator.

It remains to estimate the second summand in (6.5). The \( H^1 \)-stability and the first–order approximation property of the \( L^2 \)-projection \( \Pi \) give for \( v \in V \) with \( \|v\|_V = 1 \) and \( v^h := \Pi v \)
\[

\|v^h\|_{V_h} = \|v^h\|_V \leq \|v^h - v\|_V + \|v\|_V \leq \left( \|v^h - v\|_{L^2(\Omega)}^2 + \|\nabla (v^h - v)\|_{L^2(\Omega)} \right)^{1/2} + \|v\|_V \\
\leq \left( h_{\kappa}^2 C_{\text{approx}}^2 \|\nabla v\|_{L^2(\Omega)}^2 + C_{\text{stab}}^2 \|\nabla v\|_{L^2(\Omega)}^2 \right)^{1/2} + \|v\|_V \\
\leq \left( 1 + \sqrt{h_{\kappa}^2 C_{\text{approx}}^2 + C_{\text{stab}}^2} \right) \|v\|_V \leq C_{\text{proj}} \|v\|_V
\]

(6.8)

with some \( C_{\text{proj}} > 0 \), since \( \|\nabla v\|_{L^2(\Omega)} \leq \|v\|_V \) and since \( h_{\kappa} \) is bounded. Hence, for \( \|v\|_V = 1 \) we obtain \( \|v^h\|_{V_h} \leq C_{\text{proj}} \) and thus by using the definition of \( C^h \)
\[

\langle C(y^h), v^h \rangle_{V^*, V} = \langle C(y^h), v^h \rangle_{V^*, V_h} \leq C_{\text{proj}} \|C^h(y^h)\|_{V^*_h}.
\]

Consequently, the estimate of the summands in (6.5) yields
\[

\|C(y^h)\|_{V^*} \leq C_{\text{est}} \eta(y^h, g) + C_{\text{proj}} \|C^h(y^h)\|_{V^*_h} + \text{h.o.t.}(f) + \text{h.o.t.}(s(y))
\]

(6.10)

with \( \eta(y^h, g) \) from (6.7). The averaging estimator may then be calculated by (6.3) having regard to (6.7). If the higher order terms are not neglected, they may be integrated in the estimator-calculation.


For simplicity the error estimator is developed only for 2-dimensional spaces. Nevertheless the same theory is valid in three space dimensions. Only a few constants in some proofs will change due to larger overlaps of patches in 3D.

Let \( d \) be the (local) polynomial degree of the finite elements and let \( P_k(G) \) denote algebraic polynomials on the domain \( G \subset \mathbb{R}^2 \), of degree at most \( k \). Let \( S^d = P_d(T_h) \cap C^1(\Omega) \) be the finite element space of continuous functions on \( \Omega \) that are \( T_h \)-elementwise polynomials of degree at most \( d \) \( \in \mathbb{N} \). For generality different polynomial degrees are allowed. As in the linear finite element case \( \{ \varphi_z \}_{z \in \mathcal{N}} \) shall denote the continuous \( T_h \)-elementwise linear nodal basis functions.

We follow the analysis in [1] where the authors define a projection operator \( \mathcal{J} \) on local
polynomial spaces as follows. For each fixed node \( z \in N \setminus K \) they choose a neighboring free node \( \zeta \in K \) and thereby define a relation \( R \) on \( N \) where \( zRz \) if \( z \in K \). Then, they define \( \psi_z := \sum_{\zeta \in N, \zeta \in Rz} \varphi_{\zeta} \) and \( \Omega_z := \text{int}(\text{supp} \psi_z) \).

