Numerical Approximation of an SQP-type Method for Parameter Identification

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Abstract

This paper deals with the numerical approximation of the Levenberg-Marquardt SQP-method (LMSQP) for parameter identification problems, which has been presented and analyzed in [10]. It is shown that a Galerkin-type discretization leads to a convergent approximation and that the indefinite system arising from the Karush-Kuhn-Tucker system is well posed.

In addition, we present a multi-level version of the Levenberg-Marquardt method and discuss the simultaneous solution of the discretized KKT-system by preconditioned iteration methods for indefinite problems. From a discussion of the numerical effort we conclude that these approaches may lead to a considerable speed-up with respect to standard iterative regularization methods that eliminate the underlying state equation. The numerical efficiency of the LMSQP-method is confirmed by numerical examples.
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1 Introduction

Parameter identification denotes the procedure of determining unknown parameters appearing in an underlying state equation (usually a partial differential equation), from indirect measurements related to the solution of this equation. Such problems frequently appear in many applications, where mathematical models of physical, chemical, biological or economical processes are used (cf. e.g. [1, 12, 16] and the references there).

Since such problems are *ill-posed* in general, i.e., the parameter to be reconstructed does not depend on the observation in a stable way, regularization methods have to be used in order to compute a stable approximation of the parameter in presence of data noise. Due to the ill-posedness of the identification problem, the numerical approximation of such problems is not a simple task. The standard approach that can be found in literature is based on an a-priori elimination of the state equation, and an application of a discretized regularization method to the resulting operator equation involving the *parameter-to-output map*, which is the operator mapping the parameter to the corresponding observation. The main part in the

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evaluation of this map is the solution of the underlying state equation for given parameter, which is numerically realized by standard discretizations such as finite elements.

This approach, in particular combined with *iterative regularization methods* (cf. [17] for an overview), has been applied with success even to rather complicated parameter identification problems (cf. e.g. [9, 24, 25]). However, since this methods need a high number of direct solves (i.e., solutions of the state equation), fine discretizations of the parameter yield a considerable computational effort, which results in high CPU-times or even in the impossibility to use fine discretizations. Another drawback of this approach is that the discretizations of state and parameter are rather independent, which makes the numerical analysis extremely difficult.

Therefore, fundamentally different methods for the solution of parameter identification problems have been investigated recently, whose common idea is to avoid the a-priori elimination of the state equation (cf. [10, 20, 26]). The aim of this paper is to discuss the numerical approximation of an iterative regularization method based on the idea of sequential quadratic programming (cf. [10]). We investigate Galerkin-type discretizations in the product space for parameter, state variable and a corresponding Lagrangian variables, which leads to a sequence of well-posed indefinite systems. With this approach we are able to show convergence of the numerical approximation both for the quadratic programming problem arising in each iteration step and for the overall minimization procedure.

The general setup in this paper is as follows: we assume that we are given a noisy measurement z^δ satisfying

$$\|z - z^\delta\|_Z \le \delta, \tag{1.1}$$

where the exact data satisfy

$$z := E\hat{u}, \tag{1.2}$$

with $E \in \mathcal{L}(X, Z)$ and some $\hat{u} \in X$. Our aim is to identify the parameter $q \in Q_{ad} \subset Q$ (where Q_{ad} is a closed subset of Q with non empty interior) in the underlying equation

$$e(u, q) = f, \tag{1.3}$$

where $e : X \times Q \to X^*$ is a continuous nonlinear operator with

$$e(0, 0) = 0. \tag{1.4}$$

In this setup X, X^*, Q and Z are Hilbert spaces, and X^* can be identified with the dual of X. Finally, we assume that e is continuously Frèchet-differentiable on $X \times Q$ and that the partial derivative $e_u \in \mathcal{L}(X, X^*)$ is self-adjoint and satisfies the coercivity condition

$$\langle e_u(u, q)v, v\rangle \ge \alpha_e \|v\|_X^2, \qquad \forall (u, q, v) \in X \times Q_{ad} \times X, \tag{1.5}$$

for some $\alpha_e \in \mathbb{R}^+$.

The above setup is typical for a partial differential equation of elliptic type, which is also the main type of application we have in mind. We want to mention that the infinite-dimensional analysis carried out in the preceding paper [10] was not restricted to elliptic problems, but only assumed well-posedness of the state equation for given parameter. However, since the numerical approximation techniques for elliptic problems differ from the ones for parabolic or hyperbolic problems (cf. e.g. [32] for an overview), one cannot expect a successful unified approach to corresponding parameter identification problems. For this reason we start with an investigation of the elliptic case in this paper, but we want to mention that the numerical identification of parameters in transient equations or even mixed systems of equations is an important and challenging problem for future research.

In [10], it has been mentioned that the parameter identification problem in the above setup is an *ill-posed inverse problem* and we have proposed the following iterative regularization method based on the idea of sequential quadratic programming:

Method 1 (Levenberg-Marquardt Sequential Quadratic Programming Method). Let

$$(u_0, q_0) \in X \times Q$$

be a given initial value and let $(\beta_k)_{k\in\mathbb{N}}$ be a bounded sequence of positive real numbers. The *Levenberg-Marquardt sequential quadratic programming* (LMSQP) method consists of the iteration procedure

$$(u_{k+1}, q_{k+1}) = (\overline{u}_k, \overline{q}_k), \tag{1.6}$$

where $(\overline{u}_k, \overline{q}_k)$ is the minimizer of the quadratic programming problem

$$\frac{1}{2}\|Eu - z^\delta\|_Z^2 + \frac{\beta_k}{2}\|q - q_k\|_Q^2 \to \min_{(u,q)\in X\times Q}. \tag{1.7}$$

subject to the linear constraint

$$e(u_k, q_k) + e'(u_k, q_k)(u - u_k, q - q_k) = f. \tag{1.8}$$

The iteration procedure is stopped as soon as $k = k_*$, where

$$\|Eu_{k_*} - z^\delta\|_Z \le \tau\delta < \|Eu_k - z^\delta\|, \qquad \forall\, k < k_*, \tag{1.9}$$

with appropriately chosen $\tau > 1$.

Due to the results of [10], the LMSQP-method is a convergent regularization method, in particular the quadratic programming problems of the form (1.7), (1.8), which have to be solved in each iteration step, are well-posed. Our aim in this paper is to investigate the numerical approximation of the LMSQP-method by a Galerkin-type approach. We shall show below that this leads to an indefinite system in each iteration step, whose solution is an approximation of optimal order to the solution of (1.7), (1.8). Moreover, we show that the reconstructions obtained with the discretized LMSQP-method converge to a solution of the parameter identification problem as the noise level and the discretization size tend to zero, if an appropriate stopping rule is used, which relates the residual to the noise level and some measures for the discretization.

Moreover, we shall discuss the solution of the discretized Karush-Kuhn Tucker system, which is an indefinite linear system to be solved for the discretized equivalents of state, parameter and Lagrangian variable. The standard approaches to the solution of such discretized problems arising from partial differential equations are *reduced SQP-methods*, where state and Lagrangian variable are eliminated a-priorily. We recall the basic properties of the reduced SQP-approach, but we mainly focus on the iterative solution of the whole system with appropriate preconditioning. This promising approach has been employed recently for parameter identification (cf. [20, 26]) and optimal control problems (cf. [2, 3, 4, 5]) with good numerical results, in particular with respect to efficiency.

The paper is organized as follows: in Section 2 we investigate the numerical approximation of the LMSQP-method by a Galerkin-type approach and discuss the well-posedness, stability and approximation properties of the discretized Karush-Kuhn-Tucker (KKT) system; the convergence of the discretized solutions is shown in Section 3. Some further numerical methods and the implementation of the *outer iteration*, i.e., the SQP-iteration under the assumption that we are able to solve the quadratic optimization problems arising in each step of the LMSQP method, are examined in Section 4. We discuss the correct scaling of variables, globalization strategies as well as a multi-level approach, which leads to a further speed-up of the method. Section 5 is devoted to the *inner iteration*, i.e., the numerical solution of the discretized KKT-system. Some basic properties of this symmetric indefinite problem are studied, as well as its iterative solution with appropriate preconditioning. As a first application we investigate the identification of a potential in an elliptic boundary-value problem, where we can give quantitative error estimates in terms of the discretization sizes. Some numerical experiments related to this identification problems are presented in Section 7, before we finally conclude and give an outlook to further interesting problems related to this topic in Section 8.

2 Discretization Techniques

In the following we investigate the discretization of the LMSQP-method by a Galerkin approach. First of all, we assume that we have discretized data $z^{\delta,\eta} \in Z_\eta \subset Z$ of the form

$$z^{\delta,\eta} = R_\eta z^\delta, \tag{2.1}$$

where $R_\eta : Z \to Z_\eta$ is the orthogonal projector onto the finite-dimensional subspace Z_η. Note that we can give an error estimate for $z^{\delta,\eta}$ using (1.1) and $\|R_\eta\| = 1$, which yields

$$\delta_\eta := \|R_\eta z^\delta - z\|_Z \leq \|R_\eta(z^\delta - z)\|_Z + \|R_\eta z - z\|_Z \leq \delta + \inf_{y \in Z_\eta} \|y - z\|_Z. \tag{2.2}$$

Now let $X_h \subset X$, $Q_h \subset Q$ be finite-dimensional subspaces of X and Q, with the corresponding orthogonal projectors $P_h : X \to X_h$ and $\tilde{P}_h : Q \to Q_h$. Then we can discretize the LMSQP-Method as follows:

Method 2 (Galerkin LMSQP-Method). Let X_h, Q_h and Z_η be as above and let

$$(u_0, q_0) \in X_h \times Q_h$$

be a given initial value. Moreover, let $(\beta_k)_{k\in\mathbb{N}}$ be a bounded sequence of positive real numbers. The *Galerkin Levenberg-Marquardt sequential quadratic programming* (GLMSQP) method consists of the iteration procedure

$$(u_{k+1}, q_{k+1}) = (\overline{u}_k, \overline{q}_k), \tag{2.3}$$

where $(\overline{u}_k, \overline{q}_k) \in X_h \times Q_h$ is the minimizer of the quadratic programming problem

$$\frac{1}{2}\|R_\eta(Eu - z^\delta)\|_Z^2 + \frac{\beta_k}{2}\|q - q_k\|_Q^2 \to \min_{(u,q)\in X_h \times Q_h}, \tag{2.4}$$

subject to the linear constraint

$$\langle e(u_k, q_k) + e'(u_k, q_k)(u - u_k, q - q_k), \varphi\rangle = \langle f, \varphi\rangle, \qquad \forall\, \varphi \in X_h. \tag{2.5}$$

