Goal oriented adaptivity in the IRGNM for parameter identification in PDEs II: all-at-once formulations ‡

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Abstract. In this paper we investigate adaptive discretization of the iteratively regularized Gauss-Newton method IRGNM. All-at-once formulations considering the PDE and the measurement equation simultaneously allow to avoid (approximate) solution of a potentially nonlinear PDE in each Newton step as compared to the reduced form [22]. We analyze a least squares and a generalized Gauss-Newton formulation and in both cases prove convergence and convergence rates with a posteriori choice of the regularization parameters in each Newton step and of the stopping index under certain accuracy requirements on four quantities of interest. Estimation of the error in these quantities by means of a weighted dual residual method is discussed, which leads to an algorithm for adaptive mesh refinement. Numerical experiments with an implementation of this algorithm show the numerical efficiency of this approach, which especially for strongly nonlinear PDEs outperforms the nonlinear Tikhonov regularization considered in [21].

1. Introduction

We consider the problem of identifying a parameter q in a PDE

$$A(q,u) = f \tag{1}$$

from measurements of the state u

$$C(u) = g\,, \tag{2}$$

where $q \in Q$, $u \in V$, $g \in G$, Q, V, G are Hilbert spaces and $A\colon Q \times V \to W^*$ with W^* denoting the dual space of some Hilbert space W and $C\colon V \to G$ differential and observation operators, respectively. Among many others, for example the classical model problem of identifying the diffusion coefficient q in the linear elliptic PDE

$$-\nabla(q\nabla u) = f \text{ in } \Omega$$

from measurements of u in Ω can be cast in this form with $Q \subseteq L^\infty(\Omega)$, $V, W \subseteq H^1(\Omega)$, $G = L^2(\Omega)$, $A(q,u) = -\nabla(q\nabla u)$ and C the embedding of $H^1(\Omega)$ into $L^2(\Omega)$.

The usual approach for tackling such inverse problems is to reduce them to an operator equation

$$F(q) = g, \tag{3}$$

where $F = C \circ S$ is the composition of the parameter-to-solution map for (1)

$$\begin{array}{rcl} S\colon Q & \to & V \\ q & \mapsto & u \end{array} \tag{4}$$

with the measurement operator C. The forward operator F will then be a nonlinear operator between Q and G with typically unbounded inverse, so that recovery of q is an ill-posed problem. Since the given data g^δ are noisy with some noise level δ

$$||g - g^\delta|| \leq \delta, \tag{5}$$

regularization is needed.

We will here as in [22] consider the paradigm of the Iteratively Regularized Gauss-Newton Method (IRGNM) cf., e.g., [3, 4, 7, 18, 20, 23] and its adaptive discetization. However, instead of reducing to (3), we will simulteously consider the measurement equation and the PDE:

$$C(u) \quad = g \text{ in } G \tag{6}$$

$$A(q,u) = f \text{ in } W^* \tag{7}$$

as a system of operator equations for (q,u), which we will abbreviate by

$$\mathbf{F}(q,u) = \mathbf{g}, \tag{8}$$

where

$$\mathbf{F}\colon Q \times V \to G \times W^*\,, \quad \mathbf{F}(q,u) = \begin{pmatrix} C(u) \\ A(q,u) \end{pmatrix}\,, \qquad \text{and} \qquad \mathbf{g} = \begin{pmatrix} g \\ f \end{pmatrix} \in G \times W^*\,. \tag{9}$$

The noisy data for this all-at-once formulation is denoted by

$$\mathbf{g}^\delta = \begin{pmatrix} g^\delta \\ f \end{pmatrix} \in G \times W^*\,.$$

This will allow us to avoid a major drawback of the method in [22], namely the necessity of solving the possibly nonlinear PDE (to a certain precision) in each Newton step in order to evaluate $F(q) = C(S(q))$. Another key difference to the paper [22] is that here the u part of the previous iterate will not be subject to new discretization in the current iteration but keep its (usually coarser, hence cheaper) discretization from the previous step.

Therewith, we will arrive at iterations of the form

$$\begin{aligned} &(q^k, u^k) \\ &= \arg\min_{q,u} \|C(u^{k-1}) + C'(u^{k-1})(u - u^{k-1}) - g^\delta\|_G^2 + \alpha_k \|q - q_0\|_Q^2 + \mu_k \|u - u_0\|_V^2 \\ &\qquad + \varrho \|A'_q(q^{k-1}, u^{k-1})(q - q^{k-1}) + A'_u(q^{k-1}, u^{k-1})(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) - f\|_{W^*}^r\,. \end{aligned} \tag{10}$$

with regularization parameters $\alpha_k > 0$, $\mu_k > 0$ and the parameters $\varrho > 0$, $r \in \{1, 2\}$ determining the structure of the linearized PDE term in the Tikhonov functional. We will consider the following two cases:

- For $r = 2$, ($\varrho = 1$,) we end up with a straightforward unconstrained quadratic minimization problem so (10) yields a least squares formulation, see Section 2.
- In case $r = 1$ and ϱ sufficiently large, by exactness of the norm with exponent one as a penalty, (10) is equivalent to a Generalized Gauss-Newton type [8] form of the IRGNM

$$\begin{aligned}(q^k, u^k)\\ &= \arg\min_{q,u} \|C(u^{k-1}) + C'(u^{k-1})(u - u^{k-1}) - g^\delta\|_G^2 + \alpha_k\|q - q_0\|_Q^2 + \mu_k\|u - u_0\|_V^2\\ \text{s.t. } &A'_q(q^{k-1}, u^{k-1})(q - q^{k-1}) + A'_u(q^{k-1}, u^{k-1})(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) = f \text{ in } W^* .\end{aligned} \tag{11}$$

see Section 3.

Remark 1. *Although q^k, u^k obviously depend on δ, i.e. $q^k = q^{k,\delta}, u^k = u^{k,\delta}$, we omit the superscript δ for better readability.*

All-at-once formulations have also been considered, e.g., in [1, 2, 9, 10], however, our approach focuses on adaptive discretization using a posteriori error estimators. Additionally it differs from the previous ones in the following sense: In [9, 10] a Levenberg-Marquardt approach is considered, whereas we work with an iterative regularized Gauss-Newton approach which allows us to also prove convegergence rates (which is an involved task in a Levenberg-Marquardt setting, that has been resolved only relatively recently, [16]). Moreover we use a different regularization parameter choice in each Newton step than [9, 10]. The papers [1, 2] put more emphasis on computational aspects and applications than we do here.

For both cases $r = 1$, $r = 2$ in (10) we will investigate convergence and convergence rates in the continuous and adaptively discretized setting with discrepancy type choice of α_k (which in most of what follows will be replaced by $\frac{1}{\beta_k}$) and the overal stopping index k_*. The discretization errors with respect to certain quantities of interest will serve as refinement criteria during the Gauss-Newton iteration, where at the same time, we control the size of the regularization parameter. In order to estimate this discretization error we use goal-oriented error estimators (cf. [5, 6]).

For the least squares case we will (for the sake of completeness but not in the main strand of this paper) also provide a result on convergence with a priori parameter choice in the continuous setting, see the appendix. In Section 5, we will provide numerical results and in Section 6 some conclusions.

Throughout this paper, we will make the following assumptions:

Assumption 1. *There exists a solution $(q^\dagger, u^\dagger) \in \mathcal{B}_\rho(q_0, u_0) \subset \mathcal{D}(A) \cap (Q \times \mathcal{D}(C)) \subseteq Q \times V$ to (8), where (q_0, u_0) is some initial guess and ρ (not to be confused with the penalty parameter ϱ in (10)) is the radius of the neighborhood in which local convergence of the Newton type iterations under consideration will be shown.*

Assumption 2. *The PDE* (1) *and especially also its linearization at* (q,u) *is uniquely and stably solvable.*

Assumption 3. *The norms in* G, Q, *as well as the operator* C *and the semilinear form* $a\colon Q\times V\times W\to\mathbb{R}$ *defined by the relation* $a(q,u)(v)=\langle A(q,u),v\rangle_{W^*,W}$ *(where* $\langle .,.\rangle_{W^*,W}$ *denotes the duality pairing between* W^* *and* W*) are assumed to be evaluated exactly.*

2. A least squares formulation

Direct application of the IRGNM to (6), (7), i.e., to the all-at-once system (8) yields the iteration

$$\begin{pmatrix} q^k \\ u^k \end{pmatrix} = \begin{pmatrix} q^{k-1} \\ u^{k-1} \end{pmatrix} - \left(\mathbf{F}'(q^{k-1},u^{k-1})^*\mathbf{F}'(q^{k-1},u^{k-1}) + \begin{pmatrix} \alpha_k\,\mathrm{id} & 0 \\ 0 & \mu_k\,\mathrm{id} \end{pmatrix}\right)^{-1} \cdot \left(\mathbf{F}'(q^{k-1},u^{k-1})^*(\mathbf{F}(q^{k-1},u^{k-1})-\mathbf{g}^\delta) + \begin{pmatrix} \alpha_k(q^{k-1}-q_0) \\ \mu_k(u^{k-1}-u_0) \end{pmatrix}\right) \tag{12}$$

with regularization parameters α_k, μ_k for the q and u part of the iterates, respectively.

We will first of all show that Assumption 2 allows us to set the regularization parameter μ_k for the u part to zero. For this purpose, we introduce the abbreviations

$$K\colon V\to W^*\,,\quad K:=A'_u(q,u) \qquad \text{and} \qquad L\colon Q\to W^*\,,\quad L:=A'_q(q,u) \tag{13}$$

with Hilbert space adjoints $K^*\colon W^*\to V$ and $L^*\colon W^*\to Q$, i.e.,

$$(Lq,w^*)_{W^*}=(q,L^*w^*)_Q \qquad \forall q\in Q, w^*\in W^*\,,$$
$$(Kv,w^*)_{W^*}=(v,K^*w^*)_V \qquad \forall v\in V, w^*\in W^*\,,$$

where $(.,.)_{W^*}$ and $(.,.)_V$ denote the inner products in W^* and V.

We denote the derivate of $\mathbf{F}$ at a pair (q,u) by $\mathbf{T}$, i.e.,

$$\mathbf{T}\colon Q\times V\to G\times W^*\,,\quad \mathbf{T}=\mathbf{F}'(q,u)=\begin{pmatrix} 0 & C'(u) \\ A'_q(q,u) & A'_u(q,u) \end{pmatrix} = \begin{pmatrix} 0 & C'(u) \\ L & K \end{pmatrix} \tag{14}$$

and define the norm

$$\left\|\begin{pmatrix} q \\ u \end{pmatrix}\right\|^2_{Q\times V} := \|q\|_Q^2+\|u\|_V^2 \quad \text{and the operator norm} \quad \|T\|_{Q\times V} := \sup_{x\in Q\times V, x\neq 0} \frac{\|Tx\|_{Q\times V}}{\|x\|_{Q\times V}}\,. \tag{15}$$

for some $x\in Q\times V$ and some operator $T\colon Q\times V\to Q\times V$.

Further we define

$$\mathbf{Y}_{\alpha,\mu} := \mathbf{T}^*\mathbf{T} + \begin{pmatrix} \alpha\,\mathrm{id} & 0 \\ 0 & \mu\,\mathrm{id} \end{pmatrix} \tag{16}$$

for $\alpha>0$, $\mu\geq 0$.

Lemma 1. *Under Assumption 2*

(i) for any $\alpha > 0$, $\mu \geq 0$ the inverse $\mathbf{Y}_{\alpha,\mu}^{-1}$ of $\mathbf{Y}_{\alpha,\mu}$ exists

(ii)

$$\left\|\mathbf{Y}_{\alpha,\mu}^{-1}\mathbf{T}^*\mathbf{T}\right\|_{Q\times V} \leq 1 + \max\{\alpha,\mu\} \left\|\mathbf{Y}_{\alpha,\mu}^{-1}\right\|_{Q\times V} ,$$

(iii)

$$\left\|\mathbf{Y}_{\alpha,\mu}^{-1}\right\|_{Q\times V} \leq c_T \left(\frac{1}{\alpha} + 1\right) \tag{17}$$

for all $\alpha \in (0,1]$, $\mu \geq 0$ and some $c_T > 0$ independent of α, μ, where the bound c_T in (17) *is independent of q and u, if the operators K, K^{-1} and L, are bounded uniformly in (q,u).*

Proof. (i): With the abbreviations

$$P = L^*L + \alpha\,\mathrm{id} \quad \text{and} \quad M = C'(u)^*C'(u) + K^*K + \mu\,\mathrm{id}$$

with the Hilbert space adjoint $C'(u)^*\colon G \to V$ for $C'(u)\colon V \to G$, i.e.,

$$(C'(u)(\delta u), \varphi)_G = (\delta u, C'(u)^*\varphi)_V ,$$

we have

$$\mathbf{Y}_{\alpha,\mu} = \begin{pmatrix} P & L^*K \\ K^*L & M \end{pmatrix} .$$

Next, we will show that M is boundedly invertible. M is linear and bounded, since

$$\begin{aligned} \|Mv\|_V &\leq \|C'(u)^*C'(u)v\|_V + \|K^*Kv\|_V + \mu\|v\|_V \\ &\leq \left(\|C'(u)\|_{V\to G}^2 + \|K\|_{V\to W^*}^2 + \mu\right)\|v\|_V \leq c\|v\|_V \quad \forall v \in V \end{aligned}$$

for some constant $c > 0$. M is also positive definite: There holds

$$(Mv,v)_V = \|C'(u)v\|_G^2 + \|Kv\|_{W^*}^2 + \mu\|v\|_V^2 \geq \|Kv\|_{W^*}^2 \geq c\|v\|_V^2 \quad \forall v \in V \tag{18}$$

for some constant $c > 0$, since K is boundedly invertible due to Assumption 2.
Consequently M^{-1} exists (according to the Lax-Milgram Lemma) and we can define the Schur complement type operator

$$N := P - L^*KM^{-1}K^*L = L^*L + \alpha\,\mathrm{id} - L^*KM^{-1}K^*L .$$

We will now show that N is also invertible. Using the fact that

$$\begin{aligned} \|M^{-1/2}K^*\|_{W^*\to V}^2 &= \|KM^{-1/2}\|_{V\to W^*}^2 \\ &= \sup_{v\in V, v\neq 0} \frac{\|KM^{-1/2}v\|_{W^*}^2}{\|v\|_V^2} \\ &= \sup_{v\in V, v\neq 0} \frac{\|Kv\|_{W^*}^2}{\|M^{1/2}v\|_V^2} \\ &= \sup_{v\in V, v\neq 0} \frac{\|Kv\|_{W^*}^2}{\|C'(u)(v)\|_G^2 + \|Kv\|_{W^*}^2 + \mu\|v\|_V^2} \leq 1 \end{aligned}$$

for any $\vartheta \in Q$, we get

$$\begin{aligned}(N\vartheta, \vartheta)_Q &= (L^*L\vartheta + \alpha\vartheta - L^*KM^{-1}K^*L\vartheta, \vartheta)_Q \\ &\geq \|L\vartheta\|_{W^*}^2 + \alpha\|\vartheta\|_Q^2 - \|M^{-1/2}K^*\|_{W^*\to V}^2\|L\vartheta\|_{W^*}^2 \\ &\geq \alpha\|\vartheta\|_Q^2\,,\end{aligned} \tag{19}$$

which together with

$$\begin{aligned}\|N\vartheta\|_Q &\leq \|L^*L\vartheta\|_Q + \alpha\|\vartheta\|_Q + \|L^*KM^{-1}K^*L\vartheta\|_Q \\ &\leq \left(\|L\|_{Q\to W^*}^2 + \alpha + \|L\|_{Q\to W^*}^2\|K\|_{V\to W^*}^2\|M^{-1}\|_{V\to V}\right)\|\vartheta\|_Q \\ &\leq c\|\vartheta\|_Q \quad \forall \vartheta \in Q\end{aligned}$$

implies the existence of N^{-1}.
For

$$O_{\alpha\mu} := \begin{pmatrix} N^{-1} & -N^{-1}L^*KM^{-1} \\ -M^{-1}K^*LN^{-1} & M^{-1} + M^{-1}K^*LN^{-1}L^*KM^{-1} \end{pmatrix} \tag{20}$$

there holds

$$O_{\alpha\mu}\begin{pmatrix} P & L^*K \\ K^*L & M \end{pmatrix} = \begin{pmatrix} A & B \\ C & D \end{pmatrix}$$

with

$$\begin{aligned}A &:= N^{-1}\left(P - L^*KM^{-1}K^*L\right) = \mathrm{id} \\ B &:= N^{-1}L^*K + -N^{-1}L^*KM^{-1}M = 0 \\ C &:= -M^{-1}K^*LN^{-1}P + \left(M^{-1} + M^{-1}K^*LN^{-1}L^*KM^{-1}\right)K^*L \\ &= -M^{-1}K^*L\left[N^{-1}\left(P - L^*KM^{-1}K^*L\right) - \mathrm{id}\right] = 0 \\ D &:= -M^{-1}K^*LN^{-1}L^*K + \left(M^{-1} + M^{-1}K^*LN^{-1}L^*KM^{-1}\right)M = \mathrm{id}\,,\end{aligned}$$

we have

$$O_{\alpha\mu} = \mathbf{Y}_{\alpha,\mu}^{-1}\,. \tag{21}$$

(ii):

$$\begin{aligned}\left\|\mathbf{Y}_{\alpha,\mu}^{-1}\mathbf{T}^*\mathbf{T}\right\|_{Q\times V} &= \left\|\mathrm{id} - \mathbf{Y}_{\alpha,\mu}^{-1}\begin{pmatrix} \alpha\,\mathrm{id} & 0 \\ 0 & \mu\,\mathrm{id}\end{pmatrix}\right\|_{Q\times V} \\ &\leq 1 + \max\{\alpha,\mu\}\left\|\mathbf{Y}_{\alpha,\mu}^{-1}\right\|_{Q\times V}\end{aligned}$$