They require that for each \( z \in K \), \( \Omega_z \) is connected and \( \varphi_z \neq \psi_z \) implies that \( (\partial \Omega_z) \cap \Gamma_D \) has a positive surface measure. Then \( \{ \zeta \in N : \zeta \in Rz \} : z \in K \) is a partition of \( N \) and \( (\psi_z : z \in K) \) is a partition of unity. For each \( z \in K \) they define the degree (minimal degree allowed on \( \Omega_z \) minus one)

\[
d(z) := \max \{ k \in \mathbb{N}_0 : P_k(\Omega_z) \varphi_z \subseteq S \},
\]

where \( P_k(\Omega_z) \) denotes the set of all polynomials on \( \mathbb{R}^2 \) of total degree at most \( k \) restricted to \( \Omega_z \). The set \( S \subseteq H^1(\Omega) \) is some finite element space consisting of functions that are \( T_h \)-elementwise polynomials and globally continuous. Moreover, one requires that \( S^1_D(T_h) := \{ y \in S^1(T_h) : y|_{\Gamma_D} = 0 \} \subseteq S \), which implies that \( d(z) \) is well defined and larger than or equal to zero.

For \( g \in L^1(\Omega), z \in N \) the authors of [1] define \( g_z \in P_{d(z)}(\Omega) \) by

\[
\int_{\Omega_z} (g_z \varphi_z - g\psi_z) q_z\, dx = 0 \quad \forall q_z \in P_{d(z)}(\Omega_z),
\]

and then they define

\[
J_g := \sum_{z \in K} g_z \varphi_z \in S \cap H^1_D(\Omega).
\]

According to (cf. [1, Rem. 2.2]), \( J \) is well defined.

In the following we state a few results from [1] which are necessary to develop an estimator for the residual of the given PDE (6.1) in the presence of inexact states.

**Proposition 6.2.** There exist \( (h_T, h_\varepsilon) \)-independent constants \( C_{\text{stab}} > 0, C_{\text{approx}} > 0 \) and \( C > 0 \) such that for all \( g \in H^1_D(\Omega) \) and \( f \in L^2(\Omega) \)

1) the stability of \( J \)

\[
\|\nabla (g - Jg)\|_{L^2(\Omega)} \leq C_{\text{stab}} \|\nabla g\|_{L^2(\Omega)},
\]

2) the approximation properties of \( J \)

\[
\|h^{-1}_T(g - Jg)\|_{L^2(\Omega)} \leq C_{\text{approx}} \|\nabla g\|_{L^2(\Omega)},
\]

\[
\|h^{-1/2}_\varepsilon(g - Jg)\|_{L^2(\Gamma_N)} \leq C_{\text{approx}} \|\nabla g\|_{L^2(\Omega)},
\]

3) and the enhanced stability of \( J \)

\[
\int_{\Omega} f(g - Jg)\, dx \leq C\|\nabla g\|_{L^2(\Omega)} \left( \sum_{z \in K} h_z^2 \min_{f_z \in P_{d(z)}(\Omega_z)} \|f - f_z\|_{L^2(\Omega_z)}^2 \right)^{1/2}
\]

hold. The constants depend only on \( \Omega, \Gamma_D, \Gamma_N \), the degrees \( d(z), z \in K \), and the shapes of the elements \( T \in T_h \) and the patches \( \Omega_z, z \in K \).

For a proof see [1, Thm. 2.1].
LEMMA 6.3. Suppose $S = \{ v^h \in C(\bar{\Omega}) : \forall T \in T, v^h|_T \in P_{d(T)}(T) \}$ for positive integers $d(T), T \in T_h$, and let $d_E, E \in E$, be nonnegative integers. Then there exists a constant $C > 0$ such that for all $u^h \in S$ and each $z \in K$ we have
\[
\min_{q^h \in P_{d(z)+1}(\Omega_z)^2} \| \nabla u^h - q^h \|^2_{L^2(\Omega_z)} \leq C \sum_{E \in E_{\Omega_z}} \min_{q_E \in P_{d_E}(\omega_E)^2} \| \nabla u^h - q_E \|^2_{L^2(\omega_E)},
\]
where $E_{\Omega_z}$ is the set of edges $E \subset \bar{\Omega}_z$ with $E \not\subset \partial \Omega_z$ and $\omega_E = \bigcup_{T \in T_h, E \subset T, E \in E}$, is the union of those triangles (tetrahedra) that share the edge (face) $E$. The constant $C$ depends on the degrees $(z)$ and $d_E$ as well as on the shapes of the elements and patches but not on their diameters.

