Goal oriented adaptivity in the IRGNM for parameter identification in PDEs: I. reduced formulation

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Abstract
In this paper we study adaptive discretization of the iteratively regularized Gauss–Newton method (IRGNM) with an \textit{a posteriori} (discrepancy principle) choice of the regularization parameter in each Newton step and of the stopping index. We first of all prove convergence and convergence rates under some accuracy requirements formulated in terms of four quantities of interest. Then computation of error estimators for these quantities based on a weighted dual residual method is discussed, which results in an algorithm for adaptive refinement. Finally we extend the results from the Hilbert space setting with quadratic penalty to Banach spaces and general Tikhonov functionals for the regularization of each Newton step.

Keywords: regularization, adaptive discretization, parameter identification in PDEs, iteratively regularized Gauss–Newton method

(Some figures may appear in colour only in the online journal)

1. Introduction

Parameter identification problems in partial differential equations (PDEs) can often be written as nonlinear ill-posed operator equations

\[ F(q) = g, \] (1)
where $F$ is a nonlinear operator between Hilbert spaces $Q$ and $G$ and where the given data $g^\delta$ is noisy with the noise level $\delta$:

$$
||g - g^\delta|| \leq \delta.
$$

(2)

Throughout this paper we will assume that a solution $q^+$ to (1) exists.

In case of inverse problems for PDEs, $F$ is the composition of a parameter-to-solution map

$$
S : Q \rightarrow V
q \mapsto u
$$

with some measurement operator

$$
C : V \rightarrow G
u \mapsto g,
$$

where $V$ is an appropriate Hilbert space. Here, we will write the underlying (possibly nonlinear) PDE in its weak form:

$$
\text{for } q \in Q \text{ find } u \in V : \quad A(q, u)(v) = (f, v) \quad \forall v \in W,
$$

(3)

where $u$ denotes the PDE solution, $q$ some searched for coefficient or boundary function, and $f \in W^*$ is some given right-hand side in the dual of some Hilbert space $W$. We will assume that the PDE (3) and especially also its linearization at $(q, u)$ is uniquely and stably solvable.

For the stable solution of (1) with noisy data, we consider the iteratively regularized Gauss–Newton method (IRGNM) first of all (section 2) in the reduced form

$$
q_k^\delta = q_k^\delta - (F'(q_k^\delta)^*F(q_k^\delta) + \alpha_k I)^{-1}(F'(q_k^\delta)^*F(q_k^\delta) - g^\delta) + \alpha_k(q_k^\delta - q_0)
$$

(4)

or equivalently

$$
q_k^\delta \in \arg\min_q (T_{\alpha_k}(q)) = \arg\min_q \|F'(q_k^\delta)^*(q - q_k^\delta) + F(q_k^\delta) - g^\delta\|^2_G + \alpha_k\|q - q_0\|^2_Q.
$$

(5)

(see, e.g., [1, 17] and the references therein).

The regularization parameter $\alpha_k$ and the overall stopping index $k_*$ have to be chosen in an appropriate way in order to guarantee convergence. We will here use an inexact Newton / discrepancy principle type strategy, as it has been shown to yield convergence of the IRGNM even in a Banach space setting in [18], see also [13] for a convergence analysis in a still more general setup but with different parameter choice strategies for $\alpha_k$ and $k_*$. Our aim is to consider adaptively discretized versions of the formulations (4) defined by replacing the spaces $Q, V, W$ with finite dimensional counterparts $Q_h, V_h, W_h$ (using possibly different discretizations of $V, W$ in (9) and (8)). These should be sufficiently precise so that the convergence results from the continuous setting can be carried over, but save computational effort by using degrees of freedom only where really necessary. For this purpose we will make use of goal oriented error estimators [2, 3], that control the error in some quantities of interest $I$, which are functionals of the variables $q, u, w$ (see (7)–(9) below). We follow the concept proposed in [10], where an inexact Newton method for the computation of a regularization parameter according to the discrepancy principle is combined with adaptive refinement using goal oriented error estimators. While [10] is limited to linear inverse problems, in [15] the idea has been extended to the nonlinear case. Different from [15], we do not treat the nonlinear problem directly here, but use an iterative solution algorithm, the IRGNM (4), (5) and treat a sequence of linearized problems instead.
The exposition in this paper concentrates on a reduced formulation using the forward operator $F$, so that the obtained results largely hold for general inverse problems formulated as operator equations. In the closely related follow-up paper \cite{16} we consider some all-at-once formulations of the IRGNM that more explicitly make use of the underlying structure of the inverse problem as a combination of a PDE with additional measurements. Several of the results and methods of proof that we develop here will be useful for part II as well.

The remainder of this paper is organized as follows. In section 2 we formulate the Newton step equation as linear-quadratic optimal control problem and derive its discretization together with certain quantities of interest, whose precision will be crucial for obtaining convergence results for the overall regularized Newton iteration. This will be substantiated in the convergence and convergence rates results provided in the subsections 2.2 and 2.3. Subsection 2.4 describes computation of the required error estimators by a goal oriented approach and subsection 2.5 provides the full algorithm. The method and its analysis is extended to a setting with general data misfit and regularization terms in subsection 2.6. We conclude with a few remarks in section 3.

2. Reduced form of the discretized IRGNM

2.1. Formulation of the method

We consider the iteration rule (4) for solving the optimization problem

$$\min_{q \in Q} \|F'(q^{k-1,\delta})(q - q^{k-1,\delta}) + F(q^{k-1,\delta}) - g\|^2_G + \frac{1}{\beta_k} \|q - q_0\|^2_Q,$$

where the regularization parameter $\beta_k$ is updated in each Gauss–Newton iteration according to an inexact Newton method guaranteeing a relaxed version of the discrepancy principle (see step 15 in algorithm 3, \cite{10, 15}). Note that although the domain $D(F)$ might be a strict subset of $Q$, we need not explicitly restrict $q$ to $D(F)$ in this minimization, since we will assume that $D(F)$ contains a ball of radius $\rho$ around $q_0$ and prove that all iterates remain in this ball, cf \eqref{28}, \eqref{34}. So minimizers over $D(F)$ will automatically be minimizers over $Q$.

In \eqref{6} and in the following, we use a large parameter $\beta_k = \frac{1}{\alpha_k}$ in place of the original small regularization parameter $\alpha_k$ from \eqref{5}, since the 1-d equation to be solved (approximately) for the discrepancy principle becomes less nonlinear when considered as an equation for $\beta_k$ than it is w.r.t. $\alpha_k$.

We start with a detailed description of a single iteration step (4) for fixed (discretized) previous iterate $q^{k-1,\delta} = q_{old} \in Q$ in a continuous and later in the discretized setting actually used in computations, along with the quantities of interest required in error estimation and adaptive refinement.

Using the decomposition of the forward operator into solution and observation map, we write the optimization problem \eqref{6} equivalently as PDE constrained optimal control problem

$$\min_{(q, u_{old}, w) \in Q \times V \times V} \|C(u_{old})(w) + C(u_{old}) - g\|^2_G + \frac{1}{\beta_k} \|q - q_0\|^2_Q,$$

s.t. $A(q_{old}, u_{old})(v) = f(v) \quad \forall v \in W,$

$$A'_q(q_{old}, u_{old})(w, v) = -A'_q(q_{old}, u_{old})(q - q_{old}, v) \quad \forall v \in W,$$

since for a solution $q^{k,\delta}$ of \eqref{6} ($q^{k,\delta}, S(q_{old}), S'(q_{old})(q^{k,\delta} - q_{old}))$ solves \eqref{7}–\eqref{9}.

In most of this section we omit the superscript $\delta$ (denoting dependence on the noisy data) in order to be able to better indicate the difference between continuous and discretized quantities.

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For fixed \( q_{\text{old}} \) (the previous iterate) we consider the following quantities of interest

\[
I_1: Q \times Q \times R \to R, \quad (q_{\text{old}}, q, \beta) \mapsto \|F'(q_{\text{old}})(q - q_{\text{old}}) + F(q_{\text{old}}) - g^h\|^2_Q + \frac{1}{\beta} \|q - q_0\|^2_Q
\]

\[
I_2: Q \times Q \to R, \quad (q_{\text{old}}, q) \mapsto \|F'(q_{\text{old}})(q - q_{\text{old}}) + F(q_{\text{old}}) - g^h\|^2_G
\]

\[
I_3: Q \to R, \quad q_{\text{old}} \mapsto \|F(q_{\text{old}}) - g^h\|^2_G
\]

which for a solution \((q, u_{\text{old}}, w)\) of (7)–(9) and \(u \in V\) fulfilling

\[A(q, u)(v) = f(v) \quad \forall v \in W\]

satisfies the identities

\[
I_1(q_{\text{old}}, q, \beta) = \|C'(u_{\text{old}})(w) + C(u_{\text{old}}) - g^h\|^2_G + \frac{1}{\beta} \|q - q_0\|^2_Q
\]

\[
I_2(q_{\text{old}}, q) = \|C'(u_{\text{old}})(w) + C(u_{\text{old}}) - g^h\|^2_G
\]

\[
I_3(q_{\text{old}}) = \|C(u_{\text{old}}) - g^h\|^2_G
\]

The (continuous) quantities of interest in the \(k\)th iteration step are then defined as follows. For a solution \((q^k, u_{\text{old}}^k, w^k)\) of (7)–(9) for given \( q_{\text{old}} = q_{\text{old}}^k \) and \( \beta = \beta_k \) and \( u^k \) fulfilling

\[A(q^k, u^k)(v) = f(v) \quad \forall v \in W\]

in the \(k\)th iteration let

\[
I_{1}^k := I_1(q^k, q_{\text{old}}^k, \beta_k)
\]

\[
I_{2}^k := I_2(q_{\text{old}}^k, q^k) = \|F'(q_{\text{old}}^k)(q^k - q_{\text{old}}^k) + F(q_{\text{old}}^k) - g^h\|^2_G
\]

\[
I_{3}^k := I_3(q_{\text{old}}^k) = \|F(q_{\text{old}}^k) - g^h\|^2_G
\]

\[
I_{4}^k := I_4(q^k) = \|F(q^k) - g^h\|^2_G
\]

To formulate the quantities of interest (10) for a discrete setting, we consider finite element spaces \(Q_h, V_h, W_h\) to \(Q, V, W\), and \(S_h\) denotes the discrete solution operator of the state equation. The discretized version of the optimal control problem (7)–(9) for given \( q_{\text{old}} \in Q_h \) can then be formulated as

\[
\min_{(q, u_{\text{old}}, w) \in Q_h \times V_h \times V_h} \|C'(u_{\text{old}})(w) + C(u_{\text{old}}) - g^h\|^2_G + \frac{1}{\beta} \|q - q_0\|^2_Q
\]

subject to

\[A(q_{\text{old}}, u_{\text{old}})(v) = f(v) \quad \forall v \in W_h\]

\[A_{\delta h}(q_{\text{old}}, u_{\text{old}})(w, v) + A_{\delta h}(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}}, v) = 0 \quad \forall v \in W_h\]

Equation (16) is equivalent to \( u_{\text{old}} = S_h(q_{\text{old}}) \) and (17) is equivalent to \( w = S_{\delta h}(q_{\text{old}})(q - q_{\text{old}}) \), such that the reduced form of (15) reads

\[
\min_{q \in Q_h} \|F_h(q_{\text{old}})(q - q_{\text{old}}) + F_h(q_{\text{old}}) - g^h\|^2_G + \frac{1}{\beta} \|q - q_0\|^2_Q
\]

with \( F_h = C \circ S_h \).