(iii): From (18), (19) be get

$$\|M^{-1}\|_{V\to V} \leq \|K^{-1}\|_{W^*\to V}^2\,, \quad \|N^{-1}\|_{Q\to Q} \leq \frac{1}{\alpha}\,. \tag{22}$$

For $O_{\alpha\mu}$ (cf. (20)) this yields

$$\begin{aligned}
\|O_{\alpha\mu}\|^2_{Q\times V} &\leq \sup_{(q,u)\in Q\times V,(q,u)\neq 0} \frac{\|N^{-1}q + N^{-1}L^*KM^{-1}u\|_Q^2}{\|q\|_Q^2 + \|u\|_V^2} \\
&\quad + \sup_{(q,u)\in Q\times V,(q,u)\neq 0} \frac{\|-M^{-1}K^*LN^{-1}q + (M^{-1} + M^{-1}K^*LN^{-1}L^*KM^{-1})\, u\|_V^2}{\|q\|_Q^2 + \|u\|_V^2} \\
&\leq 2\left(\left\|N^{-1}\right\|^2_{Q\to Q} + \left\|N^{-1}L^*KM^{-1}\right\|^2_{V\to Q} \right. \\
&\quad \left. + \left\|M^{-1}K^*LN^{-1}\right\|^2_{Q\to V} + \left\|M^{-1} + M^{-1}K^*LN^{-1}L^*KM^{-1}\right\|^2_{V\to V}\right) \\
&\leq 2\left\|N^{-1}\right\|^2_{Q\to Q}(1 + \sqrt{2}\,\|L\|^2_{Q\to W^*}\,\|K\|^2_{V\to W^*}\left\|M^{-1}\right\|^2_{V\to V})^2 + 4\left\|M^{-1}\right\|^2_{V\to V} \\
&\leq \frac{2}{\alpha^2}(1 + \sqrt{2}\,\|L\|^2_{Q\to W^*}\,\|K\|^2_{V\to W^*}\left\|K^{-1}\right\|^4_{W^*\to V})^2 + 4\left\|K^{-1}\right\|^4_{W^*\to V}
\end{aligned}$$

□

Motivated by Lemma 1, we set $\mu_k = 0$ and define a regularized iteration by

$$\begin{pmatrix} q^k \\ u^k \end{pmatrix} = \begin{pmatrix} q^{k-1} \\ u^{k-1} \end{pmatrix} - \left(\mathbf{F}'(q^{k-1}, u^{k-1})^* \mathbf{F}'(q^{k-1}, u^{k-1}) + \frac{1}{\beta_k}\left(\begin{array}{cc} \mathrm{id} & 0 \\ 0 & 0 \end{array}\right)\right)^{-1} \cdot \left(\mathbf{F}'(q^{k-1}, u^{k-1})^* (\mathbf{F}(q^{k-1}, u^{k-1}) - \mathbf{g}^\delta) + \frac{1}{\beta_k}\left(\begin{array}{c} q^{k-1} - q_0 \\ 0 \end{array}\right)\right) \tag{23}$$

or equivalently $\begin{pmatrix} q^k \\ u^k \end{pmatrix}$ as solution to the unconstrained minimization problem

$$\min_{(q,u)\in Q\times V} \mathcal{T}_{\beta_k}(q,u) := \|L_{k-1}(q - q^{k-1}) + K_{k-1}(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) - f\|^2_{W^*} + \|C(u^{k-1}) + C'(u^{k-1})(u - u^{k-1}) - g^\delta\|^2_G + \frac{1}{\beta_k}\|q - q_0\|^2_Q \tag{24}$$

with the abbreviations

$$L_{k-1} = A'_q(q^{k-1}, u^{k-1}) \qquad \text{and} \qquad K_{k-1} = A'_u(q^{k-1}, u^{k-1})\,, \tag{25}$$

Here we have set $\alpha_k = \frac{1}{\beta_k}$ in order to arrive at a less nonlinear 1-d equation for determining the regularization parameter from the discrepancy principle (see (33)): Note that the part of q^k corresponding to small singular values of $\mathbf{F}'(q^{k-1}, u^{k-1})^* \mathbf{F}'(q^{k-1}, u^{k-1})$ essentially behaves like $q_0 - \beta_k \mathrm{Proj}_Q \left(\mathbf{F}'(q^{k-1}, u^{k-1})^* (\mathbf{F}(q^{k-1}, u^{k-1}) - \mathbf{g}^\delta) \right)$.

The optimality conditions of first order for (24) read

$$\begin{aligned}
0 &= \left(\mathcal{T}_{\beta_k}\right)'_q(q,u)(\delta q) \\
&= 2(L_{k-1}(q - q^{k-1}) + K_{k-1}(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) - f, L_{k-1}(\delta q))_{W^*} + 2(q - q_0, \delta q)_Q \\
0 &= \left(\mathcal{T}_{\beta_k}\right)'_u(q,u)(\delta u) \\
&= 2(L_{k-1}(q - q^{k-1}) + K_{k-1}(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) - f, K_{k-1}(\delta u))_{W^*} \\
&\quad + 2(C(u^{k-1}) + C'(u^{k-1})(u - u^{k-1}) - g^\delta, C'(u^{k-1})(\delta u))_G
\end{aligned}$$

We refer to the Appendix for a convergence and convergence rates results for (23) with a priori choice of the regularization parameters and in a continuous setting.

Here we are rather interested in a posteriori parameter choice rules and adaptive discretization. So in each step k we will replace the infinite dimensional spaces Q, V, W in (23) by finite dimensional ones $Q_h, V_h, W_h = Q_{h_k}, V_{h_k}, W_{h_k}$

$$\begin{aligned}\begin{pmatrix} q_{h_k}^k \\ u_{h_k}^k \end{pmatrix} = \arg \min_{q \in Q_h, u \in V_h} & \|L_{k-1}(q - q_{\text{old}}) + K_{k-1}(u - u_{\text{old}}) + A(q_{\text{old}}, u_{\text{old}}) - f\|_{W_h^*}^2 \\ & + \|C(u_{\text{old}}) + C'(u_{\text{old}})(u - u_{\text{old}}) - g^\delta\|_G^2 + \frac{1}{\beta_k}\|q - q_0\|_Q^2 \,. \end{aligned} \tag{26}$$

where $(q_{\text{old}}, u_{\text{old}}) = (q^{k-1}, u^{k-1}) = (q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1})$ is the previous iterate, which itself is discretized by the use of spaces $Q_{h_{k-1}}, V_{h_{k-1}}, W_{h_{k-1}}$. The discretization h_k may be different in each Newton step (typically it will get finer for increasing k), but we suppress dependence of h on k in our notation in most of what follows.
To still obtain convergence of these discretized iterates, it is essential to control the discretization error in certain quantities, which are defined, analogously to [22], via the functionals

$$\begin{aligned} I_1 &: \ Q \times V \times Q \times V \times \mathbb{R} \to \mathbb{R} \\ I_2 &: \ Q \times V \times Q \times V \to \mathbb{R} \\ I_3 &: \ Q \times V \to \mathbb{R} \\ I_4 &: \ Q \times V \to \mathbb{R} \end{aligned}$$

where we insert the previous and current iterates $(q_{\text{old}}, u_{\text{old}})$, (q, u), respectively:

$$
\begin{aligned}
&I_1(q_{\text{old}}, u_{\text{old}}, q, u, \beta)\\
&= \left\| \mathbf{F}'(q_{\text{old}}, u_{\text{old}}) \begin{pmatrix} q - q_{\text{old}} \\ u - u_{\text{old}} \end{pmatrix} + \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W^*} + \frac{1}{\beta} \left\| q - q_0 \right\|^2_Q\\
&= \left\| A'_q(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}}) + A'_u(q_{\text{old}}, u_{\text{old}})(u - u_{\text{old}}) + A(q_{\text{old}}, u_{\text{old}}) - f \right\|^2_{W^*}\\
&\quad + \left\| C'(u)(u - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta \right\|^2_G + \frac{1}{\beta} \left\| q - q_0 \right\|^2_Q\\
&I_2(q_{\text{old}}, u_{\text{old}}, q, u)\\
&= \left\| \mathbf{F}'(q_{\text{old}}, u_{\text{old}}) \begin{pmatrix} q - q_{\text{old}} \\ u - u_{\text{old}} \end{pmatrix} + \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W^*}\\
&= \left\| A'_q(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}}) + A'_u(q_{\text{old}}, u_{\text{old}})(u - u_{\text{old}}) + A(q_{\text{old}}, u_{\text{old}}) - f \right\|^2_{W^*}\\
&\quad + \left\| C'(u)(u - u_{\text{old}}) C(u_{\text{old}}) - g^\delta \right\|^2_G\\
&I_3(q_{\text{old}}, u_{\text{old}})\\
&= \left\| \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W^*}\\
&= \left\| A(q_{\text{old}}, u_{\text{old}}) - f \right\|^2_{W^*} + \left\| C(u_{\text{old}}) - g^\delta \right\|^2_G\\
&I_4(q, u)\\
&= \left\| \mathbf{F}(q, u) - \mathbf{g}^\delta \right\|^2_{G \times W^*}\\
&= \left\| A(q, u) - f \right\|^2_{W^*} + \left\| C(u) - g^\delta \right\|^2_G \,,
\end{aligned}
\tag{27}
$$

and quantities of interest

$$
\begin{aligned}
I_1^k &= I_1(q^k_{\text{old}}, u^k_{\text{old}}, q^k, u^k, \beta_k)\\
I_2^k &= I_2(q^k_{\text{old}}, u^k_{\text{old}}, q^k, u^k)\\
I_3^k &= I_3(q^k_{\text{old}}, u^k_{\text{old}})\\
I_4^k &= I_4(q^k, u^k)\,.
\end{aligned}
\tag{28}
$$

Their discrete analogs are correspondingly defined by

$$
\begin{aligned}
I_{1,h}&\colon\ Q \times V \times Q \times V \times \mathbb{R} \to \mathbb{R}\\
I_{2,h}&\colon\ Q \times V \times Q \times V \to \mathbb{R}\\
I_{3,h}&\colon\ Q \times V \to \mathbb{R}\\
I_{4,h}&\colon\ Q \times V \to \mathbb{R}
\end{aligned}
$$

$$
\begin{aligned}
& I_{1,h}(q_{\text{old}}, u_{\text{old}}, q, u, \beta) \\
& = \left\| \mathbf{F}'(q_{\text{old}}, u_{\text{old}}) \begin{pmatrix} q - q_{\text{old}} \\ u - u_{\text{old}} \end{pmatrix} + \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W_h^*} + \frac{1}{\beta} \|q - q_0\|^2_Q \\
& = \left\| A'_q(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}}) + A'_u(q_{\text{old}}, u_{\text{old}})(u - u_{\text{old}}) + A(q_{\text{old}}, u_{\text{old}}) - f \right\|^2_{W_h^*} \\
& \quad + \left\| C'(u)(u - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta \right\|^2_G + \frac{1}{\beta} \|q - q_0\|^2_Q \\
& I_{2,h}(q_{\text{old}}, u_{\text{old}}, q, u) \\
& = \left\| \mathbf{F}'(q_{\text{old}}, u_{\text{old}}) \begin{pmatrix} q - q_{\text{old}} \\ u - u_{\text{old}} \end{pmatrix} + \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W_h^*} \\
& = \left\| A'_q(q_{\text{old}}, u_{\text{old}})(q - q_{\text{old}}) + A'_u(q_{\text{old}}, u_{\text{old}})(u - u_{\text{old}}) + A(q_{\text{old}}, u_{\text{old}}) - f \right\|^2_{W_h^*} \\
& \quad + \left\| C'(u)(u - u_{\text{old}}) C(u_{\text{old}}) - g^\delta \right\|^2_G \\
& I_{3,h}(q_{\text{old}}, u_{\text{old}}) \\
& = \left\| \mathbf{F}(q_{\text{old}}, u_{\text{old}}) - \mathbf{g}^\delta \right\|^2_{G \times W_h^*} \\
& = \| A(q_{\text{old}}, u_{\text{old}}) - f \|^2_{W_h^*} + \left\| C(u_{\text{old}}) - g^\delta \right\|^2_G \\
& I_{4,h}(q, u) \\
& = \left\| \mathbf{F}(q, u) - \mathbf{g}^\delta \right\|^2_{G \times W_h^*} \\
& = \| A(q, u) - f \|^2_{W_h^*} + \left\| C(u) - g^\delta \right\|^2_G
\end{aligned}
\tag{29}
$$

and

$$
\begin{aligned}
I^k_{1,h} &= I_{1,h}(q^k_{\text{old}}, u^k_{\text{old}}, q^k_h, u^k_h, \beta_k) \\
I^k_{2,h} &= I_{2,h}(q^k_{\text{old}}, u^k_{\text{old}}, q^k_h, u^k_h,) \\
I^k_{3,h} &= I_{3,h}(q^k_{\text{old}}, u^k_{\text{old}}) \\
I^k_{4,h} &= I_{4,h}(q^k_h, u^k_h)\,.
\end{aligned}
\tag{30}
$$

At the end of each iteration step we set

$$
q^{k+1}_{\text{old}} = q^k_h \quad \text{and} \quad u^{k+1}_{\text{old}} = u^k_h\,. \tag{31}
$$

Remark 2. *Note that here neither q_{old} nor u_{old} are subject to new adaptive discretization in the current step, but they are taken as fixed quantities from the previous step. This is different from [22], where u_{old} also depends on the current discretization.*

For (28) *and* (30) *we assume that the norms in G and Q are evaluated exactly cf. Assumption 3.*

In our convergence proofs we will compare the quantities of interest $I^k_{i,h}$ with those I^k_i that would be obtained with exact computation on the infinite dimensional spaces, starting from the same $(q_{\text{old}}, u_{\text{old}}) = (q_{\text{old}\,h_{k-1}}, u_{\text{old}\,h_{k-1}})$ as the one underlying $I^k_{i,h}$. Thus, in our analysis besides the actually computed sequence $(q^k_h, u^k_h) = (q^k_{h_k}, u^k_{h_k})$ there appears an auxiliary sequence (q^k, u^k), see Figure 1.