For a proof see [1, Lem. 3.1].

LEMMA 6.4. Let $k$ and $d_E, E \in E$, be nonnegative integers and let $g^h$ be a (possibly discontinuous) piecewise polynomial on $T_h$ with local degrees on $T \in T_h$ at most $k$ and let $g^h$ be a piecewise polynomial on $E \cap \Gamma_N$ with local degrees at most $k+1$. Then,
\[
\min_{g^h \in S_{k+1}(T_h)^2} \left( \| p^h - g^h \|^2_{L^2(\Omega)} + \| h^{1/2}_E (g^h - q^h) \|^2_{L^2(\Gamma_N)} \right)
\leq C \sum_{E \in E_{\Omega \cup E_N}} \min_{q_E \in P_{d_E}(\omega_E)^2} \left( \| p^h - q_E \|^2_{L^2(\omega_E)} + h_E \| g^h - q_E \|^2_{L^2(\omega_E \cap \Gamma_N)} \right)
\]
with a constant $C > 0$ that depends on the degrees $k$ and $d_E$ as well as on the shapes of the elements and patches but not on their diameters.

For a proof see [1, Lem. 3.2].

The averaging error estimator is then defined by
(6.12)
\[
\eta_E(g^h, g) = \left( \sum_{E \in E_{\Omega \cup E_N}} \min_{q_E \in P_{d_E}(\omega_E)^2} \| p^h - q_E \|^2_{L^2(\omega_E)} \right)^{1/2} + \| h^{1/2}_E (g^h - g) \|_{L^2(\Gamma_N)} ,
\]
where $g^h$ is a piecewise polynomial on $E_N$ with local degrees at most $d_E$. The polynomial degree $d_E$ on $\omega_E$ is chosen accordingly to the elementwise degrees of $g^h$ on $\omega_E$. If problem (6.1) is a boundary control problem, then $g$ equals the control which is usually given in the finite element space which arises from the restriction of $Y_h$ onto the Neumann boundary. Then one chooses $g^h = g$. Otherwise it is reasonable to choose $g^h$ as suitable projection of $g$ onto the restriction of the finite element space to the Neumann boundary $S_{D|D}^d$. According to [1] for $g \in L^2(\Gamma_N)$ with $g|_E \in H^{d_E}(E)$ for all $E \in E$ there exists $g^h \in L^\infty(\Gamma_N)$ with $g^h|_E \in P_{d_E}(E)$ for all $E \in E_N$ such that the last summand is of higher order, i.e.
\[
\| h^{1/2}_E (g^h - g) \|_{L^2(\Gamma_N)} \leq C h^{d_E + 1/2}_E \| \partial^d_E g/\partial s^d_E \|_{L^2(\Gamma_N)}
\]
for some $C > 0$.

Now we have the tools to estimate $\| C(g^h) \|_{V^*}$. Let $Y_h = V_h = S_{D}^d$ for some $d \in \mathbb{N}$ and let $g^h \in Y_h$. Let $v \in V$ with $\| v \|_V = 1$ and let $J$ be the projection onto $Y_h$ from (6.11). Then we have
(6.13)
\[
\langle C(g^h), v \rangle = \langle C(g^h), v - Jv \rangle + \langle C(g^h), Jv \rangle.
\]
We begin with the estimation of the first summand. Let $Q$ denote the space of gradients in $L^2(\Omega)^2$ that are continuous and $T_h$-elementwise polynomials with degree at most $d$, $Q = (S_d)^2$. Set $p^h = \nabla y^h$ and let $q \in Q$. Then we obtain

\begin{equation}
\langle C(y^h), v - \mathcal{J}v \rangle = \langle y^h, v - \mathcal{J}v \rangle - (g, v - \mathcal{J}v)_{L^2(\Gamma_N)} \\
+ (s(y^h), v - \mathcal{J}v)_{L^2(\Omega)} - (f, v - \mathcal{J}v)_{L^2(\Omega)}.
\end{equation}