**Remark 1.** One can think of using different discretizations \((V_h, W_h)\) for (16) and \((\tilde{V}_h, \tilde{W}_h)\) for (17) (see algorithm 1), which we do not indicate here in order to avoid a too complicated setup that would probably not lead to much gain in computational efficiency.
Then the discrete quantities of interest in the reduced form (i.e. the discrete counterparts to (10)) are defined by

\[ I_{1,h} : Q \times Q \times \mathbb{R} \rightarrow \mathbb{R}, \quad (q_{\text{old}}, q, \beta) \mapsto \|F_h'(q_{\text{old}})(q - q_{\text{old}}) + F_h(q_{\text{old}}) - g_h^d\|_G^2 + \frac{1}{\beta} \|q - q_0\|_Q^2 \]

\[ I_{2,h} : Q \times Q \rightarrow \mathbb{R}, \quad (q_{\text{old}}, q) \mapsto \|F_h'(q_{\text{old}})(q - q_{\text{old}}) + F_h(q_{\text{old}}) - g_h^d\|_G^2 \]

\[ I_{3,h} : Q \rightarrow \mathbb{R}, \quad q_{\text{old}} \mapsto \|F_h(q_{\text{old}}) - g_h^d\|_G^2 \]

\[ I_{4,h} : Q \rightarrow \mathbb{R}, \quad q \mapsto \|F_h(q) - g_h^d\|_G^2, \]

which that consistent with (12) for a solution \((q_h, u_{\text{old},h}, w_{h})\) of the discretized problem (15)–(17) there holds

\[ I_{1,h}(q_{\text{old}}, q_h, \beta) = \|C'(u_{\text{old},h})(w_{h}) + C(u_{\text{old},h}) - g_h^d\|_G^2 + \frac{1}{\beta} \|q_h - q_0\|_Q^2 \]

\[ I_{2,h}(q_{\text{old}}, q_h) = \|C'(u_{\text{old},h})(w_{h}) + C(u_{\text{old},h}) - g_h^d\|_G^2 \]

\[ I_{3,h}(q_{\text{old}}) = \|C(u_{\text{old},h}) - g_h^d\|_G^2 \]

\[ I_{4,h}(q_h) = \|C(u_{h}) - g_h^d\|_G^2 \]

Correspondingly, the discrete quantities of interest in the \(k\)th iteration step (i.e. the discrete counterparts to (14)) for a solution \((q_h^k, u_{\text{old},h}^k, w_{h}^k)\) of (15) for given \(q_{\text{old}} = q_{\text{old}} \in Q_h\) can be formulated as

\[ I_{1,h}^k(q_{\text{old}}, q_h^k, \beta_h^k) := I_{1,h}(q_{\text{old}}, q_h^k, \beta_h) \]

\[ = \|F_h'(q_{\text{old}})(q_h^k - q_{\text{old}}) + F_h(q_{\text{old}}) - g_h^d\|_G^2 + \frac{1}{\beta_h^k} \|q_h^k - q_0\|_Q^2 \]

\[ I_{2,h}^k(q_{\text{old}}, q_h^k) := I_{2,h}(q_{\text{old}}, q_h^k) = \|F_h'(q_{\text{old}})(q_h^k - q_{\text{old}}) + F_h(q_{\text{old}}) - g_h^d\|_G^2 \]

\[ I_{3,h}^k(q_{\text{old}}) := I_{3,h}(q_{\text{old}}) = \|F_h(q_{\text{old}}) - g_h^d\|_G^2 \]

\[ I_{4,h}^k(q_h^k) := I_{4,h}(q_h^k) = \|F_h(q_h^k) - g_h^d\|_G^2, \]

where we introduced the notation \(h_k\) (replacing \(h\)), denoting the discretization in step \(k\), in order to distinguish between the possibly different discretizations during the iterative process in the following.

Note that the norms in \(G\) and in \(Q\) (and later on also the one in \(V\)) as well as the operator \(C\) and the semilinear form \(a : Q \times V \times W \rightarrow \mathbb{R}\) defined by the relation \(a(q, u)(v) = \langle A(q, u), v \rangle_{W^*,W}\) (where \(\langle \cdot, \cdot \rangle_{W^*,W}\) denotes the duality pairing between \(W^*\) and \(W\)) are assumed to be evaluated exactly.

At the end of each iteration step we set

\[ q_{\text{old}}^{k+1} := q_h^k. \]

**Remark 2.** The sequence of iterates we actually consider is the discrete one \((q_h^k)_{k \in \mathbb{N}}\), which we also update according to (21). Besides that, for theoretical purposes we keep a sequence of continuous iterates \((q^k)_{k \in \mathbb{N}}\), where each member \(q^k\) of this sequence emerges from a member \(q_{\text{old}}^k = q_{\text{old}}^{k-1}\) of the sequence of discretized iterates \((q_h^k)_{k \in \mathbb{N}}\), but *not* from \(q^{k-1}\), see figure 1. One of the reasons for the necessity of considering this auxiliary continuous iterates is the key inequality (37) in the proof of the convergence theorem below, which makes use of minimality of the iterate \(q_k\) in all of \(Q\) (and not only in the finite dimensional subspace \(Q_h\)) thus allowing for comparison to the infinite dimensional exact solution \(q^k\).

We stress once more that the discretization may be different in each iteration, as indicated by the superscripts \(h_k, h_{k-1}\) here. In order to keep the notation readable we will suppress the iteration index \(k\) in the superscript \(h_k\) whenever this is possible without causing confusion.
Figure 1. Sequence of discretized iterates and auxiliary sequence of continuous iterates.

Remark 3. In view of (21) and the last two identities in (12) one might think that $I_{3,h}^{k+1} = \|F(q_{k+1}^h) - g^h\|_G^2$ and $I_{4,h}^k = \|F(q^h_k) - g^h\|_G^2$ are the same, but this is not the case, since there holds indeed

$$u^k_h = S_h(q^k_h) = S_h(q_{old}^{k+1})$$

for $h = h_k$, i.e. with respect to the discretization from step $k$, but

$$u_{old,h}^{k+1} = S_{h,k+1}(q_{old}^{k+1})$$

for $h = h_{k+1}$, i.e. with respect to the discretization from step $k + 1$. Due to the possibly different discretizations, in general there holds

$$u^k_h \neq u_{old,h}^{k+1}.$$

Also $I_{3}^{k+1} = \|F(q_{old}^{k+1}) - g^h\|_G^2$ and $I_{4}^{k} = \|F(q^h_k) - g^h\|_G^2$ are not the same, because

$$q_{old}^{k+1} \neq q^k_h \neq q^k,$$

see figure 1.

Remark 4. Note that even the discretizations $h_k$ for fixed $k$ can differ in the different quantities of interest during one Gauss–Newton iteration cf algorithm 1. Tracking the proof of the main convergence result theorem 1 the reader can verify that only $I_{1,h}^{k}$ and $I_{2,h}^{k}$ have to be evaluated on the same mesh, since in the proof we will need the identity

$$I_{1,h}^{k} = I_{2,h}^{k} + \frac{1}{\beta_k} \|q_h^k - q_0\|^2,$$

which is guaranteed by assuming exact evaluation of the $Q$-norm $\|q_h^k - q_0\|_Q$.

In order to assess and—by adaptive refinement—to control the differences

$$|I_{i,h}^{k} - I_{i}^{k}| \leq \eta_i^k, \quad i \in \{1, 2, 3, 4\}$$

between the exact quantities of interest and their counterparts resulting from discretization, we will make use of goal oriented error estimators, which will be explained in more detail in section 2.4.
We select $\beta_k$ according to an inexact Newton condition (cf \[11, 20\]) which can be interpreted as a discrepancy principle with ‘noise level’ $\tilde{\theta} F_{h,k}$

$$\tilde{\theta} F_{h,k} \leq F_{h,k} - g,\quad (24)$$

i.e.,

$$\tilde{\theta} F_{h}(q_{old}) - g^i \leq F_{h}(q_{old})(q_h - q_{old}) + F_{h}(q_{old}) - g^i \leq \tilde{\theta} F_{h}(q_{old}) - g^i,$$

for some $0 < \tilde{\theta} \leq \tilde{\theta} < \frac{1}{2}$. Note that this regularization parameter can be computed in an efficient manner according to [10], see theorem 1 there. We mention in passing that the latter would as well allow us to use the continuous version $\tilde{\theta}$ in (24), but we prefer to formulate the condition with the discretized actually computed quantities anyway.

The overall Newton iteration is stopped according to a generalized discrepancy principle

$$k_* = \min\{k \in \mathbb{N} : \hat{F}_{h,k} \leq \tau^2 \delta^2\}.\quad (25)$$

In our convergence analysis we will use the following weak sequential closedness assumption on $F$:

$$q_n \to q \land F(q_n) \to g \Rightarrow (q \in D(F) \land F(q) = g)\quad (26)$$

for all $\{q_n\}_{n \in \mathbb{N}} \subseteq Q$ together with the tangential cone condition (also often called Scherzer condition)

$$\|F(q) - F(\tilde{q}) - F'(q)(q - \tilde{q})\|_G \leq c_r\|F(q) - F(\tilde{q})\|_G\quad \forall q, \tilde{q} \in B_{\rho}(q_0) \subseteq D(F) \subseteq Q\quad (27)$$

for some $\rho > 0, 0 < c_r < 1$, which are both typical conditions in the analysis of regularization methods for nonlinear ill-posed problems cf. e.g., [9, 17] and the references therein. This also includes the assumption that the interior of the domain of $F$ is non-empty and thus contains a ball of (sufficiently small) radius $\rho$

$$B_{\rho}(q_0) \subseteq D(F).\quad (28)$$

2.2. Convergence

**Theorem 1.** Let for the starting point $q_0^0 \in B_{\rho}(q_0)$ hold and let $F$ satisfy the weak sequential closedness condition (26) and the tangential cone condition (27) with $c_r$ sufficiently small. Let, further, $\tau > 0$ be chosen sufficiently large and $0 < \tilde{\theta} < \tilde{\theta}$ sufficiently small, such that

$$2 \left(\frac{c_r^2 + (1 + c_r)^2}{\tau^2}\right) < \tilde{\theta} \quad \text{and} \quad \frac{2\tilde{\theta} + 4c_r^2}{1 - 4c_r^2} < 1. \quad (29)$$

Finally, let for the discretization error with respect to the quantities of interest (23) hold, where $\eta_1^k, \eta_2^k, \eta_3^k, \eta_4^k$ are selected such that

$$\eta_1^k + 2c_r^2\eta_3^k \leq \left(\tilde{\theta} - 2 \left(\frac{c_r^2 + (1 + c_r)^2}{\tau^2}\right)\right)\tilde{\theta} F_{h,k} \quad (30)$$

$$\eta_3^k \leq c_1 F_{h,k} \quad \text{and} \quad \eta_2^k \to 0, \eta_3^k \to 0, \eta_4^k \to 0 \text{ as } k \to \infty \quad (31)$$

$$F_{h,k} \leq (1 + c_3)F_{h,k} + \epsilon^k \quad \text{and} \quad (1 + c_3)\frac{2\tilde{\theta} + 4c_r^2}{1 - 4c_r^2} \leq c_2 < 1 \quad (32)$$

for some constants $c_1, c_2, c_3 > 0$, and a sequence $\epsilon^k \to 0$ as $k \to \infty$. 

