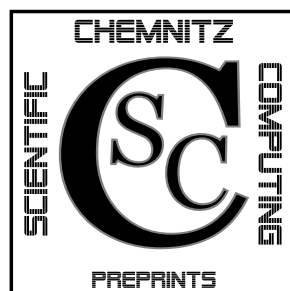Torsten Hein

On solving implicitly defined inverse problems by SQP-approaches

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Torsten Hein

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Abstract

In this paper two basic SQP-approaches for solving implicitly defined inverse problems are presented. Such problems often arises in parameter identification for differential equations. We also include regularization strategies which differ from similar problems in Optimal control. The main focus is on formulating saddle point problems for calculating the next iterate. Conditions for the unique and stable solvability of these problems are presented. The analytical considerations are illustrated by two examples including their discretizations and a numerical case study.

Contents

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1 Introduction

Let $\mathcal{Q}$, $\mathcal{U}$, $\mathcal{Y}$ and $\mathcal{Z}$ be Hilbert spaces. For given (exact) data $y \in \mathcal{Y}$ we consider the implicit defined inverse problem

$$\begin{cases} P\,u & = & y \\ E(q,u) & = & 0, \qquad (q,u) \in \mathcal{D}(E). \end{cases} \tag{1}$$

For given noisy data $y^\delta \in \mathcal{Y}$ with bound $\|y - y^\delta\|_\mathcal{Y} \le \delta$ we deal with the perturbed problem

$$\begin{cases} P\,u & = & y^\delta \\ E(q,u) & = & 0, \qquad (q,u) \in \mathcal{D}(E). \end{cases} \tag{2}$$

Thereby $E : \mathcal{D}(E) \subseteq \mathcal{Q} \times \mathcal{U} \longrightarrow \mathcal{Z}^*$ defines a nonlinear operator with domain $\mathcal{D}(E)$. Moreover, $P : \mathcal{U} \longrightarrow \mathcal{Y}$ denotes an additional linear operator. In many applications P can be considered as projection operator. If, for example, $\mathcal{U}$ is a space of functions on a domain Ω and $u \in \mathcal{U}$, then $P\,u$ might be the restriction of u to a subdomain $\Omega_1 \subset \overline{\Omega}$, where the additional observation y or y^δ is given or/and the embedding of $\mathcal{U}$ into the space $\mathcal{Y}$ with weaker norm.

There are two possibilities for treating such problems. Following the standard approach for identification problems, we replace the system (2) by a nonlinear equation

$$F(q) = y^\delta, \qquad q \in \mathcal{D}(F),$$

where the nonlinear operator $F : \mathcal{D}(F) \subseteq \mathcal{Q} \longrightarrow \mathcal{Y}$ with domain $\mathcal{D}(F)$ is given by $F = P \circ G$ and $G : \mathcal{D}(F) \subseteq \mathcal{Q} \longrightarrow \mathcal{U}$ is defined implicitly by the equation

$$E\left(q, G(q)\right) = 0, \qquad \forall q \in \mathcal{D}(F).$$

Alternatively we can deal with the constrained minimization problem

$$\begin{cases} J(u) := \dfrac{1}{2} \|P\,u - y^\delta\|_\mathcal{Y}^2 \to \min \\ \text{subject to } E(q,u) = 0, \; (q,u) \in \mathcal{D}(E), \end{cases} \tag{3}$$

which is common practice in control problems for (partial) differential equations, see e.g. [12] and the references therein. Here, often a penalty term $\alpha\,f(q)$ to the objective functional $J(u)$ is added, i.e. $J(u)$ is replaced by

$$J_\alpha(q,u) := \frac{1}{2}\|P\,u - y^\delta\|_\mathcal{Y}^2 + \alpha\,f(q).$$

The additional penalty can be considered as regularization term. As well-known from Tikhonov regularization this term provides (under some conditions to f) existence of a solution $(q_\alpha^\delta, u_\alpha^\delta)$ of (3) depending stable on the given data y^δ. But there is an important difference in identification and control problems. In order

to get an approximate solution of (2) in identification problems the regularization parameter α depending on the noise level δ is usually small. In control problems a parameter α is chosen a-priori, which is normally larger than in identification problems. So, algorithms used for control problems where the inverse of the parameter α is applied could cause numerical difficulties for small regularization parameters in identification problems.

Therefore we present some general regularization ideas for identification problems of the form (2) as it was recently done in [4], see also [5] for some numerical considerations. The analytical considerations are illustrated by two examples which deal with the identification of coefficients in an elliptic differential equation.

The paper is organized as follows: in section 2 we present some basic assumptions which we will later need in the further considerations. The third and forth section deal with two (regularized) approaches for formulating SQP-algorithms to find approximative solutions of (2). In section 5 we apply this theoretical considerations to two parameter identification problems for an elliptic differential equation. Some remarks concerning the numerical implementation of these examples are given in section 6. The paper closes with some numerical examples.

2 Basic Notations and Assumptions

Let $\mathcal{X}$ and $\mathcal{Y}$ denote Hilbert spaces with scalar products $\langle \cdot, \cdot \rangle_{\mathcal{X}}$ and $\langle \cdot, \cdot \rangle_{\mathcal{Y}}$. Moreover, $\mathcal{X}^*$ and $\mathcal{Y}^*$ are the dual spaces. Then we denote with $\langle \cdot, \cdot \rangle_{\mathcal{X}^*,\mathcal{X}}$ the duality product on $\mathcal{X}^* \times \mathcal{X}$. Let $A : \mathcal{X} \longrightarrow \mathcal{Y}$ be a linear operator. With $A^* : \mathcal{Y} \longrightarrow \mathcal{X}$ we denote the Hilbert space adjoint operator of A which is defined by

$$\langle A\,x, y \rangle_{\mathcal{Y}} = \langle x, A^*y \rangle_{\mathcal{X}} \qquad \forall\, x \in \mathcal{X},\, \forall\, y \in \mathcal{Y}.$$

The dual operator $A^\star : \mathcal{Y}^* \longrightarrow \mathcal{X}^*$ of A is given by the relation

$$\langle y, A\,x \rangle_{\mathcal{Y}^*,\mathcal{Y}} = \langle A^\star y, x \rangle_{\mathcal{X}^*,\mathcal{X}} \qquad \forall\, x \in \mathcal{X},\, \forall\, y \in \mathcal{Y}^*.$$

Remark 2.1 *Let* $R_{\mathcal{X}} : \mathcal{X}^* \longrightarrow \mathcal{X}$ *and* $R_{\mathcal{Y}} : \mathcal{Y}^* \longrightarrow \mathcal{Y}$ *denote the Riesz-Isomorphisms which identify elements of the dual spaces* $\mathcal{X}^*$ *and* $\mathcal{Y}^*$ *with elements of the spaces* $\mathcal{X}$ *and* $\mathcal{Y}$ *itself, i.e.*

$$
\begin{aligned}
\langle \tilde{x}, x \rangle_{\mathcal{X}^*,\mathcal{X}} &= \langle R_{\mathcal{X}}\tilde{x}, x \rangle_{\mathcal{X}}, \quad \forall\, \tilde{x} \in \mathcal{X}^*,\, \forall\, x \in \mathcal{X} \quad \text{and} \\
\langle \tilde{y}, y \rangle_{\mathcal{Y}^*,\mathcal{Y}} &= \langle R_{\mathcal{Y}}\tilde{y}, y \rangle_{\mathcal{Y}}, \quad \forall\, \tilde{y} \in \mathcal{Y}^*,\, \forall\, y \in \mathcal{Y}.
\end{aligned}
$$

Then we have obviously

$$A^\star = R_{\mathcal{X}}^{-1} A^* R_{\mathcal{Y}}.$$

This relation will be used later frequently.

2

Example 2.1 *We will consider a standard example in order to verify the Riesz isomorphism. Let be $\mathcal{X} = H_0^1(0,1)$, Then, as well-known, $\mathcal{X}^* = H^{-1}(0,1)$ and for $f \in \mathcal{X}^*$ the duality product is given by*

$$\langle f, x \rangle_{\mathcal{X}^*, \mathcal{X}} := \int_0^1 f\, x\, d\xi.$$

How does $y \in H_0^1(0,1)$ with $y = R_{\mathcal{X}} f$ look like? Therefore we have

$$\begin{aligned} \langle f, x \rangle_{\mathcal{X}^*, \mathcal{X}} &= \langle x, y \rangle_{\mathcal{X}} \\ &:= \int_0^1 x\, y\, d\xi + \int_0^1 x'\, y'\, d\xi \\ &= \int_0^1 (y - y'') x\, d\xi, \quad \forall\, x \in \mathcal{X}. \end{aligned}$$

Hence $R_{\mathcal{X}} : \mathcal{X}^* \longrightarrow \mathcal{X}$ is given by $R_{\mathcal{X}} f =: y$, where $y \in H_0^1(0,1)$ satisfies the (ordinary) differential equation

$$y - y'' = f \quad (\text{with } y(0) = y(1) = 0)$$

a.e. on $(0,1)$.

Moreover we need some assumptions concerning the operator E. In order to obtain a relation to classical inverse problems we assume that the condition $E(q, u) = 0$ defines a nonlinear operator mapping from a domain of the space $\mathcal{Q}$ into the space $\mathcal{U}$.