(6.14)

For the third and fourth summand in the latter expression (6.14) we use the enhanced stability of $\mathcal{J}$ from Lemma 6.2 and get

$$
\int_{\Omega} s(y^h)(v - \mathcal{J}v) \, dx \leq C \|\nabla v\|_{L^2(\Omega)} \left( \sum_{z \in N} \frac{h_z^2}{k_{z}} \min_{f_z \in P_{d-1}(\omega_z)} \|s(y^h) - f_z\|_{L^2(\Omega)}^2 \right)^{1/2}
$$

$$
= \text{h.o.t.}(s(y^h)),
$$

and, similarly, $\int_{\Omega} f(v - \mathcal{J}v) \, dx \leq \text{h.o.t.}(f)$.

We go on with the first two summands from equation (6.14), and see, using the Cauchy–Schwarz inequality, integration by parts, Gauss’ theorem, the stability property of $\mathcal{J}$, Minkowski’s theorem and the triangle inequality,

$$
\int_{\Omega} \nabla p^h \nabla (v - \mathcal{J}v) \, dx - \int_{\Gamma_N} g(v - \mathcal{J}v) \, dS(x)
$$

$$
= \int_{\Omega} (p^h - q) \nabla (v - \mathcal{J}v) \, dx + \int_{\Omega} q \nabla (v - \mathcal{J}v) \, dx - \int_{\Gamma_N} g(v - \mathcal{J}v) \, dS(x)
$$

$$
\leq \|p^h - q\|_{L^2(\Omega)} \|\nabla (v - \mathcal{J}v)\|_{L^2(\Omega)} - \int_{\Omega} (v - \mathcal{J}v) \text{div} \, q \, dx
$$

$$
+ \int_{\partial \Omega} (v - \mathcal{J}v)q \cdot \nu \, dS(x) - \int_{\Gamma_N} g(v - \mathcal{J}v) \, dS(x)
$$

$$
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + C \|\nabla v\|_{L^2(\Omega)} \left( \sum_{z \in N} \frac{h_z^2}{k_{z}} \min_{f_z \in P_{d-1}(\omega_z)} \|h_z \text{div} \, \tau (q - f_z)\|_{L^2(\omega_z)}^2 \right)^{1/2}
$$

$$
- \int_{\Gamma_N} (q \cdot \nu - g)(v - \mathcal{J}v) \, dS(x)
$$

$$
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + C \left( \sum_{z \in N} \frac{h_z^2}{k_{z}} \min_{f_z \in P_{d-1}(\omega_z)} \|h_z \text{div} \, \tau (q - f_z)\|_{L^2(\omega_z)}^2 \right)^{1/2}
$$

$$
+ \|h\bar{\iota}_{\otimes}(q \cdot \nu - g)\|_{L^2(\Gamma_N)} \|h\bar{\iota}_{\otimes}^{-1/2}(v - \mathcal{J}v)\|_{L^2(\Gamma_N)}
$$

$$
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + C \left( \sum_{z \in N} \|h_z \text{div} \, \tau (q - p^h)\|_{L^2(\omega_z)}^2 \right)^{1/2}
$$

$$
+ C \left( \sum_{z \in N} \frac{h_z^2}{k_{z}} \min_{f_z \in P_{d-1}(\omega_z)} \|h_z \text{div} \, \tau (p^h - q_z)\|_{L^2(\omega_z)}^2 \right)^{1/2} + C_{\text{approx}} \|h\bar{\iota}_{\otimes}^{1/2}(q \cdot \nu - g)\|_{L^2(\Gamma_N)}
$$

$$
\leq C_{\text{stab}} \|p^h - q\|_{L^2(\Omega)} + 3K C \|\text{div} \, \tau (q - p^h)\|_{L^2(\Omega)}
$$

$$
+ C \left( \sum_{z \in N} \frac{h_z^2}{k_{z}} \min_{f_z \in P_{d-1}(\omega_z)} \|h_z \text{div} \, \tau (p^h - q_z)\|_{L^2(\omega_z)}^2 \right)^{1/2} + C_{\text{approx}} \|h\bar{\iota}_{\otimes}^{1/2}(q \cdot \nu - g)\|_{L^2(\Gamma_N)},
$$