---
Then with $\beta_k$ and $h = h_k$ fulfilling (24) and $k_*$ selected according to (25) there holds
\[(o)\] For all $k < k_*$, $\beta_k$ satisfying (24) exists provided
\[
\|F_k'(q_{\text{old}}^k)(q_0 - q_{\text{old}}^k) + F_k(q_{\text{old}}^k) - g^k\|_G^2 \geq \tilde{\theta}\|F_k(q_{\text{old}}^k) - q^k\|_G^2. \tag{33}
\]
If (33) is violated we set $q_k^* = q_0$.
\[(i)\] for any solution $q^i \in B_{\rho}(q_0)$ of (1)
\[
\|q_k^i - q_0\|_G^2 \leq \|q^i - q_0\|_G^2 \quad \forall k < k_*, \tag{34}
\]
\[(ii)\] $k_*$ is finite.
\[(iii)\] $q_{\text{old}}^k = q_{\text{old}}^{k-1}$ converges (weakly) subsequentially to a solution of (1) as $\delta \to 0$ in the sense that it has a weakly convergent subsequence and each weakly convergent subsequence converges strongly to a solution of (1). If the solution $q^1$ to (1) is unique, then $q_{\text{old}}^k$ converges strongly to $q^i$ as $\delta \to 0$.

**Remark 5.** Condition (29) can be satisfied for $c_{tc}$ sufficiently small, which via (27) is a local restriction on the nonlinearity of $F$, and by choosing $\tau$ sufficiently large.

Conditions (30), (31) (where the right-hand side is always strictly positive by definition of the stopping index (25)) are smallness conditions on the $\eta^k_t$, whereas the first condition in (32) links the discretizations of the forward operator at $q_{\text{old}}^k = q_{\text{old}}^{k-1}$ in the old and the new iteration. The second condition in (32) is enabled by the right inequality in (29).

The algorithmic implementation of these conditions is discussed at the beginning of subsection 2.5.

**Proof.**
\[(o)\] we denote by $q(\beta)$ or $q_h(\beta)$ the minimizer of the continuous and discrete Tikhonov functional, respectively, with regularization parameter $\beta$. For all $1 \leq k < k_*$ and any solution $q^i$ of (1) we have by (23) and minimality of $q(\beta)$ for the continuous Tikhonov functional
\[
R_{i,h}(\beta) \leq R_i^h(\beta) + \eta^i_k \leq \|F'(q_{\text{old}}^k)(q^i - q_{\text{old}}^k) + F(q_{\text{old}}^k) - g^k\|_G^2 + \frac{1}{\beta}\|q^i - q_0\|_G^2 + \eta^i_k, \tag{35}
\]
where $R_{i,h}(\beta)$ denotes $R^h_i$ with $\beta_k$ replaced by $\beta$. In here, according to (2), (25) and (27), as well as the inequality $(a + b)^2 \leq 2a^2 + 2b^2$ for arbitrary $a, b \in \mathbb{R}$ we can estimate as follows
\[
\|F'(q_{\text{old}}^k)(q^i - q_{\text{old}}^k) + F(q_{\text{old}}^k) - g^k\|_G^2 \\
\leq \left(\|F'(q_{\text{old}}^k)(q^i - q_{\text{old}}^k) + F(q_{\text{old}}^k) - F(q^i)\|_G + \delta\right)^2 \\
\leq \left(\eta^i_k\|F'(q_{\text{old}}^k)\|_G + \delta\right)^2 \\
\leq \left(\eta^i_k\|g^k - F(q_{\text{old}}^k)\|_G + \delta\right)^2 \\
= (c_{tc}\sqrt{R^h_i} + (1 + c_{tc})\delta)^2 \\
\leq 2c^2_{tc}R^h_i + 2(1 + c_{tc})^2\delta^2 \\
\leq 2c^2_{tc}(R^h_i + \eta^i_k) + 2(1 + c_{tc})^2\frac{R^h_i}{\tau^2} \\
= 2\left(\frac{c^2_{tc} + (1 + c_{tc})^2}{3}\right)R^h_i + 2c^2_{tc}\tau^2. \tag{36}
\]
Hence altogether, using (29), (30), we have
\[
\limsup_{\beta \to \infty} R_{2,h}(\beta) \leq \tilde{R}_{2,h}
\]
with \(R_{2,h}(\beta)\) standing for \(R_{2,k}\) with \(\beta\) in place of \(\beta_k\). On the other hand, since \(\lim_{\beta \to 0} q_0(\beta) = q_0\), we have by (33)
\[
\lim_{\beta \to 0} R_{2,h}(\beta) = \|F_h(q_{old}^h)(q_0 - q_{old}) + F_h(q_{old}^h) - g^h\|_G^2 \geq \tilde{R}_{2,h}^k.
\]
Thus by continuity of the mapping \(\beta \mapsto R_{2,h}(\beta)\) and the intermediate value theorem the assertion follows.

(i) For \(k = 0\), (34) trivially holds, likewise if (33) is violated and we set \(q_k^0 = 0\). We make use of minimality
\[
R_{3,h}^k \leq R_1^k + \eta_1^k \leq \|F'(q_{old}^h)(q^h - q_{old}^h) + F(q_{old}^h) - g\|_G^2 + \frac{1}{\beta_k} \|q^h - q_0\|_G^2 + \eta_1^k,
\]
and (36). On the other hand, from (22), (24) it follows that
\[
R_{3,h}^k = R_{3+h}^k + \frac{1}{\beta_k} \|q_k^h - q_0\|_G^2 \geq R_{3,h}^k + \frac{1}{\beta_k} \|q^h - q_0\|_G^2 \quad \text{which together with the previous inequality and (30) gives}
\]
\[
\frac{1}{\beta_k} \|q_k^h - q_0\|_G^2 \leq R_1^k + \eta_1^k \leq \|F'(q_{old}^h)(q^h - q_{old}^h) + F(q_{old}^h) - g\|_G^2 + \frac{1}{\beta_k} \|q^h - q_0\|_G^2 + \eta_1^k \leq 2 \left( c_{r,c}^2 + \frac{(1 + c_{r,c})^2}{\theta^2} \right) R_{3,h}^k + \frac{1}{\beta_k} \|q^h - q_0\|_G^2 + \eta_1^k + 2 c_{r,c} \eta_3^k \leq \frac{\eta_3^h}{\beta_k} + \frac{1}{\beta_k} \|q^h - q_0\|_G^2,
\]
which implies (34).

(ii) Furthermore, for all \(1 \leq k < k_*\) we have by the triangle inequality as well as (27) and the fact that the upper bound in (24) always holds, no matter whether (33) holds or not,
\[
\sqrt{R_2^k} = \|F(q_k^h) - g^h\|_G \leq \|F'(q_{old}^h)(q^h - q_{old}^h) + F(q_{old}^h) - g^h\|_G + \|F'(q_{old}^h)(q^h - q_{old}^h) - F(q_{old}^h)\|_G \leq \sqrt{R_2^k} + c_{r,c} \|F(q^h) - F(q_{old}^h)\|_G \leq \sqrt{\hat{R}_{2,h}^k + \eta_3^k + c_{r,c} (R_2^k + \sqrt{R_2^k})},
\]
hence by \((a + b)^2 \leq 2a^2 + 2b^2\) for all \(a, b \in \mathbb{R}\)
\[
R_2^k \leq 2 (\hat{R}_{3,h}^k + \eta_2^k) + 2 c_{r,c} (2 R_2^k + 2 R_2^k),
\]
which implies
\[
R_2^k \leq \frac{1}{1 - 4 c_{r,c}} (2 \hat{R}_{3,h}^k + 2 \eta_2^k + 4 c_{r,c} R_2^k).
\]
With (23) and (32) we can further deduce
\[
R_{4,h}^k \leq \frac{1}{1 - 4 c_{r,c}^2} \left( (2 \tilde{R}_{3,h}^k + 4 c_{r,c} R_2^k) \tilde{R}_{3,h}^k + 2 \eta_2^k + 4 c_{r,c}^2 \eta_3^k \right) + \eta_3^k \leq 2 \tilde{R}_{3,h}^k + 4 c_{r,c}^2 \frac{1}{1 - 4 c_{r,c}^2} \left( (2 \tilde{R}_{3,h}^k + 4 c_{r,c} R_2^k) R_{2,h}^k + 2 \eta_2^k + 4 c_{r,c}^2 \eta_3^k \right) + \eta_3^k \leq c_2 R_{2,h}^k \tilde{R}_{3,h}^k + \frac{1}{1 - 4 c_{r,c}^2} \left( (2 \tilde{R}_{3,h}^k + 4 c_{r,c}^2 R_2^k) R_{2,h}^k + 2 \eta_2^k + 4 c_{r,c}^2 \eta_3^k \right) + \eta_3^k.\]
With the notation
\[
d' := \frac{1}{1 - 4\epsilon} ((2\delta + 4\epsilon)c_\delta)^r + 2n_2 + 4\epsilon^2 \eta_2 + \eta_4 \quad \forall i \in \{1, 2, \ldots, k\}
\] (38)
there follows recursively
\[
P_{k,h}^t \leq c_{k,h}^t + \sum_{j=0}^{k-1} c_{j}^t d^{k-j}.
\] (39)

Note that by the second part of (31), the second part of (32) and the fact that \( r^k \to 0 \) as \( k \to \infty \) (by definition of \( r^k \)), we have \( c_{k,h}^t + \sum_{j=0}^{k-1} c_{j}^t d^{k-j} \to 0 \) as \( k \to \infty \). So, if the discrepancy principle never got active (i.e., \( k_* = \infty \)), the sequence \((p_{k,h}^t)_{k \in \mathbb{N}}\) and therewith by assumption (31) also \((p_{k,h}^t)_{k \in \mathbb{N}}\) would be bounded by a sequence tending to zero as \( k \to \infty \), which implies that \( p_{k,h}^t \) would fall below \( \tau \delta^2 \) for \( k \) sufficiently large, thus yielding a contradiction. Hence the stopping index \( k_* < \infty \) is well-defined and finite. (Note that here we could not just argue \( p_{k,h}^t \leq (1 + c_1)p_{k,\bar{h}} + r^k \to 0 \), hence eventually smaller than \( \tau \delta \), since the estimate (39) only holds for \( k < k_* \).)