Assumption 2.1 *There exists a domain $\mathcal{D}$ and a nonlinear continuous operator $G : \mathcal{D} \subseteq \mathcal{Q} \longrightarrow \mathcal{U}$ such that G is implicitly defined by*

$$E(q, G(q)) = 0, \qquad \forall\, q \in \mathcal{D}.$$

Moreover, we suppose that E is Fréchet-differentiable with uniformly bounded partial derivatives. Additionally the inverse E_u^{-1} of the partial derivative E_u should exist and be uniformly bounded.

Assumption 2.2 *For each $(q, u) \in \mathcal{D}(E)$ the operator E is Fréchet-differentiable with partial derivatives $E_q = E_q(q, u) : \mathcal{Q} \longrightarrow \mathcal{Z}^*$ and $E_u = E_u(q, u) : \mathcal{U} \longrightarrow \mathcal{Z}^*$. They are uniformly bounded, i.e. there exist two constants $C_u, C_q > 0$ such that*

$$\|E_u\| \leq C_u \quad \text{and} \quad \|E_q\| \leq C_q \quad \forall\, (q, u) \in \mathcal{D}(E).$$

The operator $E_u^{-1} = E_u^{-1}(q, u) : \mathcal{Z}^* \longrightarrow \mathcal{U}$ exists for all $(q, u) \in \mathcal{D}(E)$ and its norm is uniformly bounded by some constant $\tilde{C}_u > 0$.

The latter assumption seems to be quite restrictive. On the other hand, this condition allows us to apply the implicit function theorem, see e.g. [9, Satz 1.4.XVII], which provides Fréchet-differentiability of the operator G.

Corollary 2.1 *The operator $G : \mathcal{D} \subseteq \mathcal{Q} \longrightarrow \mathcal{U}$ is Fréchet-differentiable for all $q \in \mathcal{D}$ with derivative*

$$G'(q) := -E_u(q, G(q))^{-1} E_q(q, G(q)), \qquad q \in \mathcal{D}.$$

For applying Newton-type methods for solving the problem (3) we have to assume twice Fréchet-differentiability of the operator E.

Assumption 2.3 *For each $(q, u) \in \mathcal{D}(E)$ the operator E is twice continuously Fréchet differentiable with second Fréchet-derivative $E'' = E''(q, u) : (\mathcal{Q} \times \mathcal{U})^2 \longrightarrow \mathcal{Z}^*$ satisfying*

$$\|E''[(q, u), (p, v)]\|_{\mathcal{Z}^*} \leq C_{(2)} \sqrt{\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2} \sqrt{\|p\|_{\mathcal{Q}}^2 + \|v\|_{\mathcal{U}}^2}, \quad \forall (q, u), (p, v) \in \mathcal{Q} \times \mathcal{U},$$

for some constant $C_{(2)} > 0$.

Finally we can suppose that $\|P u\|_{\mathcal{Y}}$ is bounded from below.

Assumption 2.4 *There exists a constant $C_p \geq 0$ such that $\|P u\|_{\mathcal{Y}} \geq C_p \|u\|_{\mathcal{U}}$.*

Note, that the trivial case $C_p = 0$ is included in this assumption.

3 Linearization of the constraints

Let the iterate $(q_k, u_k) \in \mathcal{D}(E)$ be given. We linearize the constraint

$$E(q_k + \Delta q, u_k + \Delta u) \approx E(q_k, u_k) + E_q \Delta q + E_u \Delta u, \quad \Delta q \in \mathcal{Q}, \ \Delta u \in \mathcal{U}$$

with derivatives $E_q(q_k, u_k) =: E_q : \mathcal{Q} \longrightarrow \mathcal{Z}^*$ and $E_u(q_k, u_k) =: E_u : \mathcal{U} \longrightarrow \mathcal{Z}^*$ by supposing $(q + \Delta q, u + \Delta u) \in \mathcal{D}(E)$. Moreover, we introduce an additional regularization term to the functional J. In particular, we replace J by

$$J_k(\Delta q, \Delta u) := \frac{1}{2} \|P(u_k + \Delta u) - y^\delta\|_{\mathcal{Y}}^2 + \frac{\alpha_k}{2} \|\Delta q - q_k^*\|_{\mathcal{Q}}^2$$

where $\alpha_k > 0$ denotes a regularization parameter. The element $q_k^* \in \mathcal{Q}$ should be of the form

$$q_k^* := \eta(q^* - q_k)$$

with a-priori guess $q^* \in \mathcal{Q}$ and $\eta = 0$ or $\eta = 1$. We consider different regularization strategies:

(i) $\eta = 0$ coincides with the Levenberg-Marquardt algorithm,

(ii) $\eta = 1$ and $\alpha_k = \alpha = \text{const.}$ is the classical Tikhonov regularization and

(iii) $\eta = 1$ and $\alpha_k \leq \alpha_{k-1}$ corresponds with an iterative regularized Gauss-Newton scheme.

For the application of (i) and (iii) as regularization methods we need an additional criterion for stopping the iteration, see e.g. [4] for the Levenberg-Marquardt approach and [2] for the iterative regularized Gauss-Newton algorithm. Then we replace (3) by the linear-quadratic problem

$$\begin{cases} J_k(\Delta q, \Delta u) \to \min \\ \text{subject to } E(q_k, u_k) + E_q \Delta q + E_u \Delta u = 0. \end{cases} \tag{4}$$

The iteration is given now as follows: find a solution $(\Delta q, \Delta u) \in \mathcal{Q} \times \mathcal{U}$ of (4) with corresponding Lagrangian multiplier $\lambda \in \mathcal{Z}$ and calculate the next iterate

$$q_{k+1} := q_k + \Delta q \quad \text{and} \quad u_{k+1} := u_k + \Delta u.$$

A modification is presented in [11]. Here, for given q_{k+1}, the next iterate u_{k+1} is estimated by the equation

$$E(q_{k+1}, u_{k+1}) = 0.$$

Hence, all iterates (q_k, u_k) satisfy the equation $E(q, u) = 0$, which means that this modifaction can be considered as corrector step for a predictor-corrector algorithm following a path of feasible solutions.

The corresponding Lagrangian functional $L : \mathcal{Q} \times \mathcal{U} \times \mathcal{Z} \longrightarrow \mathbb{R}$ is given by

$$L(\Delta q, \Delta u, \lambda) := J_k(\Delta q, \Delta u) + \langle E(q_k, u_k) + E_q \Delta q + E_u \Delta u, \lambda \rangle_{\mathcal{Z}^*, \mathcal{Z}}.$$

In order to solve (4) we introduce the following bilinear forms

$$\begin{array}{llll}
a_q(\cdot, \cdot) : \mathcal{Q} \times \mathcal{Q} \longrightarrow \mathbb{R} & : & a_q(q, p) := \langle q, p \rangle_{\mathcal{Q}}, & q, p \in \mathcal{Q}, \\
a_u(\cdot, \cdot) : \mathcal{U} \times \mathcal{U} \longrightarrow \mathbb{R} & : & a_u(u, v) := \langle Pu, Pv \rangle_{\mathcal{Y}}, & u, v \in \mathcal{U}, \\
b_q(\cdot, \cdot) : \mathcal{Q} \times \mathcal{Z} \longrightarrow \mathbb{R} & : & b_q(q, z) := \langle E_q q, z \rangle_{\mathcal{Z}^*, \mathcal{Z}}, & q \in \mathcal{Q}, z \in \mathcal{Z} \quad \text{and} \\
b_u(\cdot, \cdot) : \mathcal{U} \times \mathcal{Z} \longrightarrow \mathbb{R} & : & b_u(u, z) := \langle E_u u, z \rangle_{\mathcal{Z}^*, \mathcal{Z}}, & u \in \mathcal{U}, z \in \mathcal{Z}.
\end{array}$$

Moreover, we define the functionals

$$\begin{array}{llll}
f_q \in \mathcal{Q}^* & : & \langle f_q, q \rangle_{\mathcal{Q}^*, \mathcal{Q}} := \langle q, q_k^* \rangle_{\mathcal{Q}}, & q \in \mathcal{Q}, \\
f_u \in \mathcal{U}^* & : & \langle f_u, u \rangle_{\mathcal{U}^*, \mathcal{U}} := \langle Pu, y^\delta - Pu_k \rangle_{\mathcal{Y}}, & u \in \mathcal{U},
\end{array}$$

and $g := -E(q_k, u_k) \in \mathcal{Z}^*$. Then we can write the weak formulation of the KKT-system as

$$\begin{array}{llll}
\langle L_{\Delta q}, p \rangle_{\mathcal{Q}^*, \mathcal{Q}} & = & \alpha_k a_q(\Delta q, p) + b_q(p, \lambda) - \alpha_k \langle f_q, p \rangle_{\mathcal{Q}^*, \mathcal{Q}} & = & 0, \quad \forall p \in \mathcal{Q}, \\
\langle L_{\Delta u}, v \rangle_{\mathcal{U}^*, \mathcal{U}} & = & a_u(\Delta u, v) + b_u(v, \lambda) - \langle f_u, v \rangle_{\mathcal{U}^*, \mathcal{U}} & = & 0, \quad \forall v \in \mathcal{U}, \quad (5) \\
\langle L_\lambda, z \rangle_{\mathcal{Z}^*, \mathcal{Z}} & = & b_q(\Delta q, z) + b_u(\Delta u, z) - \langle g, z \rangle_{\mathcal{Z}^*, \mathcal{Z}} & = & 0, \quad \forall z \in \mathcal{Z}.
\end{array}$$