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since \( h_z \leq Kh_T \), \( z \in T \in T_h \), for some \( K > 0 \) and \( \text{vol}(\cup_{z \in \mathcal{N}} \omega_z) \leq 3\text{vol}(\Omega) \). A \( T_h \)-elementwise inverse estimate shows

\[
\| h_T \text{div}_T (p^h - q) \|_{L^2(T)} \leq C_{\text{inv}} \| p^h - q \|_{L^2(T)} \quad \forall T \in T_h,
\]

and

\[
\| h_z \text{div}_T (p^h - q_z) \|_{L^2(\omega_z)} \leq C_{\text{inv}} \| p^h - q_z \|_{L^2(\omega_z)} \quad \forall z \in \mathcal{N},
\]

for some \( C_{\text{inv}} > 0 \). Hence, we obtain

\[
a(y^h, v - Jv) - (g, v - Jv)_{L^2(\Gamma_N)} \leq C_{\text{stab}} \| p^h - q \|_{L^2(\Omega)} + 3KC_{\text{inv}} \| p^h - q \|_{L^2(\Omega)}
\]

\[
+ CC_{\text{inv}} \left( \sum_{z \in \mathcal{N}} \min_{q_z \in \mathcal{P}_d(\omega_z)} \| p^h - q_z \|_{L^2(\omega_z)}^2 \right) \leq \frac{1}{2}
\]

\[
+ C_{\text{approx}} \| h_z^{1/2} (q \cdot \nu - g^h) \|_{L^2(\Gamma_N)} + C_{\text{approx}} \| h_z^{1/2} (g^h - g) \|_{L^2(\Gamma_N)}
\]

\[+ \text{h.o.t.} (s(y^h)) + \text{h.o.t.}(u^h) \]

All this together gives, using Lemma 6.3 and Lemma 6.4, and minimizing over the arbitrarily chosen \( q \in Q \),

\[
\langle C(y^h), v - Jv \rangle \leq (C_{\text{stab}} + 3KC_{\text{inv}}) \min_{q \in Q} \| \nabla y^h - q \|_{L^2(\Omega)}
\]

\[
+ CC_{\text{inv}} \left( \sum_{z \in \mathcal{N}} \min_{q_z \in \mathcal{P}_d(\omega_z)} \| \nabla y^h - q_z \|_{L^2(\omega_z)}^2 \right) \leq \frac{1}{2}
\]

\[
+ C_{\text{approx}} \| h_z^{1/2} (q \cdot \nu - g^h) \|_{L^2(\Gamma_N)} + \| h_z^{1/2} (g^h - g) \|_{L^2(\Gamma_N)}
\]

\[+ \text{h.o.t.} (s(y^h)) + \text{h.o.t.}(u^h) \]

\[
\leq \tilde{C}_{\text{est}} \left( \sum_{E \in \Omega} \min_{q_E \in \mathcal{P}_{dE}(\omega_E)^2} \| \nabla y^h - q_E \|_{L^2(\omega_E)}^2 \right) \leq \frac{1}{2}
\]

\[
+ C_{\text{approx}} \| h_z^{1/2} (g^h - g) \|_{L^2(\Gamma_N)} + \text{h.o.t.} (s(y^h)) + \text{h.o.t.}(u^h)
\]

\[
\leq C_{\text{est}} \eta_E(y^h, g) + \text{h.o.t.} (s(y^h)) + \text{h.o.t.}(u^h).
\]