We assume the knowledge about bounds η^k_i on the error in the quantities of interest due to discretization

$$
|I^k_{i,h} - I^k_i| \le \eta^k_i\,, \quad i \in \{1, 2, 3, 4\}\,, \tag{32}
$$

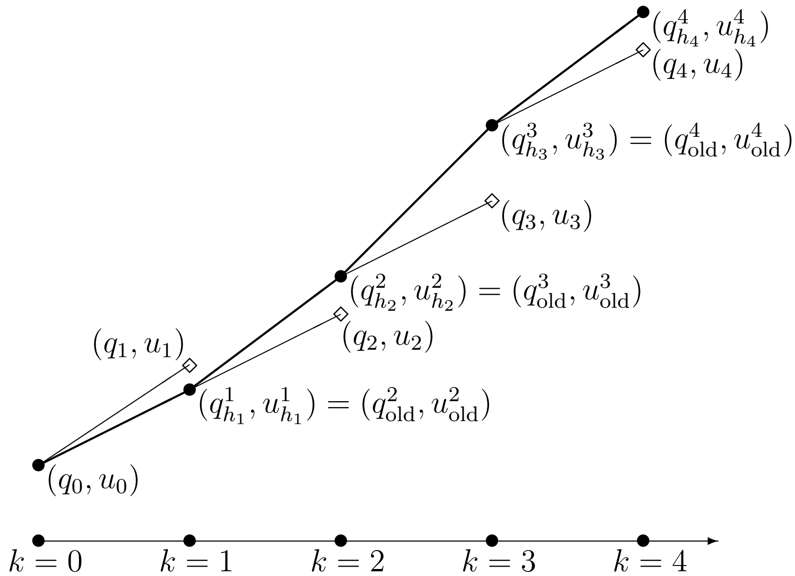

Figure 1. Sequence of discretized iterates and auxiliary sequence of continuous iterates for the all-at-once formulation of IRGNM

(which can, at least partly, be computed by goal oriented error estimators, see e.g., [5, 6, 14, 21] and Section 4) and refine adaptively according to these bounds. On the other hand, we will now impose conditions on such upper bounds for the discretization error that enable to prove convergence and convergence rates results, see Assumption 7 below.

Additionally, we will make some assumptions on the forward operator

Assumption 4. *Let the reduced forward operator* $\mathbf{F}$ *be continuous and weakly sequentially closed, i.e.*

$$\begin{aligned}&(q_n \rightharpoonup q \wedge u_n \rightharpoonup u \wedge C(u_n) \to g \wedge A(q_n, u_n) \to f)\\&\Rightarrow (u \in \mathcal{D}(C) \wedge (q,u) \in \mathcal{D}(A) \wedge C(u) = g \wedge A(q,u) = f)\end{aligned}$$

for all sequences $((q_n, u_n))_{n\in\mathbb{N}} \subseteq Q \times V$.

We also transfer the usual tangential cone condition to the all-at once setting from this section, which yields

Assumption 5. *Let*

$$\begin{aligned}&\|C(u) - C(\bar{u}) - C'(u)(u-\bar{u})\|_G\\&\qquad + \|A(q,u) - A(\bar{q},\bar{u}) - A'_q(q,u)(q-\bar{q}) - A'_u(q,u)(u-\bar{u})\|_{W^*}\\&\le c_{tc}\left(\|C(u) - C(\bar{u})\|_G + \|A(q,u) - A(\bar{q},\bar{u})\|_{W^*}\right)\end{aligned}$$

hold for all $(q,u), (\bar{q},\bar{u}) \in \mathcal{B}_\rho(q_0,u_0) \subset (Q \times V)$ *and some* $0 < c_{tc} < 1$.

The choice of the regularization parameter β_k will be done a posteriori according to an inexact Newton /discrepancy principle, which with the quantities introduced above reads as

$$\underline{\tilde{\theta}} I^k_{3,h} \le I^k_{2,h} \le \tilde{\bar{\theta}} I^k_{3,h}\,. \tag{33}$$

A discrepancy type principle will also be used for the choice of the overall stopping index

$$k_* = \min\{k \in \mathbb{N} \ : \ I^k_{3,h} \leq \tau^2\delta^2\}. \tag{34}$$

The parameters used there have to satisfy the following assumption.

Assumption 6. *Let τ be chosen sufficiently large and $\underline{\tilde{\theta}} < \tilde{\bar{\theta}}$ sufficiently small (see* (33),(34)*), such that*

$$2\left(c_{tc}^2 + \frac{(1+c_{tc})^2}{\tau^2}\right) < \underline{\tilde{\theta}} \quad \textit{and} \quad \frac{2\tilde{\bar{\theta}} + 4c_{tc}^2}{1-4c_{tc}^2} < 1\,. \tag{35}$$

Therewith, we can also formulate our conditions on precision in the quantities of interest:

Assumption 7. *Let for the discretization error with respect to the quantities of interest estimate* (32) *hold, where η_1^k, η_2^k, η_3^k, η_4^k are selected such that*

$$\eta_1^k + 4c_{tc}^2\eta_3^k \leq \left(\underline{\tilde{\theta}} - 2\left(2c_{tc}^2 + \frac{(1+2c_{tc})^2}{\tau^2}\right)\right) I^k_{3,h} \tag{36}$$

$$\eta_3^k \leq c_1 I^k_{3,h} \quad \textit{and} \quad \eta_2^k \to 0\,,\ \eta_3^k \to 0\,,\ \eta_4^k \to 0 \ \textit{as}\ k \to \infty \tag{37}$$

$$I^k_{3,h} \leq (1+c_3)I^{k-1}_{4,h} + r^k \quad \textit{and} \quad (1+c_3)\frac{2\tilde{\bar{\theta}} + 4c_{tc}^2}{1-4c_{tc}^2} \leq c_2 < 1 \tag{38}$$

for some constants $c_1, c_2, c_3 > 0$, and a sequence $r^k \to 0$ as $k \to \infty$ (where the second condition in (38) *is possible due to the right inequality in* (35)*).*

Exactly along the lines of the proofs of Theorems 1 and 2 in in [22], replacing F there by $\mathbf{F}$ according to (9), we therewith obtain convergence and convergence rates results:

Theorem 1. *Let for the starting point $(q^0_{\mathrm{old}}, u^0_{\mathrm{old}}) \in \mathcal{B}_\rho((q_0, u_0))$ hold, let the Assumptions 1, 2, 3, 4 and 5 with c_{tc} sufficiently small be satisfied and let Assumption 6 hold. For the quantities of interest* (28) *and* (30)*, let, further, the estimate* (32) *hold with η_i satisfying Assumption 7.*

Then with β_k, $h = h_k$ fulfilling (33)*, k_* selected according to* (34)*, and $(q^k_{h_k}, u^k_{h_k})$ defined by* (26) *there holds*

(o) For all $k < k_*$, a parameter β_k satisfying (33) *with $I^k_{2,h}$, $I^k_{3,h}$ according to* (29), (30) *exists provided*

$$\left\| \mathbf{F}'(q_{\mathrm{old}}, u_{\mathrm{old}}) \begin{pmatrix} q_0 - q_{\mathrm{old}} \\ u_0 - u_{\mathrm{old}} \end{pmatrix} + \mathbf{F}(q_{\mathrm{old}}, u_{\mathrm{old}}) - \mathbf{g}^\delta \right\|^2_{G\times W_h^*} \geq \tilde{\bar{\theta}}\, \left\|\mathbf{F}(q_{\mathrm{old}}, u_{\mathrm{old}}) - \mathbf{g}^\delta\right\|^2_{G\times W_h^*}\,. \tag{39}$$

If (39) *is violated we set $(q^k_{h_k}, u^k_{h_k}) = (q_0, u_0)$.*

(i)

$$\|q^k_{h_k} - q_0\|^2_Q + \|u^k_{h_k} - u_0\|^2_V \leq \|q^\dagger - q_0\|^2_Q + \|u^\dagger - u_0\|^2_V \qquad \forall 0 \leq k \leq k_*\,; \tag{40}$$

(ii) k_* *is finite;*

(iii) $(q_h^{k_*}, u_h^{k_*}) = (q_{h_{k_*(\delta)}}^{k_*(\delta),\delta}, u_{h_{k_*(\delta)}}^{k_*(\delta),\delta})$ *converges (weakly) subsequentially to a solution of* (8) *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* (8). *If the solution* $(q^\dagger, u^\dagger)$ *to* (8) *is unique, then* $(q_h^{k_*}, u_h^{k_*})$ *converges strongly to* $(q^\dagger, u^\dagger)$ *as* $\delta \to 0$.

For proving rates, as usual (cf. e.g. [4, 11, 18, 23]) source conditions are assumed

Assumption 8. *Let*

$$(q^\dagger - q_0, u^\dagger - u_0) \in \mathcal{R}\left(\kappa\left(\mathbf{F}'(q^\dagger, u^\dagger)^*\mathbf{F}'(q^\dagger, u^\dagger)\right)\right)$$

(cf. Assumption 1) hold with some $\kappa\colon \mathbb{R}^+ \to \mathbb{R}^+$ *such that* κ^2 *is strictly monotonically increasing on* $(0, \|\mathbf{F}(q^\dagger, u^\dagger)\|^2_{Q\times V}]$, ϕ *defined by* $\phi^{-1}(\lambda) = \kappa^2(\lambda)$ *is convex and* ψ *defined by* $\psi(\lambda) = \kappa(\lambda)\sqrt{\lambda}$ *is strictly monotonically increasing on* $(0, \|\mathbf{F}(q^\dagger, u^\dagger)\|^2_{Q\times V}]$. *Here, for some selfadjoint nonnegative operator* A, *the operator function* $\kappa(A)$ *is defined via functional calculus based on the spectral theorem (cf. e.g. [11]).*

Theorem 2. *Let the conditions of Theorem 1 and additionally the source condition Assumption 8 be fulfiled.*

Then there exists a $\bar{\delta} > 0$ *and a constant* $\bar{C} > 0$ *independent of* δ *such that for all* $\delta \in (0, \bar{\delta}]$ *the convergence rates*

$$\|q_{\mathrm{old}}^{k_*} - q^\dagger\|_Q^2 + \|u_{\mathrm{old}}^{k_*} - u^\dagger\|_V^2 = \mathcal{O}\left(\frac{\delta^2}{\psi^{-1}(\bar{C}\delta)}\right). \tag{41}$$

are obtained.

Remark 3. *We compare the source conditions for the reduced formulation from [22] with the forward operator* $F = C \circ S$ *containing the control-to-state map* S *for the PDE* (1)

$$q^\dagger - q_0 \in \mathcal{R}\left(\kappa\left(F'(q^\dagger)^* F'(q^\dagger)\right)\right)$$

with Assumption 8 for the all-at-once formulation, exemplarily for the case $\kappa(\lambda) = \sqrt{\lambda}$, *i.e., we compare*

$$q^\dagger - q_0 \in \mathcal{R}\left(F'(q^\dagger)^*\right) \tag{42}$$

with

$$(q^\dagger - q_0, u^\dagger - u_0) \in \mathcal{R}\left(\mathbf{F}'(q^\dagger, u^\dagger)^*\right). \tag{43}$$

For this purpose we use the abbreviations

$$u^\dagger = S(q^\dagger), \quad K_\infty = A'_u(q^\dagger, u^\dagger), \quad L_\infty = A'_q(q^\dagger, u^\dagger), \quad C_\infty = C'(u^\dagger)$$

so that we can write

$$F'(q^\dagger) = -C_\infty {K_\infty}^{-1} L_\infty, \quad \mathbf{F}'(q^\dagger, u^\dagger) = \begin{pmatrix} 0 & C_\infty \\ L_\infty & K_\infty \end{pmatrix}$$

Therewith, (42) *becomes*

$$\exists \bar{g} \in \mathcal{N}(F'(q^\dagger)^*)^\perp \subseteq G: \quad q^\dagger - q_0 = -L_\infty^* K_\infty^{-*} C_\infty^* \bar{g} \tag{44}$$

and (43) *reads*

$$\exists (\tilde{g}, \tilde{f}) \in \mathcal{N}(\mathbf{F}'(q^\dagger, u^\dagger)^*)^\perp \subseteq G \times W^*: \quad q^\dagger - q_0 = -L_\infty^* \tilde{f} \text{ and } u^\dagger - u_0 = C_\infty^* \tilde{g} + K_\infty^* \tilde{f}, \tag{45}$$

respectively. These two conditions are not directly equivalent to each other, but it is readily checked that

$$\begin{aligned} \exists \bar{g}, \hat{g} \in \mathcal{N}(C_\infty^*)^\perp : q^\dagger - q_0 = -L_\infty^* K_\infty^{-*} C_\infty^* \bar{g} \\ \text{and } u^\dagger - u_0 = C_\infty^* \hat{g} \end{aligned} \tag{46}$$

is equivalent to

$$\begin{aligned} \exists (\tilde{g}, \tilde{f}) \in \mathcal{N}(C_\infty^*)^\perp \times \mathcal{N}(K_\infty^*)^\perp : q^\dagger - q_0 = -L_\infty^* \tilde{f} \text{ and } u^\dagger - u_0 = C_\infty^* \tilde{g} + K_\infty^* \tilde{f} \\ \text{and } K_\infty^* \tilde{f} \in \mathcal{R}(C_\infty^*) \end{aligned} \tag{47}$$

via setting $(\tilde{f}, \tilde{g}) = (-K_\infty^{-*} C_\infty^* \bar{g}, \hat{g} + \bar{g})$ *for the implication* (46) $\Rightarrow$ (47) *and* $(\bar{g}, \hat{g}) = (-C_\infty^{-*} K_\infty^* \tilde{f}, \tilde{g} + C_\infty^{-*} K_\infty^* \tilde{f})$ *for the implication* (47) $\Rightarrow$ (46). *The additional condition as compared to* (44), (45) $v \in \mathcal{R}(C_\infty^*)$ *for* $v = u^\dagger - u_0$, *or* $v = K_\infty^* \tilde{f}$ *seems to be not too restrictive, as the simple (linear) example of identifying the source* q *in the elliptic boundary value problem*

$$\begin{cases} -\Delta u = q \text{ in } \Omega \\ u = 0 \text{ on } \partial\Omega \end{cases}$$

from measurements of u *in the smooth domain* Ω *shows: Here we have*

$$\begin{aligned} &V = W = H_0^1(\Omega), \quad G = L^2(\Omega), \quad Q = L^2(\Omega), \\ &K_\infty = -\Delta, \quad L_\infty = id_{L^2(\Omega) \to H^{-1}(\Omega)}, \quad C_\infty = id_{H_0^1(\Omega) \to L^2(\Omega)} \end{aligned}$$

the latter two being the respective embedding operators, so that we get

$$\begin{array}{lll} K_\infty^* : H^{-1}(\Omega) \to H_0^1(\Omega) & L_\infty^* : H^{-1}(\Omega) \to L^2(\Omega) & C_\infty^* : L^2(\Omega) \to H_0^1(\Omega) \\ K_\infty^* = (-\Delta)^{-1} & L_\infty^* = (-\Delta)^{-1} & C_\infty^* = (-\Delta)^{-1} \end{array}$$

(note that we take Hilbert space adjoints here). Thus for $q^\dagger \in L^2(\Omega)$ *we have* $u^\dagger \in H^2(\Omega) \cap H_0^1(\Omega)$, *hence by a choice* $u_0 \in H^2(\Omega) \cap H_0^1(\Omega)$, *the difference* $u^\dagger - u_0$ *will typically be an element of* $H^2(\Omega) \cap H_0^1(\Omega)$ *so that the condition* $u^\dagger - u_0 = C_\infty^* \hat{g}$ *for some* $\hat{g} \in G = L^2(\Omega)$ *from* (46) *is trivially satisfied. However the condition* $K_\infty^* \tilde{f} \in \mathcal{R}(C_\infty^*)$, *i.e.,* $(-\Delta)^{-1} \tilde{f} \in (-\Delta)^{-1}(L^2(\Omega))$, *meaning that* $\tilde{f}$ *lies in* $L^2(\Omega)$ *(and not only in its natural space* $H^{-1}(\Omega)$*) is somewhat more restictive. So condition* (43) *appears to be weaker than* (42) *in this example.*

Remark 4. *The error estimators* η_i^k, $i \in \{1, \ldots, 4\}$ *can in principle be computed using a dual weighted residual approach. However, the appearence of the dual norm* $\| \cdot \|_{W^*}$ *complicates things considerably. For this reason, the presented least squares formulation will not be implemented and we only refer to Section 4.2.1 in [25] for more details concerning the error estimators for this section.*

3. A Generalized Gauss-Newton formulation

A drawback of the unconstrained formulation (24) is the necessity of computing the W^*-norm of the (linearized) residual and especially of computing error estimators for this quantity of interest. Besides, a rescaling of the state equation (7) changes the solution of the optimization problem. Moreover, depending on the given inverse problem and its application, in some cases, it does not make sense to only minimize the residual of the linearized state equation, instead of setting it to zero.