Introducing the operators $A_u : \mathcal{U} \longrightarrow \mathcal{U}^*$ and $A_q : \mathcal{Q} \longrightarrow \mathcal{Q}^*$ via

$$a_u(u,v) = \langle A_u u, v \rangle_{\mathcal{U}^*, \mathcal{U}} \quad \text{and} \quad a_q(q,p) = \langle A_q q, p \rangle_{\mathcal{Q}^*, \mathcal{Q}},$$

we can rewrite (5) as operator equation

$$\begin{pmatrix} \alpha_k A_q & 0 & E_q^\star \\ 0 & A_u & E_u^\star \\ E_q & E_u & 0 \end{pmatrix} \begin{pmatrix} \Delta q \\ \Delta u \\ \lambda \end{pmatrix} = \begin{pmatrix} \alpha_k f_q \\ f_u \\ g \end{pmatrix}. \tag{6}$$

Remark 3.1 *Using the corresponding Riesz-Isomorphisms we have $A_u = R_{\mathcal{U}}^{-1} P^* P$, $A_q = R_{\mathcal{Q}}^{-1}$, $f_q = R_{\mathcal{Q}}^{-1} q_k^*$ and $f_u = R_{\mathcal{U}}^{-1} P^*(y^\delta - P u_k)$. Multiplying the first row with $R_{\mathcal{Q}}$ and second with $R_{\mathcal{U}}$ we obtain with $\tilde{\lambda} := R_{\mathcal{Z}}^{-1} \lambda \in \mathcal{Z}^*$ the equation*

$$\begin{pmatrix} \alpha_k I_{\mathcal{Q}} & 0 & E_q^* \\ 0 & P^* P & E_u^* \\ E_q & E_u & 0 \end{pmatrix} \begin{pmatrix} \Delta q \\ \Delta u \\ \tilde{\lambda} \end{pmatrix} = \begin{pmatrix} \alpha_k q_k^* \\ P^*(y^\delta - P u_k) \\ g \end{pmatrix} \tag{7}$$

By defining the bilinear forms $a(\cdot, \cdot) : (\mathcal{Q} \times \mathcal{U})^2 \longrightarrow \mathbb{R}$, and $b(\cdot, \cdot) : (\mathcal{Q} \times \mathcal{U}) \times \mathcal{Z} \longrightarrow \mathbb{R}$ as

$$a((q,u),(p,v)) := \alpha_k a_q(q,p) + a_u(u,v) \quad \text{and} \quad b((q,u),z) := b_q(q,z) + b_u(u,z)$$

for $(q,u),(p,v) \in \mathcal{Q} \times \mathcal{U}$, $z \in \mathcal{Z}$ as well as

$$\langle f, (q,u) \rangle := \langle f_q, q \rangle_{\mathcal{Q}^*, \mathcal{Q}} + \langle f_u, u \rangle_{\mathcal{U}^*, \mathcal{U}},$$

we can formulate (5) also as classical saddle point problem

$$\begin{aligned} a((\Delta q, \Delta u),(p,v)) + b((p,v),\lambda) &= \langle f, (p,v) \rangle, & \forall (p,v) \in \mathcal{Q} \times \mathcal{U}, \\ b((\Delta q, \Delta u),z) &= \langle g, z \rangle_{\mathcal{Z}^*, \mathcal{Z}}, & \forall z \in \mathcal{Z}. \end{aligned} \tag{8}$$

We use this relation to show the unique solvability of the system (5).

Lemma 3.1 *Suppose the assumptions 2.1, 2.2 and 2.4 to be hold. Then the bilinear-form $a(\cdot, \cdot)$ is bounded and satisfies the kernel ellipticity with respect to $b(\cdot, \cdot)$, i.e.*

$$a((q,u),(q,u)) \geq c_1 \left(\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2 \right), \quad \forall (q,u) : b(q,u) = 0$$

for some constant $c_1 > 0$ and

$$|a((q,u),(p,v))| \leq c_2 \sqrt{\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2} \sqrt{\|p\|_{\mathcal{Q}}^2 + \|v\|_{\mathcal{U}}^2}, \quad \forall (q,u),(p,v) \in \mathcal{Q} \times \mathcal{U},$$

for another constant $c_2 > 0$.

PROOF. First we note, that $b(q, u) = 0$ implies $u = -E_u^{-1} E_q q$ which gives $\|u\|_{\mathcal{U}} \leq \|E_u^{-1} E_q\| \|q\|_{\mathcal{Q}}$ and hence $\|q\|_{\mathcal{Q}} \geq \|E_u^{-1} E_q\|^{-1} \|u\|_{\mathcal{U}}$. Then we have

$$
\begin{aligned}
a\left((q, u), (q, u)\right) &= \alpha_k \|q\|_{\mathcal{Q}}^2 + \|P u\|_{\mathcal{Y}}^2 \\
&\geq \alpha_k \gamma \|q\|_{\mathcal{Q}}^2 + \left(\frac{\alpha(1 - \gamma)}{\|E_u^{-1} E_q\|^2} + C_p^2 \right) \|u\|_{\mathcal{U}}^2
\end{aligned}
$$

for all $\gamma \in (0, 1)$. For $\alpha_k > C_p^2$ we choose γ such that

$$
\alpha_k \gamma = \frac{\alpha(1 - \gamma)}{\|E_u^{-1} E_q\|^2} + C_p^2 \quad \Leftrightarrow \quad \gamma = \frac{\alpha_k + \|E_u^{-1} E_q\|^2 C_p^2}{\alpha_k (\|E_u^{-1} E_q\|^2 + 1)} < 1
$$

and we obtain

$$
a\left((q, u), (q, u)\right) \geq \min \left\{ \alpha_k, \frac{\alpha_k + \|E_u^{-1} E_q\|^2 C_p^2}{(\|E_u^{-1} E_q\|^2 + 1)} \right\} \left(\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2 \right).
$$

Moreover

$$
\begin{aligned}
|a\left((q, u), (p, v)\right)| &\leq \alpha_k \|q\|_{\mathcal{Q}} \|p\|_{\mathcal{Q}} + \|P\|^2 \|u\|_{\mathcal{U}} \|v\|_{\mathcal{U}} \\
&\leq \max \left\{ \alpha_k, \|P\|^2 \right\} \left(\|q\|_{\mathcal{Q}} + \|u\|_{\mathcal{U}} \right) \left(\|p\|_{\mathcal{Q}} + \|v\|_{\mathcal{U}} \right) \\
&\leq 2 \max \left\{ \alpha_k, \|P\|^2 \right\} \sqrt{\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2} \sqrt{\|p\|_{\mathcal{Q}}^2 + \|v\|_{\mathcal{U}}^2}.
\end{aligned}
$$

The proof is complete. ■

For the proof of the LBB-condition we follow directly [4, Theorem 2.3].

Lemma 3.2 *The bilinear form $b(\cdot, \cdot)$ satisfies the LBB-condition*

$$
\inf_{\lambda \in \mathcal{Z}} \sup_{(q, u) \in \mathcal{Q} \times \mathcal{U}} \frac{b\left((q, u), \lambda\right)}{\|(q, u)\|_{\mathcal{Q} \times \mathcal{U}} \|\lambda\|_{\mathcal{Z}}} \geq \beta > 0.
$$

PROOF. We set $u := E_u^{-1} \lambda$ and $q = 0$. Then

$$
\begin{aligned}
\inf_{\lambda \in \mathcal{Z}} \sup_{(q, u) \in \mathcal{Q} \times \mathcal{U}} \frac{b\left((q, u), \lambda\right)}{\|(q, u)\|_{\mathcal{Q} \times \mathcal{U}} \|\lambda\|_{\mathcal{Z}}} &\geq \inf_{\lambda \in \mathcal{Z}} \frac{b\left((0, E_u^{-1} \lambda), \lambda\right)}{\|E_u^{-1} \lambda\|_{\mathcal{U}} \|\lambda\|_{\mathcal{Z}}} \\
&= \inf_{\lambda \in \mathcal{Z}} \frac{\|\lambda\|_{\mathcal{Z}}^2}{\|E_u^{-1} \lambda\|_{\mathcal{U}} \|\lambda\|_{\mathcal{Z}}} \geq \frac{1}{\|E_u^{-1}\|} =: \beta. \quad ■
\end{aligned}
$$

Applying both lemmas we have the unique solvability of the KKT-system (5) respectively the saddle-point problem (7), see e.g. [3].

Corollary 3.1 *The system (5) admits a unique solution $(\Delta q, \Delta u) \in \mathcal{Q} \times \mathcal{U}$ with corresponding Lagrange multiplier $\lambda \in \mathcal{Z}$, which depend stable on $(f_q, f_u, g) \in \mathcal{Q}^* \times \mathcal{U}^* \times \mathcal{Z}^*$.*

In the present paper we do not deal with questions concerning the local convergence of the iterates $(q_k, u_k) \in \mathcal{Q} \times \mathcal{U}$ to a solution of the problem (3). The local convergence of Lagrange-Newton methods and possible ways of globalization of the convergence is a topic of its own. We refer to [1] for further readings, see also the books [12] and [10] for discussing the finite-dimensional case including discussions of globalization strategies.