Now, we come to the second summand of (6.13). Using proposition 6.2, we obtain as in (6.8) in the linear finite element case, with projection operator \( J \) instead of \( \Pi \),

\[
\| Jv \|_V \leq \left( 1 + \sqrt{\frac{h_T^2}{\Omega} C_{\text{approx}}^2 + C_{\text{stab}}^2} \right) \| v \|_V \leq C_{\text{proj}} \| v \|_V,
\]

for some \( C_{\text{proj}} > 0 \). Thus, we get

\[
\langle C(y^h, u^h), Jv \rangle \leq C_{\text{proj}} \sup_{\| v^h \|_{V^h} = 1} \langle C(y^h, u^h), v^h \rangle \leq C_{\text{proj}} \| C(\cdot, u^h) \|_{V^h}.
\]

Hence, the estimations of the first and second summand in (6.13) yield

\[
\| C(y^h) \|_{V^*} \leq C_{\text{est}} \eta_E(y^h, g) + C_{\text{proj}} \| C(\cdot, u^h) \|_{V^h} + \text{h.o.t.}(s(y^h)) + \text{h.o.t.}(u^h).
\]

(6.15)
If the higher order terms are not neglected, they may be estimated with the following lemma and integrated in the estimator–calculation.

**Lemma 6.5.** For all $z \in \mathcal{N}$ there exists an $h_z$–independent constant $C > 0$ such that, if $f|_{\omega_z} \in H^d(\omega_z)$, $d \geq 1$, we have $(D^d f)(\partial^d f)|_{\partial_z} = d$ denotes the vector of all partial derivatives of order $d$)

$$\min_{f_z \in \mathcal{T}_{d-1}(\omega_z)} \|f - f_z\|_{L^2(\omega_z)} \leq C h_z^d \|D^d f\|_{L^2(\omega_z)}.$$ 

For a proof see [1, Lem. 4.1].

### 6.2. Residual Based Error Estimators for Inexact States.

Using the same idea from the previous section on averaging estimates we obtain the required estimation for the residual in the given semilinear elliptic PDE (6.1).

**Remark 6.6.** Recall the following properties of the quasi-interpolation operator $I_h$: Let $v \in H^1(\Omega)$, let $\omega_T$ denote the patch around a triangle $T \in \mathcal{T}_h$ and let $\omega_E$ denote the patch around an edge $E \in \mathcal{E}$. Then there exists $C > 0$ such that

1. $\|v - I_h v\|_{L^2(T)} \leq C h_T \|\nabla v\|_{L^2(\omega_T)}$
2. $\|v - I_h v\|_{L^2(E)} \leq C h_E^{1/2} \|\nabla v\|_{L^2(\omega_E)}$
3. $\|\nabla(v - I_h v)\|_{L^2(T)} \leq C \|\nabla v\|_{L^2(\omega_T)}$

Using finite overlap property 3 yields $\|\nabla(v - I_h v)\|_{L^2(\omega_T)} \leq C \|\nabla v\|_{L^2(\omega_T)}$ for some $C > 0$. For a proof see [30]. Now we follow the analysis in [17, pp. 287-289] and use the same arguments. Recall that we do not have Galerkin orthogonality since we do not assume that $y^h$ is an exact solution of $C^h(y^h) = 0$. To be able to use the same techniques, again we devide the residual into two parts

$$\langle C(y^h), v \rangle_{V^*,V} = \langle C(y^h), v - I_h v \rangle_{V^*,V} + \langle C(y^h), I_h v \rangle_{V^*,V}$$

for $v \in V$ and then take the supremum over all testfunctions $v \in V$ with norm 1. We begin with the estimation of the first summand. Observe that

$$\langle C(y), v - I_h v \rangle_{V^*,V} = \sum_{T \in \mathcal{T}} (r_T(v, v - I_h v)_{L^2(T)} + \sum_{E \in \mathcal{E}} (r_E(v, v - I_h v)_{L^2(E)}$$