(iii) With (2), (23), (31) and definition of \( k_* \), we have
\[
\|F(q_{old}^{k(h)}) - g\|_Q \leq \sqrt{1 + \frac{c_1}{\tau}} + \delta \leq \sqrt{P_{k,h}^t + n_3^k + \delta} \leq (1 + c_1) c_{k,h}^t + \delta
\] (40)
as \( \delta \to 0 \). Thus, due to (ii) (34) \( q_{old}^{k(h)} \) has a weakly convergent subsequence \((q_{old}^{k(h)})_{k \in \mathbb{N}}\) and due to the weak sequential closeness of \( F \) and (40) the limit \( q^* \in B_\epsilon(q_0) \) of every weakly convergent subsequence is a solution to \( F(q) = g \).

Strong convergence of \((q_{old}^{k(h)})_{k \in \mathbb{N}}\) to \( q^* \) follows from the standard argument
\[
\|q_{old}^{k(h)} - q^*\|_Q = \|q_{old}^{k(h)} - q_0\|_Q^2 + \|q^* - q_0\|_Q^2 - 2 \langle q_{old}^{k(h)} - q_0, q^* - q_0 \rangle_Q \leq \|q^* - q_0\|_Q^2 \text{ by weak convergence}
\]
(with \( \langle \ldots \rangle_Q \) denoting the scalar product in \( Q \)), where we have used the fact that in (34) we can replace \( q^k \) by \( q^* \) since the latter solves (1).

\[\]

### 2.3. Convergence rates

To prove convergence rates we will consider Hilbert space source conditions
\[
\exists s \in Q \text{ s.t. } q^l - q_0 = f(F'(q^*)^*F'(q^*))s,
\] (41)
with \( f : [0, \infty) \to [0, \infty) \) satisfying
\[
f(0) = 0, \quad f^2 \text{ strictly monotonically increasing}
\]
\[
\phi \text{ convex, where } \phi := (f^2)^{-1} \text{ i.e., } \phi^{-1}(\lambda) = f^2(\lambda) \quad \text{and}
\]
\[
\Theta : \lambda \mapsto f(\lambda) \sqrt{\lambda} \text{ strictly monotonically increasing.}
\]
Examples of functions \( f \) satisfying (42) are Hölder type \( f(\lambda) = \lambda^\nu, \nu > 0 \) or logarithmic type \( f(\lambda) = \ln(1 + \lambda)^p, \lambda \in (0, 1/e], p > 0 \) functions.

If (41) holds, then we have by Jensen’s inequality
\[
|\langle q^l - q_0, q - q^* \rangle_Q| = |\langle s, f(F'(q^*)^*F'(q^*)) (q - q^*) \rangle_Q| \leq \|s\|_Q \|q - q^*\|_Q f(\frac{\|F'(q^*) (q - q^*)\|_Q^2}{\|q - q^*\|_Q^2})
\] (43)

Using estimate (34) from the proof of theorem 1, as well as the definition of the stopping index according to the discrepancy principle, we can therefore make use of theorem 1 in [15] to obtain
Theorem 2. Let the conditions of theorem 1 and additionally the source condition (41) for some function $f$ with (42) be fulfilled. Then there exists a $\bar{\delta} > 0$ and a constant $\bar{C} > 0$ independent of $\delta$ such that for all $\delta \in (0, \bar{\delta}]$

$$\|q_h^k - q^+\|^2_Q \leq \frac{\bar{C}^2 \delta^2}{\Theta^{-1}(\frac{\bar{C}}{2\|s\|_Q} \delta)} = 4\|s\|^2 f^2(\Theta^{-1}(\frac{\bar{C}}{2\|s\|_Q} \delta)) \quad (44)$$

where $\Theta(\lambda) := f(\lambda)\sqrt{\lambda}$.

Proof. The assertion follows from theorem 1 in [15] using the estimate (34) and

$$\|F(q_h^k) - g^\delta\|_G \leq \sqrt{I_{3,h}^k + N_{3,h}^k} \leq \sqrt{1 + c_1^3 I_{3,h}^k} \leq \sqrt{1 + c_1 \tau \delta}.$$ \hfill \Box

Remark 6. If $f$ satisfies the condition

$$t \mapsto \frac{f(t)}{\sqrt{t}} \text{ monotonically decreasing}, \quad (45)$$

then for all $C > 0$ the inequality

$$f(\Theta^{-1}(Ct)) \leq \max\{\sqrt{C}, 1\} f(\Theta^{-1}(t)) \quad (t \geq 0) \quad (46)$$

holds, which implies that we can conclude from (44) the optimal rates

$$\|q_h^k - q^+\|_Q \leq C \left( f^2(\Theta^{-1}(\delta)) \right) = C \left( \frac{\delta^2}{\Theta^{-1}(\delta)} \right). \quad (47)$$

The restriction (45) corresponds to the typical saturation phenomenon of Tikhonov regularization in combination with the discrepancy principle, see e.g., [9].

2.4. Computation of the error estimators

The computation of the error estimators $\eta_1^k, \eta_2^k, \eta_3^k$ and $\eta_4^k$ is done similarly to [10]. The only difference lies in the fact that in $I_1$ we have three variables subject to discretization, namely $q, u_{old}$ and $w$ instead of only two ($q$ and $u$) as usual, which leads to the following error estimators. In this section we omit the iteration index $k$ for simplicity. The previous iterate $q_{old}$ is fixed and not subject to new discretization and the dependence on $\beta$ is not important for error estimation, so we neglect $q_{old}, \beta$ as arguments.

2.4.1. Error estimator for $I_1$. We consider

$$I_1(q, u_{old}, w) = \|C'(u_{old})(w) + C(u_{old}) - g^\delta\|^2_Q + \frac{1}{\beta} \|q - q_0\|^2_Q,$$

(where $I_1$ actually stands for $I_1^k$ with the superscript skipped and should not to be confused with the functional $I_1$ from section 2.1.) and define the Lagrange functional

$$L(q, u_{old}, v, v_{old}) := I_1(q, u_{old}, w) + A'(q_{old}, u_{old})(w)(v) + A'(q_{old}, u_{old})(q - q_{old})(v) + A(q_{old}, u_{old})(v_{old}) - f(v_{old}).$$
Proposition 1. Let $X = Q \times V \times V \times W \times W$ and $X_h = Q_h \times V_h \times V_h \times W_h \times W_h$. Let $x = (q, u_{old}, w, v, v_{old}) \in X$ be a stationary point of $L$, i.e.,

$$x_h \in X_h : \quad L(x)(dx) = 0 \quad \forall dx \in X$$

and let $x_h = (q_h, u_{old,h}, w_h, v_h, v_{old,h}) \in X_h$ be a discrete stationary point of $L$, i.e.,

$$L(x_h)(dx) = 0 \quad \forall dx \in X_h.$$

Then there holds

$$I_1(q, u_{old}, w) - I_1(q_h, u_{old,h}, w_h) = \frac{1}{2} L'(x_h)(x - x_h) + R,$$

for an arbitrary $x_h \in X_h$ and

$$R = \frac{1}{2} \int_0^1 L''(x_s)(e_s, e_s, e_s) s(s - 1) \, ds$$

with $e_s := x - x_h$.

Proof. cf [10] and [2].

Explicitly such stationary points can be computed by solving the equations

$$u_{old} \in V : \quad A(q_{old}, u_{old})(dv_{old}) = f(dv_{old}) \quad \forall dv_{old} \in W$$

$$w \in V : \quad A'_w(q_{old}, u_{old})(dw) = -A'_w(q_{old}, u_{old})(q - q_{old})(dw) \quad \forall dw \in V$$

$$v \in W : \quad A'_v(q_{old}, u_{old})(dv) = -I'_{1,u}(q, u_{old}, w)(dv) \quad \forall dv \in V$$

$$v_{old} \in W : \quad A'_v(q_{old}, u_{old})(dv)(v_{old}) = -I'_{1,u}(q, u_{old}, w)(dv) \quad \forall dv \in V$$

$$q \in Q : \quad I'_{1,q}(q, u_{old}, w)(dq) = -A'_q(q_{old}, u_{old})(dq)(v) \quad \forall dq \in Q$$

and their discrete counterparts.

Obviously, we do not actually compute continuous stationary points, but (as in [10]) we choose $\tilde{x}_h = \psi_{hx}$ with a suitable interpolation operator $\psi_h : X \to X_h$ and approximate the interpolation error using an operator $\pi_h : X_h \to X_h$ with $X_h \neq X_h$, such that $x - \pi_h x$ has a better local asymptotical behavior than $x - \psi_{hx}$. Then the error estimator $\eta_1$ for $I_1$ can be computed as

$$I_1 - I_{1,h} = I_1(q, u_{old}, w) - I_1(q_h, u_{old,h}, w_h) \approx \frac{1}{2} L'(x_h)(\pi_h x_h - x_h) = \eta_1$$

(cf [2]).

Remark 7. Please note that the equations (48)/(50)–(56) are solved anyway in the process of solving the optimization problem (7)–(9).

Although these error estimators are known to work efficiently in practice (see, e.g., [3]), they are not reliable, i.e., the conditions $\eta_i \geq |I_1 - I_{1,h}|$ ($i = 1, 2, 3, 4$) cannot be guaranteed in a strict sense in our computations, since we have to neglect the remainder term $R$ and use an approximation for $x - \tilde{x}_h$. Since our analysis is kept rather general, it is not restricted to dual-weighted-residual (DWR) estimators and would also work with a reliable error estimator. However, since they are based on residuals which are computed in the optimization process, the additional costs for estimation are very low, which makes the DWR error estimators tailored for our purposes.
2.4.2. Error estimator for $I_2$. We consider

$$I_2(u_{\text{old}},w) = \|C(u_{\text{old}})(w) + C(u_{\text{old}}) - g\|^2_C$$

and for $x_1 := (q_1, u_{\text{old},1}, w_1, v_1, v_{\text{old}}^1) \in X$ we define the auxiliary Lagrange functional

$$M(x, x_1) := I_2(u_{\text{old}},w) + L'(x)(x_1).$$

By doing so, we combine information on the quantity of interest $I_2$ (whose precision is to be assessed) with information on the underlying minimization problem (represented by the gradient of the Lagrangian $L$) into one functional. Indeed this allows us to conclude a similar result to proposition 1 for the difference $I(u_{\text{old}},w) - I(u_{\text{old},h},w_h)$ for stationary points $y = (x, x_1) \in X \times X$ and $y_h = (x_h, x_h^1) \in X_h \times X_h$ of $M$ (cf [3]). Such a discrete stationary point $y_h$ can be computed by solving the equations (48)/(50)–(56) and

$$x_h^1 \in X_h: \quad L''(y_h)(x_h^1, dx) = -I'_{2,w}(u_{\text{old},h},w_h)(dw) - I'_{2,u}(u_{\text{old},h},w_h)(dw) \quad \forall dx \in X_h,$$

(57)

(where $dx = (dq_{\text{old}}, du, dw, dv, dv_{\text{old}})$). The error estimator $\eta_2$ for $I_2$ can then be computed by

$$I_2 - I_{2,h} = I_2(u_{\text{old}},w) - I_2(u_{\text{old},h},w_h) \approx \frac{1}{2} M'(y_h)(\pi_h y_h - y_h) = \eta_2.$$

Remark 8. Once the optimality system (48)/(50)–(56) has been solved, computation of the auxiliary variable $x_h^1$ in $y_h = (x_h, x_h^1)$ only requires solution of a system (57) with the Hessian of the Lagrangian as a system matrix, which will be available (possibly even in a factorized or well preconditioned form) if the optimality system (48)/(50)–(56) has been solved by Newton’s method, thus only requiring minor additional effort.