4 Direct Lagrange approach

In a second variant we apply the Lagrange method directly to the problem (3). Then the Lagrangian functional is defined by

$$L(q, u, \lambda) := \frac{1}{2}\|P\,u - y^\delta\|_{\mathcal{Y}}^2 + \langle E(q, u), \lambda \rangle_{\mathcal{Z}^*, \mathcal{Z}}$$

Again let the iterate $(q_k, u_k, \lambda_k) \in \mathcal{Q} \times \mathcal{U} \times \mathcal{Z}$ be given. Then the weak formulation of the KKT-system reads as

$$
\begin{aligned}
\langle L_q, p \rangle_{\mathcal{Q}^*, \mathcal{Q}} &= \langle E_q p, \lambda_k \rangle_{\mathcal{Z}^*, \mathcal{Z}} &&= 0, \quad \forall p \in \mathcal{Q}, \\
\langle L_u, v \rangle_{\mathcal{U}^*, \mathcal{U}} &= \langle P\,v, P\,u_k - y^\delta \rangle_{\mathcal{Y}} + \langle E_u v, \lambda_k \rangle_{\mathcal{Z}^*, \mathcal{Z}} &&= 0, \quad \forall v \in \mathcal{U}, \\
\langle L_\lambda, \mu \rangle_{\mathcal{Z}^*, \mathcal{Z}} &= \langle E(q_k, u_k), \mu \rangle_{\mathcal{Z}^*, \mathcal{Z}} &&= 0, \quad \forall \mu \in \mathcal{Z},
\end{aligned}
$$

which is in general a nonlinear system. We also can write abstractly

$$
\begin{aligned}
L_q &= E_q^\star \lambda_k && \in \mathcal{Q}^*, \\
L_u &= R_{\mathcal{U}}^{-1} P^* (P\,u_k - y^\delta) + E_u^\star \lambda_k && \in \mathcal{U}^*, \\
L_\lambda &= E(q_k, u_k) && \in \mathcal{Z}^*.
\end{aligned}
$$

There are two possible ways to formulate the Newton iteration. First the next iterate is given as

$$q_{k+1} := q_k + \Delta q, \ u_{k+1} := u_k + \Delta u \ \text{ and } \ \lambda_{k+1} := \lambda_k + \Delta\lambda,$$

where $(\Delta q, \Delta u, \Delta\lambda)$ solves the linear system

$$
\begin{pmatrix} L_{qq} & L_{qu} & E_q^\star \\ L_{uq} & L_{uu} & E_u^\star \\ E_q & E_u & 0 \end{pmatrix}
\begin{pmatrix} \Delta q \\ \Delta u \\ \Delta\lambda \end{pmatrix}
= -\begin{pmatrix} L_q \\ L_u \\ E(q_k, u_k) \end{pmatrix}. \tag{9}
$$

Thereby the operators are defined as follows:

$$
\begin{aligned}
L_{qq} : \mathcal{Q} &\longrightarrow \mathcal{Q}^* &:& \quad \langle L_{qq} q, p \rangle_{\mathcal{Q}^*, \mathcal{Q}} = \langle E_{qq}(q, p), \lambda_k \rangle_{\mathcal{Z}^*, \mathcal{Z}}, && \forall\, p, q \in \mathcal{Q}, \\
L_{uu} : \mathcal{U} &\longrightarrow \mathcal{U}^* &:& \quad \langle L_{uu} u, v \rangle_{\mathcal{U}^*, \mathcal{U}} = \langle E_{uu}(u, v), \lambda_k \rangle_{\mathcal{Z}^*, \mathcal{Z}} + \langle P\,u, P\,v \rangle_{\mathcal{Y}}, && \forall\, u, v \in \mathcal{U}, \\
L_{qu} : \mathcal{U} &\longrightarrow \mathcal{Q}^* &:& \quad \langle L_{qu} u, q \rangle_{\mathcal{Q}^*, \mathcal{Q}} = \langle E_{qu}(q, u), \lambda_k \rangle_{\mathcal{Z}^*, \mathcal{Z}}, && \forall\, q \in \mathcal{Q}, \forall\, u \in \mathcal{U},
\end{aligned}
$$

and $L_{uq} := L_{qu}^\star : \mathcal{Q} \longrightarrow \mathcal{U}^*$. Moreover

$$E''(q_k, u_k)[(q, u), (p, v)] := E_{qq}(q, p) + E_{qu}(q, v) + E_{qu}(p, u) + E_{uu}(u, v)$$

for $q, p \in \mathcal{Q}$, $u, v \in \mathcal{U}$ denotes the second derivative of the operator $E(q, u)$ at the point (q_k, u_k). Here, $E_{qq} : \mathcal{Q} \times \mathcal{Q} \longrightarrow \mathcal{Z}^*$, $E_{uu} : \mathcal{U} \times \mathcal{U} \longrightarrow \mathcal{Z}^*$ and $E_{qu} = E_{uq} : \mathcal{Q} \times \mathcal{U} \longrightarrow \mathcal{Z}^*$. Then the Newton iteration can be alternatively written as

$$q_{k+1} := q_k + \Delta q, \ u_{k+1} := u_k + \Delta u \ \text{ and } \ \lambda_{k+1} := \lambda$$

where $(\Delta q, \Delta u)$ solves the linear-quadratic problem

$$\begin{cases} \dfrac{1}{2}\|P(u_k + \Delta u) - y^\delta\|_{\mathcal{Y}}^2 + \dfrac{1}{2}\langle E''(q_k, u_k)[(\Delta q, \Delta u), (\Delta q, \Delta u)], \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}} \to \min \\ \text{subject to } E(q_k, u_k) + E_q \Delta q + E_u \Delta u = 0. \end{cases}$$
(10)

with corresponding Lagrange multiplier $\lambda \in \mathcal{Z}$. This approach allows us to add the regularization term $\frac{\alpha_k}{2}\|\Delta q - q_k^*\|_{\mathcal{Q}}^2$ again. Then the solution of (10) is equivalent to the problem

$$\begin{aligned} \alpha_k a_q(\Delta q, p) + \langle E_{qq}(\Delta q, p) + E_{qu}(p, \Delta u), \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}} + b_q(p, \lambda) \\ = \alpha_k \langle f_q, p\rangle_{\mathcal{Q}^*, \mathcal{Q}}, \qquad &\forall\, p \in \mathcal{Q}, \\[4pt] a_u(\Delta u, v) + \langle E_{uu}(\Delta u, v) + E_{uq}(\Delta q, v), \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}} + b_u(v, \lambda) \\ = \langle f_u, v\rangle_{\mathcal{U}^*, \mathcal{U}}, \qquad &\forall\, v \in \mathcal{U}, \\[4pt] b_q(\Delta q, z) + b_u(\Delta u, z) \quad = \langle g, z\rangle_{\mathcal{Z}^*, \mathcal{Z}}, \qquad &\forall\, z \in \mathcal{Z}, \end{aligned}$$
(11)

or alternatively with $\lambda := \lambda_k + \Delta\lambda$

$$\begin{aligned} \alpha_k a_q(\Delta q, p) + \langle E_{qq}(\Delta q, p) + E_{qu}(p, \Delta u), \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}} + b_q(p, \Delta\lambda) \\ = \alpha_k \langle f_q, p\rangle_{\mathcal{Q}^*, \mathcal{Q}} - b_q(p, \lambda_k), \qquad &\forall\, p \in \mathcal{Q}, \\[4pt] a_u(\Delta u, v) + \langle E_{uu}(\Delta u, v) + E_{uq}(\Delta q, v), \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}} + b_u(v, \Delta\lambda) \\ = \langle f_u, v\rangle_{\mathcal{U}^*, \mathcal{U}} - b_u(v, \lambda_k), \qquad &\forall\, v \in \mathcal{U}, \\[4pt] b_q(\Delta q, z) + b_u(\Delta u, z) \quad = \langle g, z\rangle_{\mathcal{Z}^*, \mathcal{Z}}, \qquad &\forall\, z \in \mathcal{Z}, \end{aligned}$$
(12)

Last equation is in fact the weak formulation of (9) with added regularization term.

Comparing (11) with (5) we see, that we can also obtain (5) from (11) by ignoring the second derivatives of the operator E.

Again we are interested in the kernel ellipticity of the bilinear form

$$\tilde{\alpha}((q, u), (p, v)) := \alpha((q, u), (p, v)) + \langle E''((q, u), (p, v)), \lambda_k\rangle_{\mathcal{Z}^*, \mathcal{Z}}, \quad (q, u), (p, v) \in \mathcal{Q} \times \mathcal{U},$$

with respect to the bilinear form $b(\cdot, \cdot)$. In opposite to Lemma 3.1 we need now a condition to the regularization parameter α_k for proving the kernel ellipticity.