with the elementwise residuals $r_T(y) = (-\Delta y + s(y) - f)|_T$ of the PDE and the jumps $r_E(y) = [v_E \cdot \nabla y]_E$ of the (discontinuous) normal derivative of $y$ across the edges $E$. Hence, using the standard arguments we obtain for $v \in V$ with $\|v\|_V = 1$

$$\langle C(y), v - I_h v \rangle_{V^*,V} \leq C_{\text{est}} \eta(y)$$

where

$$\eta^2(y) = \sum_{T \in \mathcal{T}} \eta^2_T(y) \quad \text{and} \quad \eta^2_T(y) = \sum_{T \in \mathcal{T}} \eta^2_T(y) = \sum_{T \in \mathcal{T}} \eta^2_T(y) + \frac{1}{2} \|r_E(y)\|_{L^2(E)}^2.$$

It remains to estimate the second summand in (6.16). Using the properties from Remark 6.6 of the Clément interpolation operator we see that

$$\|I_h v\|_V \leq \|I_h v - v\|_V + \|v\|_V \leq \left(\|I_h v - v\|_{L^2(\omega)}^2 + \|v\|_{L^2(\omega)}^2\right)^{1/2} + \|v\|_V \leq \left(\|I_h v\|_{L^2(\omega)}^2 + \|v\|_{L^2(\omega)}^2\right)^{1/2} + \|v\|_V \leq C_{\text{proj}} \|v\|_V.$$
for $v \in V$ with $\|v\|_V = 1$. Consequently, we obtain
\[
\|C(y)\|_{V^*} \leq C_{\text{est}} \eta(y) + C_{\text{proj}} \|C^h(y)\|_{V^*_h}.
\]

7. Numerical Results.

7.1. A Distributed Optimal Control Problem.

**Problem 7.1.** We consider the following problem
\[
\min_{y \in H^1_0(\Omega), u \in L^2(\Omega)} f(y, u) := \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2
\]
\[\text{s.t.} \quad -\Delta y + y^3 = u \quad \text{in } \Omega,
\]
\[y = 0 \quad \text{on } \partial \Omega,
\]
where $\Omega \subset \mathbb{R}^2$ is a polygonal domain, $y_d \in H^1_0(\Omega)$ and $\alpha > 0$.

The cost function and the constraint operator in the weak formulation are twice continuously Fréchet differentiable. These functions and their derivatives are bounded on a bounded subset $D \subset Y \times U$. Moreover, the theory of maximal monotone operators guarantees that there exists a unique solution operator for this PDE that is uniformly bounded. Hence, the required assumptions for algorithm 3.9 are satisfied. It is furthermore well known that this optimization problem has a solution.

7.1.1. Estimators for the convergence conditions. We are in the situation to use error estimators as in section 6 for the infinite dimensional norm of the residual in the PDE constraint.

The Lagrangian function is given by
\[
l(y, u, \lambda) = \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Omega)}^2 + \langle \lambda, C(y, u) \rangle_{H^1_0(\Omega), H^{-1}(\Omega)}.
\]

Thus, the $u$–gradient of the Lagrangian reads $l_u(y, u, \lambda) = (\alpha u - \lambda, \cdot)_{L^2(\Omega)}$. Hence, the norm of the $u$–gradient of the Lagrangian is easy to evaluate following Riesz representation theorem: $\|l_u(y, u, \lambda)\|_{L^2(\Omega)^*} = \|\alpha u - \lambda\|_{L^2(\Omega)}$. Thus, the convergence condition on the $u$–gradient of the Lagrangian (3.31) is always satisfied since we calculate exact $L^2$–norms for a given discrete control $u^h$ and discrete adjoint state $\lambda^h$.

The $y$–gradient of the Lagrangian $l(y, u, \lambda)$ is given by
\[
l_y(y, u, \lambda) = (y - y_d, \cdot)_{L^2(\Omega)} + a(\lambda, \cdot) + (3\lambda y^2, \cdot)_{L^2(\Omega)}.
\]

Again, the residual in the adjoint equation can be estimated with the techniques from section 6.