To avoid the computation of second order information in (57) we would like to refer to [3], where (57) is replaced by an approximate equation of first order.

2.4.3. Error estimator for $I_3$. For $I_3$ we again proceed similarly to the sections 2.4.1 and 2.4.2, i.e. we consider

$$I_3(u_{\text{old}}) = \|C(u_{\text{old}}) - g\|^2_C$$

and define the auxiliary Lagrangian

$$N(x, x_2) := I_3(u_{\text{old}}) + L'(x)(x_2),$$

again combining the current quantity of interest with information on the minimization problem. As there holds again a similar results to proposition 1, we compute a discrete stationary point $\chi_h = (x_h, x_h^2) \in X_h \times X_h$ of $N$ by solving the equations (48)/(50)–(56) and

$$x_h^2 \in X_h: \quad L''(y_h)(x_h^2, dx) = -I'_{3,u}(u_{\text{old},h}) (du_{\text{old}}) \quad \forall dx \in X_h,$$

and compute the error estimator for $I_3$ as

$$I_3 - I_{3,h} = I_3(u_{\text{old}}) - I_3(u_{\text{old},h}) \approx \frac{1}{2} N'(\chi_h)(\pi_h \chi_h - \chi_h) = \eta_3.$$

Note that concerning the efficient computation of the required auxiliary variable $x_h^3$ in $\chi_h = (x_h, x_h^2)$ an analogous of remark 8 holds.
2.4.4. Error estimator for $I_4$. Different to the other error estimates, the bound on the error in $I_4$ only appears in connection with the very weak assumption $\eta_4^k \to 0$ as $k \to \infty$, which may be satisfied in practice without refining explicitly with respect to $\eta_4$, but simply, by refining with respect to the other error estimators $\eta_1, \eta_2$, and especially $\eta_3$. Another way to make sure that $\eta_4^k \to 0$ as $k \to \infty$, is, of course, to refine globally every now and then, although this is admittedly, not a very efficient solution.

If one does not want to rely on such practically motivated speculations and actually wants to compute an error estimator for $I_4$, one has to include the decoupled constraint

$$A(q, u)(v) = f(v) \quad \forall v \in W$$

in the definition of the Lagrangian $L$ in subsection 2.4.1. In that case we redefine the Lagrange functional in subsection 2.4.1 as

$$L(q, u_{\text{old}}, w, v, v_{\text{old}}, u, z) := I_1(q, u_{\text{old}}, w) + A_q(q_{\text{old}}, u_{\text{old}})(w)(v) + A_u(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}})(v) + A_q(q_{\text{old}}, u_{\text{old}})(v_{\text{old}}) - f(v_{\text{old}}) + A(q, u)(z) - f(z),$$

and the spaces $X := Q \times V \times V \times W \times V \times W$ and $X_h := Q_h \times V_h \times V_h \times W_h \times V_h \times W_h$. Then we consider

$$I_4(u) := \|C(u) - g\|^2_G$$

and define the auxiliary Lagrange functional

$$K(x, x_3) := I_4(u) + L'(x)(x_3)$$

for $x, x_3 \in X$. Then again (as in the subsections 2.4.1, 2.4.2 and 2.4.3) we could estimate the difference $I_4(u) - I_4(u_h)$ by computing a discrete stationary point $\tilde{\xi}_h = (x_h, x_3^h)$ of $K$, that means we would solve the equations $(48)/(50)–(56)$ and

$$x_3^h \in X_h : \quad L''(x_h)(x_3^h, dx) = -I_4'(u_h)(dx) \quad \forall dx = (dq, du, dz) \in X_h,$$

with $X_h := Q_h \times V_h \times V_h \times W_h \times V_h \times W_h$ and compute the error estimator $\eta_4$ for $I_4$ by

$$I_4 - I_{4,h} = I_4(u) - I_4(u_h) \approx \frac{3}{4}K''(\tilde{\xi}_h)(\pi u_h - \tilde{\xi}_h) = \eta_4.$$  

Again, according to remark 8, computation of $x_3^h$ in $\tilde{\xi}_h = (x_h, x_3^h)$ would be computable at low additional cost.

2.5. Algorithm

As mentioned and justified in subsection 2.4.4, we neglect $\eta_4^k$ and the condition $\eta_4^k \to 0$ and $\eta_3^k \to 0$ as $k \to \infty$ from (31) in the following algorithm.

In order to verify the condition (30) more easily, we split (30) into

$$\eta_4^k \leq c_4 I_{4,h}^k \quad \text{with} \quad c_4 = \frac{1}{2} \bigg( \bar{p} - 2 \left( c_{rf}^2 + \frac{(1 + c_{rf})^2}{\tau^2} \right) \bigg),$$

and

$$\eta_3^k \leq c_3 I_{3,h}^k \quad \text{with} \quad c_3 = \frac{1}{4c_{rf}^2} \bigg( \bar{p} - 2 \left( c_{rf}^2 + \frac{(1 + c_{rf})^2}{\tau^2} \right) \bigg).$$

Additionally we combine the inequality in (31), the first inequality in (32) and (59), since there holds

$$I_{4,h}^k \leq I_4^k + \eta_3^k \quad \text{and} \quad I_{4,h}^{k-1} \geq I_4^{k-1} - \eta_4^{k-1},$$

such that the condition

$$\eta_3^k + (1 + c_3)\eta_4^{k-1} \leq (1 + c_3)I_4^{k-1} - I_4^k + I_4^k$$

(60)
implies the first inequality in (32). As mentioned in remark 3, \( R^k_3 \) and \( R^{k-1}_3 \) only differ in the discretization level, which motivates the assumption that for small \( h \), we have \( R^k_3 \approx R^{k-1}_3 \) and \( \eta^k_3 \approx \eta^{k-1}_3 \), such that instead of (60) we check whether

\[
\eta^k_3 \leq \frac{c_3}{2(1 + c_3)} R^{k}_3,h + \frac{r^k}{2(1 + c_3)}.
\]

Thus, as a combination of the inequality in (31), (61) and (59), we formulate

\[
\eta^k_3 \leq \min \left\{ c_1, c_5, \frac{c_3}{2(1 + c_3)} \right\} R^{k}_3,h.
\]

In the statement ‘refine grids according to the error estimator …’ within the algorithms below, refinement of the spaces \( Q_h V_h \) and \( W_h \) is supposed to be done in principle separately according to the corresponding contributions within the error estimators. Namely, e.g., for \( I_3 \), the estimator

\[
\eta_1 := \frac{1}{2} L'(x_0)(x - \tilde{x}_h),
\]

from (49) being a Euclidean inner product between two vectors, comes as a sum of contributions corresponding to the different components of \( x_h = (q_h, u_{old,h}, u_h, v_h, v_{old,h}) \), as well as locally for each basis element (e.g. finite element) of the finite dimensional spaces used. In case it should be necessary to use equal spaces \( W_h = V_h \), e.g. in the context of Ritz–Galerkin methods for elliptic PDEs, we use the stronger accuracy criterion for doing a common refinement of both spaces.

The main algorithm is illustrated in a flowchart in figure 2 and explicitly given in algorithm 1.

**Algorithm 1. Reduced form of discretized IRGNM**

1: Choose \( \tau, \tau_\beta, \tilde{\delta}, \tilde{\beta} \) such that \( 0 < \tilde{\beta} \leq \tilde{\delta} < 1 \) and (29) holds, \( \tilde{\delta} = (\tilde{\beta} + \tilde{\delta})/2 \) and \( \max\{1, \tilde{\delta}\} < \tau_\beta \leq \tau \) and choose the constants \( c_1, c_2 \) and \( c_3 \), such that the second part of (32) is fulfilled.

2: Choose a discretization \( h = h_0 \) and starting value \( q_0^h = q^h_0 \) (not necessarily coinciding with \( q_0 \) in the regularization term) and set \( q_{old}^0 = q_0^h \).

3: Determine \( u_{old}^0 = u_{old,h_0}^0, I_3^0 = I_{3,h_0}^0 \) and \( \eta_3^0 = \eta_{3,h_0}^0 \) by applying algorithm 2 with \( m = 0 \) (and \( h = h_0 \)).

4: Set \( h_1^0 = h_0 \).

5: **while (62) is violated do**

6: Refine grids according to the error estimator \( \eta^0_3 \), such that we obtain a finer discretization \( h_1^0 \).

7: Determine \( u_{old}^0 = u_{old,h_1}, I_3^0 = I_{3,h_1}^0 \) and \( \eta_3^0 = \eta_{3,h_1}^0 \) by applying algorithm 2 with \( h = h_1^0 \) and \( m = 0 \).

8: Set \( k = 0 \) and \( h = h_1^0 \) (possibly different from \( h_0 \)).

9: **while \( I_{3,h}^k \geq \tau^2 \tilde{\delta}^2 \) do**

10: Set \( h = h_{k+1} \).

11: With \( q_{old}^k, u_{old}^k \) fixed, apply algorithm 3 starting with the current mesh \( h(= h_1^k) \) to obtain a regularization parameter \( \beta_k \) and a possibly different discretization \( h_2^k \) such that (24) holds and the corresponding \( w_h^k = w_{h_2}^k, q_h^k = q_{h_2}^k \).

12: Set \( h = h_1^k \).

13: Evaluate error estimator \( \eta_1^k = \eta_1^h(h_1^k) \).

14: Set \( h_{k+1} = h_{1}^k \).

15: **while (58) is violated do**
16:  Refine grids according to the error estimator $\eta_3$, such that we obtain a finer discretization $h_{k}^3$.
17:  Set $h = h_{3}^3$.
18:  With $q_{old}^k$ and $u_{old}^k$ fixed, determine $q_h^k = q_{h,3}^k$ and $w_h^k = w_{h,3}^k$ by solving (63).
19:  Set $q_{old}^{k+1} = q_h^k$.
20:  Determine $u_{old}^{k+1} = u_{old,h,3}^{k+1} = u_{h,3}^{k+1}$, and $\eta_3^{k+1} = \eta_{3,h,3}^{k+1}$ by applying algorithm 2 with $m = k + 1$ and $h = h_{3}^3$.
21:  while (62) is violated
22:  Refine grid according to the error estimator $\eta_3^{k+1}$, such that we obtain a finer discretization $h_{k+1}^3$.
23:  Determine $u_{old}^{k+1} = u_{old,h,3}^{k+1}$, $I_{h,3}^{k+1}$, and $\eta_3^{k+1} = \eta_{3,h,3}^{k+1}$ by applying algorithm 2 with $m = k + 1$ and $h = h_{3}^3$.
24:  Set $h_{k+1}^3 = h_{3}^3$ (i.e. use the current mesh as a starting mesh for the next iteration).
25:  Set $k = k + 1$.