Lemma 4.1 *Suppose the assumptions 2.1-2.4 to be hold. Then the bilinear-form $\tilde{a}(\cdot, \cdot)$ is bounded, i.e.*

$$|\tilde{a}\left((q, u), (p, v)\right)| \leq c_4 \sqrt{\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2} \sqrt{\|p\|_{\mathcal{Q}}^2 + \|v\|_{\mathcal{U}}^2}.$$

for some constant $c_4 > 0$. Moreover, the kernel ellipticity

$$\tilde{a}\left((q, u), (q, u)\right) \geq c_3 \left(\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2\right), \quad \forall (q, u) : b(q, u) = 0$$

is satisfied, if

$$c_3 := \min\left\{\alpha_k, \frac{\alpha_k + \|E_u^{-1} E_q\|^2 C_p^2}{(\|E_u^{-1} E_q\|^2 + 1)}\right\} - \|E''\| \, \|\lambda_k\|_{\mathcal{Z}} > 0.$$

PROOF. We have by definition of $\tilde{a}(\cdot, \cdot)$ and Lemma 3.1

$$\tilde{a}\left((q, u), (q, u)\right) \geq \left(c_1 - \|E''\| \, \|\lambda_k\|_{\mathcal{Z}}\right) \left(\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2\right)$$

and

$$|\tilde{a}\left((q, u), (p, v)\right)| \leq \left(c_2 + \|E''\| \, \|\lambda_k\|_{\mathcal{Z}}\right) \sqrt{\|q\|_{\mathcal{Q}}^2 + \|u\|_{\mathcal{U}}^2} \sqrt{\|p\|_{\mathcal{Q}}^2 + \|v\|_{\mathcal{U}}^2}.$$

This proves the lemma. ■

Again it follows now that the unique solutions $(\triangle q, \triangle u, \triangle \lambda) \in \mathcal{Q} \times \mathcal{U} \times \mathcal{Z}$ of (11) and $(\triangle q, \triangle u, \lambda) \in \mathcal{Q} \times \mathcal{U} \times \mathcal{Z}$ of (12) depend stable on the corresponding right hand sides.

We also refer to [6] for numerical algorithms for solving the system (11) or (12) efficiently and for the discussion of some modifications of the iteration procedure. Furthermore, pre-conditioning strategies for the systems (11) and (12) were discussed in [7] for solving these systems with Krylov methods. Note, that the efficiency of the suggested pre-conditioner strongly depends on the choice of the regularization parameter α_k. In particular, the parameter α_k should not be chosen too small, which probably contradicts regularization strategies when the noise-level δ is small.

5 Two Examples

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with sufficiently smooth boundary $\partial\Omega$. We consider the elliptic equation

$$\begin{cases} -\text{div}\,(q\nabla u) + c\,u &= f, & \text{on } \Omega, \\ q\dfrac{\partial u}{\partial \nu} &= 0, & \text{on } \Gamma_N, \\ u &= 0, & \text{on } \Gamma_D, \end{cases} \tag{13}$$

with $\partial\Omega = \Gamma_N \cup \Gamma_D$ and $f \in L^2(\Omega)$ is a given source. Moreover, $q, c \in H^2(\Omega)$ are two additional parameters. Thereby we use, that the space $H^2(\Omega)$ is continuously embedded in the space $L^\infty(\Omega)$ for two-dimensional domains $\Omega \subset \mathbb{R}^2$. Here, we assume

$$c \in \mathcal{D}_1 := \left\{ c \in H^2(\Omega) \; : \; 0 < C_1 \leq c \leq C_2 < \infty \ \text{ a.e. on } \ \Omega \right\}$$

and

$$q \in \mathcal{D}_2 := \left\{ q \in H^2(\Omega) \; : \; 0 < C_3 \leq q \leq C_4 < \infty \ \text{ a.e. on } \ \Omega \right\}.$$

For given $c \in \mathcal{D}_1$ and $q \in \mathcal{D}_2$, the weak solution $u \in \mathcal{V}$ of (13) is given by

$$a(u, v; c, q) = \langle f, v \rangle, \qquad \forall\, v \in \mathcal{V}. \tag{14}$$

where

$$\mathcal{V} := \left\{ u \in H^1(\Omega) \; : \; u \equiv 0 \text{ auf } \Gamma_D \right\}$$

is a Hilbert space associated with H^1-scalar product. Moreover, the bilinear form $a(\cdot, \cdot; c, q) : \mathcal{V} \times \mathcal{V} \longrightarrow \mathbb{R}$ is defined via

$$a(u, v; c, q) := \int_\Omega q \nabla u \, \nabla v \, d\xi + \int_\Omega c\, u\, v \, d\xi, \qquad u, v \in \mathcal{V},$$

and $f \in \mathcal{V}^*$ as

$$\langle f, v \rangle := \int_\Omega f\, v \, d\xi, \qquad v \in \mathcal{V}.$$

Now two possible inverse problems can be formulated: Assume one of the functions c or q to be unknown. Then we try to determine this function approximately by an additional (noisy) measurement y^δ on $\Omega_1 \subseteq \Omega$. We discuss both variants.

a) Determining the reaction term

First, we suppose that the function $c \in \mathcal{D}_1$ has to be identified, whereas $q = q^* \in \mathcal{D}_2$ is a given function. We set $\mathcal{Q} = H^2(\Omega)$, $\mathcal{U} = \mathcal{Z} = \mathcal{V}$ and $\mathcal{Y} = L^2(\Omega_1)$. The domain $\mathcal{D}_1 \subset \mathcal{Q}$ denotes the set of admissible parameters. The operator P is the projection operator onto Ω_1, i.e. $P u = u|_{\Omega_1}$ for $\mathcal{U} \in \mathcal{V}$. Following the Lagrange approach in Section 4 we define the Lagrangian functional as

$$L(c, u, \lambda) := \frac{1}{2} \int_{\Omega_1} \left(u - y^\delta \right)^2 d\xi + \langle E(c, u), \lambda \rangle$$

with

$$\langle E(c, u), \lambda \rangle := a(u, \lambda; c, q^*) - \langle f, \lambda \rangle.$$

We consider derivatives. Let the iterate (c_k, u_k, λ_k) be given. Again we formulate the quadratic problem (10) and add the regularization term $\frac{\alpha_k}{2} \| \Delta c - c_k^* \|_{L^2}^2$. Note,

that this choice differs from the regularization terms in the previous sections since we consider the L^2-norm instead the H^2-norm. In order to formulate the equation (5) we have the bilinear forms

$$a_c(c, p) = \int_\Omega c\, p \, d\xi, \qquad c, p \in \mathcal{Q},$$

$$a_u(u, v) = \int_{\Omega_1} u\, v \, d\xi, \qquad u, v \in \mathcal{V},$$

$$b_c(c, z) = \int_\Omega c\, u_k\, z \, d\xi, \qquad c \in \mathcal{Q},\ z \in \mathcal{V}, \quad \text{and}$$

$$b_u(u, z) = a(u, z; c_k, q^*), \qquad u, v \in \mathcal{V}.$$

For the second derivatives we have $E_{cc} = 0 = E_{uu}$ and

$$\langle E_{cu}(c, u), \lambda_k \rangle = \int_\Omega c\, u\, \lambda_k \, d\xi, \qquad c \in \mathcal{Q},\ u \in \mathcal{V}.$$

Hence, for the iteration

$$c_{k+1} := c_k + \Delta c, \ u_{k+1} := u_k + \Delta u \ \text{ and } \ \lambda_{k+1} := \lambda$$

we have to find a solution $(\Delta c, \Delta u, \lambda)$ of the problem

$$\alpha_k \int_\Omega \Delta c\, p \, d\xi + \int_\Omega p\, \Delta u\, \lambda_k \, d\xi + \int_\Omega p\, u_k\, \lambda \, d\xi$$
$$= \alpha_k \int_\Omega p\, c_k^* \, d\xi, \qquad \forall\, p \in \mathcal{Q},$$

$$\int_\Omega \Delta c\, v\, \lambda_k \, d\xi + \int_{\Omega_1} \Delta u\, v \, d\xi + a(v, \lambda; c_k, q^*) \qquad\qquad (15)$$
$$= \int_{\Omega_1} v(y^\delta - u_k) \, d\xi, \qquad \forall\, v \in \mathcal{V},$$

$$\int_\Omega \Delta c\, u_k\, z \, d\xi + a(\Delta u, z; c_k, q^*) = \langle f, z \rangle - a(u_k, z; c_k, q^*), \qquad \forall\, z \in \mathcal{V}.$$

We discuss a discretization approach of the problem. Let $\mathcal{V}_n := \mathrm{span}\{\varphi_1, \ldots, \varphi_n\} \subset \mathcal{V}$ and $\mathcal{Q}_m := \mathrm{span}\{\psi_1, \ldots, \psi_m\} \subset \mathcal{Q}$ be subspaces and

$$u \approx \sum_{i=1}^n u_i \varphi_i, \ z \approx \sum_{i=1}^n z_i \varphi_i, \ \text{ and } \ c \approx \sum_{i=1}^m c_i \psi_i.$$

Moreover, we set $\underline{u} := (u_1, \ldots, u_n)^T$, $\underline{z} := (z_1, \ldots, z_n)^T \in \mathbb{R}^n$ and $\underline{c} := (c_1, \ldots, c_m)^T \in \mathbb{R}^m$.