Note that the constraint (2.5) can be rewritten in operator form as

$$P_h^* K_k P_h(u-u_k) + P_h^* L_k \tilde{P}_h(q-q_k) = P_h^*(f-e(u_k,q_k)), \tag{2.6}$$

to be solved for $(u,q) \in X_h \times Q_h$, with the notation

$$K_k : X \to X^*, \qquad K_k u = e_u(u_k,q_k)u, \quad \forall\, u \in X, \tag{2.7}$$
$$L_k : Q \to X^*, \qquad L_k q = e_q(u_k,q_k)q, \quad \forall\, q \in Q, \tag{2.8}$$

and $P_h^* : X_h^* \to X^*$ is the adjoint of P_h. Under the assumption (1.5), we obtain that

$$\langle P_h^* K_k P_h v, v\rangle = \langle K_k P_h v, P_h v\rangle = \langle K_k v, v\rangle \geq \alpha_e \|v\|_X^2 \tag{2.9}$$

for all $v \in X_h$, i.e., the discrete bilinear form associated with the operator $P_h^* K_k P_h$ is coercive on X_h. This implies by the Lax-Milgram theorem, that (2.6) is uniquely solvable with respect to u for given $q \in Q_h$. Consequently, in an analogous way to the proof of Proposition 2.1 in [10] we may show the following result on the well-posedness of the quadratic programming problem that has to be solved in each step of Method 2:

Proposition 2.1. *Let e be continuously Frèchet-differentiable, let (1.5) hold and let $\beta_k > 0$. Then the quadratic programming problem (2.4), (2.5) has a unique solution $(\overline{u}_k, \overline{q}_k) \in X_h \times Q_h$, which is also the only local minimum.*

2.1 The Discretized Karush-Kuhn-Tucker System

In [10], the Karush-Kuhn-Tucker system for the infinite-dimensional version of the LMSQP-method has been derived and analyzed in the framework of linear saddle point problems. Now we will discuss the discretized analogue of this system, namely the first-order optimality conditions for the quadratic programming problem (2.4), (2.5).

The Lagrangian of (2.4), (2.5) is given by

$$\begin{aligned}\mathcal{L}_k(u,q;\lambda) &= \frac{1}{2}\|R_\eta(Eu-z^\delta)\|_Z^2 + \frac{\beta_k}{2}\|q-q_k\|_Q^2 + \\ &\quad +\langle \lambda, e'(u_k,q_k)(u-u_k, q-q_k) + e(u_k,q_k) - f\rangle,\end{aligned} \tag{2.10}$$

for $(u,q,\lambda) \in X_h \times Q_h \times X_h$. Since P_h and $\tilde{P}_h$ are equal to the identity on X_h and Q_h, respectively, we can rewrite the Lagrangian as

$$\begin{aligned}\mathcal{L}_k(u,q;\lambda) &= \frac{1}{2}\|R_\eta(EP_h u-z^\delta)\|_Z^2 + \frac{\beta_k}{2}\|\tilde{P}_h(q-q_k)\|_Q^2 + \\ &\quad +\langle P_h\lambda, K_k P_h(u-u_k) + L_k\tilde{P}_h(q-q_k) + e(u_k,q_k) - f\rangle,\end{aligned} \tag{2.11}$$

with the operators K_k and L_k defined by (2.7), (2.8). The KKT-system can now be deduced by computing the partial derivatives of the Lagrangian with respect to u, q and λ, i.e., $(u_{k+1}-u_k, q_{k+1}-q_k, \lambda_{k+1})$ solves the linear saddle-point problem

$$\begin{pmatrix} P_h^* E^* R_\eta^* R_\eta E P_h & 0 & P_h^* K_k^* P_h \\ 0 & \beta_k \tilde{P}_h^* \tilde{P}_h & \tilde{P}_h^* L_k^* P_h \\ P_h^* K_k P_h & P_h^* L_k \tilde{P}_h & 0 \end{pmatrix} \begin{pmatrix} u \\ q \\ \lambda \end{pmatrix} = \begin{pmatrix} P_h^* E^* R_\eta^* R_\eta (z^\delta - Eu_k) \\ 0 \\ P_h^*(f-e(u_k,q_k)) \end{pmatrix}. \tag{2.12}$$

As in [10], we define the symmetric bilinear form $a_k : (X \times Q)^2 \to \mathbb{R}$ by

$$a_k^\eta(u,q;\varphi,\sigma) := \langle R_\eta E u, R_\eta E\varphi\rangle_Z + \beta_k \langle q,\sigma\rangle_Q \tag{2.13}$$

and the bilinear form $b_k : (X \times Q) \times X \to \mathbb{R}$ by

$$b_k(u,q;\lambda) := \langle K_k u, \lambda\rangle + \langle L_k u, \lambda\rangle. \tag{2.14}$$

Moreover, we use the right-hand sides

$$\begin{aligned} f_k &:= f - e(u_k,q_k) \quad &\in X^*, \qquad &(2.15)\\ g_k^\eta &:= (E^* R_\eta^* R_\eta (z^\delta - E u_k), 0) \quad &\in X^* \times Q. \qquad &(2.16) \end{aligned}$$

Then the KKT-system (2.12) can be interpreted as the Galerkin approximation of an indefinite variational problem, i.e., $(u,q,\lambda) \in X_h \times Q_h \times X_h$ is the solution of

$$\begin{aligned} a_k^\eta(u,q;\varphi,\sigma) + b_k(\varphi,\sigma;\lambda) &= \langle g_k^\eta, (\varphi,\sigma)\rangle, \qquad &\forall\ (\varphi,\sigma) \in X_h \times Q_h, \qquad &(2.17)\\ b_k(u,q;\mu) &= \langle f_k, \mu\rangle, \qquad &\forall\ \mu \in X_h. \qquad &(2.18) \end{aligned}$$

In an analogous way to the proof of Theorem 2.3 in [10] we can show that the bilinear form a satisfies the kernel-ellipticity condition on $X_h \times Q_h$, i.e., there exists a constant $\alpha_a > 0$ such that

$$a_k^\eta(u,q;u,q) \geq \alpha_a \|(u,q)\|^2, \quad \forall\ (u,q) \in \mathcal{K}_b^h := \{\ (v,s) \in X_h \times Q_h \mid b(v,s;\lambda) = 0,\ \forall\ \lambda \in X_h\ \},$$

and that b satisfies the LBB-condition

$$\inf_{\lambda \in X_h} \sup_{(u,q) \in X_h \times Q_h} \frac{b_k(u,q;\lambda)}{\|(u,q)\|\ \|\lambda\|} \geq \alpha_b,$$

for some $\alpha_b > 0$. This implies the following well-posedness result (cf. [7, 8]) for the discretized problem (2.17), (2.18):

Theorem 2.2. *Let e be continuously Frèchet-differentiable, let* (1.5) *hold and let $\beta_k > 0$. Then the indefinite system* (2.17), (2.18) *has a unique solution $(u,q,\lambda) \in X_h \times Q_h \times X_h$, which depends continuously on the right-hand sides f_k and g_k^η.*

Since the constants α_a and α_b are the same as in the corresponding infinite-dimensional conditions in $X \times Q$, they are in particular independent of the discrete subspaces X_h and Q_h. This allows to deduce an approximation result for the solutions of (2.17), (2.18) to the solution $(u,q,\lambda) \in X \times Q \times X$ of the infinite-dimensional KKT-System, given in variational form as

$$\begin{aligned} a_k(u,q;\varphi,\sigma) + b_k(\varphi,\sigma;\lambda) &= \langle g_k, (\varphi,\sigma)\rangle, \qquad &\forall\ (\varphi,\sigma) \in X \times Q, \qquad &(2.19)\\ b_k(u,q;\mu) &= \langle f_k, \mu\rangle, \qquad &\forall\ \mu \in X, \qquad &(2.20) \end{aligned}$$

with a_k given by

$$a_k(u,q;\varphi,\sigma) := \langle Eu, E\varphi\rangle_Z + \beta_k \langle q,\sigma\rangle_Q, \tag{2.21}$$

b_k, f_k as above and g_k defined by

$$g_k := (E^*(z^\delta - E u_k), 0) \in X^* \times Q. \tag{2.22}$$

Theorem 2.3. *Suppose that the assumptions of Theorem 2.2 are satisfied and let*

$$(u_h, q_h, \lambda_h) \in X_h \times Q_h \times X_h$$

denote the unique solution of (2.17), (2.18). *Then there exists a constant* $c > 0$ *independent of* X_h *and* Q_h *such that*

$$\|(u - u_h, q - q_h, \lambda - \lambda_h)\| \leq c \left(r^\delta_{\eta,h} + \inf_{(v,s,\mu) \in X_h \times Q_h \times X_h} \|(u - v, q - s, \lambda - \mu)\| \right), \tag{2.23}$$

where (u, q, λ) *denotes the unique solution of* (2.19), (2.20) *and*

$$r^\delta_{\eta,h} := \|(R_\eta - I) z^\delta\|_Z + \sup_{v \in X_h, \|v\|=1} \|(R_\eta - I) E v\|_Z. \tag{2.24}$$

Proof. First, let $(\tilde{u}_h, \tilde{q}_h, \tilde{\lambda}_h)$ denote the solution of (2.17), (2.18) with a^η_k, g^η_k replaced by a_k, g_k. Then Theorem 2.1 in [8] implies the existence of a constant $c_1 > 0$ (independent of X_h and Q_h) such that

$$\|(u - \tilde{u}_h, q - \tilde{q}_h, \lambda - \tilde{\lambda}_h)\| \leq c_1 \inf_{(v,s,\mu) \in X_h \times Q_h \times X_h} \|(u - v, q - s, \lambda - \mu)\|.$$