A formulation that is much better tractable is obtained by defining $(q^k, u^k) = (q^{k,\delta}, u^{k,\delta})$ as a solution to the PDE constrained minimization problem (11), i.e.,

$$\min_{(q,u)\in Q\times V} \mathcal{T}_{\beta_k}(q,u) := \|C(u^{k-1}) + C'(u^{k-1})(u-u^{k-1}) - g^\delta\|_G^2 + \frac{1}{\beta_k}\left(\|q-q_0\|_Q^2 + \|u-u_0\|_V^2\right) \tag{48}$$

$$\text{s.t.} \quad L_{k-1}(q-q^{k-1}) + K_{k-1}(u-u^{k-1}) + A(q^{k-1},u^{k-1}) = f \qquad \text{in } W^* \tag{49}$$

(see also [9], [10]) with the abbreviations (25). Here we again set the regularization parameter to the reciprocal of some value β_k in order to decrease nonlinear dependence of $(q^{k,\delta}, u^{k,\delta})$ on this parameter. Note that this time we also need a nonzero regularization parameter for the u term, cf. Remark 6. Thus, altogether we set $\alpha_k = \mu_k = \frac{1}{\beta_k}$ in (11).

We consider the Lagrangian $\mathcal{L}\colon Q\times V\times W \to \mathbb{R}$

$$\mathcal{L}(q,u,z) := \mathcal{T}_{\beta_k}(q,u) + \langle f - A(q^{k-1},u^{k-1}) - L_{k-1}(q-q^{k-1}) - K_{k-1}(u-u^{k-1}), z\rangle_{W^*,W}$$

and formulate the optimality conditions of first order for (48), (49):

$$\mathcal{L}'_z(q,u,z)(\delta z) = \langle f - A(q^{k-1},u^{k-1}) - L_{k-1}(q-q^{k-1}) - K_{k-1}(u-u^{k-1}), \delta z\rangle_{W^*,W} = 0\,, \tag{50}$$

$$\mathcal{L}'_u(q,u,z)(\delta u) = 2(C(u^{k-1}) + C'(u^{k-1})(u-u^{k-1}) - g^\delta, C'(u^{k-1})(\delta u))_G + \tfrac{2}{\beta_k}(u-u_0,\delta u)_V - \langle K_{k-1}\delta u, z\rangle_{W^*,W} = 0\,, \tag{51}$$

$$\mathcal{L}'_q(q,u,z)(\delta q) = \tfrac{2}{\beta_k}(q-q_0,\delta q)_Q - \langle L_{k-1}\delta q, z\rangle_{W^*,W} = 0 \tag{52}$$

for all $\delta q \in Q$, $\delta u \in V$, $\delta z \in W$.

We assume boundedness of the operators $A(q,u), L_{k-1}, K^*_{k-1}, K^{-1}_{k-1}, C(u)$ and $C'(u)$ in the following sense.

Assumption 9. *There holds*

$$\sup_{(q,u)\in\mathcal{B}_\rho(q_0,u_0)} \|A(q,u)\|_{W^*} + \|A'_q(q,u)\|_{Q\to W^*} + \|A'_u(q,u)^*\|_{W^*\to V} < \infty$$

$$\sup_{(q,u)\in\mathcal{B}_\rho(q_0,u_0)} \|A'_u(q,u)^{-1}\|_{W^*\to V} < \infty$$

and

$$\sup_{u\in\mathcal{B}_\rho(u_0)} \{\|C(u)\|_G + \|C'(u)\|_{V\to G}\} < \infty\,.$$

In order to make use of equivalence of (48), (49) with an unconstrained but penalized problem of the form (10) with $r = 1$, the following lemma will serve as tool for unformly bounding the the adjoint variable and therewith the penalty parameter ϱ.

Lemma 2. *Under Assumption 9 and provided* $(q^{k-1}, u^{k-1}) \in \mathcal{B}_\rho(q_0, u_0)$, $\beta_k \geq \beta_{\min} > 0$ *for a stationary point* $(q^k, u^k, z^k) \in Q \times V \times W$ *of* $\mathcal{L}$ *(cf.* (50) - (52)*) there holds the estimate*

$$\|z^k\|_W \leq c_{\text{adj}} \left(\sqrt{\|q^{k-1} - q_0\|_Q^2 + \|u^{k-1} - u_0\|_V^2} + 1 \right) , \tag{53}$$

with a constant c_{adj} *independent of* k.

Proof. To formulate the optimality system (50)-(52) in a matrix-vector form, we introduce another dual variable $p \in W^*$ defined by

$$p = J_{W^*} z \in W^* \tag{54}$$

via the map J_{W^*}, which maps $z \in W$ to the Riesz representation $J_{W^*} z \in W^*$ of the linear functional $W^* \to \mathbb{R}$, $w^* \mapsto w^*(z)$, such that

$$\mathcal{L}(q, u, z) = \mathcal{T}_{\beta_k}(q, u) + (f - A(q^{k-1}, u^{k-1}) - L_{k-1}(q - q^{k-1}) - K_{k-1}(u - u^{k-1}), p)_{W^*} .$$

Using the abbreviations (25) and

$$C_{k-1} := C'(u^{k-1}) , \quad r_{k-1}^f := A(q^{k-1}, u^{k-1}) - f , \quad r_{k-1}^g := C(u^{k-1}) - g^\delta \tag{55}$$

the optimality system (50)-(52) can be written as

$$\begin{aligned}
\mathcal{L}'_z(q, u, z)(\delta z) &= \langle -r_{k-1}^f - L_{k-1}(q - q^{k-1}) - K_{k-1}(u - u^{k-1}), \delta z \rangle_{W^*, W} = 0 , \\
\mathcal{L}'_u(q, u, z)(\delta u) &= 2(r_{k-1}^g + C_{k-1}(u - u^{k-1}), C_{k-1}\delta u)_G + \tfrac{2}{\beta_k}(u - u_0, \delta u)_V - (K_{k-1}\delta u, p)_{W^*} \\
&= (2C_{k-1}^*[r_{k-1}^g + C_{k-1}(u - u^{k-1})] + \tfrac{2}{\beta_k}(u - u_0) - K_{k-1}^* p, \delta u)_V = 0 , \\
\mathcal{L}'_q(q, u, z)(\delta q) &= \tfrac{2}{\beta_k}(q - q_0, \delta q)_Q - (L_{k-1}\delta q, p)_{W^*} = (\tfrac{2}{\beta_k}(q - q_0) - L_{k-1}^* p, \delta q)_Q = 0
\end{aligned}$$

for all $\delta q \in Q$, $\delta u \in V$ and $\delta z \in W$, or equivalently as

$$\begin{aligned}
q^k &= q_0 + \frac{\beta_k}{2} L_{k-1}^* p^k \\
u^k &= \left[\frac{2}{\beta_k} \operatorname{id} + 2C_{k-1}^* C_{k-1} \right]^{-1} \left(2C_{k-1}^* \left(C_{k-1}(u^{k-1}) - r_{k-1}^g \right) + \frac{2}{\beta_k} u_0 + K_{k-1}^* p^k \right) \\
u^k &= K_{k-1}^{-1} \left(L_{k-1} q^{k-1} + K_{k-1} u^{k-1} - r_{k-1}^f - L_{k-1} q^k \right) .
\end{aligned}$$

Upon elimination of q^k and u^k this yields

$$\begin{aligned}
&\left[\frac{2}{\beta_k} \operatorname{id} + 2C_{k-1}^* C_{k-1} \right]^{-1} \left(2C_{k-1}^* \left(C_{k-1}(u^{k-1}) - r_{k-1}^g \right) + \frac{2}{\beta_k} u_0 + K_{k-1}^* p^k \right) \\
&= K_{k-1}^{-1} \left(L_{k-1} q^{k-1} + K_{k-1} u^{k-1} - r_{k-1}^f - L_{k-1} \left(q_0 + \frac{\beta_k}{2} L_{k-1}^* p^k \right) \right) ,
\end{aligned}$$

which we reformulate as

$$
\begin{aligned}
&-\frac{\beta_k}{2}K_{k-1}^{-1}L_{k-1}L_{k-1}^*p^k - \left[\frac{2}{\beta_k}\,\mathrm{id} + 2C_{k-1}^*C_{k-1}\right]^{-1}K_{k-1}^*p^k \\
&= \left[\frac{2}{\beta_k}\,\mathrm{id} + 2C_{k-1}^*C_{k-1}\right]^{-1}\left(2C_{k-1}^*\left(C_{k-1}(u^{k-1}) - r_{k-1}^g\right) + \frac{2}{\beta_k}u_0\right) \\
&\quad - K_{k-1}^{-1}\left(L_{k-1}(q^{k-1}-q_0) + K_{k-1}u^{k-1} - r_{k-1}^f\right)
\end{aligned}
$$

and finally

$$
\begin{aligned}
&-\left[\frac{1}{\beta_k}\,\mathrm{id} + C_{k-1}^*C_{k-1}\right]\beta_kK_{k-1}^{-1}L_{k-1}L_{k-1}^*p^k - K_{k-1}^*p^k \\
&= 2C_{k-1}^*\left(C_{k-1}(u^{k-1}) - r_{k-1}^g\right) + \frac{2}{\beta_k}u_0 \\
&\quad - 2\left[\frac{1}{\beta_k}\,\mathrm{id} + C_{k-1}^*C_{k-1}\right]K_{k-1}^{-1}\left(L_{k-1}(q^{k-1}-q_0) + K_{k-1}u^{k-1} - r_{k-1}^f\right) .
\end{aligned}
$$

With

$$
C_{\beta_k} := \left(\frac{1}{\beta_k}\,\mathrm{id} + C_{k-1}^*C_{k-1}\right)^{1/2}
$$

this is equivalent to

$$
\begin{aligned}
&-\beta_kC_{\beta_k}^2K_{k-1}^{-1}L_{k-1}L_{k-1}^*p^k - K_{k-1}^*p^k \\
&= 2C_{k-1}^*\left(C_{k-1}(u^{k-1}) - r_{k-1}^g\right) + \frac{2}{\beta_k}u_0 \\
&\quad - 2C_{\beta_k}^2K_{k-1}^{-1}\left(L_{k-1}(q^{k-1}-q_0) + K_{k-1}u^{k-1} - r_{k-1}^f\right) ,
\end{aligned}
$$

which upon premultiplication with $C_{\beta_k}^{-1}$ becomes

$$
\begin{aligned}
&-\left(\beta_kC_{\beta_k}K_{k-1}^{-1}L_{k-1}(K_{k-1}^{-1}L_{k-1})^*C_{\beta_k} + \mathrm{id}\right)C_{\beta_k}^{-1}K_{k-1}^*p^k \\
&= -2C_{\beta_k}^{-1}C_{k-1}^*r_{k-1}^g + \frac{2}{\beta_k}C_{\beta_k}^{-1}(u_0 - u^{k-1}) + 2C_{\beta_k}K_{k-1}^{-1}\left(L_{k-1}(q_0 - q^{k-1}) + r_{k-1}^f\right) \\
&\quad + \left[2C_{\beta_k}^{-1}C_{k-1}^*C_{k-1} - 2C_{\beta_k} + \frac{2}{\beta_k}C_{\beta_k}^{-1}\right]u^{k-1} \\
&= -2C_{\beta_k}^{-1}C_{k-1}^*r_{k-1}^g + \frac{2}{\beta_k}C_{\beta_k}^{-1}(u_0 - u^{k-1}) + 2C_{\beta_k}K_{k-1}^{-1}\left(L_{k-1}(q_0 - q^{k-1}) + r_{k-1}^f\right) \\
&\quad + \left[2C_{\beta_k}^{-1}\left(\frac{1}{\beta_k}\,\mathrm{id} + C_{k-1}^*C_{k-1}\right) - 2C_{\beta_k}\right]u^{k-1} \\
&= -2C_{\beta_k}^{-1}C_{k-1}^*r_{k-1}^g + \frac{2}{\beta_k}C_{\beta_k}^{-1}(u_0 - u^{k-1}) + 2C_{\beta_k}K_{k-1}^{-1}\left(L_{k-1}(q_0 - q^{k-1}) + r_{k-1}^f\right) .
\end{aligned}
$$

Since $\beta_kC_{\beta_k}K_{k-1}^{-1}L_{k-1}(K_{k-1}^{-1}L_{k-1})^*C_{\beta_k} = \beta_k(C_{\beta_k}K_{k-1}^{-1}L_{k-1})(C_{\beta_k}K_{k-1}^{-1}L_{k-1})^*$ is positive semidefinite, we can conclude

$$
\begin{aligned}
&\left\|C_{\beta_k}^{-1}K_{k-1}^*p^k\right\|_V \\
&\leq \left\|-2C_{\beta_k}^{-1}C_{k-1}^*r_{k-1}^g + \frac{2}{\beta_k}C_{\beta_k}^{-1}(u_0 - u^{k-1}) + 2C_{\beta_k}K_{k-1}^{-1}\left(L_{k-1}(q_0 - q^{k-1}) + r_{k-1}^f\right)\right\|_V ,
\end{aligned}
$$

and with the estimates

$$\|C_{\beta_k}^{-1}C_{k-1}^*\|_{G\to V}\leq 1\,,\quad \|C_{\beta_k}^{-1}\|_V\leq \beta_k^{\frac{1}{2}}\,,\qquad \text{and}\quad \|C_{\beta_k}\|_V\leq\left(\frac{1}{\beta_k}+\|C_{k-1}\|_{V\to G}^2\right)^{\frac{1}{2}}$$

we have

$$\begin{aligned}\left\|K_{k-1}^*p^k\right\|_V &\leq \left\|C_{\beta_k}C_{\beta_k}^{-1}K_{k-1}^*p^k\right\|_V\\ &\leq\left(\frac{1}{\beta_k}+\|C_{k-1}\|_{V\to G}^2\right)^{\frac{1}{2}}\left\|C_{\beta_k}^{-1}K_{k-1}^*p^k\right\|_V\\ &\leq 2\left(\frac{1}{\beta_k}+\|C_{k-1}\|_{V\to G}^2\right)^{\frac{1}{2}}\Big\{\|r_{k-1}^g\|+\frac{1}{\sqrt{\beta_k}}\|u_0-u^{k-1}\|_V\\ &\qquad+\left(\frac{1}{\beta_k}+\|C_{k-1}\|_{V\to G}^2\right)^{\frac{1}{2}}\|K_{k-1}^{-1}\left(L_{k-1}(q_0-q^{k-1})+r_{k-1}^f\|\right)\Big\}\,,\end{aligned}$$

which by Assumption 9 and $(q^{k-1},u^{k-1})\in\mathcal{B}_\rho(q_0,u_0)$ yields (53). □

We will prove inductively that the iterates indeed remain in $\mathcal{B}_\rho(q_0,u_0)$, and even in $\mathcal{B}_{\hat\rho}(q_0,u_0)$ with $\hat\rho=\sqrt{\|q^\dagger-q_0\|^2+\|u^\dagger-u_0\|^2}$, see estimate (69) below. Thus, due to Lemma 2, which remains valid in the discretized setting (58), we get uniform boundedness of the dual variables by some sufficiently large ϱ, namely by any

$$\varrho\geq c_{\mathrm{adj}}\left(\sqrt{\|q^\dagger-q_0\|_Q^2+\|u^\dagger-u_0\|_V^2}+1\right)\,. \tag{56}$$

Hence we can use exactness of the norm with exponent one as a penalty (cf., e.g., Theorem 5.11 in [13]), which implies that a solution (q^k,u^k) of (48), (49) coincides with the unique solution of the unconstrained minimization problem (10) with $r=1$, $\alpha_k=\mu_k=\frac{1}{\beta_k}$, i.e.,

$$\begin{aligned}\min_{(q,u)\in Q\times V}\varrho\|A_q'(q^{k-1},u^{k-1})(q-q^{k-1})+A_u'(q^{k-1},u^{k-1})(u-u^{k-1})+A(q^{k-1},u^{k-1})-f\|_{W^*}\\ +\|C(u^{k-1})+C'(u^{k-1})(u-u^{k-1})-g^\delta\|_G^2+\frac{1}{\beta_k}(\|q-q_0\|_Q^2+\|u-u_0\|_V^2)\,,\end{aligned} \tag{57}$$

for ϱ larger than the norm of the dual variable.