7.1.2. Numerical Results for the Distributed Optimal Control Problem. For the test problem 7.1 we used the following configuration: $\Omega = L$-shaped domain, $\alpha = 1 \times 10^{-4}$, $y_d = 1$. We used preconditioned Krylov solvers as iterative solvers with incomplete Cholesky factorizations in the preconditioner on the KKT-system of the tangential step and in the quasi-normal step. We calculated both with linear finite elements and the averaging ZZ-estimator and with quadratic finite elements and the averaging estimator proposed by Bartels and Carstensen. We show the results for quadratic finite elements and the averaging estimator of Bartels and Carstensen.

In figure 7.1 we see a table of error estimators with the iteration number in the first column, the error estimator for the constraint in the second column, the error
estimator for the adjoint state in the third column, the norm of the inexact reduced gradient in the fourth column, the degrees of freedom in the fifth column and the degrees of freedom one would need to achieve the same accuracy on uniformly refined meshes in the sixth column.

<table>
<thead>
<tr>
<th>It.</th>
<th>$\eta_{C,h}(x_k)$</th>
<th>$\eta_{L^2,h}(\lambda_k + \Delta \lambda_k)$</th>
<th>$|g_k|_{L^2}$</th>
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<th>Uniform DOF</th>
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</tbody>
</table>

**Fig. 7.1. Table of error estimators**

The same accuracy on uniform meshes would here require more than 20 times the degrees of freedom on our adaptively refined meshes.

In figure 7.2 we see the last grid produced by the multilevel SQP algorithm as well as the optimal control and the optimal state.

**Fig. 7.2. Last (9th) grid, optimal control, optimal state**

### 7.2. A Boundary Control Problem

**Problem 7.2.** We consider the following problem taken from [2].

$$\min_{y \in H^1(\Omega), u \in L^2(\Gamma_C)} f(y, u) := \frac{1}{2} \|y - y_d\|_{L^2(\Gamma_O)}^2 + \frac{\alpha}{2} \|u\|_{L^2(\Gamma_C)}^2$$

s.t.  

$$-\Delta y + y^3 - y = 1 \quad \text{in} \ \Omega,$$

$$\partial_n y = 0 \quad \text{on} \ \partial \Omega \setminus \Gamma_C,$$

$$\partial_n y = u \quad \text{on} \ \Gamma_C.$$

where $\alpha = 1e - 4$, $y_d = 1$, $\partial_n$ denotes the normal derivative, $\Omega$ is a T-shaped domain, $\Gamma_C$ bottom boundary of $T$, $\Gamma_O$ upper boundary of $T$, i.e. $T = \text{int}([1/4, 3/4] \times [0, 1/2] \cup [0, 1] \times [1/2, 3/4])$, $\Gamma_O = [0, 1] \times \{3/4\}$, $\Gamma_C = [1/4, 3/4] \times \{0\}$. Again we used preconditioned Krylov solvers as iterative solvers with incomplete Cholesky
factorizations in the preconditioner on the KKT-system of the tangential step and in the quasi-normal step. We calculated with quadratic finite elements and the averaging estimator from Bartels and Carstensen.

In figure 7.3 we see a table of error estimators with the iteration number in the first column, the error estimator for the constraint in the second column, the error estimator for the adjoint state in the third column, the norm of the inexact reduced gradient in the fourth column and the degrees of freedom in the fifth column.

<table>
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<tr>
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<th>$\eta_{C,h}(x_k)$</th>
<th>$\eta_{L_{\mu,h}}(\lambda_k + \Delta \lambda_k)$</th>
<th>$|\hat{y}<em>k|</em>{U^*}$</th>
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</table>

Fig. 7.3. Table of error estimators

In figure 7.4 we see the last grid produced by the multilevel SQP algorithm as well as the optimal control and the optimal state.

Fig. 7.4. Last (8th) grid, optimal control, optimal state

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