Moreover, the stable dependence of the solutions of (2.17), (2.18) on the right-hand side implies the existence of $c_2 > 0$ with

$$\begin{aligned}
&\|(u_h - \tilde{u}_h, q_h - \tilde{q}_h, \lambda_h - \tilde{\lambda}_h)\| \\
&\quad \leq c_2 \left(\sup_{v \in X_h, \|v\|=1} \langle g^\eta_k - g_k, (v, 0) \rangle + \sup_{\varphi \in X_h, \|\varphi\|=1} |a^\eta_k(\tilde{u}_h, \tilde{q}_h, \varphi) - a_k(\tilde{u}_h, \tilde{q}_h, \varphi)| \right) \\
&\quad \leq c_2 \left(\sup_{v \in X_h, \|v\|=1} \langle Ev, (R^*_\eta R_\eta - I)(z^\delta - E u_k) \rangle + \sup_{\varphi \in X_h, \|\varphi\|=1} \langle E\varphi, (R^*_\eta R_\eta - I) E \tilde{u}_h \rangle \right) \\
&\quad \leq c_2 \|E\| \, \|(R_\eta - I) z^\delta\|_Z + c_3 \sup_{v \in X_h, \|v\|=1} \|(R_\eta - I) E v\|_Z,
\end{aligned}$$

and with the triangle inequality we may conclude (2.23). □

Theorem 2.3 provides an error estimate for the solutions of the discretized saddle-point problem (2.17), (2.18), consisting of two parts corresponding to the numerical approximation in the image space Z and in the pre-image spaces X and Q. An obvious estimate for the first term is

$$r^\delta_{\eta,h} \leq \inf_{y \in Z_\eta} \|y - z^\delta\|_Z + \sup_{v \in X_h, \|v\|_X=1} \inf_{\tilde{y} \in Z_\eta} \|\tilde{y} - Ev\|_Z,$$

which possibly does not lead to a quantitative estimate, since there is no additional information on the smoothness of the noisy data. An alternative estimate is

$$r^\delta_{\eta,h} \leq \delta + \inf_{y \in Z_\eta} \|y - z\|_Z + \sup_{v \in X_h, \|v\|_X=1} \inf_{\tilde{y} \in Z_\eta} \|\tilde{y} - Ev\|_Z.$$

The infimum of $\|y - z\|_Z$ can usually be estimated more easily, since the exact data z are smoother due to the fact that $\hat{u}$ is the solution of the state equation for some parameter $\hat{q}$. E.g., if the state equation is of elliptic type with solution $\hat{u} \in H^1(\Omega)$, $E : H^1(\Omega) \to L^2(\Omega)$

is the embedding operator, and R_η results from a standard finite element discretization on a grid with fineness η, then we have at least

$$\inf_{y\in Z_\eta} \|y-z\| = \mathcal{O}(\eta).$$

Another important observation is that the last term vanishes if the discrete spaces Z_η and X_h are equal, which can be achieved in some applications.

The second term in (2.23) shows that the Galerkin approximation of the KKT-system is of optimal order in $X_h \times Q_h \times X_h$; it can be estimated by standard methods for finite element discretizations; quantitative estimates can be obtained using the regularity of the iterates. This part depends of course strongly on the specific application.

3 Convergence Analysis

In this section we will analyze the Galerkin LMSQP method with respect to convergence, i.e., the convergence of the reconstruction obtained with an appropriate stopping rule as the noise level and the measure for the discretization fineness tend to zero. With $\eta = 0$, $h = 0$ we will identify the infinite-dimensional case, i.e., $X_0 = X$, $Q_0 = Q$ and $Z_0 = Z$. We assume that the discrete subspaces satisfy

$$\bigcup_{h>0} X_h = X, \qquad \bigcup_{\eta>0} Z_\eta = Z, \qquad \bigcup_{h>0} Q_h = Q.$$

If we denote by e_k and f_k the error terms

$$(e_k, f_k) := (P_h(u_k - \hat{u}), \tilde{P}_h(q_k - \hat{q})), \tag{3.1}$$

we can rewrite the Karush-Kuhn-Tucker system (2.12) as

$$\begin{pmatrix} P_h^* E^* R_\eta^* R_\eta E P_h & 0 & P_h^* K_k^* P_h \\ 0 & \beta_k \tilde{P}_h^* \tilde{P}_h & \tilde{P}_h^* L_k^* P_h \\ P_h^* K_k P_h & P_h^* L_k \tilde{P}_h & 0 \end{pmatrix} \begin{pmatrix} e_{k+1} \\ f_{k+1} \\ \lambda_{k+1} \end{pmatrix} = \begin{pmatrix} P_h^* E^* R_\eta^* R_\eta (z^\delta - E P_h \hat{u}) \\ \beta_k \tilde{P}_h^* \tilde{P}_h (q_k - \hat{q}) \\ r_k \end{pmatrix} \tag{3.2}$$

where the r_k denotes the remainder

$$r_k := P_h^* \left(e(\hat{u}, \hat{q}) - e(u_k, q_k) + e'(u_k, q_k)(P_h e_k, \tilde{P}_h f_k) \right). \tag{3.3}$$

As in [10], we require a condition on the nonlinearity, which is summarized in the following:

Assumption 1. Let (1.5) be satisfied and define the remainder $r(u,q)$ by

$$r(u,q) \ := \ e(\hat{u},\hat{q}) - e(u,q) - e'(u,q)(\hat{u} - u, \hat{q} - q). \tag{3.4}$$

Then we assume that there exists a constant $\gamma_1 < 1$ such that

$$\|Ee_u(u,q)^{-1} r(u,q)\|_Z \le \gamma_1 \|Eu - z\|_Z, \qquad \forall\ (u,q) \in B_{2\zeta}(u_0) \times B_{2\rho}(q_0), \tag{3.5}$$

and that there exists a solution $(\hat{u},\hat{q}) \in B_\zeta(u_0) \times B_\rho(q_0)$ of the parameter identification problem.

If we define the discretization measures ϵ_h, κ_h by

$$\epsilon_h = \|E(I-P_h)\hat{u}\|_Z, \qquad \kappa_h = c_{\zeta,\rho}\|(I-\tilde{P}_h)\hat{q}\|_Q, \tag{3.6}$$

where

$$c_{\zeta,\rho} = \sup_{(u,q)\in B_{2\zeta}(u_0)\times B_{2\rho}(q_0)} \|Ee_u(u,q)^{-1}e_q(u,q)\|_Z, \tag{3.7}$$

and ϵ_η by

$$\epsilon_\eta = \gamma_1\zeta^{-1}\sup_{\|v\|_X=1}\|(R_\eta - I)Ev\|_Z. \tag{3.8}$$

Then for all $(u,q)\in B_{2\zeta}(u_0)\times B_{2\rho}(q_0)$, the estimate

$$\|R_\eta Ee_u(u,q)^{-1}r_h(u,q)\|_Z \le \gamma_1\|R_\eta(Eu-z)\|_Z + \epsilon_\eta + \epsilon_h + \kappa_h \tag{3.9}$$

holds, where

$$r_h(u,q) := e(\hat{u},\hat{q}) - e(u,q) - e'(u,q)(P_h\hat{u}-u, \tilde{P}_h\hat{q}-q). \tag{3.10}$$

Remark 1. If X_h, Z_η and Q_h are standard finite-element spaces on some triangulations, then ϵ_h, ϵ_η and κ_h can be estimated by the approximation error of these elements. In particular, if the discretization parameter (i.e., the maximal size of a triangle) tends to zero and if the triangulation is regular, one can guarantee that ϵ_h, ϵ_η and κ_h tend to zero (cf. [32] for further details).

For the choice of the stopping index we use a numerical version of (1.9), which involves the discretization measures defined above:

$$\|R_\eta(Eu_{k_*} - z^\delta)\|_Z \le \tau(\delta_\eta + 2\epsilon_h + \kappa_h) < \|R_\eta(Eu_k - z^\delta)\|_Z, \qquad \forall\, k < k_*. \tag{3.11}$$

For an appropriate choice of τ, this allows us to prove the following monotonicity property of the iterates:

Lemma 3.1. *Let Assumption 1 be fulfilled, let the noise be bounded by* (1.1), *and assume that*

$$\beta_0^{-1}(\|Ee_0\|_Z - \delta - \epsilon_h)^2 + \|f_0\|_Q^2 \le \rho^2. \tag{3.12}$$

In addition, β_k is chosen such that $\beta_k \le \beta_{k-1}$ for all $k\in\mathbb{N}$ and that

$$\overline{\gamma}_1 := \gamma_1\sup_{k\in\mathbb{N}}\sqrt{\frac{\beta_{k-1}}{\beta_k}} < 1, \tag{3.13}$$

and the stopping index k_* is chosen according to the generalized discrepancy principle (3.11) *with*

$$\tau > 1 + \frac{\gamma_1 + \overline{\gamma}_1}{\gamma_1(1-\overline{\gamma}_1)}, \tag{3.14}$$

then $q_k \in B_{2\rho}(q_0)$ and the estimates

$$\begin{aligned}(\|R_\eta Ee_{k+1}\|_Z - \delta - \epsilon_h)^2 + \beta_k\|f_{k+1}\|_Q^2 + \beta_k\|q_{k+1}-q_k\|_Q^2 \\ \le (\gamma_1\|R_\eta Ee_k\|_Z + \delta + \epsilon_\eta + 2\epsilon_h + \kappa_h)^2 + \beta_k\|f_k\|_Q^2\end{aligned} \tag{3.15}$$

and

$$\beta_k^{-1}(\|R_\eta Ee_{k+1}\|_Z - \delta - \epsilon_h)^2 + \|f_{k+1}\|_Q^2 \le \beta_{k-1}^{-1}(\|R_\eta Ee_k\|_Z - \delta - \epsilon_h)^2 + \|f_k\|_Q^2 \tag{3.16}$$

hold for all $k < k_*$.