The penalty formulation (57) of (48), (49) will be used in the convergence proofs only. For a practical implementation we will directly discretize (48), (49).

The discrete version of (48), (49) reads

$$\min_{(q,u)\in Q_{h_k}\times V_{h_k}}\|C(u_{\mathrm{old}})+C'(u_{\mathrm{old}})(u-u_{\mathrm{old}})-g^\delta\|_G^2+\frac{1}{\beta_k}\left(\|q-q_0\|_Q^2+\|u-u_0\|_{V_{h_k}}^2\right) \tag{58}$$

$$\text{s.t.}\quad L_{k-1}(q-q_{\mathrm{old}})+K_{k-1}(u-u_{\mathrm{old}})+A(q_{\mathrm{old}},u_{\mathrm{old}})=f\qquad \text{in } W_{h_k}^*\,, \tag{59}$$

where $(q_{\mathrm{old}},u_{\mathrm{old}})=(q^{k-1},u^{k-1})=(q_{h_{k-1}}^{k-1},u_{h_{k-1}}^{k-1})$ is the previous iterate and we assume again that the norms in G and W as well as A and C are evaluated exactly (cf. Assumption 3).

With ϱ chosen sufficiently large such that (56) holds, we define the quantities of interest as follows

$$\begin{aligned}
I_1 \colon\ V \times Q \times V \times \mathbb{R} \to \mathbb{R}\,, \quad & (u_{\text{old}}, q, u, \beta) \mapsto \left\| C'(u_{\text{old}})(u - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta \right\|_G^2 \\
& \qquad + \frac{1}{\beta} \left(\|q - q_0\|_Q^2 + \|u - u_0\|_V^2 \right) \\
I_2 \colon\ V \times V \to \mathbb{R}\,, \quad & (u_{\text{old}}, u) \mapsto \left\| C'(u_{\text{old}})(u - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta \right\|_G^2 \\
I_3 \colon\ Q \times V \to \mathbb{R}\,, \quad & (q_{\text{old}}, u_{\text{old}}) \mapsto \left\| C(u_{\text{old}}) - g^\delta \right\|_G^2 + \varrho \left\| A(q_{\text{old}}, u_{\text{old}}) - f \right\|_{W^*} \\
I_4 \colon\ Q \times V \to \mathbb{R}\,, \quad & (q, u) \mapsto \left\| C(u) - g^\delta \right\|_G^2 + \varrho \left\| A(q, u) - f \right\|_{W^*}
\end{aligned} \tag{60}$$

(cf. (27)) and

$$\begin{aligned}
I_1^k &= I_1(u_{\text{old}}^k, q^k, u^k, \beta_k) \\
I_2^k &= I_2(u_{\text{old}}^k, u^k) \\
I_3^k &= I_3(q_{\text{old}}^k, u_{\text{old}}^k) \\
I_4^k &= I_4(q^k, u^k)\,,
\end{aligned} \tag{61}$$

(cf. (28)), where q_{old}^k, u_{old}^k are fixed from the previous step and q^k, u^k are coupled by the linearized state equation (49) (or (50) respectively) for $q^{k-1} = q_{\text{old}}^k$ and $u^{k-1} = u_{\text{old}}^k$.

Consistently, the discrete counterparts to (60) and (61) are

$$\begin{aligned}
I_{1,h} \colon\ V \times Q \times V \times \mathbb{R} \to \mathbb{R}\,, \quad & (u_{\text{old}}, q, u, \beta) \mapsto \left\| C'(u_{\text{old}})(u - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta \right\|_G^2 \\
& \qquad + \frac{1}{\beta} \left(\|q - q_0\|_Q^2 + \|u - u_0\|_{V_{h_k}}^2 \right) \\
I_{2,h} \colon\ V \times V \to \mathbb{R}\,, \quad & (u_{\text{old}}, u) \mapsto I_2(u_{\text{old}}, u) \\
I_{3,h} \colon\ Q \times V \to \mathbb{R}\,, \quad & (q_{\text{old}}, u_{\text{old}}) \mapsto \left\| C(u_{\text{old}}) - g^\delta \right\|_G^2 + \varrho \left\| A(q_{\text{old}}, u_{\text{old}}) - f \right\|_{W_{h_k}^*} \\
I_{4,h} \colon\ Q \times V \to \mathbb{R}\,, \quad & (q, u) \mapsto \left\| C(u) - g^\delta \right\|_G^2 + \varrho \left\| A(q, u) - f \right\|_{W_{h_k}^*}
\end{aligned} \tag{62}$$

and

$$\begin{aligned}
I_{1,h}^k &= I_{1,h}(u_{\text{old}}^k, q_{h_k}^k, u_{h_k}^k, \beta_k) \\
I_{2,h}^k &= I_{2,h}(u_{\text{old}}^k, u_{h_k}^k) \\
I_{3,h}^k &= I_{3,h}(q_{\text{old}}^k, u_{\text{old}}^k) \\
I_{4,h}^k &= I_{4,h}(q_{h_k}^k, u_{h_k}^k)
\end{aligned} \tag{63}$$

(cf. (30)), where q_{old}^k, u_{old}^k are fixed from the previous step, since (like in (31)) we set $q_{\text{old}}^{k+1} = q_{h_k}^k$ and $u_{\text{old}}^{k+1} = u_{h_k}^k$ at the end of each iteration step.

Remark 5. *Here, as compared to (28), we have removed the W^*-norms in the definition of I_1^k and I_2^k.*

The W^*-norm still appears in I_3^k, but only in connection with the old iterate $(q_{\text{old}}^k, u_{\text{old}}^k)$, such that the only source of error in I_3^k is the evaluation of the W^* norm. That means that with respect to Section 2, we have replaced the problematic expression

$$\|E(q,u)\|_{W^*} - \|E(q_h,u_h)\|_{W_h^*}$$

(cf. Remark 4) by an expression of the form

$$\|E(q_{\text{old}},u_{\text{old}})\|_{W^*} - \|E(q_{\text{old}},u_{\text{old}})\|_{W_h^*}\ , \tag{64}$$

For the very typical case $W = V = H_0^1(\Omega)$ *(see Section 5), we can indeed estimate such an error using goal oriented error estimators:*

Let $v \in V$, $v_h \in V_h$ *solve the equations*

$$\begin{aligned}(\nabla v, \nabla\varphi)_{L^2(\Omega)} &= \langle E(q_{\text{old}},u_{\text{old}}),\varphi\rangle_{V^*,V} \quad \forall\varphi\in V\,,\\ (\nabla v_h, \nabla\varphi)_{L^2(\Omega)} &= \langle E(q_{\text{old}},u_{\text{old}}),\varphi\rangle_{V^*,V} \quad \forall\varphi\in V_h\,,\end{aligned}$$

where $(.,.)_{L^2(\Omega)}$ *denotes the scalar product in* $L^2(\Omega)$ *and* $\langle .,.\rangle_{V^*,V}$ *denotes the duality pairing between* V^* *and* V*. Then there holds*

$$\|E(q_{\text{old}},u_{\text{old}})\|_{V^*} = \|\nabla v\|_{L^2(\Omega)} \quad \text{and} \quad \|E(q_{\text{old}},u_{\text{old}})\|_{V_h^*} = \|\nabla v_h\|_{L^2(\Omega)}\ .$$

We define the functional

$$\Psi(v) := \|\nabla v\|_{L^2(\Omega)}$$

and the Lagrangian

$$L(v,w) := \Psi(v) + \langle E(q_{\text{old}},u_{\text{old}}),w\rangle_{V^*,V} - (\nabla v,\nabla w)_{L^2(\Omega)}\,.$$

Let (v,w) *and* (v_h,w_h) *be continuous and discrete stationary points of* L*, i.e.*

$$\begin{aligned}L_v'(v,w)(\varphi) &= (\|\nabla v\|_{L^2(\Omega)})^{-1}(\nabla v,\nabla\varphi)_{L^2(\Omega)} - (\nabla\varphi,\nabla w)_{L^2(\Omega)} = 0 && \forall\varphi\in V\,, && (65)\\ L_w'(v,w)(\varphi) &= \langle E(q_{\text{old}},u_{\text{old}}),\varphi\rangle_{V^*,V} - (\nabla v,\nabla\varphi)_{L^2(\Omega)} = 0 && \forall\varphi\in V\,,\\ L_v'(v_h,w_h)(\varphi) &= (\|\nabla v_h\|_{L^2(\Omega)})^{-1}(\nabla v_h,\nabla\varphi)_{L^2(\Omega)} - (\nabla\varphi,\nabla w_h)_{L^2(\Omega)} = 0 && \forall\varphi\in V_h\,, && (66)\\ L_w'(v_h,w_h)(\varphi) &= \langle E(q_{\text{old}},u_{\text{old}}),\varphi\rangle_{V^*,V} - (\nabla v_h,\nabla\varphi)_{L^2(\Omega)} = 0 && \forall\varphi\in V_h\,.\end{aligned}$$

Then (by (65) *and* (66)*) we have*

$$w = (\|\nabla v\|_{L^2(\Omega)})^{-1}v \qquad \text{and} \qquad w_h = (\|\nabla v_h\|_{L^2(\Omega)})^{-1}v_h\,. \tag{67}$$

For the error (64) *then holds*

$$\begin{aligned}&\|E(q_{\text{old}},u_{\text{old}})\|_{V^*} - \|E(q_{\text{old}},u_{\text{old}})\|_{V_h^*}\\ &\quad= \Psi(v)-\Psi(v_h)\\ &\quad= \tfrac12 L'(v_h,w_h)(v-\tilde{v_h},w-\tilde{w_h}) + R\\ &\quad= \tfrac12(\|\nabla v_h\|_{L^2(\Omega)})^{-1}(\nabla v_h,\nabla(v-\tilde{v_h}))_{L^2(\Omega)} - \tfrac12(\nabla(v-\tilde{v_h}),\nabla w_h)_{L^2(\Omega)}\\ &\qquad\quad+\tfrac12\langle E(q_{\text{old}},u_{\text{old}}),w-\tilde{w_h}\rangle_{V^*,V} - \tfrac12(\nabla v_h,\nabla(w-\tilde{w_h}))_{L^2(\Omega)} + R\\ &\quad= \tfrac12(\|\nabla v_h\|_{L^2(\Omega)})^{-1}(\nabla v_h,\nabla(v-\tilde{v_h}))_{L^2(\Omega)} - \tfrac12(\|\nabla v_h\|_{L^2(\Omega)})^{-1}(\nabla(v-\tilde{v_h}),\nabla v_h)_{L^2(\Omega)}\\ &\qquad\quad+\tfrac12\langle E(q_{\text{old}},u_{\text{old}}),w-\tilde{w_h}\rangle_{V^*,V} - \tfrac12(\nabla v_h,\nabla(w-\tilde{w_h}))_{L^2(\Omega)} + R\\ &\quad= \tfrac12\langle E(q_{\text{old}},u_{\text{old}}),w-\tilde{w_h}\rangle_{V^*,V} - \tfrac12(\nabla v_h,\nabla(w-\tilde{w_h}))_{L^2(\Omega)} + R\end{aligned}$$

for arbitrary $\tilde{v}_h, \tilde{w}_h \in V_h$*, where* R *is a third order remainder term (see e.g. [5, 6], Section 4). Please note that due to the relation* (67) *no additional system of equations has to be solved in order to obtain the additional variable* w_h*.*

Another way to deal with the discretization error in I_3^k *is the following: Tracking the full convergence proof of Theorem 3 in [25] (Theorem 4.11 there) the reader can realize that the discretization for* $I_{3,h}^k$ *does not have to be the same as for* $I_{1,h}^k$*,* $I_{2,h}^k$*, such that* $I_{3,h}^k$ *could be evaluated on a very fine separate mesh, such that* η_3^k *could be neglected. This alternative is of course, more costly, but since everything else is still done on the adaptively refined (coarser) mesh, the proposed method could still lead to an efficient algorithm.*

The W^**-norm also appears in* I_4^k*, and unfortunately, in combination with the current* q *and* u*, which are subject to discretization, such that in principle we face the same situation as in the least squares formulation from Section 2 (cf. Remark 4). Since, however,* η_4^k *only appears in connection with the very weak assumption* $\eta_4^k \to 0$ *as* $k \to \infty$ *(cf.* (37)*), as in [22], we save ourselves the computational effort of computing an error estimator for* I_4^k*.*

Like in Section 2 we need the weak sequential closedness of $\mathbf{F}$, i.e. Assumption 4 and the following tangential cone condition (cf. Assumption 5).

Assumption 10. *There exist* $0 < c_{tc} < 1$ *and* $\rho > 0$ *such that*

$$\begin{aligned}
&\|C(u) - C(\bar{u}) - C'(u)(u - \bar{u})\|_G \leq c_{tc}\|C(u) - C(\bar{u})\|_G \\
&\|A(q,u) - A(\bar{q},\bar{u}) - A'_q(q,u)(q - \bar{q}) - A'_u(q,u)(u - \bar{u})\|_{W^*} \\
&\leq 4c_{tc}^2\|A(q,u) - A(\bar{q},\bar{u})\|_{W^*} ,
\end{aligned}$$

holds for all $(q,u), (\overline{q},\overline{u}) \in \mathcal{B}_\rho(q_0,u_0) \subset Q \times V$ *(cf. Assumption 1).*

By means of Lemma 2 and the Assumptions 4, 10, we can now formulate a convergence result like in Theorems 1 and 3 in [22] and Theorem 1 here for (48), (49).

Theorem 3. *Let for the starting point* $(q_{\text{old}}^0, u_{\text{old}}^0) \in \mathcal{B}_\rho((q_0,u_0))$ *hold, let the Assumptions 1, 2, 3, 4 and 10 with* c_{tc} *sufficiently small be satisfied and let Assumption 6 hold. For the quantities of interest* (61) *and* (63)*, let, further, the estimate* (32) *hold with* η_i *satisfying Assumption 7.*

Then with β_k*,* $h = h_k$ *fulfilling* (33)*,* k_* *selected according to* (34)*, and* $(q_{h_k}^k, u_{h_k}^k)$ *defined as the primal part of a KKT point of* (58)*,* (59) *there holds*

(o) There exists a $\beta_{\min} > 0$ *independent of* δ *such that for all* $k < k_*$*, a parameter* $\beta_k \geq \beta_{\min}$ *satisfying* (33) *with* $I_{2,h}^k$*,* $I_{3,h}^k$ *according to* (62)*,* (63) *exists provided*

$$\left\|C'(u_{\text{old}})(u_0 - u_{\text{old}}) + C(u_{\text{old}}) - g^\delta\right\|_G^2 \geq \tilde{\tilde{\theta}} \left\|C(u_{\text{old}}) - g^\delta\right\|_G^2 + \varrho \left\|A(q_{\text{old}},u_{\text{old}}) - f\right\|_{W_{h_k}^*} . \tag{68}$$

If (68) *is violated we set* $(q_{h_k}^k, u_{h_k}^k) = (q_0, u_0)$*.*

(i)

$$\|q_{h_k}^k - q_0\|^2 + \|u_{h_k}^k - u_0\|^2 \leq \|q^\dagger - q_0\|^2 + \|u^\dagger - u_0\|^2 \qquad \forall 0 \leq k \leq k_* ; \tag{69}$$

(i') The adjoint states z^k are bounded, i.e.

$$\|z^k\|_W \leq c_{\mathrm{adj}}(\sqrt{\|q^\dagger - q_0\|^2 + \|u^\dagger - u_0\|^2} + 1) \qquad \forall 0 \leq k \leq k_* \,;$$

(ii) k_* is finite;

(iii) $(q_h^{k_*}, u_h^{k_*}) = (q_{h_{k_*(\delta)}}^{k_*(\delta),\delta}, u_{h_{k_*(\delta)}}^{k_*(\delta),\delta})$ converges (weakly) subsequentially to a solution of (8) 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 (8). If the solution $(q^\dagger, u^\dagger)$ to (8) is unique, then $(q_h^{k_*}, u_h^{k_*})$ converges strongly to $(q^\dagger, u^\dagger)$ as $\delta \to 0$.