For the given data we introduce a slight modification. We assume $\mathcal{Y}_N \subseteq \mathcal{V}_n$ with $\mathcal{Y}_N := \mathrm{span}\{\varphi_{i_1}, \ldots, \varphi_{i_N}\}$. Then the projection operator is given as matrix $P \in \mathbb{R}^{N \times n}$ such that

$$P\,\underline{u} = (u_{i_1}, \ldots, u_{i_N})^T \in \mathbb{R}^N.$$

This approach can be motivated as follows: the discrete data $\underline{y} = (y_1, \ldots, y_N)^T \in \mathbb{R}^N$ is given on N measurement points, which coincide with nodes $P_{i_1}, \ldots, P_{i_N}$ of the FE-mesh. Hence, we set

$$y^\delta := \sum_{j=1}^{N} y_j \varphi_{i_j},$$

whereas the projection in the space $\mathcal{V}_n$ of functions we interprete as

$$P\,u = P\left(\sum_{i=1}^{n} u_i \varphi_i\right) := \sum_{j=1}^{N} u_{i_j} \varphi_{i_j}.$$

We introduce the following notations

$$K = (k_{ij}) \in \mathbb{R}^{n \times n} \quad : \quad k_{ij} := \int_\Omega q^* \, \nabla \varphi_i \, \nabla \varphi_j \, d\xi,$$

$$Q = (q_{ij}) \in \mathbb{R}^{m \times m} \quad : \quad q_{ij} := \int_\Omega \psi_i \, \psi_j \, d\xi,$$

$$M_k = \left(m_{ij}^{(k)}\right) \in \mathbb{R}^{n \times n} \quad : \quad m_{ij}^{(k)} := \int_\Omega \psi_k \, \varphi_i \, \varphi_j \, d\xi, \quad 1 \le k \le m,$$

$$\tilde{M} = (\tilde{m}_{kj}) \in \mathbb{R}^{n \times n} \quad : \quad \tilde{m}_{kj} := \begin{cases} \int_\Omega \varphi_k \, \varphi_j \, d\xi, & j, k \in \{i_1, \ldots, , i_N\}, \\ 0 & \text{else.} \end{cases}$$

Moreover we have the matrices

$$
\begin{aligned}
M(\underline{u}) &:= (M_1 \underline{u}, \ldots, M_m \underline{u}) \in \mathbb{R}^{n \times m}, \\
\hat{M}(\underline{c}) &:= \sum_{i=1}^{m} c_i M_i \in \mathbb{R}^{n \times n} \quad \text{and} \\
A(\underline{c}) &:= K + \hat{M}(\underline{c}) \in \mathbb{R}^{n \times n},
\end{aligned}
$$

and finally

$$\underline{f} = (f_1, \ldots, f_n)^T \in \mathbb{R}^n \quad \text{with} \quad f_i := \langle f, \varphi_i \rangle, \ 1 \le i \le n.$$

Then we can write the problem (15) as equation system

$$
\begin{pmatrix}
\alpha_k Q & M(\underline{\lambda}_k)^T & M(\underline{u}_k)^T \\
M(\underline{\lambda}_k) & \tilde{M} & A(\underline{c}_k)^T \\
M(\underline{u}_k) & A(\underline{c}_k) & 0
\end{pmatrix}
\begin{pmatrix}
\Delta \underline{c} \\
\Delta \underline{u} \\
\underline{\lambda}
\end{pmatrix}
=
\begin{pmatrix}
\alpha_k Q \, \underline{c}_k^* \\
\tilde{M} \, P^T \left(\underline{y}^\delta - P \, \underline{u}_k \right) \\
\underline{f} - A(\underline{c}_k) \underline{u}_k
\end{pmatrix}
\qquad (16)
$$

or in terms of $(\Delta \underline{c}, \Delta \underline{u}, \Delta \underline{\lambda})$

$$
\begin{pmatrix}
\alpha_k Q & M(\underline{\lambda}_k)^T & M(\underline{u}_k)^T \\
M(\underline{\lambda}_k) & \tilde{M} & A(\underline{c}_k)^T \\
M(\underline{u}_k) & A(\underline{c}_k) & 0
\end{pmatrix}
\begin{pmatrix}
\Delta \underline{c} \\
\Delta \underline{u} \\
\Delta \underline{\lambda}
\end{pmatrix}
=
\begin{pmatrix}
\alpha_k Q \, \underline{c}_k^* - M(\underline{u}_k)^T \underline{\lambda}_k \\
\tilde{M} \, P^T \left(\underline{y}^\delta - P \, \underline{u}_k \right) - A(\underline{c}_k)^T \underline{\lambda}_k \\
\underline{f} - A(\underline{c}_k) \underline{u}_k
\end{pmatrix} .
\qquad (17)
$$

One of those equations has to be solved in each iteration step.

b) Determining the diffusion term

Now we assume that the function $q \in \mathcal{D}_2$ has to be identified, whereas $c = c^* \in \mathcal{D}_2$ is the given function. We again set $\mathcal{Q} := H^2(\Omega)$, $\mathcal{U} = \mathcal{Z} := \mathcal{V}$ and $\mathcal{Y} := L^2(\Omega_1)$. The domain $\mathcal{D}_2 \subset \mathcal{Q}$ denotes now the set of admissible parameters. We can define the Lagrangian functional as

$$
L(q, u, \lambda) := \frac{1}{2} \int_{\Omega_1} \left(u - y^\delta \right)^2 d\xi + \langle \tilde{E}(q, u), \lambda \rangle
$$

with

$$
\langle \tilde{E}(q, u), \lambda \rangle := a(u, \lambda; c^*, q) - \langle f, \lambda \rangle.
$$

We consider derivatives. Let the iterate (q_k, u_k, λ_k) be given. Again we formulate the quadratic problem (10) and add the regularization term $\frac{\alpha_k}{2} \| \Delta q - q_k^* \|_{L^2}^2$. We have for the bilinear forms

$$
\begin{aligned}
a_q(q, p) &= \int_\Omega q \, p \, d\xi, & q, p \in \mathcal{Q}, \\
a_u(u, v) &= \int_{\Omega_1} u \, v \, d\xi, & u, v \in \mathcal{V}, \\
b_q(q, z) &= \int_\Omega q \, \nabla u_k \, \nabla z \, d\xi, & c \in \mathcal{Q},\ z \in \mathcal{V}, \quad \text{and} \\
b_u(u, z) &= a(u, z; c^*, q_k), & u, v \in \mathcal{V}.
\end{aligned}
$$

For the second derivatives we derive $\tilde{E}_{qq} = 0 = \tilde{E}_{uu}$ and

$$
\langle \tilde{E}_{qu}(q, u), \lambda_k \rangle = \int_\Omega q \, \nabla u \, \nabla \lambda_k \, d\xi, \qquad q \in \mathcal{Q},\ u \in \mathcal{V}.
$$

14

Hence, for the iteration

$$q_{k+1} := q_k + \Delta q, \ u_{k+1} := u_k + \Delta u \ \text{ and } \ \lambda_{k+1} := \lambda$$

we have to find a solution $(\Delta q, \Delta u, \lambda)$ of the problem

$$
\alpha_k \int_\Omega \Delta q\, p\, d\xi + \int_\Omega p\, \nabla(\Delta u)\, \nabla \lambda_k\, d\xi + \int_\Omega p\, \nabla u_k\, \nabla \lambda\, d\xi
$$
$$
= \alpha_k \int_\Omega p\, q_k^*\, d\xi, \qquad\qquad \forall\, p \in \mathcal{Q},
$$

$$
\int_\Omega \Delta q\, \nabla v\, \nabla \lambda_k\, d\xi + \int_{\Omega_1} \Delta u\, v\, d\xi + a(v, \lambda; c^*, q_k) \tag{18}
$$
$$
= \int_{\Omega_1} v(y^\delta - u_k)\, d\xi, \qquad\qquad \forall\, v \in \mathcal{V},
$$

$$
\int_\Omega \Delta q\, \nabla u_k\, \nabla z\, d\xi + a(\Delta u, z; c^*, q_k) = \langle f, z \rangle - a(u_k, z; c^*, q_k), \quad \forall\, z \in \mathcal{V}.
$$

By the same discretization approach as above we define

$$
M = (m_{ij}) \in \mathbb{R}^{n \times n} \ : \ m_{ij} := \int_\Omega c^*\, \varphi_i\, \varphi_j\, d\xi,
$$

$$
Q = (q_{ij}) \in \mathbb{R}^{m \times m} \ : \ q_{ij} := \int_\Omega \psi_i\, \psi_j\, d\xi,
$$

$$
K_k = \left(k_{ij}^{(k)} \right) \in \mathbb{R}^{n \times n} \ : \ k_{ij}^{(k)} := \int_\Omega \psi_k\, \nabla \varphi_i\, \nabla \varphi_j\, d\xi, \quad 1 \le k \le m.
$$

Moreover we have the matrices

$$
\begin{aligned}
K(\underline{u}) &:= (K_1 \underline{u}, \ldots, K_m \underline{u}) \in \mathbb{R}^{n \times m}, \\
\hat{K}(\underline{q}) &:= \sum_{i=1}^{m} q_i K_i \in \mathbb{R}^{n \times n} \quad \text{and} \\
A(\underline{q}) &:= M + \hat{K}(\underline{q}) \in \mathbb{R}^{n \times n},
\end{aligned}
$$

As well the matrices Q and $\tilde{M}$ as the vector $\underline{f}$ we can left unchanged. Then we can write the problem (18) as equation system

$$
\begin{pmatrix}
\alpha_k Q & K(\underline{\lambda}_k)^T & K(\underline{u}_k)^T \\
K(\underline{\lambda}_k) & \tilde{M} & A(\underline{q}_k)^T \\
K(\underline{u}_k) & A(\underline{q}_k) & 0
\end{pmatrix}
\begin{pmatrix}
\Delta \underline{q} \\
\Delta \underline{u} \\
\underline{\lambda}
\end{pmatrix}
=
\begin{pmatrix}
\alpha_k Q\, \underline{q}_k^* \\
\tilde{M}\, P^T \left(\underline{y}^\delta - P\, \underline{u}_k \right) \\
\underline{f} - A(\underline{q}_k) \underline{u}_k
\end{pmatrix}
\tag{19}
$$

or in terms of $(\vartriangle\underline{q}, \vartriangle\underline{u}, \vartriangle\underline{\lambda})$

$$\begin{pmatrix} \alpha_k Q & K(\underline{\lambda}_k)^T & K(\underline{u}_k)^T \\ K(\underline{\lambda}_k) & \tilde{M} & A(\underline{q}_k)^T \\ K(\underline{u}_k) & A(\underline{q}_k) & 0 \end{pmatrix} \begin{pmatrix} \vartriangle\underline{q} \\ \vartriangle\underline{u} \\ \vartriangle\underline{\lambda} \end{pmatrix} = \begin{pmatrix} \alpha_k Q\, \underline{q}_k^* - K(\underline{u}_k)^T \underline{\lambda}_k \\ \tilde{M}\, P^T \left(\underline{y}^\delta - P\, \underline{u}_k \right) - A(\underline{q}_k)^T \underline{\lambda}_k \\ \underline{f} - A(\underline{q}_k)\underline{u}_k \end{pmatrix} \tag{20}$$

Again we have to solve one of these equations in each iteration.