Proof. Assume that $q_k \in B_{2\rho}(q_0)$. Then, with (3.2) and

$$\lambda_{k+1} = -(P_h^* K_k^* P_h)^{-1} P_h^* E^* R_\eta^* R_\eta (Eu_{k+1} - z^\delta)$$

we deduce the identity

$$\begin{aligned}
2\|R_\eta E e_{k+1}\|_Z^2 &+ \beta_k \|f_{k+1}\|_Q^2 + \beta_k \|q_{k+1} - q_k\|_Q^2 \\
&= 2\|R_\eta E e_{k+1}\|_Z^2 + \beta_k \|f_k\|_Q^2 + 2\beta_k \langle f_{k+1}, q_{k+1} - q_k \rangle \\
&= 2\langle R_\eta (z^\delta - EP_h \hat{u}), R_\eta E e_{k+1} \rangle_Z + \beta_k \|f_k\|_Q^2 \\
&\quad + 2\langle R_\eta (Eu_{k+1} - z^\delta), R_\eta E P_h (P_h^* K_k P_h)^{-1} P_h^* r_h(u_k, q_k) \rangle_Z .
\end{aligned}$$

The noise bound (1.1) implies that

$$\|R_\eta (z^\delta - P_h \hat{u})\|_Z \le \|R_\eta (z^\delta - z)\|_Z + \|E(I - P_h)\hat{u}\|_Z \le \delta + \epsilon_h,$$

and using the Cauchy-Schwarz inequality together with (3.9) we obtain the estimate

$$\begin{aligned}
(\|R_\eta E e_{k+1}\|_Z - \delta - \epsilon_h)^2 &+ \beta_k \|f_{k+1}\|_Q^2 + \beta_k \|q_{k+1} - q_k\|_Q^2 \\
&\le (\gamma_1 \|R_\eta E e_k\|_Z + \delta + \epsilon_\eta + 2\epsilon_h + \kappa_h)^2 + \beta_k \|f_k\|_Q^2 .
\end{aligned}$$

(3.16) follows from dividing (3.15) by β_k and the fact that

$$\sqrt{\frac{\beta_{k-1}}{\beta_k}} (\gamma_1 \|R_\eta E e_k\|_Z + \delta + \epsilon_\eta + 2\epsilon_h + \kappa_\eta) \le \|R_\eta E e_k\|_Z - \delta - \epsilon_h .$$

By induction we can now show that $q_k \in B_\rho(q_0)$ for $k < k_*$ and τ satisfying (3.14). □

In an analogous way to the proof of Lemma 3.2 in [10] we can prove the following statement on the finiteness of the stopping index k_* if $\delta > 0$:

Lemma 3.2. *Under the assumptions of Lemma 3.1, the discrepancy principle* (3.11) *yields a finite stopping index k_* if*

$$\delta_{\eta,h} := \delta + \epsilon_\eta + 2\epsilon_h + \kappa_h > 0, \tag{3.17}$$

and τ is chosen according to (3.14).

One observes that in the above estimates, the term $\delta_{\eta,h}$ now plays the same role as the noise level δ in the infinite-dimensional setup. Therefore it is also possible to prove convergence as $\delta_{\eta,h} \to 0$ in the same way as convergence in the infinite-dimensional case for $\delta \to 0$ (cf. [10, Theorem 3.5]). Consequently, we do not give the detailed convergence proof, but refer to [10] for further details on the technique of the proof. We only recall the basic assumptions on e and give the final convergence result, where we use the notation $(u_k^{\delta,\eta,h}, q_k^{\delta,\eta,h})$ for the iteration according to (2.12) with initial value $(P_h u_0, \tilde{P}_h q_0)$, noise level δ and discretization parameter h and η.

Assumption 2. In addition to Assumption 1, assume that e is of the form

$$e(u,q) = A(u) + N(u,q), \qquad \forall\ (u,q) \in X \times Q, \tag{3.18}$$

with continuously Frèchet-differentiable (nonlinear) operators $A : X \to X^*$ and $N : X \times Q \to X^*$, such that

$$N(u,.) \in \mathcal{L}(Q, X^*), \qquad \forall\, u \in X. \tag{3.19}$$

Moreover, we assume that A and N satisfy the nonlinearity conditions

$$\|Ee_u(u,q)^{-1}A'(v)w\|_{X^*} \le \gamma_2 \|Ew\|_{X^*}, \quad \forall\, (u,v,w,q) \in B_{2\zeta}(u_0)^2 \times X \times B_{2\rho}(q_0), \tag{3.20}$$

and

$$\|Ee_u(u,q)^{-1}N_u(v,s)w\|_{Y} \le \gamma_3 \|Ew\|_{Y}, \quad \forall\, (u,v,w,q,s) \in B_{2\zeta}(u_0)^2 \times X \times B_{2\rho}(q_0)^2, \tag{3.21}$$

for some positive constants γ_2 and γ_3.

Theorem 3.3 (Convergence). *Let Assumption 2 and* (3.12) *be fulfilled with ζ, ρ sufficiently small, and let the noise be bounded by* (1.1)*. Moreover, let β_k be chosen such that $\beta_k \le \beta_0$ for all $k \in \mathbb{N}$ and that* (3.13) *is satisfied. If the perturbed iteration is stopped with $k_* = k_*(\delta, R_\eta z^\delta, h)$ according to the generalized discrepancy principle* (3.11) *with $\tau = \tau(h,\eta)$ (uniformly bounded in h and η) satisfying* (3.14)*, then*

$$(q^{\delta,\eta,h}_{k_*(\delta,R_\eta z^\delta,h)}, u^{\delta,\eta,h}_{k_*(\delta,R_\eta z^\delta,h)}) \to (\overline{q}, \overline{u}), \qquad \text{in } X \times Q, \quad \text{as } \max\{\delta_\eta, \epsilon_h, \kappa_h\} \to 0, \tag{3.22}$$

where $(\overline{u}, \overline{q})$ is a solution of (1.3) *with $E\overline{u} = z$.*

Proof. Analogous to the proof of Theorem 3.5 in [10]. □

4 Numerical Realization of the SQP-Iteration

In the following we want to discuss some numerical methods and variants for the 'outer iteration', i.e., the Galerkin LMSQP algorithm under the assumption that we are able to solve the discretized KKT-system numerically. The 'inner iteration', namely the numerical solution of the indefinite system (2.12) will be investigated in Section 5.

4.1 Scaling of State Variable, Parameter and Lagrangian Variable

The performance of an iteration algorithm often depends crucially on the way the problem is formulated. Scaling is a well-known technique for reformulating an optimization problem whose main objective is twofold: on the one hand all the variables should be of similar magnitude, on the other hand also the value of the derivatives should all be of similar size. In unconstrained optimization, a problem should be rescaled in such a way, that changes of the iterate in one direction do not result in by far larger changes of the value of the objective than changes in another direction. In constrained optimization the above statements are also true for each constraint. Additionally the set of constraints should be well balanced with respect to each other such that each constraint has equal weight. Furthermore the set of constraints should be balanced with respect to the objective. As scaling is of high practical importance for any optimization problem, many aspects can be found in monographs on optimization (cf. e.g. [19, 30]).

We want to consider only the last aspect in this context, i.e., the scaling of the state constraint with respect to the objective which is also of high importance for achieving fast convergence of the outer iteration. For the inner iteration, the aspect of scaling can be included in the construction of a good preconditioner. The outer iteration of an SQP method tries to attain two goals at the same time: feasibility of the iterate with respect to the state constraint and optimality of the iterate with respect to the objective. One aspect dominating the other results usually in bad convergence properties: If the feasibility aspect dominates, only very small changes of the iterate are possible in order to ensure "almost" feasibility. If the optimality aspect dominates, any violation of the state constraint is reduced too slowly.

For the LMSQP method in the form of (2.4),(2.5) it turned out that in many situations the feasibility aspect is strongly dominating. Using line search methods for globalization (see also Subsection 4.2) this results usually in step lengths much smaller than one. Replacing the state constraint by a preconditioned state constraint leads to a better balanced formulation and to much faster convergence. Furthermore a step length parameter equal to one is accepted in almost all steps. Another aspect of this kind of rescaling is treated in Subsection 6.2.

4.2 Globalization Strategies

The LMSQP method is a variant of Newton's method and therefore only locally convergent (see also the analysis in Section 3). For this reason, globalization strategies, such as *trust region methods* or *line search strategies* (which are the two most popular classes of globalization techniques in optimization), are needed.

The basic idea of trust region methods is to add an additional constraint on the maximal increment to the quadratic optimization problem for the correction step of the current iterate, i.e. instead of (2.4), (2.5) one would solve (2.4), (2.5) and $\|(u-u_k, q-q_k)\| \leq \epsilon_k$ with ϵ_k chosen appropriately. Trust region methods have been successfully applied to PDE constrained optimization problems (see e.g. [14, 38]), often using a reduced SQP approach. We want to mention that a similar effect as with trust-region methods could be reached in principle by controlling the penalty parameter β_k, which also restricts the step size and produced good numerical results (see Example 7.1). For a comprehensive overview of trust region methods we refer to Conn et. al. [13].

In the code used for two-dimensional problems (cf. [10] and Example 7.2), we use a line search algorithm for globalization. In contrast to trust region methods, the calculation of the increment is split into two phases: first of all, a search direction is determined, and secondly the estimation of a step length parameter indicating how far into the search direction one should go. For the computation of the search direction we solve the optimization problem (2.4) and (2.5). In order to determine the step length we cannot use the objective itself as a criterion (as in unconstrained optimization), but have to use a merit function which balances the minimization of the objective with the feasibility with respect to the state constraint. Applied to a discretized optimization problem of the form

$$\tilde{J}(V,S) \rightarrow \min_{(V,S)\in\mathbb{R}^m\times\mathbb{R}^n},$$

subject to an equation constraint of the form

$$\tilde{e}(V,S) = \tilde{f},$$

possible choices are the l^1-merit function

$$\Phi(V,S) = \tilde{J}(V,S) + \kappa\|\tilde{e}(V,S) - \tilde{f}\|_{l^1}$$

and its variants, and the augmented Lagrangian

$$\Phi(V,S,\Lambda) = \tilde{J}(V,S) + \Lambda^T(\tilde{e}(V,S) - \tilde{f}) + \frac{\kappa}{2}\|\tilde{e}(V,S) - \tilde{f}\|_{l^2}^2,$$

where Λ is an estimate of the Lagrangian variable corresponding to the discretized equation constraint. Both merit functions are exact in the sense that for κ sufficiently large, minimizers of the original constrained optimization problem also minimize the merit function.