We mention in passing that this is a new result also in the continuous case $\eta_i^k = 0$.

Proof. The results (o),(i),(ii),(iii) follow from Theorem 3 and Lemma 1 in [22], replacing F there by $\mathbf{F}$ according to (9) as well as q there by $\begin{pmatrix} q \\ u \end{pmatrix}$, setting

$$\begin{aligned} \mathcal{S}\left(\begin{pmatrix} y_C \\ y_A \end{pmatrix}, \begin{pmatrix} \tilde{y}_C \\ \tilde{y}_A \end{pmatrix}\right) &= \|y_C - \tilde{y}_C\|_G^2 + \varrho\|y_A - \tilde{y}_A\|_{W^*} \,, \\ \mathcal{R}\left(\begin{pmatrix} q \\ u \end{pmatrix}\right) &= \|q - q_0\|_Q^2 + \|u - u_0\|_V^2 \,, \\ c_{\mathcal{S}} &= 2 \,, \end{aligned} \tag{70}$$

and choosing the topologies $\tau_{G\times W^*}$ and $\tau_{Q\times V}$ as the strong norm topology on $G \times W^*$ and the weak topology on $Q \times V$, respectively, to meet the continuity and (strict) convexity requirements of Theorem 3 and Lemma 1 in [22].
Item (i') follows from (i) via Lemma 2 within the induction proof of Theorem 3 in [22].
A full convergence proof of Theorem 3 without making use of the equivalence of (58) to the discrete version of (57) can be found in Section 4.2.2 of [25]. □

The convergences rates from Theorem 4 in [22] also hold for the all-at-once formulation (8), due to equivalence with (57) which we formulate in the following theorem.

Instead of source conditions we use variational source conditions (cf., e.g., [12, 19, 20, 27]) due to the nonquadratic data fidelity term in (57).

Assumption 11. *Let*

$$\begin{aligned} &|(q^\dagger - q_0, q - q^\dagger)_Q + (u^\dagger - u_0, u - u^\dagger)_V| \\ &\leq \; c\sqrt{\|q - q^\dagger\|_Q^2 + \|u - u^\dagger\|_V^2}\,\kappa\left(\frac{\|C(u) - C(u^\dagger)\|_G^2 + \varrho\|A(q,u) - A(q^\dagger, u^\dagger)\|_{W^*}}{\|q - q^\dagger\|_Q^2 + \|u - u^\dagger\|_V^2}\right) \,, \\ &\qquad\qquad (q,u) \in \mathcal{D}(A) \,,\; u \in \mathcal{D}(C) \,, \end{aligned}$$

with ϱ sufficiently large (cf. (56)) and independent from q, u, hold with some $\kappa\colon \mathbb{R}^+ \to \mathbb{R}^+$ such that κ^2 is strictly monotonically increasing on $(0, \|\mathbf{F}(q^\dagger, u^\dagger)\|_{Q\times V}^2]$, ϕ defined by $\phi^{-1}(\lambda) = \kappa^2(\lambda)$ is convex and ψ defined by $\psi(\lambda) = \kappa(\lambda)\sqrt{\lambda}$ is strictly monotonically increasing on $(0, \|\mathbf{F}(q^\dagger, u^\dagger)\|_{Q\times V}^2]$.

Theorem 4. *Let the conditions of Theorem 3 and additionally the variational inequality Assumption 11 be fulfilled.*

Then there exists a $\bar{\delta} > 0$ and a constant $\bar{C} > 0$ independent of δ such that for all $\delta \in (0, \bar{\delta}]$ the convergence rates

$$\|q_{\text{old}}^{k_*} - q^\dagger\|_Q^2 + \|u_{\text{old}}^{k_*} - u^\dagger\|_V^2 = \mathcal{O}\left(\frac{\delta^2}{\psi^{-1}(\bar{C}\delta)}\right), \tag{71}$$

with $q_{\text{old}}^{k_*} = q_{\beta_{k_*-1},h_{k*-1}}^{\delta,k_*-1}$, $u_{\text{old}}^{k_*} = u_{\beta_{k_*-1},h_{k*-1}}^{\delta,k_*-1}$ are obtained.

Proof. With (70) the rate follows directly from Theorem 4 in [22] due to Theorem 3 (especially (69)) and the fact that, with (5), (32), (37) and the definition of k_*, we have

$$\|C(u_{\text{old}}^{k_*}) - g\|_G^2 + \varrho\|A(q_{\text{old}}^{k_*}, u_{\text{old}}^{k_*}) - f\|_{W^*} \leq \tilde{\tau}^2\delta^2 \tag{72}$$

with $\tilde{\tau} = \sqrt{2\left((1+c_1)\tau^2+1\right)}$. □

Remark 6. *In fact, no regularization of the u part would be needed for proving just stability of the single Gauss-Newton steps, since by Assumption 2 the terms $\varrho\|A_q'(q^{k-1}, u^{k-1})(q - q^{k-1}) + A_u'(q^{k-1}, u^{k-1})(u - u^{k-1}) + A(q^{k-1}, u^{k-1}) - f\|_{W^*}$ and $\frac{1}{\beta_k}\|q - q_0\|_Q^2$ in (57) as regularization term together ensure weak compactness of the level sets of the Tikhonov functional (cf. Item 6 in Assumption 2 in [22]). However, we require even uniform boundedness of $u_{h_k}^k$ in order to uniformly bound the dual variable and come up with a penalty parameter ϱ that is independent of k, cf. the discrete version of Lemma 2. Using the equality constraint (49) (for $q^{k-1} = q_{h_{k-1}}^{k-1}$) together with the tangential cone condition Assumption 10 for $c_{tc}^2 < \frac{1}{8}$ would only enable to bound $A(q^k, u^k) - f$:*

$$\begin{aligned}
&\|A(q^k, u^k) - f\|_{W^*} \\
&\quad = \|L_{h,k-1}(q^k - q_{h_{k-1}}^{k-1}) + K_{h,k-1}(u^k - u_{h_{k-1}}^{k-1}) + A(q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1}) - A(q^k, u^k)\|_{W^*} \\
&\quad \leq 4c_{tc}^2\|A(q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1}) - A(q^k, u^k)\|_{W^*} \\
&\quad \leq 4c_{tc}^2\|A(q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1}) - f\|_{W^*} + 4c_{tc}^2\|A(q^k, u^k) - f\|_{W^*},
\end{aligned}$$

such that

$$\|A(q^k, u^k) - f\|_{W^*} \leq \frac{4c_{tc}^2}{1 - 4c_{tc}^2}\|A(q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1}) - f\|_{W^*}.$$

However, without error estimators on the difference between $\|A(q^k, u^k) - f\|_{W^*}$ and $\|A(q_{h_k}^k, u_{h_k}^k) - f\|_{W^*}$ (note that η_4^k only yields an estimate on $\|A(q^k, u^k) - f\|_{W^*} - \|A(q_{h_k}^k, u_{h_k}^k) - f\|_{W_{h_k}^*}$), this does not give a recursion

$$\|A(q_{h_k}^k, u_{h_k}^k) - f\|_{W^*} \leq c\|A(q_{h_{k-1}}^{k-1}, u_{h_{k-1}}^{k-1}) - f\|_{W^*}$$

(from which, by uniform boundedness of $q_{h_k}^k$ and Assumption 9 we could conclude uniform boundedness of $u_{h_k}^k$).

Thus, in order to obtain uniform boundedness of $u_{h_k}^k$ we introduce the term $\frac{1}{\beta_k}\|u - u_0\|_V^2$ here for theoretical purposes. For our practical computations we will assume that the error by discretization between $\|A(q^k, u^k) - f\|_{W^*}$ and $\|A(q_{h_k}^k, u_{h_k}^k) - f\|_{W^*}$ is small enough so that the mentioned gap in this argument for uniform boundedness of $u_{h_k}^k$ can be neglected and the part $\frac{1}{\beta_k}\|u - u_0\|_V^2$ of the regularization term is omitted.

4. Computation of the error estimators

Since – different to [22] – u_{old} ist not subject to new discretization in the kth step here, the computation of the error estimators via a dual weighted residual approach (DWR) is easier here and can be done exactly as in [14] and [21]. Thus we omit the arguments q_{old} and u_{old} in the quantities of interest in this section and we also omit the iteration index k and the explicit dependence on β.

Appearance of the dual norm $\|\cdot\|_{W^*}$ makes evaluation of the error estimators for the least squares method from Section 2 problematic (we refer to Remark 4 above and to Section 4.2.1 in [25] for a possible workaround). This is why we only comment on computation or the estimators for the generalized Gauß-Newton method from Section 2 in more detail.

Error estimator for I_1: We consider

$$I_1(q,u) = \left\|C'(u_{\text{old}})(u-u_{\text{old}}) + C(u_{\text{old}}) - g^\delta\right\|_G^2 + \alpha(\|q-q_0\|_G^2 + \|u-u_0\|_V^2)$$

and the Lagrange functional

$$\mathcal{L}(q,u,z) \coloneqq I_1(q,u) + h(z) - B(q,u)(z)\,, \tag{73}$$

with $h \in W^*$ and $B(q,u) \in W^*$ defined as

$$h \coloneqq f - A(q_{\text{old}},u_{\text{old}}) - A'_q(q_{\text{old}},u_{\text{old}})(q_{\text{old}}) - A'_u(q_{\text{old}},u_{\text{old}})(u_{\text{old}})$$

and

$$B(q,u) \coloneqq A'_q(q_{\text{old}},u_{\text{old}})(q) + A'_u(q_{\text{old}},u_{\text{old}})(u)\,.$$

There holds a similar result to Proposition 1 in [22](see also [14]), which allows to estimate the difference $I_1(q,u) - I_1(q_h,u_h)$ by computing a discrete stationary point $x_h = (q_h,u_h,z_h) \in X_h = Q_h \times V_h \times W_h$ of $\mathcal{L}$. This is done by solving the equations

$$z_h \in W_h: \qquad A'_u(q_{\text{old}},u_{\text{old}})(du)(z_h) = I'_{1,u}(q_h,u_h)(du) \qquad \forall du \in V_h \tag{74}$$

$$u_h \in V_h: \qquad A'_q(q_{\text{old}},u_{\text{old}})(q_h)(dz) + A'_u(q_{\text{old}},u_{\text{old}})(u_h)(dz) = h(dz) \qquad \forall dz \in W_h \tag{75}$$

$$q_h \in Q_h: \qquad I'_q(q_h,u_h)(dq) = A'_q(q_{\text{old}},u_{\text{old}})(dq)(z_h) \qquad \forall dq \in Q_h \tag{76}$$

Then the error estimator η_1 for I_1 can be computed as

$$I_1 - I_{1,h} = I_1(q,u) - I_2(q_h,u_h) \approx \frac{1}{2}\mathcal{L}'(x_h)(\pi_h x_h - x_h) = \eta_1 \tag{77}$$

(cf. [22, 21, 14]).

Remark 7. *Please note that the equations* (74)-(76) *are solved anyway in the process of solving the optimization problem* (48), (49).

Error estimator for I_2: The computation of the error estimator for I_2 can be done similarly to the computation of η_2 in [22] (or η^I in [14]) by means of the Lagrange functional $\mathcal{L}$. We consider

$$I_2(u) \coloneqq \left\|C'(u_{\text{old}})(u-u_{\text{old}}) + C(u_{\text{old}}) - g^\delta\right\|_G^2$$

and compute a discrete stationary point $y_h \coloneqq (x_h, x_h^1) \in X_h \times X_h$ of the auxiliary Lagrange functional

$$\mathcal{M}(y) \coloneqq I_2(u) + \mathcal{L}'(x)(x_1)$$

(which combines information on the quantity of interest I_2 with information on the underlying minimization problem via $\mathcal{L}$) by solving the equations

$$\begin{aligned} x_h \in X_h : \quad & \mathcal{L}'(x_h)(dx_1) = 0 && \forall dx_1 \in X_h \\ x_h^1 \in X_h : \quad & \mathcal{L}''(x_h)(x_h^1, dx) = -I_2'(u_h)(du) && \forall dx \in X_h \end{aligned} \tag{78}$$

(79)

(with $dx = (dq, du, dz)$ and $dx_1 = (dq_1, du_1, dz_1)$). Then we compute the error estimator for I_2 by

$$\eta_2 \coloneqq \frac{1}{2}\mathcal{M}'(y_h)(\pi_h y_h - y_h) \approx I_2(u) - I_2(u_h) = I_2 - I_{2,h}\,. \tag{80}$$

Remark 8. *Once the optimality system* (50)-(52) *has been solved, computation of the auxiliary variable x_h^1 only requires solution of a system* (78) *with the Hessian of the Lagrangian as a system matrix, which will can be done at very low additional effort if the optimality system* (50)-(52) *has been solved by Newton's method. To avoid the computation of second order information in* (78) *we would like to refer to [6], where* (78) *is replaced by an approximate equation of first order.*

Error estimator for I_3: In Remark 5, we already mentioned that the W^* norm in I_3 can be evaluated on a separate very fine mesh, so that we will neglect the difference between $\|A(q_{\text{old}}, u_{\text{old}}) - f\|_{W^*}$ and $\|A(q_{\text{old}}, u_{\text{old}}) - f\|_{W_h^*}$. This implies that we do not need to compute the error estimator η_3, since $I_3 = I_{3,h}$, so that (38), and the first part of (37) is trivially fullfilled.

Error estimator for I_4: We also mentioned in Remark 5 that we will not compute η_4, as the error $|I_4 - I_{4,h}|$ needs to be controlled only through the very weak assumption $\eta_4^k \to 0$ as $k \to \infty$ (cf. (37)), which in practice we will simply make sure by altogether decreasing the mesh size in the course of the iteration.

These error estimators are known to work efficiently in practice (see, e.g., [6]). 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 taylored to our purposes. However, they are not reliable, i.e., the conditions $\eta_i \geq |I_i - I_{i,h}|$ $(i = 1, 2, 3, 4)$ cannot be guaranteed in a strict sense in our computations, since we have to neglect certain terms, see the approximation in (77), (80). We mention in passing that our analysis is kept rather general so that it is not restricted to DWR estimators and would also work with different reliable error estimators.

4.1. Algorithm

Since we only know about the existence of an upper bound $\bar{\varrho} = \sup_{k \leq k_*} \|z^k\|_W$ of the adjoint states (cf. item (i') in Theorem 3), but not its value, we choose ϱ (cf. (56)) heuristically, i.e.

in each iteration step we set $\varrho = \varrho_k = \max\{\varrho_{k-1}\,, \|z^k_{h_k}\|_{W_{h_k}}\}$ for the discrete counterpart $z^k_{h_k}$ of z^k.

Remark 9. *Theoretically one should use $\varrho = \|z^k_{h_k}\|_{W_H}$ on a very fine discretization H in order to get a better approximation to $\|z^k\|_W$. However, since we only need the correct order of magnitude and not the exact value, we just use the current mesh h_k.*

In view of Remark 6 we omit the part $\frac{1}{\beta_k}\|u-u_0\|_V^2$ of the regularization term. Also, as motivated in Section 4, we assume $\eta_3^k = 0$ for all k, such that we neither compute η_3 nor η_4.

Thus we only check for the condition

$$\eta_1^k \le \left(\underline{\tilde{\theta}} - 2\left(2c_{tc}^2 + \frac{(1+2c_{tc})^2}{\tau^2}\right)\right) I^k_{3,h} \tag{81}$$

on η_1^k in Assumption 7.