Algorithm 2. Evaluation of $P^m_{3,h}$
1:  Determine
$$u_{old}^m \in V_h : \quad A(q_{old}^m, u_{old}^m) = f(v) \quad \forall v \in W_h.$$ 
2:  Evaluate $P^m_{3,h}$ according to (20).
3:  Evaluate error estimator $\eta_3^m$.

Algorithm 3. Inexact Newton method for the determination of a regularization parameter for
the IRGNM subproblem from [10]
1:  Set $\delta_h = \sqrt{\theta k_{3,h}^3 / \gamma \beta}$.
2:  Compute a Lagrange triple $x_h = (q_h, w_h, z_h)$ to the linear-quadratic minimization problem
$$\min_{q(w), w \in Q_h \times V_h} \| C'(u_{old}^k)(w) + C(u_{old}^k) - \delta \|^2_{L} + \frac{1}{\beta} \| q - q_{old} \|^2_{G}$$
subject to
$$A_h(q_{old}^k, u_{old}^k)(w), v) + A_h(q_{old}^k, u_{old}^k)(q - q_{old}^k)(v)$$
$$+ A(q_{old}^k, u_{old}^k)(v) - f(v) = 0 \quad \forall v \in W_h.$$ (63)
3:  Evaluate $i_h = I_{h,2}^k = \| C'(u_{old}^k)(w)_h) + C(u_{old}^k) - \delta \|^2_{L} - G.$
4:  while $i_h > (\tau_2^2 + \frac{\epsilon_2^2}{\beta}) \delta_h^2$ do
5:  Evaluate $i_h$ (cf [10]).
6:  Evaluate error estimator for $i(\beta) = I(w(\beta))$ with $I: \beta \mapsto I_2(u_{old}^k, w)$ (cf [10]).
7:  while accuracy requirements (cf [10]) are violated do
8:  Refine with respect to the corresponding error estimator.
9:  Compute a Lagrange triple $x_h = (q_h, w_h, z_h)$ to (63).
10:  Evaluate $i_h = I_{h,2}^k = \| C'(u_{old}^k)(w)_h) + C(u_{old}^k) - \delta \|^2_{L} - G.$
11:  Evaluate $i_h$ (cf [10]).
12:  Evaluate error estimator for $i(\beta) = I(w(\beta))$ with $I: \beta \mapsto I_2(u_{old}^k, w)$ (cf [10]).
13:  Evaluate error estimator for $i(\beta) = I(w(\beta))$ (cf [10]).
14:  Update $\beta$ according to an inexact Newton method (cf [10]) $\beta \gets \beta - \frac{i_h}{\delta_h}$.
15:  Compute a Lagrange triple $x_h = (q_h, w_h, z_h)$ to (63).
16:  Evaluate $i_h = I_{h,2}^k = \| C'(u_{old}^k)(w)_h) + C(u_{old}^k) - \delta \|^2_{L} - G.$
Figure 2. Illustration of algorithm 1. The arrows within the blocks point to variables that are computed in this step.

Remark 9. Algorithm 3 corresponds to the algorithm from [10] with the following replacements:

| in [10] | here |
|---------|------|
| $q$     | $q = q_0$ |
| $T$     | $F'(q_{old}^k)$ |
| $g^0$   | $g = F(q_{old}^k) + F'(q_{old}^k)(q_{old}^k)$ |
| $\tau^2 \delta^2$ | $\delta \hat{H}_{\tau, h}$ |
| $(\tau - \bar{\tau})^2 \delta^2$ | $\delta \hat{H}_{\bar{\tau}, h}$ |
| $(\tau + \bar{\tau})^2 \delta^2$ | $\delta \hat{H}_{\bar{\tau}, h}$ |
With respect to loops and the solution of PDEs and optimization problems, the algorithm has the following form. (We do not display the refinement loops on lines 5, 15, 22 of algorithm 1 and on line 8 of algorithm 3 but only the iteration loops.)

Algorithm 4. Loops in reduced form of discretized IRGNM

1: \textbf{while} \cdots (Newton iteration) \textbf{do}
2: \quad Apply algorithm from \cite{10}, \textit{i.e.}
3: \textbf{while} \cdots (Iteration for $\beta_k$) \textbf{do}
4: \quad Solve linear-quadratic optimization problem (i.e. solve linear PDE).
5: \quad Update $\beta$ and refine eventually.
6: \quad Solve nonlinear PDE.

In contrast with the nonlinear Tikhonov method

$$\min_{q \in Q} \| F(q) - g^\delta \|_G^2 + \frac{1}{\beta} \| q - q_0 \|_Q^2$$

investigated in \cite{15} (cf algorithm 5 below), we have one additional loop, but we only have to solve a linear-quadratic optimization problem instead of a nonlinear problem. On the other hand, we still have to solve (at least) one nonlinear PDE in each outer loop (see lines 3, 19, and 24 of algorithm 1). For this reason we doubt whether algorithm 1 pays off with respect to computation time as compared to the method in \cite{15}. Therefore we do not implement this algorithm, but consider more efficient modifications in \cite{16} (part II of this paper).

Algorithm 5. Loops in inexact Newton method (for Tikhonov regularized nonlinear problems)

1: \textbf{while} \cdots (Iteration for $\beta$) \textbf{do}
2: \quad Solve nonlinear optimization problem (i.e. solve nonlinear PDE).
3: \quad Update $\beta$ and refine eventually.

2.6. Extension to more general data misfit and regularization terms

Motivated by the increasing use of nonquadratic, non-Hilbert space misfit and regularization terms for modeling, e.g., sparsity of the solution, or non-Gaussian data noise (cf, e.g., \cite{6, 19} for Tikhonov regularization, and \cite{13} for the IRGNM), we now extend our results to a more general setting. To this purpose we consider a more general version of (15):

$$\min_{\vartheta \in Q} T_\beta(\vartheta) := S(F'(q^k_{old})(q - q^k_{old} + F(q^k_{old}), g^\delta) + \frac{1}{\beta} R(q) \quad (64)$$

with quantities of interest (cf (10))

$$\begin{align*}
I^1_k &:= S(F'(q^k_{old})(q^k - q^k_{old}) + F(q^k_{old}), g^\delta) + \frac{1}{\beta} R(q^k) \\
I^2_k &:= S(F'(q^k_{old})(q^k - q^k_{old}) + F(q^k_{old}), g^\delta) \\
I^3_k &:= S(F(q^k_{old}), g^\delta) \\
I^4_k &:= S(F(q^k), g^\delta)
\end{align*} \quad (65)$$

and their discrete counterparts (cf (18))

$$\min_{\vartheta \in Q_h} T_{\beta,h}(\vartheta) := S(F'(q^k_{old})(q - q^k_{old} + F_h(q^k_{old}), g^\delta) + \frac{1}{\beta} R(q) \quad (66)$$
with
\[
\begin{align*}
I_{1,h}^k & := S(F_h'(q_{old}^h)(q_h^k - q_{old}^h) + F_h(q_{old}^h), g'\big) + \frac{1}{\beta} R(q_h^k) \\
I_{2,h}^k & := S(F_h'(q_{old}^h)(q_h^k - q_{old}^h) + F_h(q_{old}^h), g') \\
I_{3,h}^k & := S(F_h(q_{old}^h), g') \\
I_{4,h}^k & := S(F_h(q_{old}^h), g')
\end{align*}
\] (67)
(cf (20)).

The data misfit and regularization functionals \( S \) and \( R \) should satisfy:

**Assumption 1.** Let \( S : G \times G \to \mathbb{R} \) and \( R : Q \to \mathbb{R} \) have the following properties.

(i) The mapping \( y \mapsto S(y, g^q) \) is convex.

(ii) \( S \) is symmetric, i.e. \( S(y, \tilde{y}) = S(\tilde{y}, y) \) for all \( y, \tilde{y} \in G \).

(iii) \( S \) is positive definite, i.e. \( S(y, \tilde{y}) \geq 0 \) and \( S(y, y) = 0 \) for all \( y, \tilde{y} \in G \).

(iv) There exists a constant \( c_S \) such that for all \( y, \tilde{y}, \tilde{y} \in G \)
\[ S(y, \tilde{y}) \leq c_S (S(y, \tilde{y}) + S(\tilde{y}, \tilde{y})). \]

(v) The regularization functional \( R \) is proper (i.e. the domain of \( R \) is non-empty) and convex.

Where the domain of an functional \( R : M \to \mathbb{R} \) should be understood as
\[
\mathcal{D}(R) := \{ m \in M | R(m) \neq \infty \}.
\]

**Remark 10.** In fact, it suffices to require \( S(y, y) = 0 \) only for \( y = g \), i.e. for the exact data in item (iii) of assumption 1, but since (iii) is a more "natural" assumption in terms of general functional properties, we stick with the stronger assumption (iii).

We refer once more to [13] where convergence and convergence rates for the IRGNM have already been established in an even more general (continuous) setting and mention that we here consider a somewhat simpler situation with stronger assumptions on \( S, R \), since our main intention is to demonstrate transferability of the adaptive discretization concept. Moreover, note that we rely on a different choice of the regularization parameter here. The results obtained here will allow us to easily establish convergence rates results for an exact penalty formulation of an all-at-once formulation of the IRGNM in [16] (part II of this paper).

We discuss convergence in a Banach space setting to emphasize the generality of the subsequent results. To this purpose we introduce the **Bregman distance**
\[
D_R^q(q, \tilde{q}) := R(q) - R(\tilde{q}) - \langle \xi, q - \tilde{q} \rangle_Q, \quad q \in Q
\] (68)
with some \( \xi \in \partial R(q) \subset Q^* \), which coincides with \( \frac{1}{2} \| q - q^j \|_Q^2 \) for \( R(q) = \frac{1}{2} \| q - q_0 \|_Q^2 \) and \( \xi = q^j - q_0 \) in a Hilbert space \( Q \).

Well-definedness (i.e. for every \( g^l \in G \) and \( \beta_h > 0 \) there exists a solution \( q_{old}^h \) to (66)) and stable dependence on the data (i.e. for every fixed \( \beta_h > 0 \) the solution \( q_{old}^h \) depends continuously on \( g^l \)) can be shown under the following assumptions (cf. e.g., assumption 1.32 in [19] or remark 2.1 in [13]).

**Assumption 2.**

(i) \( Q \) and \( G \) are Banach spaces, with which there are associated topologies \( \tau_Q \) and \( \tau_G \), which are weaker than the norm topologies.

(ii) The mapping \( y \mapsto S(y, g^q) \) is sequentially lower semi-continuous with respect to \( \tau_G \).

(iii) \( F'(q_{old}^h) : Q \to G \) is continuous with respect to the topologies \( \tau_Q \) and \( \tau_G \).