A crucial property in the design of a merit function is that it should accept step length one close to a solution in order to preserve the quadratic convergence of the SQP method. The augmented Lagrangian works well, as long as the estimate for the Lagrangian multiplier is accurate enough, whereas the l^1-merit function sometimes suffers from the so-called "Marathos-effect", i.e. it does not accept unit step length and therefore causes a slow-down of the convergence. A strategy to overcome this difficulty using a second order correction can be found in [30]; nevertheless, it performed very well in our numerical experiments (see Example 7.2).

4.3 Nested Multi-Level Optimization Techniques

Important tools for the efficient numerical approximation of infinite-dimensional optimization problems are *multi-level optimization methods*. In the nested multi-level setup, one starts the optimization procedure at a coarse level $X_{h_1} \times Q_{h_1}$, where the iteration procedure can be carried out efficiently. If an appropriate stopping rule is satisfied, one interpolates the state and parameter obtained in this way to a finer level $X_{h_2} \times Q_{h_2}$ (for $h_2 < h_1$), serving now as a starting value on this level. This procedure is repeated until the finest level is reached. Usually, nested space are used in this approach, i.e., $X_{h_1} \subset X_{h_2}$, $Q_{h_1} \subset Q_{h_2}$ (for $h_2 < h_1$), which leads to simple interpolation operators. Since one cannot choose the discretization of the data arbitrarily in general , we consider only the case of fixed η here, but a multi-level approach in η can be realized in an analogous way, if necessary.

Nested multi-level methods outperform standard discretization techniques in many cases (cf. e.g. [21, 22, 29]); usually a considerable number of iterations is needed on the coarse level only , where the numerical effort per iteration is very low. On the finest levels, the stopping rule is often satisfied already after one iteration step and so the overall effort is less than for a direct discretization on the finest level. For the Galerkin LMSQP method, we can formulate a multi-level algorithm as follows:

Algorithm 4.1 (Nested Multi-Level Galerkin LMSQP). Given a decreasing sequence $\{h_\ell\}_{\ell=1,\dots,L}$ with nested spaces $X_{h_\ell} \subset X_{h_{\ell+1}}$, $Q_{h_\ell} \subset Q_{h_{\ell+1}}$ (e.g. $h_\ell = 2^{-\ell}h_0$), and a non-increasing sequence τ_ℓ satisfying (3.14), the nested multi-level Galerkin LMSQP method consists of the following iterative procedure:

1. Set $\ell = 1$, $h = h_1$ and start with $(u_0^\ell, q_0^\ell) \in X_h \times Q_h$.

2. Perform the Galerkin LMSQP method until the stopping criterion (3.11) is satisfied with stopping index $k_*(\ell)$.

3. If $\ell = L$ stop the iteration, else prolongate the iterate $(u_{k_*}^\ell, q_{k_*}^\ell)$ to the finer level $X_{h_{\ell+1}} \times Q_{h_{\ell+1}}$, which results in a new starting value $(u_0^{\ell+1}, q_0^{\ell+1})$. Set $h = h_{\ell+1}$, $\ell = \ell+1$ and go to step 2.

The analysis in Section 3 shows that for $\beta_0^\ell \geq \beta_{k_*(\ell-1)}^{\ell-1}$, the estimate

$$\begin{aligned}(\beta_{k_*(\ell)}^\ell)^{-1}\|R_\eta E e_{k_*(\ell)}^\ell\|_Z^2 + \|f_{k_*(\ell)}^\ell\|_Q^2 + \sum_{j=0}^{k_*(\ell)-1} \|q_{j+1}^\ell - q_j^\ell\|_Q^2 \\ \leq (\beta_0^\ell)^{-1}\|R_\eta E e_0^\ell\|_Z^2 + \|f_0^\ell\|_Q^2 \\ \leq (\beta_{k_*(\ell-1)}^{\ell-1})^{-1}\|R_\eta E e_{k_*(\ell-1)}^{\ell-1}\|_Z^2 + \|f_{k_*(\ell-1)}^{\ell-1}\|_Q^2 + \theta_\ell\end{aligned}$$

holds, where θ_ℓ is the error corresponding to the interpolation of the iterates from level $\ell-1$ to level ℓ, i.e.,

$$\theta_\ell = (\beta_0^\ell)^{-1}\left(\|R_\eta E e_0^\ell\|_Z^2 - \|R_\eta E e_{k_*(\ell-1)}^{\ell-1}\|_Z^2\right) + \left(\|f_0^\ell\|_Q^2 - \|f_{k_*(\ell-1)}^{\ell-1}\|_Q^2\right). \tag{4.1}$$

This monotonicity estimate corresponds very well to the intuition that only few iterations are needed on the fine levels, in particular if β_k^ℓ is decreasing, which leads to

$$\|R_\eta E e_{k_*(\ell)}^\ell\|_Z^2 \leq \beta_{k_*(\ell)}^\ell \left((\beta_0^\ell)^{-1}\tau_{\ell-1}\delta_{\eta,h_{\ell-1}} + \|f_{k_*(\ell-1)}^{\ell-1}\|_Q^2 + \theta_\ell\right).$$

For a fine level with small β, we can expect that

$$\beta_{k_*(\ell)}^\ell(\beta_0^\ell)^{-1}\tau_{\ell-1}\delta_{\eta,h_{\ell-1}} \approx \tau_\ell\delta_{\eta,h_\ell},$$

and the second term $\beta_{k_*(\ell)}^\ell(\|f_{k_*(\ell-1)}^{\ell-1}\|_Q^2+\theta_\ell)$ can be expected to be negligible. I.e., the stopping rule at level ℓ is probably satisfied with $k_*(\ell)=1$.

Under typical conditions, where X_{h_ℓ} and Q_{h_ℓ} correspond to standard finite-element spaces on different refinement levels of an initial triangulation of a domain Ω, one can show that at least $\theta_\ell = \mathcal{O}(h_{\ell-1})$, and consequently

$$\sum_{\ell=2}^{L}\theta_\ell \leq ch_1(1+\sum_{j=0}^{L-2} r^j) \leq ch_1\frac{2-r}{1-r}$$

for some constant $c \in \mathbb{R}_+$, where

$$r = \max_{1\leq\ell\leq L-1}\frac{h_{\ell+1}}{h_\ell} < 1.$$

Together with the above estimate one can show with a standard proof technique that the pair $(u_{k_*(L)}^L, q_{k_*(L)}^L)$ converges to a solution $(\overline{u},\overline{q})$ of the parameter identification problem for $\delta_{\eta,h_L} \to 0$.

5 Numerical Solution of the KKT-System

In the following we will discuss the numerical solution of the discretized KKT-system (2.12) for fixed iteration number k. We have seen above that the Galerkin-type approximation (2.12) of the original KKT-system is stable and convergent, now we discuss some of its structural properties, which are important for the application of iterative solution methods and for the construction of preconditioners.

Choosing bases

$$\Phi = (\varphi_1, \ldots, \varphi_m)^T \in X_h^m, \qquad \Sigma = (\sigma_1, \ldots, \sigma_n)^T \in Q_h^n, \tag{5.1}$$

of the finite-dimensional subspaces X_h and Q_h, we may represent $(u, q, \lambda) \in X_h \times Q_h \times X_h$ via

$$u = V^T \Phi, \qquad q = S^T \Sigma, \qquad \lambda = \Lambda^T \Phi, \tag{5.2}$$

with coordinate vectors $V, \Lambda \in \mathbb{R}^m$ and $S \in \mathbb{R}^n$. In order to transform (2.12) into a linear system for V, S and Λ, we define the matrices

$$G := (\langle E\varphi_j, E\varphi_i \rangle_Z)_{i,j=1,\ldots,m} \qquad H := (\langle \sigma_j, \sigma_i \rangle_Q)_{i,j=1,\ldots,n} \tag{5.3}$$

$$K := (\langle K_k \varphi_j, \varphi_i \rangle)_{i,j=1,\ldots,m} \qquad L := (\langle L_k \sigma_j, \varphi_i \rangle)_{i=1,\ldots,m; j=1,\ldots,n} \tag{5.4}$$

and the vectors

$$f_1 := (\langle z^{\delta,\eta} - Eu_k, E\varphi_i \rangle_Z)_{i=1,\ldots,m}, \qquad f_3 := (\langle f - e(u_k, q_k), \varphi_i \rangle)_{i=1,\ldots,m}. \tag{5.5}$$

This allows us to rewrite the discretized KKT-system (with penalty parameter $\beta = \beta_k$) as

$$\begin{pmatrix} G & 0 & K^T \\ 0 & \beta H & L^T \\ K & L & 0 \end{pmatrix} \begin{pmatrix} V \\ S \\ \Lambda \end{pmatrix} = \begin{pmatrix} f_1 \\ 0 \\ f_3 \end{pmatrix}, \tag{5.6}$$

respectively as

$$MX = F, \tag{5.7}$$

where M is the matrix in (5.6) and

$$X = \begin{pmatrix} V \\ S \\ \Lambda \end{pmatrix} \qquad F = \begin{pmatrix} f_1 \\ 0 \\ f_3 \end{pmatrix}.$$

The structural properties of M and its sub-matrices will be examined in the following section.