For simplicity, we evaluate $I^k_{3,h}$ on the current mesh instead of a very fine mesh as explained in Remark 5.

For computing β_k, $h = h_k$ fulfilling (33), we can resort to the Algorithm from [14], which also contains refinement with respect to the quantity of interest $I^k_{2,h}$ and repeated solution of

$$\begin{aligned} &\min_{(q,v)\in Q_h\times V_h} \|C'(u^k_{\text{old},h})(v) + C(u^k_{\text{old},h}) - g^\delta\|_G^2 + \frac{1}{\beta_k}\|q-q_0\|_Q^2 \\ &\text{s.t.}\quad A'_u(q^k_{\text{old}}, u^k_{\text{old},h})(v)(\varphi) + A'_q(q^k_{\text{old}}, u^k_{\text{old},h})(q-q^k_{\text{old}})(\varphi) + A(q^k_{\text{old}}, u^k_{\text{old},h})(\varphi) - f(\varphi) = 0 \\ &\hspace{30em}\forall \varphi\in W_h \end{aligned} \tag{82}$$

for $(q,v)\in Q_h\times V_h$.

The presented Generalized Gauss-Newton formulation can be implemented according to the following Algorithm 1.

Algorithm 1. *Generalized Gauss-Newton Method*

1: *Choose τ, τ_β, $\tilde{\tau}_\beta$, $\underline{\tilde{\theta}}$, $\overline{\tilde{\theta}}$ such that $0 < \underline{\tilde{\theta}} \le \overline{\tilde{\theta}} < 1$ and Assumption 6 holds. $\tilde{\theta} = (\underline{\tilde{\theta}} + \overline{\tilde{\theta}})/2$ and $\max\{1\,,\tilde{\tau}_\beta\} < \tau_\beta \le \tau$, and choose c_1, c_2 and c_3, such that the second part of* (38) *is fulfilled.*
2: *Choose a discretization $h = h_0$ and starting value $q_h^0 (= q_{h_0}^0)$ (not necessarily coinciding with q_0 in the regularization term) and set $q^0_{\text{old}} = q^0_h$.*
3: *Choose starting value $u^0_h (= u^0_{h_0})$ (e.g. by solving the PDE $A(q^0_{\text{old}}, u^0_{\text{old}}) = f$) and set $u^0_{\text{old}} = u^0_h$.*
4: *Compute the adjoint state $z^0_h (= z^0_{h_0})$ (see* (51)*), evaluate $\|z^0_h\|_{W_h}$, set $\varrho_0 = \|z^0_h\|_{W_h}$. and evaluate $I^0_{3,h}$ (cf.* (30)*).*
5: *Set $k = 0$ and $h = h^1_0 = h_0$.*
6: ***while** $I^k_{3,h} > \tau^2\delta^2$ **do***
7:     *Set $h = h^1_k$.*
8:     *Solve the optimization problem* (82)
9:     *Set $h^2_k = h^1_k$ and $\delta^2_\beta = \tilde{\theta} I^k_{3,h}$.*

if $I_{2,h}^k > \left(\tau_\beta^2 + \frac{\tilde{\tau}_\beta^2}{2}\right)\delta_\beta^2$ **then**
  With q_{old}^k, u_{old}^k *fixed, apply the Algorithm from [14] (with quantity of interest* I_2^k *and noise level* $\delta_\beta^2 = \tilde{\theta} I_{3,h}^k$*) starting with the current mesh* $h(= h_k^1)$ *to obtain a regularization parameter* β_k *and a possibly different discretization* h_k^2 *such that* (33) *holds; Therwith, also the corresponding* $v_h^k = v_{h_k^2}^k$, $q_h^k = q_{h_k^2}^k$ *according to* (82) *are computed.*
Set $h = h_k^2$.
Evaluate the error estimator η_1^k *(cf.* (28),(30)*).*
Set $h_k^3 = h_k^2$.
if (81) *is violated* **then**
  Refine grid with respect to η_1^k *such that we obtain a finer discretization* h_k^3.
  Solve the the optimization problem (82) *and evaluate* η_1^k.
else
  Set $q_{\text{old}}^{k+1} = q_h^k$, $u_{\text{old}}^{k+1} = u_{\text{old}}^k + v_h^k$.
Set $h = h_k^3$.
Compute the adjoint state $z_h^{k+1}(= z_{h_k^3}^{k+1})$ *(see* (51)*), evaluate* $\|z_h^{k+1}\|_{W_h}$*, set* $\varrho_k = \max\{\varrho_{k-1}, \|z_h^{k+1}\|_{W_h}\}$*. and evaluate* $I_{3,h}^{k+1}$.
Set $h_{k+1}^1 = h_k^3$ *(i.e. use the current mesh as a starting mesh for the next iteration).*
Set $k = k+1$.

To provide a more intuitive impression of Algorithm 1 as compared to those from [21] and [22], we only sketch the structure of the loops in these algorithms below:

Algorithm 2. *Loops in Nonlinear Tikhonov Method from [21]*

while $\cdots$ *(Iteration for* β*)* **do**
  Solve nonlinear optimization problem (i.e. solve nonlinear PDE).
  Update β *and refine eventually.*

Algorithm 3. *Loops in reduced form of discretized IRGNM from [22]*

while $\cdots$ *(Newton iteration)* **do**
  Apply algorithm from [14], i.e.
  while $\cdots$ *(Iteration for* β_k*)* **do**
    Solve linear-quadratic optimization problem (i.e. solve linear PDE).
    Update β *and refine eventually.*
  Solve nonlinear PDE.

Algorithm 4. *Loops in Algorithm 1 above*

while $\cdots$ *(Newton iteration)* **do**
  Apply algorithm from [14], i.e.
  while $\cdots$ *(Iteration for* β_k*)* **do**
    Solve linear-quadratic optimization problem (i.e. solve linear PDE).
    Update β *and refine eventually.*
  Solve linear PDE.

The structure of the loops in Algorithm 4 (i.e., Algorithm 1) is the same as in Algorithm 3 (the one from [22]), but here, we only have to solve linear PDEs, which justifies the drawback of one additional loop in comparison to Algorithm 2 (the one from [21]). This motivates the implementation and promises a gain of computation time for strongly nonlinear problems, which will be considered in terms of numerical tests in Section 5.

5. Numerical Results

For illustrating the performance of the proposed method according to Algorithm 1, we apply it to the example PDE

$$\begin{cases} -\Delta u + \zeta u^3 = q & \text{in } \Omega \\ \qquad\qquad u = 0 & \text{on } \partial\Omega \end{cases},$$

where we aim to identify the parameter $q \in Q = L^2(\Omega)$ from noisy measurements $g^\delta \in G$ of the state $u \in H_0^1(\Omega)$ in $\Omega = (0,1)^2 \subset \mathbb{R}^2$, where $\zeta > 0$ is a given constant. As for the measurements we consider two cases:

(i) via point functionals in n_m uniformly distributed points ξ_i, $i = 1, 2, \ldots, n_m$ and perturbed by uniformly distributed random noise of some percentage $p > 0$. Then the observation space is chosen as $G = \mathbb{R}^{n_m}$ and the observation operator is defined by $(C(v))_i = v(\xi_i)$ for $i = 1, \ldots, n_m$.

(ii) via L^2-projection. Then $G = L^2(\Omega)$, $C = \mathrm{id}$, and

$$g^\delta = g + \delta \frac{r}{\|r\|_{L^2(\Omega)}} = g + p\,\|g\|_{L^2(\Omega)} \frac{r}{\|r\|_{L^2(\Omega)}},$$

where r denotes some uniformly distributed random noise and p the percentage of perturbation. The exact state $u^\dagger$ is simulated on a very fine mesh with 1050625 nodes and equally sized quadratic cells, and we denote the corresponding finite element space by V_{h_L}. In order to evaluate $\left\|C(u) - g^\delta\right\|_{L^2(\Omega)} = \left\|u - g^\delta\right\|_{L^2(\Omega)}$ on coarser meshes and the corresponding finite element spaces V_{h_l} with $l = 0, 1, \ldots, L$ during the optimization algorithm, g^δ has to be transferred from V_{h_L} to the current grid V_{h_l}. As usual in the finite element context, this is done by the L^2-projection as the restriction operator.

We consider configurations with three different exact sources $q^\dagger$:

(a) A Gaussian distribution

$$q^\dagger = \frac{c}{2\pi\sigma^2} \exp\left(-\frac{1}{2}\left(\left(\frac{sx-\mu}{\sigma}\right)^2 + \left(\frac{sy-\mu}{\sigma}\right)^2\right)\right)$$

with $c = 10$, $\mu = 0.5$, $\sigma = 0.1$, and $s = 2$.

(b) Two Gaussian distributions added up to one distribution

$$q^\dagger = q_1 + q_2,$$

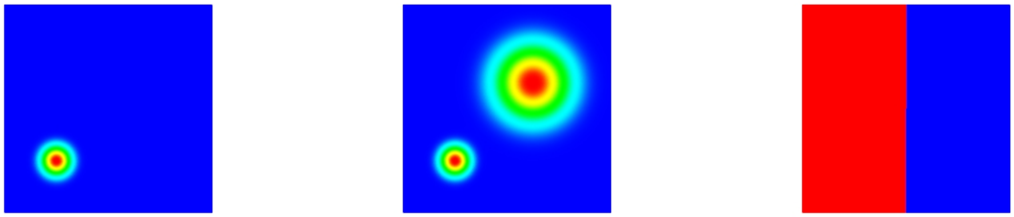

Figure 2. Exact source distribution/control $q^\dagger$. FLTR: (a),(b),(c)

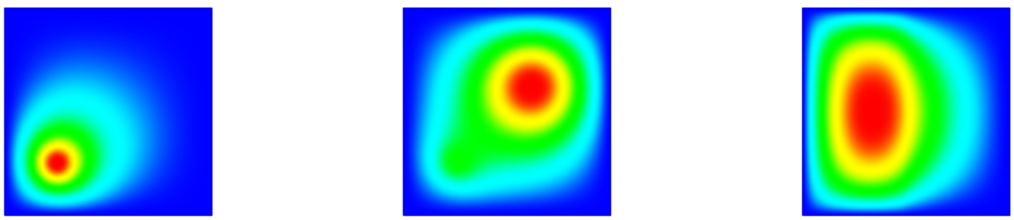

Figure 3. Exact states $u^\dagger$ with $\zeta = 1000$. FLTR: configuration (a),(b),(c)

where

$$q_1 = \frac{c_1}{2\pi\sigma^2} \exp\left(-\frac{1}{2}\left(\left(\frac{s_1 x - \mu}{\sigma}\right)^2 + \left(\frac{s_1 y - \mu}{\sigma}\right)^2\right)\right),$$

$$q_2 = \frac{c_2}{2\pi\sigma^2} \exp\left(-\frac{1}{2}\left(\left(\frac{s_2 x - \mu}{\sigma}\right)^2 + \left(\frac{s_2 y - \mu}{\sigma}\right)^2\right)\right)$$

with $\sigma = 0.1$, $\mu = 0.5$, $s_1 = 2$, $s_2 = 0.8$, $c_1 = 1$, and $c_2 = 1$.

(c) The step function

$$q^\dagger = \begin{cases} 0 & \text{for } x \geq \frac{1}{2} \\ 1 & \text{for } x < \frac{1}{2} \,. \end{cases}$$

Figure 2 shows the exact source distributions $q^\dagger$.

The exact states corresponding to these controls with $\zeta = 1$ are displayed in Figure 3. A comparison with the exact controls in Figure 2 shows the ill-posedness of the problem: Due to the diffusive nature of the PDE, the state gives a strongly blurred image of the control in each of these examples.

The concrete choice of the parameters for the numerical tests is as follows: $c_{tc} = 10^{-7}$, $\tilde{\tilde{\theta}} = 0.4999$, $\underset{\sim}{\tilde{\theta}} = 0.2$, $\tau = 5$, $\tau_\beta = 1.66$, $\tilde{\tau}_\beta = 1$, $(c_2 = 0.9999,\ c_3 = 0.0001)$. Here c_{tc} is not necessarily the true nonlinearity parameter (which we did not attempt to compute for our examples) but only one which is chosen for the implementation of the smallness conditions on the error estimators in Assumption 7. The coarsest (starting mesh) consists of 25 nodes and 16 equally sized squares, the inital values for the control and the state are $q_0 = 0$ and $u_0 = 0$ and we start with a regularization parameter $\beta = 10$.

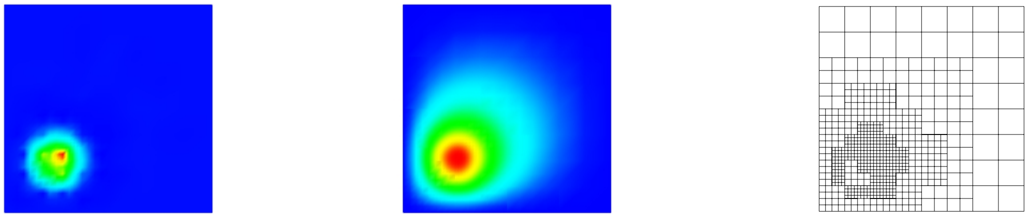

Figure 4. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (a)(i), $\zeta = 1$, 1% noise using (GGN)

Considering the numerical tests, we are mainly interested in saving computation time compared to the Algorithm from [21], where the inexact Newton method for the determination of the regularization parameter β is applied directly to the nonlinear problem, instead of the linearized subproblems (82). That is why besides the numerical results for the Generalized Gauss-Newton (GGN) method presented in section 3, we also present the results from the "Nonlinear Tikhonov" (NT) Algorithm from [21].

For the exact source (a), point measurements (i), $\zeta = 1$ and 1% noise, we present the reconstructions obtained by Algorithm 1 (GGN). Despite the linearizations, the algorithm detects the location of the source very well and refines the mesh accordingly.

Taking a look at Figure 5 the reader can track the behavior of Algorithm 1 (GGN). The algorithm goes from right to left in Figure 5, where the quantities of interest I_2 and I_3 (or rather their discrete counterparts $I_{3,h}$ and $I_{2,h}$) are rather large. The noise level for the inner iteration $\tilde{\theta}I_{3,h}$ is about 0.68 in the beginning. For this noise level the stopping criterion for the β–algorithm (step 10 and 11 in Algorithm 1) is already fulfilled, such that only one Gauss–Newton step is made without refining or updating β. This decreases the noise level $\tilde{\theta}I_{3,h}$ to about 0.41. Then the β–algorithm comes into play, with one refinement step and three β–steps, which in total reduces $I_{2,h}$ from 1.340 to 0.48, with which the β–algorithm terminates. The subsequent run of the β–algorithm (with a smaller noise level of 0.25) consists of one refinement step and two β enlargement steps and so on. Finally, after 7 Gauss–Newton iterations, both quantites of interest $I_{2,h}$ and $I_{3,h}$ fulfill the required smallness conditions such that the whole Gauss–Newton Algorithm terminates. (The fact that it looks like the line for I_2 touches the one for I_3 is just a coincidence.)