(iv) \( R : Q \to (-\infty, +\infty] \) is proper, convex and \( \tau_Q \)-lower semi-continuous.
(v) \( \mathcal{D} := \mathcal{D}(F) \cap \mathcal{D}(\mathcal{R}) \neq \emptyset \) is closed with respect to \( \tau_{\mathcal{Q}} \).

(vi) For every \( C > 0 \) the set
\[
\mathcal{C}(C) := \{ q \in \mathcal{D} : \mathcal{R}(q) \leq C \},
\]
is \( \tau_{\mathcal{Q}} \)-sequentially compact in the following sense: every sequence \((q_n)_{n \in \mathbb{N}}\) in \( \mathcal{C}(C) \) has a subsequence, which is convergent in \( \mathcal{Q} \) with respect to the \( \tau_{\mathcal{Q}} \)-topology.

**Remark 11.** For Hilbert spaces \( \mathcal{Q} \) and \( \mathcal{G} \) and the choice \( S(y, \tilde{y}) := \frac{1}{2} \| y - \tilde{y} \|_{\mathcal{G}}^2 \) and \( \mathcal{R}(q) := \frac{1}{2} \| q - q_0 \|_{\mathcal{G}}^2 \) assumptions 1 and 2 are obviously fulfilled. As for examples in a real Banach spaces setting, we refer to [6, 13, 14, 18, 19].

Consistently the conditions (26) and (27) on \( F \) are generalized to the following two assumptions.

**Assumption 3.** Let the reduced forward operator \( F \) be continuous with respect to \( \tau_{\mathcal{Q}}, \tau_{\mathcal{G}} \) and satisfy
\[
(q_n \rightarrow q \land S(F(q_n), g) \rightarrow 0 \Rightarrow (q \in \mathcal{D}(F) \land F(q) = g)
\]
for all \((q_n)_{n \in \mathbb{N}} \subseteq \mathcal{Q} \).

**Assumption 4.** Let the generalized tangential cone condition
\[
S(F(q), F(\tilde{q}) + F'(\tilde{q})(q - \tilde{q})) \leq c_{ic}^2 S(F(q), F(\tilde{q}))
\]
hold for all \( q, \tilde{q} \in \mathcal{Q} \) in the level set \( \{ q \in \mathcal{Q} : \mathcal{R}(q) \leq \mathcal{R}(q^\dagger) \} \) for some \( 0 < c_{ic} < 1 \).

For proving convergence rates, the source condition (41) is replaced by assumption 5.

**Assumption 5.** Let the multiplicative variational inequality
\[
|\langle \xi, q - q^\dagger \rangle_{\mathcal{G}^*, \mathcal{G}}| \leq c_{ic}^2 \mathcal{D}_{\mathcal{R}}^2(q, q^\dagger)^{1/2} \left( \frac{S(F(q), F(q^\dagger))}{\mathcal{D}_{\mathcal{R}}^2(q, q^\dagger)} \right)
\]
for all \( q \in \mathcal{D}(F) \) hold.

Based on this groundwork, we can now formulate a convergence theorem similar to theorem 1:

**Theorem 3.** Let assumption 2 be satisfied, let for the starting point \( \mathcal{R}(q^0_k) \leq \mathcal{R}(q^\dagger_k) \) hold, and let \( F \) be continuous and satisfy assumptions 3, 4 with \( c_{ic} \) sufficiently small. Let, further, \( \tau > 0 \) be chosen sufficiently large such that
\[
c_{ic} \left( c_{ic}^2 \mathcal{D}^2 + \frac{1 + c_{ic}^2}{\tau^2} \right) < \frac{\tilde{\theta}}{2} \quad \text{and} \quad 0 < \frac{c_{ic} \mathcal{R} + c_{ic}^2}{1 - c_{ic}^2} < 1
\]
and let
\[
S(g, g^\delta) \leq \delta^2.
\]
Finally, let for the discretization error with respect to the quantities of interest (65), (67) estimates (23) hold, where \( \eta_1^k, \eta_2^k, \eta_3^k, \eta_4^k \) are selected such that
\[
\eta_1^k + c_{ic}^2 \eta_3^k \eta_4^k \leq \left( \frac{\theta - c_{ic} \left( c_{ic}^2 \mathcal{D}^2 + \frac{1 + c_{ic}^2}{\tau^2} \right) \eta_4^2}{\eta_3^k} \right) \eta_3^k.
\]
as well as (31), the first part of (32) and
\[(1 + c_3)\frac{c_5\delta + c_6^2\tau^2}{1 - c_5^{2}\tau^2} \leq c_2 < 1 \quad (73)\]
hold for some constants \(c_1, c_2, c_3 > 0\), and a sequence \(i^k \to 0\) as \(k \to \infty\), where (73) is possible due to the right inequality in (70).

Then with \(\beta_k\) and \(h = h_k\) fulfilling (24) and \(k_\ast\) selected according to (25) with \(I_{2,h}^k, I_{3,h}^k\) according to (67), there holds:

(i) For all \(k < k_\ast\),
\[R(q_k^\delta) \leq R(q^\delta) \quad \forall k < k_\ast, \quad (74)\]

(ii) \(k_\ast\) is finite,
(iii) \(q_{k_\ast}^\delta = q_{k_\ast - 1}^\delta\) converges (weakly) subsequentially to a solution of (1) as \(\delta \to 0\) in the sense that it has a \(\tau_0\) convergent subsequence and each \(\tau_0\) convergent subsequence converges to a solution of (1). If the solution \(q^\delta\) to (1) is unique, then \(q_{k_\ast}^\delta\) converges with respect to \(\tau_0\) to \(q^\delta\) as \(\delta \to 0\).

**Proof.** The proof basically follows the lines of the proof of theorem 1, where we have to replace the specific fitting and regularization terms by \(S\) and \(R\).

(i) For all \(k < k_\ast\) and any solution \(q^\delta\) of (1) we have by (23) and minimality of \(q^\delta\)
\[R_{1,h}^k \leq R_1^k + \eta_1^k \leq S(F'(q_{\text{old}}^k)(q^k - q_{\text{old}}^k) + F(q_{\text{old}}^k), g^k) + \frac{1}{\beta_k} R(q^\delta) + \eta_1^k. \quad (75)\]

In here, according to (71), (25) and assumption 4, as well as the inequality \((a + b)^2 \leq 2a^2 + 2b^2\) for arbitrary \(a, b \in \mathbb{R}\) we can estimate as follows
\[S(F'(q_{\text{old}}^k)(q^k - q_{\text{old}}^k) + F(q_{\text{old}}^k), g^k) \leq c_S \left( S(g, F'(q_{\text{old}}^k)(q^k - q_{\text{old}}^k) + F(q_{\text{old}}^k)) + \delta^2 \right)
\leq c_S \left( c_S^{-1} S(g, F(q_{\text{old}}^k)) + \delta^2 \right)
\leq c_S \left( c_S^{-1} c_S^{-1} (I_{3,h}^k + \eta_1^k) + c_S (1 + c_S c_{\tau_0}^2) \right)^\frac{1}{\tau_0^2}
\leq c_S \left( c_S c_{\tau_0}^2 + \frac{1 + c_S c_{\tau_0}^2}{\tau_0^2} \right) I_{3,h}^k + c_S c_{\tau_0}^2 \eta_1^k. \quad (76)\]

On the other hand, from (24) and the fact that \(I_{2,h}^k = I_{2,h}^k + \frac{1}{\beta_k} R(q_k^\delta)\) (cf (22)) there follows that
\[R_{1,h}^k = I_{2,h}^k + \frac{1}{\beta_k} R(q_k^\delta) \geq \tilde{R}_{1,h}^k + \frac{1}{\beta_k} R(q_k^\delta), \quad (77)\]
which together with the previous inequality and (72) gives
\[\tilde{R}_{3,h}^k + \frac{1}{\beta_k} R(q_k^\delta) \leq I_{2,h}^k + \frac{1}{\beta_k} R(q_k^\delta)
\leq S(F'(q_{\text{old}}^k)(q^k - q_{\text{old}}^k) + F(q_{\text{old}}^k), g^k) + \frac{1}{\beta_k} R(q^\delta) + \eta_1^k
\leq c_S \left( c_S c_{\tau_0}^2 + \frac{1 + c_S c_{\tau_0}^2}{\tau_0^2} \right) I_{3,h}^k + c_S c_{\tau_0}^2 \eta_1^k + \frac{1}{\beta_k} R(q^\delta) + \eta_1^k
\leq \tilde{R}_{3,h}^k + \frac{1}{\beta_k} R(q^\delta),\]
which implies (74).
(ii) Furthermore, for all $k < k_*$ we have by the triangle inequality as well as assumption 4 and (24)

$$I_k^t = S(F(q^k), g^k) \leq c_S (S(F(q^k_{old}), g^k) + \|S(F(q^k_{old}), F(q^k))\|
\leq c_S (I_k^t + c_S^2 S(F(q^k), F(q^k))) \leq c_S (\tilde{I}_k^t + c_S^2 S(F(q^k), g^k)) + c_S^2 (I_k^t + \tilde{I}_k^t), \quad (78)$$

which implies

$$I_k^t \leq \frac{1}{1 - c_S^2 c_{ic}} \left( c_S \tilde{I}_k^t + c_S c_{ic}^2 I_k^t \right).$$

With (23) and (32) we can further deduce

$$I_{k,h}^t \leq \frac{1}{1 - c_S^2 c_{ic}} (c_S \tilde{I}_{k,h}^t + c_S c_{ic}^2 I_{k,h}^t) \leq c_S \tilde{I}_{k,h}^t + c_S c_{ic}^2 I_{k,h}^t + \eta^t_k$$

With the notation

$$d^t := \frac{1}{1 - c_S^2 c_{ic}} (r^t + c_S \eta^t_1 + c_S c_{ic}^2 \eta^t_1) \quad \forall i \in \{1, 2, \ldots, k\} \quad (79)$$

there follows recursively

$$I_{k,h}^t \leq c_S \tilde{I}_{k,h}^t + \sum_{j=0}^{k-1} c_S^j d^{t-j}. \quad (80)$$

Note that by the second part of (31), the second part of (32) and the fact that $r^t \to 0$ as $k \to \infty$ (by definition of $r^t$), we have $c_S \tilde{I}_{k,h}^t \to 0$ as $k \to \infty$. So, if the discrepancy principle never got active (i.e., $k_* = \infty$), the sequence $(I_{k,h}^t)_{k \in \mathbb{N}}$ and therewith by assumption (31) also $(\tilde{I}_{k,h}^t)_{k \in \mathbb{N}}$ would be bounded by a sequence tending to zero as $k \to \infty$, which implies that $I_{k,h}^t$ would fall below $\tau^2 \delta^2$ for $k$ sufficiently large, thus yielding a contradiction. Hence the stopping index $k_* < \infty$ is well-defined and finite.