5.1 The System Matrix M

Due to the well-posedness result on the discretized KKT-system (2.12) (cf. Theorem 2.2), we may conclude that the system matrix M is regular. In order to obtain further insight into the structure of M, we investigate the properties of the sub-matrices G, H, K and L:

Proposition 5.1. *The matrices $K \in \mathbb{R}^{m\times m}$ and $H \in \mathbb{R}^{n\times n}$ are symmetric positive definite, and the matrix $G \in \mathbb{R}^{m\times m}$ is symmetric positive semi-definite. If, in addition, the operator E is injective on X_h, then G is regular, too.*

Proof. Let u and q be as in (5.2), then there exist constants $c_1(h)$ and $c_2(h)$ such that

$$\|u\|_X \geq c_1(h)|V|, \qquad \|q\|_Q \geq c_2(h)|S|,$$

where $|.|$ denotes the euclidean norm in $\mathbb{R}^n$ and $\mathbb{R}^m$, respectively. Thus, we have

$$V^T K V = \langle K_k u, u \rangle \geq \alpha_e \|u\|_X^2 \geq \alpha_e c_1(h)^2 |V|^2,$$

and

$$S^T H S = \|q\|_Q^2 \geq c_2(h)^2 |S|^2.$$

Moreover, the identity

$$V^T G V = \|Eu\|_Z^2 \geq 0$$

implies that G is positive semi-definite and regular under the assumption that E is injective on X_h. The symmetry of the matrices G, H and K can be verified in a similar way, using the symmetry of scalar products and the self-adjointness of the operator K_k. $\square$

The matrix $L \in \mathbb{R}^{m \times n}$ is difficult to analyze, it is neither symmetric nor regular in general (in particular if $n \neq m$). However, some fundamental properties of M (such as its regularity) rely rather on G, H and K than on L. Moreover, the classical splitting of a symmetric saddle-point problem as

$$\begin{pmatrix} G & 0 & K^T \\ 0 & H_\beta & L^T \\ K & L & 0 \end{pmatrix} = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ KG^{-1} & LH_\beta^{-1} & I \end{pmatrix} \begin{pmatrix} G & 0 & 0 \\ 0 & H_\beta & 0 \\ 0 & 0 & -C \end{pmatrix} \begin{pmatrix} I & 0 & G^{-1}K^T \\ 0 & I & H_\beta^{-1}L^T \\ 0 & 0 & I \end{pmatrix},$$

where $H_\beta := \beta H$ and C is the Schur-complement

$$C := KG^{-1}K^T + \beta^{-1} L H^{-1} L^T, \tag{5.8}$$

is possible if we only know that G and H are regular. In particular, we may conclude that M has $n+m$ positive and m negative eigenvalues.

5.2 Reduced SQP Approaches

The basic idea of reduced SQP-methods is the a-priori elimination of the equality constraint, which can be written in matrix form as

$$KV + LS = f_3, \tag{5.9}$$

which is equivalent to an elimination of V and Λ in (5.6).

Due to Proposition 5.1, K is a regular, symmetric matrix and thus, we may compute

$$V = K^{-1}(f_3 - LS), \tag{5.10}$$
$$\Lambda = K^{-T}(f_1 - GV), \tag{5.11}$$

which yields after some calculations the $n \times n$-system

$$M_r S = g \tag{5.12}$$

with

$$M_r := H + L^T K^{-T} G K^{-1} L \tag{5.13}$$
$$g := L^T K^{-T} (G K^{-1} f_3 - f_1). \tag{5.14}$$

The reduced SQP-approach seems of particular interest if $n \ll m$, which is a frequently used discretization strategy for parameter identification and optimal control problems (cf. e.g. [35, 36, 37]). The original matrix M is an indefinite matrix of size $(2m+n) \times (2m+n)$, while the reduced system matrix M_r in (5.12) is of size $n \times n$. However, M_r is not a sparse matrix even if all the sub-matrices of M are sparse, since it involves the inverse of K. Moreover, the evaluation of M_r is more expensive than the evaluation of the original system matrix M, since it involves the solution of two systems of the form

$$KW = g, \tag{5.15}$$

with different right-hand sides g, while for the evaluation of M only direct evaluations of K are needed, which are very cheap for typical finite element discretization of the state constraint. In practice, one usually tries to compensate this disadvantage of reduced SQP-methods by using a Broyden-type update for the reduced system matrix instead of the exact matrix M_r, which leads to efficient optimization algorithms for small n.

5.3 Simultaneous Solution of the KKT-System

Recently, the simultaneous solution of KKT-systems by iterative methods has been investigated, in particular in connection with optimal control problems (cf. [2, 4, 5, 20]). Compared to the reduced SQP-approach, a simultaneous solution strategy has the obvious advantage that the allocation and evaluation of the system matrix M is much cheaper than of M_r. The pay-off is that M is indefinite and larger than M_r, which might cause additional effort. However, the main effort in the reduced SQP-approach is related to the evaluation or assembly of the system matrix M_r, respectively, and therefore a simultaneous solution of the KKT-system can result in a tremendous speed-up of the SQP-method, in particular for fine discretizations.

At a first glance, it seems rather straight-forward to solve (5.7) by a standard iterative method for indefinite systems such as inexact Uzawa methods (cf. [6, 15]) or Krylov-subspace methods such as GMRES (cf. [34]), MINRES (cf. [31]) and QMR (cf. [18]). However, in the case of large-scale problems, we have to expect a large condition number (note that β is usually small and that M is singular for $\beta = 0$) and a complicated eigenvalue pattern of the matrix M, which might cause iterative methods to diverge or to need a high number of iterations. Therefore, an appropriate preconditioning technique seems necessary for any of the methods. We do not go into details here, but refer to the forthcoming paper [11] for a discussion of preconditioners.

In the following we distinguish two types of solvers that seem appropriate for the solution of the indefinite system (5.7) and discuss their basic properties with respect to the special structure of M.

Inexact Uzawa Iterations

Inexact Uzawa methods and similar iteration procedures have been developed for the solution of the classical Stokes system and similar problems (cf. [32] for an overview). The classical Uzawa method is just a gradient method for the dual of the corresponding Lagrange functional, the inexact Uzawa method can be interpreted as a preconditioned version (cf. [32]). Following the exposition by Zulehner [39], we can write an inexact Uzawa method for a system of the form (5.6) as

$$\hat{A} \begin{pmatrix} V_{j+1} - V_j \\ S_{j+1} - S_j \end{pmatrix} = \begin{pmatrix} f_1 - GV_j - K\Lambda_j \\ -\beta H S_j - L\Lambda_j \end{pmatrix}, \tag{5.16}$$

followed by

$$\hat{C}(\Lambda_{j+1} - \Lambda_j) = f_3 - KV_{j+1} - LS_{j+1}, \tag{5.17}$$

where $\hat{A}$ is a preconditioner for the diagonal matrix

$$A := \begin{pmatrix} G & 0 \\ 0 & \beta H \end{pmatrix}, \tag{5.18}$$

and $\hat{C}$ is a preconditioner for the Schur-complement C defined by (5.8). In terms of (5.7) we can write the inexact Uzawa iteration as

$$X_{k+1} = (I - \hat{M}^{-1}M)X_k + \hat{M}^{-1}F, \tag{5.19}$$

where $\hat{M}$ is a preconditioner for the system matrix, given by

$$\hat{M} = \begin{pmatrix} \hat{A} & 0 \\ B & \hat{C} \end{pmatrix}, \tag{5.20}$$

with $B = \begin{pmatrix} K & L \end{pmatrix}$.

A convergence analysis of this method is available only in the case when A is a regular matrix (cf. [6, 39]), which means that we have to assume that G is regular. The latter is true e.g. if the data z represent distributed data for the state, i.e., E is an embedding operator. In this case, the structure of A is rather simple and it is not a difficult task to construct a preconditioner, even exact preconditioning seems possible (note that G is just a mass matrix for a typical finite element discretization). Since the matrices G and H do not change during the SQP-iteration we may even compute decompositions in a preprocessing step. The construction of a preconditioner for the Schur-complement C is more difficult and must take into account the specific nature of the underlying state equation.

Krylov-Subspace Methods

The Krylov-subspace methods GMRES and QMR are variants of the CG-algorithm that are applicable to indefinite problems, too. The basic idea of such methods is a defect minimization in the Krylov-subspace

$$\mathcal{K}_k(M; X_1) = \{X_1, MX_1, \ldots, M^{k-1}X_1\}, \tag{5.21}$$

generated by X_1, in the k-th iteration step. Since preconditioned CG-methods are probably the most successful class of iteration methods for positive definite systems, such methods seem very attractive also in the indefinite case, although additional difficulties may arise (cf. e.g. [34]).

The convergence analysis in [34] and [18] shows that the error bounds obtained for both methods are essentially the same, and mainly dependent on the eigenvalue distribution and the condition number of the system matrix M. Therefore, appropriate preconditioning is again of high importance, in this case also with the possibility that G is singular. We refer to [11] for a detailed discussion of this problem.

6 Application to Potential Reconstruction

As a first application we investigate the identification of the potential q in the elliptic boundary value problem

$$-\Delta u + qu = f \qquad \text{in } \Omega, \tag{6.1}$$
$$u = 0 \qquad \text{on } \partial\Omega, \tag{6.2}$$

from a state observation in $L^2(\Omega)$, which is a well-studied problem in literature (cf. e.g. [33]). In [10], it has been shown that in the setup (d denotes the space dimension)

$$X = H_0^1(\Omega), \qquad X^* = H^{-1}(\Omega), \qquad Q = H^d(\Omega), \qquad Z = L^2(\Omega), \tag{6.3}$$

the operators

$$e : X \times Q \to X^*, (u,q) \mapsto (-\Delta u + qu) \tag{6.4}$$
$$E : X \to Z, u \mapsto u, \tag{6.5}$$

satisfy all assumptions needed for the convergence analysis of the LMSQP-method. Now we shall study a concrete finite-element discretization of the KKT-system and the derivation of estimates for the numerical errors ϵ_η, ϵ_h and κ_h.