6 Aspects of the implementation

We assume a FE discretization of the problem (14). We have two triangular meshes $\mathcal{T}_1 := \{T_1^{(1)}, \ldots, T_m^{(1)}\}$ and $\mathcal{T}_2 := \{T_1^{(2)}, \ldots, T_{m'}^{(2)}\}$, where $\mathcal{T}_2$ is a refinement of $\mathcal{T}_1$. That means, that for each $1 \le k \le m'$ exists an index $1 \le p(k) \le m'$ such that $\mathrm{int}(T_k^{(2)}) \subseteq \mathrm{int}(T_{p(k)}^{(1)})$. The mesh $\mathcal{T}_2$ has nodes P_j, $1 \le j \le n$.

As basis of $\mathcal{V}_n$ we choose the hat functions φ_j, $1 \le j \le n$, which are piecewise linear on each triangle $T_j^{(2)}$ and

$$\varphi_i(P_j) = \delta_{ij}, \quad 1 \le i, j \le n.$$

Moreover, as ansatz function for the space $\mathcal{Q}_m$ we choose the characteristic functions of the triangles of the mesh $\mathcal{T}_1$, i.e.

$$\psi_j := \chi_{T_j^{(1)}}, \quad 1 \le j \le m.$$

Let $\underline{u} \in \mathbb{R}^n$ and $\underline{c} \in \mathbb{R}^m$ be given vectors. For an effective calculation of the matrices $M(\underline{u}) = (M_1\underline{u}, \ldots, M_m\underline{u}) \in \mathbb{R}^{n \times m}$ and $\hat{M}(\underline{c}) = \sum c_i M_i \in \mathbb{R}^{n \times n}$ an element-wise consideration of the mesh can be used. Let $M^{(k)}$ denotes the element matrix of the triangle $T_k^{(2)}$ corresponding to the mass matrix of the triangulation $\mathcal{T}_2$. Let $\mathrm{meas}(T_k^{(2)})$ be the area of $T_k^{(2)}$, then

$$M^{(k)} = \frac{\mathrm{meas}(T_k^{(2)})}{12} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}.$$

The triangle $T_k^{(2)}$ has the vertices P_{k_1}, P_{k_2} and P_{k_3}. Then the vectors

$$b_k = \begin{pmatrix} b_1^k \\ b_2^k \\ b_3^k \end{pmatrix} := M^{(k)} \begin{pmatrix} u_{k_1} \\ u_{k_2} \\ u_{k_3} \end{pmatrix} = \frac{\mathrm{meas}(T_k^{(2)})}{12} \begin{pmatrix} 2u_{k_1} + u_{k_2} + u_{k_3} \\ u_{k_1} + 2u_{k_2} + u_{k_3} \\ u_{k_1} + u_{k_2} + 2u_{k_3} \end{pmatrix}$$

are calculated and b_j^k, $1 \le j \le 3$, is added on the element $(p(k), k_j)$ of $M(\underline{u})$. The construction of $\hat{M}(\underline{c})$ can be described quite effective since the parameter c

is constant on each triangle $T_k^{(2)}$ by construction. Hence we multiply each $M^{(k)}$ with $c_{p(k)}$ and add the entries of this 3×3-matrix on the corresponding entries of the matrix $\hat{M}(\underline{c})$.

The matrices $K(\underline{u}) \in \mathbb{R}^{n \times m}$ and $\hat{K}(\underline{q}) \in \mathbb{R}^{n \times n}$ for given $\underline{u} \in \mathbb{R}^n$ and $\underline{q} \in \mathbb{R}^m$ can be treated similarly. Since the ansatz functions φ_j, $1 \leq j \leq m$, are piecewise linear their gradients $\nabla \varphi_j$, $1 \leq j \leq m$, are constant on each triangle. For the triangle $T_k^{(2)}$ with vertices $P_{k_i} = (x_{k_i}, y_{k_i})^T$ we have

$$\nabla \varphi_{k_1} \equiv \frac{1}{2 \operatorname{meas}(T_k^{(2)})} \begin{pmatrix} y_{k_2} - y_{k_3} \\ x_{k_3} - x_{k_2} \end{pmatrix}, \quad \nabla \varphi_{k_2} \equiv \frac{1}{2 \operatorname{meas}(T_k^{(2)})} \begin{pmatrix} y_{k_3} - y_{k_1} \\ x_{k_1} - x_{k_3} \end{pmatrix}$$

and

$$\nabla \varphi_{k_3} \equiv \frac{1}{2 \operatorname{meas}(T_k^{(2)})} \begin{pmatrix} y_{k_1} - y_{k_2} \\ x_{k_2} - x_{k_1} \end{pmatrix}$$

on $T_k^{(2)}$. Hence for the element matrix $K^k = (k_{ij})$ we have

$$k_{ij} := \operatorname{meas}(T_k^{(2)}) (\nabla \varphi_{k_i})^T \nabla \varphi_{k_j}, \quad 1 \leq i, j \leq 3.$$

Then the vectors

$$\tilde{b}_k = \begin{pmatrix} \tilde{b}_1^k \\ \tilde{b}_2^k \\ \tilde{b}_3^k \end{pmatrix} := K^{(k)} \begin{pmatrix} u_{k_1} \\ u_{k_2} \\ u_{k_3} \end{pmatrix}$$

are calculated and $\tilde{b}_j^k$, $1 \leq j \leq 3$, is added on the element $(p(k), k_j)$ of $K(\underline{u})$. The construction of $\hat{K}(\underline{q})$ can be done analogously by using that the parameter q is constant on each triangle $T_k^{(2)}$ by construction. We multiply each $K^{(k)}$ with $q_{p(k)}$ and add the entries of this 3×3-matrix on the corresponding entries of the matrix $\hat{K}(\underline{q})$.

7 Some numerical results

We present some numerical examples. In particular we deal with the situation that the function c is unknown whereas the function q is given in (13). The L-shaped domain Ω is given as in Figure 1, which is the same situation as in the numerical case studies in [8]. Thereby Ω is decomposed into three disjoint sub-domains Ω_j $j = 1, 2, 3$. For the source function f in the differential equation (13) we choose the constant function $f(\xi) \equiv 50$, $\xi \in \Omega$. The function q is assumed to be piecewise constant, i.e.

$$q(\xi) := \begin{cases} 1, & \xi \in \Omega_1, \\ 3, & \xi \in \Omega_2, \\ 4, & \xi \in \Omega_3. \end{cases}$$
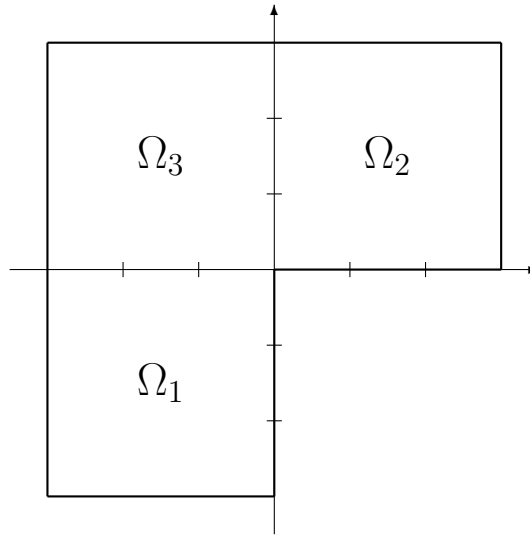
17

Figure 1: Domain Ω

Figure 2: Choice of the boundary conditions
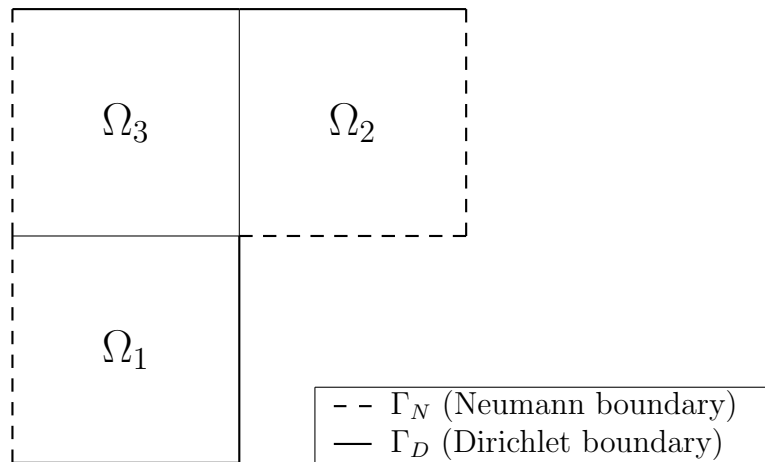
The boundary $\Gamma = \partial\Omega$ of Ω is decomposed into a Neumann boundary Γ_N and a Dirichlet boundary Γ_D as presented in Figure 2. For the choice of the function $c^\dagger$ which has to be identified we take

$$c^\dagger(x,y) := \begin{cases} 2-x, & (x,y) \in \Omega_1, \\ 1-x+y & (x,y) \in \Omega_2, \\ 2+x & (x,y) \in \Omega_3. \end{cases}$$

This function is continuously on each of these three sub-domains Ω_j, $j = 1, 2, 3$, but has jumps on the boundary. The discretization of this function is given by $\underline{c}^\dagger = (c_1, \ldots, c_m)^T \in \mathbb{R}^m$, where the entries c_j of the vector contain the values of the function $c^\dagger$ at the mid points of the corresponding triangles of the mesh $\mathcal{T}_1$.