(iii) With (71), (23), (31) and definition of $k_*$, we have

$$S(F(q^k_{old}), g) \leq c_S (S(F(q^k_{old}), g^k) + \delta^2) \leq c_S (I_{k,h}^t + \delta^2) \leq c_S ((1 + c_1) I_{k,h}^t + \delta^2) \leq c_S ((1 + c_1) \tau^2 + 1) \delta^2 \to 0 \quad (81)$$

as $\delta \to 0$. By (i), (ii) and (69) in assumption 2 $q^k_{old} = q^k_{h_{k-1}}$ has a $\tau_0$ convergent subsequence $(q^k_{old(h_{k-1})})_{k \in \mathbb{N}}$ and due to assumption 3 and (81), the limit of every $\tau_0$ convergent subsequence is a solution to $F(q) = g$.

It is readily checked that (like in the case of $\mathcal{R}$, $S$ being defined by squared Hilbert space norms as considered in theorem 1 of [15]) any approximation $\tilde{q}$ of a solution $q'$ of $F(q) = g$ with $\|g - g'\| \leq \delta$ such that

$$\mathcal{R}(\tilde{q}) \leq \mathcal{R}(q') \quad \text{and} \quad S(F(\tilde{q}), g') \leq \tilde{\epsilon}^2 \delta^2$$
with \( \tilde{\tau} \) independent of \( \delta \), as well as the variational inequality (5) holds, satisfies the rate estimate

\[
D^\delta R(\tilde{q}_h, q^*) \leq \frac{C^2 \delta^2}{\Theta^{-1} (\frac{\tilde{\tau}}{c})} = c^2 f^2 (\Theta^{-1} (\frac{\tilde{\tau}}{c})),
\]

with \( C^2 = c_\delta (\tilde{\tau}^2 + 1) \).

Hence we directly obtain from (74) and the definition of \( k^* \) according to (25) the following rates result.

**Theorem 4.** Let the conditions of theorem 3 and additionally the variational inequality (5) for some function \( f \) with (42) be fulfilled.

Then there exists a \( \tilde{\delta} > 0 \) and a constant \( \tilde{C} > 0 \) independent of \( \delta \) such that for all \( \delta \in (0, \tilde{\delta}] \)

\[
D^\delta R(\tilde{q}_h, q^*) \leq \frac{C^2 \delta^2}{\Theta^{-1} (\frac{\tilde{\tau}}{c})} = c^2 f^2 \left( \Theta^{-1} \left( \frac{\tilde{\tau}}{c} \right) \right),
\]

where \( \Theta(\lambda) := f(\lambda)/\sqrt{\lambda} \).

**Proof.** The proof can be done analogously to the proof of theorem 1 in [15] with the same replacements as in the proof of theorem 3. \( \square \)

**Remark 12.** So far we have not commented on well-definedness of the regularization parameter \( \beta_k \) by (24) with \( \beta_{h_1}, \beta_{h_2} \) according to (67) yet. As a matter of fact, this can be shown analogously to lemma 1 and theorem 3 in [18] under some additional assumptions on \( S \) and \( R \). For simplicity of exposition we will only do so for the continuous setting.

**Lemma 1.** Let assumptions 1–4 be satisfied with lower semicontinuity replaced by continuity in items (ii), (iv) of assumption 2 and convexity by strict convexity in item (v) of assumption 1. Moreover, assume that

\[
c_S \left( c_S \frac{\tau^2}{c} + \frac{1 + c_S \tau^2}{\tau^2} \right) < \frac{\tilde{\tau}}{\tilde{\nu}} < \frac{\tilde{\nu}}{\tilde{\tau}}
\]

(cf (70)), that \( k < k_* \), and that for the (then existent and unique) minimizer \( q_0 \) of \( R \)

\[
S(F(q^k_{\text{old}})(q_0 - q^k_{\text{old}}) + F(q^k_{\text{old}}), g^k) \geq \tilde{\nu} S(F(q^k_{\text{old}}), g^k)
\]

and (71) holds. Then there exists \( \beta_k \) such that

\[
\tilde{\nu} S(F(q^k_{\text{old}}), g^k) \leq S(F'(q^k_{\text{old}})(q^k - q^k_{\text{old}}) + F(q^k_{\text{old}}), g^k) \leq \tilde{\nu} S(F(q^k_{\text{old}}), g^k).
\]

**Proof.** We denote by \( \Psi \) the real function \( \beta \mapsto S(F(q^k_{\text{old}})(q(\beta) - q^k_{\text{old}}) + F(q^k_{\text{old}}), g^k) \) where \( q(\beta) \) is the (under the stated conditions existent and unique) minimizer of the Tikhonov functional \( T_\beta(q) := S(F'(q^k_{\text{old}})(q - q^k_{\text{old}}) + F(q^k_{\text{old}}), g^k) + \frac{1}{\beta} R(q) \). Since by minimality of \( q_0 \) and of \( q(\beta) \) we have

\[
\Psi(\beta) + \frac{1}{\beta} R(q_0) \leq \Psi(\beta) + \frac{1}{\beta} R(q(\beta)) = T_\beta(q(\beta)) \leq T_\beta(q^k)
\]

\[
= S(F'(q^k_{\text{old}})(q^* - q^k_{\text{old}}) + F(q^k_{\text{old}}), g^k) + \frac{1}{\beta} R(q^*)
\]
we can conclude, using the generalized triangle inequality for \( S \), the generalized tangential cone condition assumption 4, as well as the definition of \( k_* \) that

\[
\limsup_{\beta \to \infty} \Psi(\beta) \leq S(F'(q^1_\text{old})(q' - q^1_\text{old}) + F(q^1_\text{old}), g^1) \\
\leq c_S \left( c_S c_t^2 + \frac{1 + c_S c_t^2}{\tau^2} \right) S(F(q^1_\text{old}), g^1) \\
\leq \tilde{\Psi}_1 S(F(q^1_\text{old}), g^1).
\]

On the other hand we have, again by minimality,

\[
\frac{1}{\beta} \mathcal{R}(q(\beta)) \leq \Psi(\beta) + \frac{1}{\beta} \mathcal{R}(q(\beta)) \\
= T_\beta(q(\beta)) \leq T_\beta(q_0) \\
= S(F'(q^k_\text{old})(q_0 - q^k_\text{old}) + F(q^k_\text{old}), g^k) + \frac{1}{\beta} \mathcal{R}(q_0)
\]

hence (by minimality of \( q_0 \) for \( \mathcal{R} \))

\[
0 \leq \limsup_{\beta \to 0} (\mathcal{R}(q(\beta)) - \mathcal{R}(q_0)) \leq \limsup_{\beta \to 0} \beta S(F'(q^1_\text{old})(q_0 - q^1_\text{old}) + F(q^1_\text{old}), g^1) = 0
\]

i.e.

\[
\mathcal{R}(q(\beta)) \to \mathcal{R}(q_0) \text{ as } \beta \to 0.
\]

Hence by the compactness assumption assumption 2 (vi) on level sets of \( \mathcal{R} \), every subsequence of \( q(\beta) \) has a \( \tau_Q \) convergent subsequence whose limit by weak lower semicontinuity of \( \mathcal{R} \) and the estimate above is a minimizer of \( \mathcal{R} \) and hence by strict convexity of \( \mathcal{R} \) coincides with \( q_0 \). Thus, by a subsequence–subsequence argument \( q(\beta) \to q_0 \) in \( \tau_Q \) as \( \beta \to 0 \), hence by assumption 2 (ii), (iii) we have

\[
\liminf_{\beta \to 0} \Psi(\beta) = \liminf_{\beta \to 0} S(F'(q^k_\text{old})(q(\beta) - q^k_\text{old}) + F(q^k_\text{old}), g^k) \\
\geq S(F'(q^k_\text{old})(q_0 - q^k_\text{old}) + F(q^k_\text{old}), g^k) \geq \tilde{\Psi}_1 S(F(q^k_\text{old}), g^k)
\]

where the latter inequality was just assumed to hold, cf (84).

Now we show continuity of \( \Psi \). For fixed \( \beta \in (0, \infty) \) and any sequence \( (\beta^n)_{n \in \mathbb{N}} \) converging to \( \beta \) (which implies \( \frac{1}{2} \beta \leq \beta^n \leq 2 \beta \) for all sufficiently large \( n \)) we have by minimality

\[
\frac{1}{2\beta} \mathcal{R}(q(\beta^n)) \leq T_{\beta^n}(q(\beta^n)) \leq \mathcal{T}_{\beta^n}(q(\beta^n)) \leq \Psi(\beta) + \frac{2}{\beta} \mathcal{R}(q(\beta))
\]

hence by assumption 2 (vi) every subsequence of \( q(\beta^n) \) has a \( \tau_Q \) convergent subsequence. The limit of every \( \tau_Q \) convergent subsequence of \( q(\beta^n) \) by assumption 2 (ii), (iii), (iv) and

\[
T_{\beta^n}(q(\beta^n)) \to T_{\beta^n}(q(\beta)) \to T_{\beta}(q(\beta))
\]

is a minimizer of \( T_{\beta} \). By uniqueness of this minimizer and a subsequence–subsequence argument the whole sequence \( q(\beta^n) \) converges to \( q(\beta) \) in \( \tau_Q \) as \( n \to \infty \). Continuity of \( F'(q^k_\text{old}), S(\cdot, g^k) \), and \( \mathcal{R} \) implies \( \Psi(\beta^n) \to \Psi(\beta) \) as \( n \to \infty \).

Using the intermediate value theorem, we conclude from

\[
\limsup_{\beta \to \infty} \Psi(\beta) \leq \tilde{\Psi}_1 S(F(q^k_\text{old}), g^k) \leq \tilde{\Psi}_1 S(F(q^k_\text{old}), g^k) \leq \liminf_{\beta \to 0} \Psi(\beta)
\]

that a \( \beta \in (0, \infty) \) satisfying \( \tilde{\Psi}_1 S(F(q^k_\text{old}), g^k) \leq \Psi(\beta) \leq \tilde{\Psi}_1 S(F(q^k_\text{old}), g^k) \) exists.

Note that lower semicontinuity \( S(\cdot, g^k) \), and \( \mathcal{R} \) would only imply \( \liminf_{n \to \infty} \Psi(\beta^n) \geq \Psi(\beta) \) for any sequence \( \beta^n \to \beta \), i.e., lower semicontinuity of \( \Psi \), which would not allow us to apply the intermediate value theorem. \( \square \)
In case (84) is violated and therefore well-definedness of the choice of $\beta_k$ cannot be guaranteed, like in [18] we set the iterate to $q_0$, which formally corresponds to setting $\beta_k = 0$ and implies that the crucial estimates (74) (trivially) and (78) (by violation of (84)) hold for such iterates.

3. Conclusions and remarks

In this paper we consider the iteratively regularized Gauss–Newton method and its adaptive discretization by means of goal oriented error estimators. Our aim is to recover convergence as in the continuous setting for discretized hence approximate computations. The key result is that control of a small number (four) of real valued quantities per Newton step suffices to guarantee convergence and convergence rates. While we have studied the problem in a reduced form here, using the parameter-to-solution map, the related paper [16] (part II of this paper) develops and studies all-at-once formulations. Numerical tests are provided in part II of this paper [16].

Finally we point out that the convergence and convergence rates results obtained here do not only apply to identification problems in PDEs, but also to more general operator equations.

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