6.1 Error Estimates for the Discretized KKT-System

In this case we can write the whole KKT-system in classical form as

$$-\Delta v + q_k v + s u_k = f \qquad \text{in } \Omega, \tag{6.6}$$
$$-\Delta\lambda + q_k\lambda + u - z^\delta = 0 \qquad \text{in } \Omega, \tag{6.7}$$
$$\beta L_d s + u_k\lambda = 0 \qquad \text{in } \Omega, \tag{6.8}$$

again with homogenous Dirichlet boundary conditions upon v and λ on $\partial\Omega$, where L_d is a dimension-dependent differential operator of order $2d$ corresponding the norm in $H^d(\Omega)$, e.g., we have

$$L_1 q = -q_{xx} + q \tag{6.9}$$
$$L_2 q = \Delta(\Delta q + q) + q, \tag{6.10}$$

supplemented by homogenous boundary conditions up to order $d-1$. If $f \in L^2(\Omega)$ and $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$, a standard elliptic regularity argument shows that $\hat{u}, u_k \in H^2(\Omega) \cap H_0^1(\Omega)$, for all $k \in \mathbb{N}$. In the same way we can show that $\lambda_k \in H^2(\Omega) \cap H_0^1(\Omega)$ and $s_k \in H^{2d}(\Omega)$. This additional regularity can be employed to derive standard error estimates for finite-element discretizations of the KKT-system (2.12).

If we use piecewise linear finite elements on regular triangulations $\mathcal{T}_\eta$ and $\mathcal{T}_h$ for the discretization spaces Z_η and X_h, where η and h represent the fineness of the grids, then a classical approximation result for finite elements (cf. [32, p.96]) implies that

$$\epsilon_\eta = \mathcal{O}(\eta^2) \qquad \text{and} \qquad \epsilon_h = \mathcal{O}(h). \tag{6.11}$$

Of course, one could also use piecewise constant elements on $\mathcal{T}_\eta$, which would yield $\epsilon_\eta = \mathcal{O}(\eta)$. However, in practical applications a higher-order approximation in η is often desirable, since

η can be significantly larger than a reasonable choice of h. A canonical approximation of the parameter q is a finite element space of order greater or equal d on a regular triangulation $\mathcal{T}_{\tilde{h}} \subset \mathcal{T}_h$; under a-priori assumptions on the exact solution $\hat{q}$ one can obtain quantitative estimates for κ_h in terms $\tilde{h}$. At a first glance it seems surprising that one needs a-priori assumptions on the parameter, but not on the state in order to derive error estimates. However, due to the ill-posedness of the identification problem with respect to the parameter q, such a-priori knowledge seems to be necessary. The approximation of the state corresponds rather to the approximation of the underlying elliptic state equation, which is well-posed with respect to u and yields further regularity. We finally want to mention that according to the theory developed above, one could choose $\mathcal{T}_{\tilde{h}}$ independent of $\mathcal{T}_h$, but this would cause unnecessary complications in the implementation of the method.

We note that alternatively one can use the space $Q = L^2(\Omega)$ for $d \leq 3$, which yields $L_d = I$, i.e., (6.8) becomes

$$\beta s + u_k \lambda = 0. \tag{6.12}$$

An appropriate discretization strategy is e.g. to choose Q_h as the space of piecewise constant elements on an underlying grid $\mathcal{T}_{\tilde{h}}$. The advantage of this approach is that elements of order greater than one, which are necessary for $Q = H^d(\Omega)$ ($d \geq 2$), can be avoided.

6.2 Structure of the System Matrix

For the potential identification problem, some parts of the system matrix M in (5.6) are well-understood. First of all, G is an L^2-mass matrix and it is positive definite if the triangulations $\mathcal{T}_\eta$ and $\mathcal{T}_h$ coincide, which we assume in the following. The eigenvalues of G are then all of order h^d. The matrix H is the stiffness matrix for the differential operator L_d, with minimal eigenvalue of order h^d and maximal eigenvalue of order h^{-d}.

The matrix K is the sum of a stiffness matrix for the Laplacian and a weighted mass matrix (with weight q_k in the L^2-scalar product), where one can expect the first part in this sum to be dominating. Thus, the stiffness matrix $\hat{K}$ for the Laplacian will be a good preconditioner for K. The maximal and minimal eigenvalues of K and $\hat{K}$ are of order h^{d-2} and h^d, respectively. The remaining part in the system matrix, namely the matrix L, is difficult to understand, since its elements are weighted L^2-scalar products of basis functions of different finite element spaces. However, the spectral norm of L can be estimated, it is of order $\tilde{h}^d$.

The construction of preconditioners for G and H is well-investigated, even exact preconditioning seems to be applicable. For K it seems reasonable to use a preconditioner $\hat{K}$ for the Laplacian, e.g. a multi-grid preconditioner. With preconditioning for K, the system matrix can be transformed to

$$\tilde{M} = \begin{pmatrix} G & 0 & K\hat{K}^{-1} \\ 0 & \beta H & L^T\hat{K}^{-1} \\ \hat{K}^{-1}K & \hat{K}^{-1}L & 0 \end{pmatrix}, \tag{6.13}$$

with the corresponding Schur-complement

$$\tilde{C} = \hat{K}^{-1}KG^{-1}K\hat{K}^{-1} + \beta^{-1}\hat{K}^{-1}LH^{-1}L^T\hat{K}^{-1}. \tag{6.14}$$

If $\hat{K}$ is an appropriate preconditioner for K, then we can estimate the minimal eigenvalue by

$$\lambda_{min}(\tilde{C}) \geq \lambda_{min}(\hat{K}^{-1}KG^{-1}K\hat{K}^{-1}) = \mathcal{O}(h^{-d}), \tag{6.15}$$

and the maximal eigenvalue by

$$\begin{aligned} \lambda_{max}(\tilde{C}) &\leq \|\hat{K}^{-1}KG^{-1}K\hat{K}^{-1}\|_2 + \beta^{-1}\|\hat{K}^{-1}LH^{-1}L^T\hat{K}^{-1}\|_2 && (6.16)\\ &= \mathcal{O}\left(h^{-d}(1+\beta^{-1}h^{-2d}\tilde{h}^{2d})\right). && (6.17) \end{aligned}$$

Hence, the condition number of $\tilde{C}$ is independent of h, but only depends on β and $\frac{\tilde{h}}{h}$. One observes that the condition number is decreasing as $\tilde{h}$ tends to h from above (note that usually $\tilde{h} \geq h$). For the Uzawa iteration, one can choose the preconditioner $\hat{C}$ in this case as a multiple of $\hat{K}^{-1}KG^{-1}K\hat{K}^{-1}$ or even of G^{-1}. If $\tilde{h} \gg h$, the Uzawa iteration seems not to be optimal, in this case one can apply either a reduced SQP-approach or use Krylov-subspace methods with different preconditioning strategies. For the details on the latter we refer to [11].

7 Numerical Experiments

In order to test our theoretical results, we numerically solve some model problems, which have already been investigated with respect to the convergence behavior of the LMSQP-method in [10].

Example 7.1. Our first example is the identification of the potential q in (6.1), (6.2) from a state observation $u \in L^2(\Omega)$, with $\Omega = (0,1)$, $g = 0$ and

$$f(x) = \frac{1}{2} + \sin x, \qquad x \in \Omega.$$

The exact potential is given by

$$q(x) = x(1-x),$$

which is an element of $Q = H^1(\Omega)$. This problem was implemented in the software-system MATLAB.

The data are generated by solving the state equation on a fine grid and subsequent interpolation to a coarser grid; the noise is an additive high-frequency perturbation. We used uniform grids with m nodes for the discretization of the state u and the Lagrange-parameter λ and n nodes for the parameter q, i.e., $h = (m-1)^{-1}$ and $\tilde{h} = (n-1)^{-1}$. The parameters β_k are chosen according to $\beta_{k+1} = 0.9\beta_k$, with $\beta_0 = 10^{-6}$, which lead to convergence of the method even for starting value $q \equiv 0$.

The KKT-system (5.6) is solved by the QMR method, using an Uzawa-type preconditioner as described in Section 6.2, with $\hat{A} = A$, $\hat{K}$ a preconditioner for the Laplacian and $\hat{C} = G^{-1}$. The convergence results for the overall LMSQP-method have been shown in [10] and compared to a Levenberg-Marquardt method following the feasible path. It turned out that both methods lead to almost the same iteration sequence q_k. In particular, the number of iterations needed until the stopping rule is satisfied, is the same for both methods. Now we compare the numerical efficiency of the LMSQP-method with feasible path approaches, namely the Levenberg-Marquardt method (LM) on the feasible path (with the same Galerkin discretization as for LMSQP and solution of the Gauss-Newton system by a preconditioned CG-method) and a Broyden-type variant of the Levenberg-Marquardt method (cf. [23] for further details).

m	n	LMSQP	LM	Broyden
201	41	0.07	1.37	0.51
201	101	0.18	3.44	1.34
201	201	0.36	6.94	2.88
401	201	0.51	24.83	9.09
401	401	1.39	50.39	20.48
801	401	2.61	193.21	70.69
801	801	5.66	392.54	158.69
1601	801	7.91	1564.50	600.66
1601	1601	22.86	3144.40	1356.60

Table 1: CPU-time (in seconds) needed for the LMSQP-method, the LM-method and a Broyden-type variant of the LM-method.

For this sake we choose different discretization levels (fixed during the iteration) and measure the CPU-time needed for the LMSQP-method, until the stopping rule is satisfied (for fixed noise level δ). From the results shown in Table 1 one observes that the LMSQP-method with simultaneous solution of the KKT-system outperforms the feasible-path approaches for all different discretizations. Since the LMSQP and the LM-method need the same number of outer iterations, the difference in the numerical effort is caused by the fact that the effort for the evaluation of the system matrix in the LM-method is significantly higher than evaluation and preconditioning of the system matrix in the simultaneous LMSQP-method. Obviously, the gain in the numerical effort for the evaluation of the system matrix increases with the number of discretization points, which explains the extremely large CPU-time for the LM-method at the finest discretization level ($m = 1601$). For small m and n, the Broyden-variant is much faster than the LM-method, which is again caused by the fact that the evaluation of the system matrix can be carried out efficiently. However, the number of iterations needed for the Broyden-type variant is much larger than for the other two methods, which use the full information about the derivatives.