The numerical realization was done with aid of the PARTIAL-DIFFERENTIAL-EQUATION TOOLBOX in MATLAB. The presented calculation times were obtained on the CASE-computers at the Faculty of Mathematics at the Chemnitz University of Technology.

For the numerical results presented below the mesh $\mathcal{T}_2$ for calculating the solutions $\underline{u}$ of the differential equation (13) has $n = 8433$ nodes. The data $\underline{y}$ was given on the nodes of a coarser mesh with $N = 1928$ nodes. The unknown parameter c is discretized on the mesh $\mathcal{T}_1$ with $m = 1032$ triangles.

In a first example we assume exact data $\underline{y}$ to be given. We want to compare the Levenberg-Marquardt method with the Tikhonov regularization approach with respect to speed of convergence and regularization error depending on the regularization parameter α. We apply the system (11) for calculating the next iterates. The iteration was stopped, when the tolerance

$$\|\underline{y} - P\,\underline{u}_k\| \leq TOL1 = 10^{-6} \quad \text{or} \quad \|\triangle \underline{c}\| \leq TOL2 = 10^{-6} \tag{21}$$

was reached. The obtained solutions we denoted with $\underline{c}_\alpha$. The corresponding results were given below in Table 1 for the Levenberg-Marquardt scheme and in Table 2 and 3 for Tikhonov regularization with different a-priori guess $\underline{c}^*$. As we can see the Levenberg-Marquardt algorithm provides better approximation $\underline{c}_\alpha$ of the unknown function $\underline{c}^\dagger$ than Tikhonov regularization since no regularization errors occur. On the other hand for choosing the the parameter α too large the number of iterations grows rapidly. For Tikhonov regularization we can see the increasing regularization error with respect to growing regularization parameter α. Comparing the results in Table 2 where the a-priori guess $\underline{c}^* \equiv 0$ was chosen with the results of Table 3 obtained with $\underline{c}^* \equiv 1$, we can see the dependence of the regularization error on this function. So we can expect better results by improving the a-priori guess $\underline{c}^*$.

In further calculations we deal with noisy data. Here, we replace the exact data $\underline{y}$ by noisy data $\underline{y}^\delta$, where $\delta > 0$ describes the relative size of the perturbation, i.e.

$$\|\underline{y} - \underline{y}^\delta\| \leq \delta\,\|\underline{y}\|.$$

In a first step we calculate an unregularized solution $\underline{c}^\delta$ with the Levenberg-Marquardt algorithm. The (sufficiently small) chosen parameter α does not influence the obtained results much. Table 4 shows the relative errors of the obtained solutions $\underline{c}^\delta$ for different noise levels. The size of the errors shows the ill-posedness of the problem under consideration. In order to introduce regulariza-

α	#iter.	time (sec.)	rel.err.
10^{-12}	3	14.6	$1.52 \cdot 10^{-7}$
10^{-11}	3	14.5	$1.51 \cdot 10^{-6}$
10^{-10}	3	14.5	$1.57 \cdot 10^{-5}$
10^{-9}	5	23.6	$1.80 \cdot 10^{-5}$
10^{-8}	23	106.3	$3.42 \cdot 10^{-5}$
10^{-7}	198	¿1000	$4.12 \cdot 10^{-5}$

Table 1: Levenberg-Marquardt method for exact data and different α

α	#iter.	time (sec.)	rel.err.
10^{-12}	3	14.6	$1.81 \cdot 10^{-5}$
10^{-10}	4	19.0	$1.83 \cdot 10^{-3}$
10^{-8}	4	19.2	$5.22 \cdot 10^{-2}$
10^{-6}	5	23.1	$1.48 \cdot 10^{-1}$
10^{-4}	4	5.6	$2.59 \cdot 10^{-1}$
10^{-2}	5	4.7	$3.92 \cdot 10^{-1}$

Table 2: Tikhonov regularization for exact data and different α, $\underline{c}^* \equiv 0$

α	#iter.	time (sec.)	rel.err.
10^{-12}	3	14.6	$7.12 \cdot 10^{-6}$
10^{-10}	4	19.1	$6.94 \cdot 10^{-4}$
10^{-8}	4	19.2	$2.27 \cdot 10^{-2}$
10^{-6}	5	22.0	$5.93 \cdot 10^{-2}$
10^{-4}	4	5.8	$1.10 \cdot 10^{-1}$
10^{-2}	5	4.7	$1.65 \cdot 10^{-1}$

Table 3: Tikhonov regularization for exact data and different α, $\underline{c}^* \equiv 1$

δ	rel.err.
10^{-6}	$1.03 \cdot 10^{-3}$
10^{-5}	$1.07 \cdot 10^{-2}$
10^{-4}	$1.02 \cdot 10^{-1}$
10^{-3}	1.01
10^{-2}	10.6

Table 4: unregularized solutions depending on the noise level

	$\underline{c}^* \equiv 0$		$\underline{c}^* \equiv 1$	
δ	α	rel.err.	α	rel.err.
10^{-6}	10^{-11}	$9.52 \cdot 10^{-4}$	10^{-11}	$9.91 \cdot 10^{-4}$
10^{-5}	10^{-10}	$9.43 \cdot 10^{-3}$	10^{-10}	$9.97 \cdot 10^{-3}$
10^{-4}	10^{-8}	$7.87 \cdot 10^{-2}$	10^{-7}	$5.45 \cdot 10^{-2}$
10^{-3}	10^{-5}	$2.08 \cdot 10^{-1}$	10^{-4}	$1.08 \cdot 10^{-1}$
10^{-2}	10^{-3}	$3.17 \cdot 10^{-1}$	10^{-3}	$1.40 \cdot 10^{-1}$

Table 5: Tikhonov regularization for noisy data, different a priori guesses $\underline{c}^*$

tion strategies we first apply Tikhonov regularization. For different noise level δ and regularization parameter α solutions $\underline{c}_\alpha^\delta$ where calculated. The regularization parameter α were chosen such that for a sequence $\{\alpha_j\}$ with

$$\alpha_0 := 0.1, \qquad \alpha_j := 0.1\,\alpha_{j-1}, \quad j \geq 2,$$

and regularized solutions $\{\underline{c}_{\alpha_j}^\delta\}$ we have $\alpha = \alpha_k$ with

$$\left\| \underline{c}_\alpha^\delta - \underline{c}^\dagger \right\| = \min_j \left\| \underline{c}_{\alpha_j}^\delta - \underline{c}^\dagger \right\|.$$

In Table 5 the relative errors with corresponding regularization parameter α were presented for both a-priori guesses $\underline{c}^* \equiv 0$ and $\underline{c}^* \equiv 1$. By applying Tikhonov regularization we could reduce the approximation errors caused by the use of noisy data $\underline{y}^\delta$. As in the noiseless case in the case $\underline{c}^* \equiv 1$ we obtained better approximations of the unknown parameter $\underline{c}^\dagger$. Using the Levenberg-Marquardt algorithm as regularization method we have to introduce a stopping criterion depending on the noise-level δ. We apply the discrepancy principle by Morozov which stops the iteration as soon as

$$\| P\,\underline{y}_k^\delta - \underline{y}^\delta \| \leq \delta \| \underline{y}^\delta \|.$$

where $\underline{c}_k^\delta$ denotes the actual iterate and $\underline{y}_k^\delta$ is the corresponding (numerical) solution of the differential equation (13), i.e. $\underline{y}_k^\delta$ satisfies

$$A(\underline{c}_k^\delta)\,\underline{y}_k^\delta = \underline{f}.$$

Hence, for verifying the stopping criterion we have to solve an additional differential equation in each iteration step. The results were given in Table 7. Again the calculations were performed for different parameters α. Choosing the parameter α too small the stopping criterion becomes active after one or two iterations which gives worse approximations than for a slower convergence with a larger parameter α. Again the parameter α is specified with yields the smallest relative approximation error. Comparing the results of Table 5 for $\underline{c}^* \equiv 1$ and Table 7 the obtained approximation errors are nearly the same for the different noise levels in both regularization methods.

δ	α	rel.err.
10^{-6}	10^{-12}	$1.00 \cdot 10^{-3}$
10^{-5}	10^{-9}	$4.03 \cdot 10^{-2}$
10^{-4}	10^{-6}	$6.29 \cdot 10^{-2}$
10^{-3}	10^{-4}	$1.02 \cdot 10^{-1}$
10^{-2}	10^{-2}	$1.54 \cdot 10^{-1}$

Table 6: Levenberg-Marquardt regularization for noisy data

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