Finally, we investigate the spectral condition of the system matrix M as well as of the matrix $\tilde{M}$ defined by (6.13), where we use a preconditioner for the Laplacian as $\hat{K}$. ¿From the left picture in Figure 1, which shows the condition number as a function of the discretization size h (in logarithmic scale) for fixed $\beta = 10^{-5}$, one observes that the condition number of M grows quadratically with h^{-1}, while the condition number of $\tilde{M}$ is much smaller and almost independent of h. The second part of Figure 1 shows a plot of the condition numbers vs. the parameter β in doubly logarithmic scale, from which it seems that the growth of the condition number as $\beta \to 0$ is slower for $\tilde{M}$ than for the original matrix M. In both cases, the condition number seems to be a convex function of β, which has a unique minimum at some $\overline{\beta}$. However, this value $\overline{\beta}$ is rather large and values of β that are significantly larger than $\overline{\beta}$ are not of interest for our purpose, since they would cause a tremendous slow-down of the outer iteration. Therefore we can focus our attention to the case $\beta < \overline{\beta}$, where the condition number increases in a monotonically with β^{-1}.

Example 7.2. Our second numerical example is the identification of the conductivity $q \in$

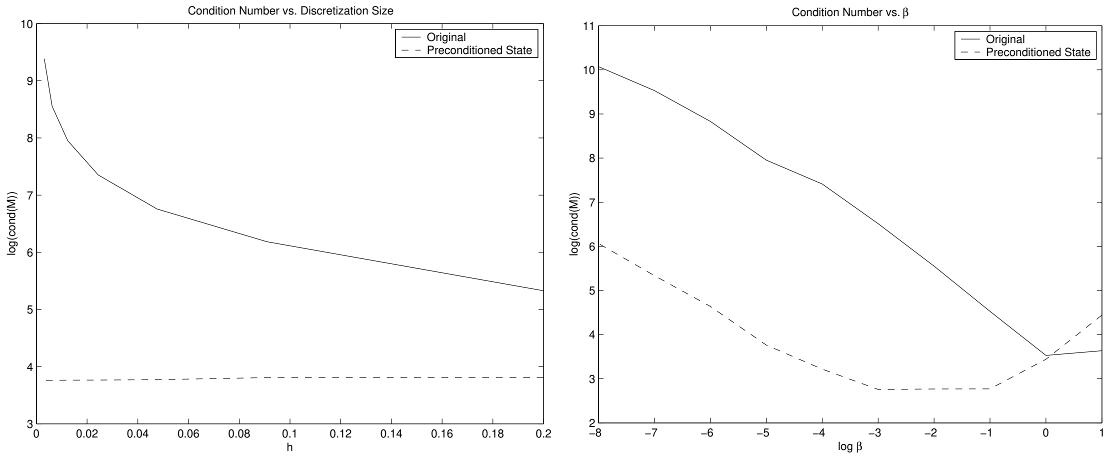

Figure 1: Plot of the spectral condition of the matrix M vs. the discretization size h (in logarithmic scale, left) and vs. the parameter β (in doubly logarithmic scale, right). The solid line shows the condition number of the original matrix M, the dashed line of the matrix $\tilde{M}$ with preconditioned state equation.

$L^\infty(\Omega)$ in

$$-\text{ div } (q\nabla u) = f \qquad \text{in } \Omega, \tag{7.1}$$

$$u = g \qquad \text{on } \partial\Omega. \tag{7.2}$$

from a state observation $u \in L^2(\Omega)$. The domain Ω is a ball in $\mathbb{R}^2$ with missing first quadrant, i.e., in radial coordinates

$$\Omega = \{\ (r\cos\theta, r\sin\theta)\ |\ r \in [0,1), \theta \in (\pi/2, 2\pi)\ \}. \tag{7.3}$$

The exact parameter to be reconstructed is $\hat{q} \equiv 1$, the right-hand side in (7.1) is given by

$$f = \frac{3\pi}{4}\big(3\pi\cos(\frac{3\pi}{2}r) + \frac{2}{r}\sin(\frac{3\pi}{2}r)\big) \qquad \text{with } r = \sqrt{x^2+y^2}.$$

The corresponding solution of the state equation is $\hat{u} = \cos(\frac{3\pi}{2}r)$. The data are generated using the exact solution $\hat{u}$ perturbed by uniformly distributed random noise. For the discretization we used triangular finite elements with piecewise quadratic shape functions for the state u and the Lagrange parameter λ and piecewise constant shape functions for the parameter q. The results were calculated using the finite element code FEPP [27], developed at the Department for Analysis and Computational Mathematics of the University of Linz.

We want to mention that this identification problem is quite challenging not only due to the complicated geometry, but also due to the fact that q is not identifiable along a level line in the interior, where u attains an extremum. This does not destroy the theoretical identifiability results, because it is a set of Lebesgue-measure zero, but it can be expected to create numerical difficulties.

Results for exact data can be found in Table 2. The good performance of the method with respect to both, CPU time and number of outer iterations can be observed clearly. Especially for problems with fine discretizations of the parameter q, this method can still be realized efficiently, while classical approaches do not yield results in reasonable time. A plot

Level	dim q	dim u	avg QMR it	SQP it	time
2	92	215	200	9	8 sec
3	368	797	200	4	15 sec
4	1472	3065	180	5	77 sec
5	5888	12017	142	6	450 sec

Table 2: CPU-time and number of inner (QMR) and outer (SQP) iterations for exact data

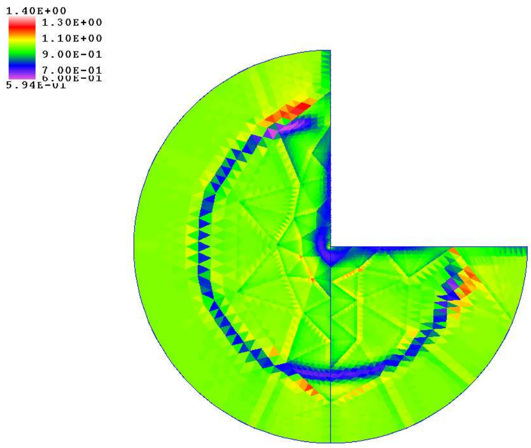

Figure 2: Parameter distribution for exact data at level 4

of the parameter q can be found in Figure 2, from which one observes that the parameter is reconstructed very well except in a neighborhood of the level curve $\{\nabla u = 0\}$.

Additional speed-up can be gained using a multi-level approach as described in Subsection 4.3. We used nested spaces for q and u by subdividing each triangular element into four smaller elements, when refining the mesh. Table 3 presents results for this approach. It can be seen that on fine discretization levels one SQP step is sufficient for fulfilling the stopping criterion, which corresponds very well to the theoretical predictions made in Section 4.3. A comparison of the results to the ones in Table 2 shows that for fixed discretization level, the solution of the identification problem on level 5 is only slightly faster than the identification of q on level 6 (with about the fourfold number of parameters) using a multi-level approach. A plot of

Level	dim q	dim u	avg QMR it	SQP it	time	acc. time
2	92	215	200	9	8 sec	8 sec
3	368	797	200	4	15 sec	23 sec
4	1472	3065	175	2	24 sec	47 sec
5	5888	12017	80	1	47 sec	94 sec
6	23552	47585	121	1	425 sec	520 sec

Table 3: CPU-time per level, accumulated time and number of inner (QMR) and outer (SQP) iterations for exact data using a nested multi-level approach

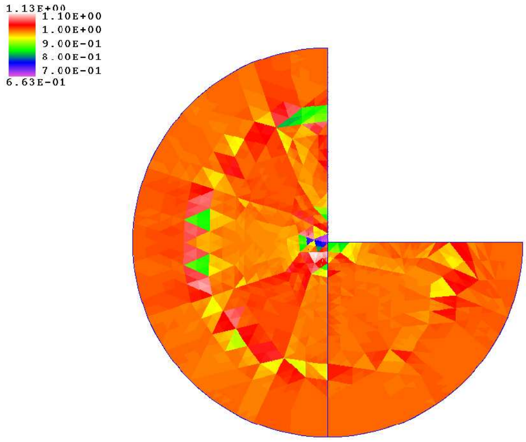

Figure 3: Parameter distribution for exact data at level 4 using a nested multi-level approach

the parameter can be found in Figure 3. Here the approximation of the parameter in the area where it can not identified is by far better than in the classical approach using only one discretization level (compare Figure 2).

8 Conclusions and Outlook

We have developed a framework for Galerkin-type approximations of the LMSQP-method for parameter identification problems in elliptic partial differential equations and we have discussed the implementation of the Galerkin LMSQP-method with iterative solution of the KKT-system. The numerical results show that the resulting iteration method clearly outperforms state-of-the-art methods for iterative regularization and provides a tool for the efficient solution of identification problems with fine discretizations. Moreover, we have developed a multi-level version of the Galerkin-LMSQP method, which yields a further speed-up.

The crucial point for the possibility to obtain an efficient implementation of the LMSQP-method is the preconditioning of the KKT-system, which is then solved iteratively as an indefinite problem in the product space for state, parameter and Lagrangian variable. The construction of such preconditioners is not a simple task and has not been discussed in detail in the present paper, but will be investigated in [11], where different preconditioning techniques will be compared.

Other numerical aspects to be investigated in future research are adaptive discretization strategies and fast parallel solvers based on domain-decomposition techniques. The adaptive discretization of optimal control problems, which is a closely related subject, has been discussed by Becker et al. [3]; possibly the ideas of this work can be carried over to identification problems, too. The parallel solution of optimal control problems has been investigated by Lions and Pironneau [28] in the case of quadratic problems; recently Biros and Ghattas [4, 5] performed a numerical study of a parallel solver with an SQP-method for the outer and preconditioned Krylov-subspace methods for the inner iteration. Many of their ideas seem to be applicable also for parameter identification problems that are solved with the LMSQP-method, which rises the hope that efficient parallel versions of the LMSQP-method can be designed also for large-scale identification problems such as impedance tomography.

Finally, we want to recall that the framework of this problem does not apply to transient problems of parabolic or hyperbolic type. Since numerical methods for different types of partial differential equations have many type-specific features in general, it is not surprising that also the numerical treatment of parameter identification problems should depend on the type of the underlying state equation. However, it seems possible to construct efficient and convergent discretized methods at least in the case of parabolic equations, which is an important task for future research.

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