In Table 1 we present the respective results (i.e., Example (a) (i), 1% noise) for different choices of ζ (first column). In the second and fifth column in Table 1 one can see the relative control error (83), in the third and sixth column is the number of nodes in the adaptively refined mesh, and in the forth and seventh column one can see the regularization parameter obtained by (GGN) and (NT) respectively. The eighth column shows the gain with respect to computation time using (GGN) instead of (NT). The reduction of computation time is about the same for all ζ, where the computation times in general are higher (thus more representative) for larger ζ. The same holds for the number of nodes and the relative control error. Only the obtained regularization parameter is larger, the larger ζ is. At the same time, it yields a smaller control error, which is somewhat surprising, since (GGN)

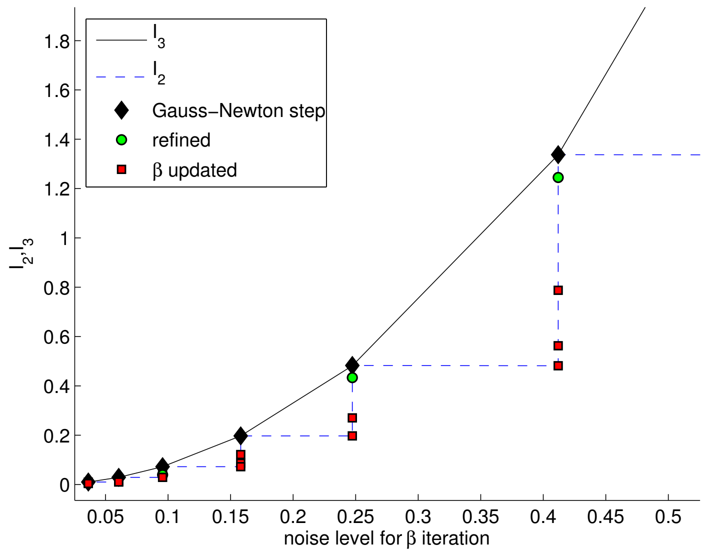

Figure 5. GGN algorithm for Example (a)(i) with $\zeta = 1$ and 1% noise using (GGN)

Table 1. Algorithm 1 (GGN) versus (NT) for (a)(i) for different choices of ζ with 1% noise. CTR: Computation time reduction using (GGN) instead of (NT)

ζ	GN			NT			CTR
	error	β	# nodes	error	β	# nodes	
1	0.395	4899	781	0.456	3085	38665	98%
10	0.395	5155	769	0.452	3194	38377	99%
100	0.393	7579	761	0.443	4999	31967	95%
1000	0.421	17445	677	0.475	11463	44413	99%

only works with the linearized state equation. However, (GGN) seems to finds a better regularization parameter, which causes a better reconstruction.

Due to the mentioned larger and consequently more significant computation times, we consider $\zeta = 1000$ or $\zeta = 100$ in the following.

To see that the algorithm behaves similarly when considering an L^2 tracking type functional, i.e., configuration (ii), we present the corresponding reconstruction and the adaptively refined mesh produced by Algorithm 1 (GGN) in Figure 6. The mesh is much coarser than with (NT) (only 137 instead of 1305 nodes), which causes a saving of computation time of 99%. The regularization parameter is slightly smaller and the relative control error (83) is a bit larger, see Table 2.

The results for a different exact source distribution (b) can be found in Figure 7 for point measurements (i) and in Figure 8 for the L^2–projection alternative (ii).

In both cases (GGN) produces much coarser meshes than (NT), especially for (i), which leads to a remarkable reduction of computation time, which can be read out of Table 2. The obtained regularization parameter is larger than for (NT), which explains

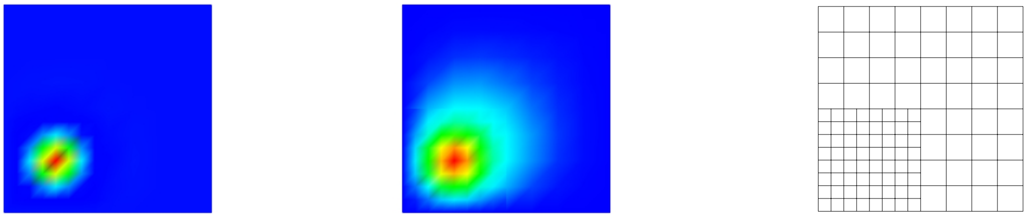

Figure 6. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (a)(ii), $\zeta = 1000$, 1% noise using (GGN)

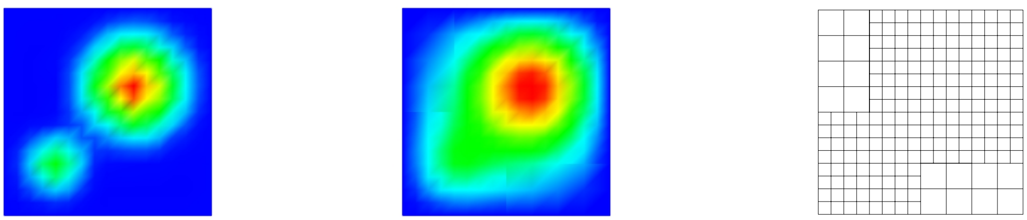

Figure 7. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (b)(i), $\zeta = 1000$, 1% noise using (GGN)

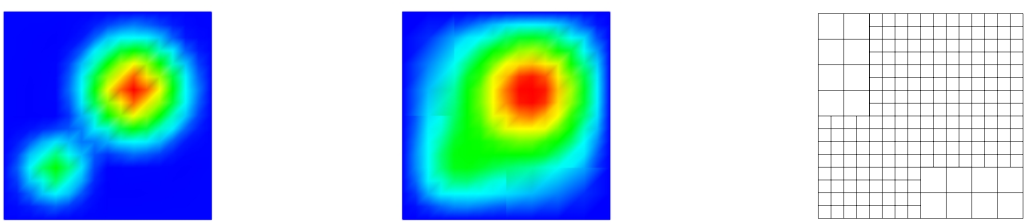

Figure 8. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (b)(ii), $\zeta = 1000$, 1% noise using (GGN)

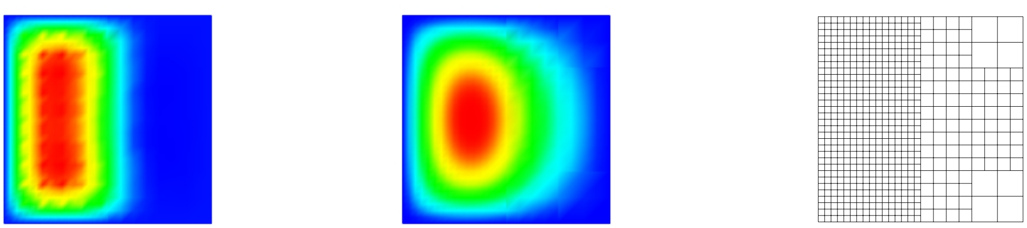

Figure 9. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (c)(i), $\zeta = 1000$, 1% noise using (GGN)

the smaller control error.

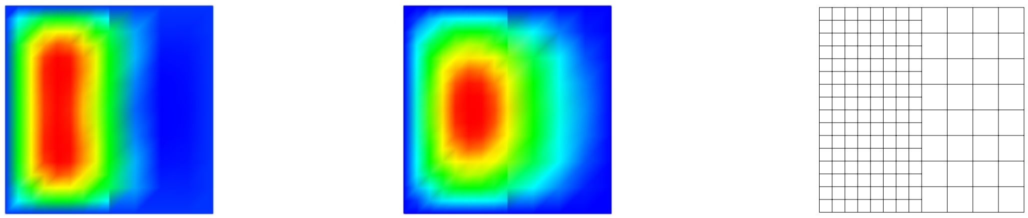

Figure 10. FLTR: reconstructed control, reconstructed state, adaptively refined mesh for Example (c)(ii), $\zeta = 1000$, 1% noise using (GGN)

Table 2. Algorithm 1 (GGN) versus (NT) with $\zeta = 1000$ and 1% noise.
CTR: Computation time reduction using (GGN) instead of (NT)

Example	GN			NT			CTR
	error	β	# nodes	error	β	# nodes	
(a) (i)	0.421	17445	677	0.475	11463	44413	99%
(a)(ii)	0.318	3449334	137	0.302	4368044	1305	53%
(b) (i)	0.225	1764	241	0.300	947	20231	98%
(b)(ii)	0.247	243290	241	0.276	151048	761	33%
(c) (i)	0.431	396	673	0.450	261	11785	91%
(c)(ii)	0.467	36831	189	0.461	42541	651	28%

The same observations can be made for the reconstruction of the source (c), see Figure 9 and Figure 10. In this example refinement is obviously not done optimally, since refinement in the left hand part should be coarser as well. The reason for this behaviour probably lies in the fact the intial guess $q_0 = 0$ and the source $q^\dagger$ have different values on the boundary in this region and thus violate the source condition. Moreover, for such a piecewise constant function total variation regularization would most probably yield much better results than L^2 regularization.

The key results of the previous test configuration for (GGN) as well as (NT) are collected in Table 2.

We come back to the example source (a) and examine the results for different noise levels. In Figure 11 and Figure 12 we display the reconstructions of the control and the state obtained by (GGN) for configuration (i) with $\zeta = 100$ for the noise levels 1%, 2%, and 4%.

The corresponding refined meshes can be found in Figure 13.

In Table 3 we list the relative control error

$$\frac{\left\|q_h^{k_*} - q^\dagger\right\|_Q^2}{\|q^\dagger\|_Q}, \tag{83}$$

the computed final regularization parameter β, and the number of nodes in the obtained mesh for $p = 0.5\%$, $p = 1\%$, $p = 2\%$, $p = 4\%$, and $p = 8\%$ and come to following natural

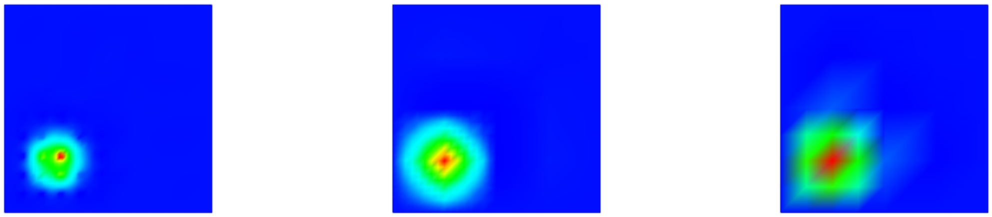

Figure 11. Reconstructed control for Example (a)(i), $\zeta = 100$ for different noise levels. FLTR: 1%, 2%, 4% noise using (GGN)

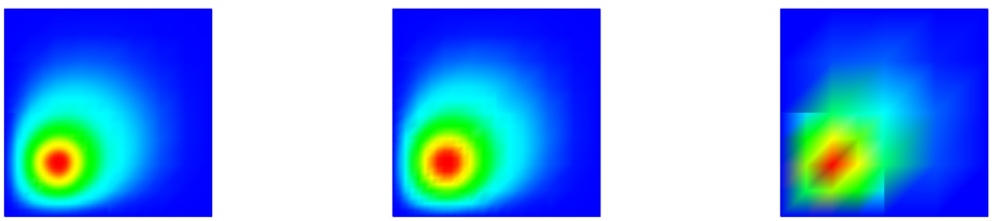

Figure 12. Reconstructed state for Example (a)(i), $\zeta = 100$ for different noise levels. FLTR: 1%, 2%, 4% noise using (GGN)

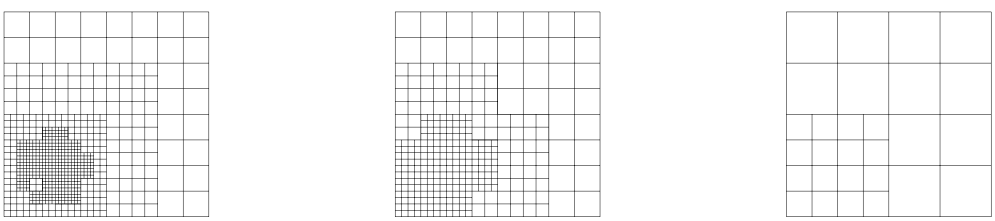

Figure 13. Adaptively refined mesh for Example (a)(i), $\zeta = 100$ for different noise levels. FLTR: 1%, 2%, 4% noise using (GGN)

Table 3. Different noise levels for Example (a)(i), $\zeta = 100$ using (GGN)

noise	error	β	# nodes
0.5%	0.360	13689	761
1%	0.393	7579	761
2%	0.549	1748	361
4%	0.770	817	41
8%	1.03	53	41

conclusion: The more noise, the worse the reconstruction, the stronger the regularization, the coarser the mesh.

6. Conclusions and Remarks

In this paper we consider all-at-once formulations of the iteratively regularized Gauss-Newton method and their adaptive discretizations using a posteriori error estimators. This allows us to consider only the linearized PDE (instead of the full potentially nonlinear one) as a constraint in each Newton step, which safes computational effort. Alternatively, in a least squares approach, the measurement equation and the PDE are treated simultaneously via unconstrained minimization of the squared residual. In both cases we show convergence and convergence rates which we carry over to the discretized setting by controlling precision only in four real valued quantities per Newton step. The choices of the regularization parameters in each Newton step and of the overall stopping index are done a posteriori, via a discrepancy type principle. From the numerical tests we have seen, that the presented method yields reasonable reconstructions and can even lead to a large reduction of computation time compared to similar non-iterative methods.

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Appendix

For proving convergence rates of the iterates according to (23), we consider source conditions of the form

$$\exists (s,v) \in Q \times V \text{ s.t. } (q^\dagger - q_0, u^\dagger - u_0) = \kappa(\mathbf{F}'(q^\dagger, u^\dagger)^* \mathbf{F}'(q^\dagger, u^\dagger))(s,v)\,. \tag{84}$$

with $\kappa = \kappa_\nu$ or $\kappa = \kappa_p$ as in the following Lemma. The case $\kappa = \kappa_\nu$ with $\nu = 0$ corresponds to the pure convergence case without rates. Using the interpolation inequality and Lemma

3.13 in [18] we immediately get the following result, that is crucial for convergence and convergence rates.

Lemma 3. *Under Assumption 2 we have for $\alpha > 0$ $\mu \in [0, \alpha]$, as well as any $\nu \in [0, 1]$ and any $p > 0$*

$$\alpha \left\| \left(\mathbf{T}^*\mathbf{T} + \begin{pmatrix} \alpha I & 0 \\ 0 & \mu I \end{pmatrix} \right)^{-1} \kappa_\nu(\mathbf{T}^*\mathbf{T}) \right\| \leq C_\nu \alpha^\nu \tag{85}$$

$$\alpha \left\| \left(\mathbf{T}^*\mathbf{T} + \begin{pmatrix} \alpha I & 0 \\ 0 & \mu I \end{pmatrix} \right)^{-1} \kappa_p(\frac{1}{e\|\mathbf{T}\|^2}\mathbf{T}^*\mathbf{T}) \right\| \leq C_p f_p(\alpha) \tag{86}$$

where $\kappa_\nu(\lambda) = \lambda^\nu$, $\kappa_p(\lambda) = \ln(\frac{1}{\lambda})^{-p}$, $\lambda \in (0, 1/e]$.

Therewith, the following convergence and convergence rates result with a priori chosen sequence α_k and stopping index k_* follow directly along the lines of the proofs of Theorem 2.4 in [7] and Theorem 4.7 in [18], see also Theorem 4.12 in [23]:

Theorem 5. *Let β_k be a positive sequence decreasing monotonically to zero and satisfying*

$$\sup_{k \in \mathbb{N}} \frac{\beta_{k+1}}{\beta_k} < \infty \,,$$

and let $k_* = k_*(\delta)$ be chosen according to

$$k_* \to \infty \qquad \text{and} \qquad \eta \geq \delta \beta_{k_*}^{\frac{1}{2}} \to 0 \;\; \text{as} \;\; \delta \to 0$$

and

$$\eta \beta_{k_*}^{-\nu-\frac{1}{2}} \leq \delta < \eta \beta_k^{-\nu-\frac{1}{2}} \,, \qquad 0 \leq k < k_* \,,$$

in case of (84) with $\kappa(\lambda) = \lambda^\nu$, $\nu \in (0, 1]$ or

$$\frac{\eta}{\beta_{k_*}} \leq \delta < \frac{\eta}{\beta_k} \,, \qquad 0 \leq k < k_* \,,$$

in case of (84) with $\kappa(\lambda) = \ln(\frac{1}{\lambda})^{-p}$, $p > 0$ respectively.

(i) If (84) holds with $\kappa(\lambda) = \lambda^\nu$, $\nu \in [0, \frac{1}{2}]$ or $\kappa(\lambda) = \ln(\frac{1}{\lambda})^{-p}$, $p > 0$, we assume that

$$\begin{aligned} \mathbf{F}'(\tilde{q}, \tilde{u}) &= R((\tilde{q}, \tilde{u}), (q, u))\mathbf{F}'(q, u) + Q((\tilde{q}, \tilde{u}), (q, u)) \\ \|I - R((\tilde{q}, \tilde{u}), (q, u))\| &\leq c_R \\ \|Q((\tilde{q}, \tilde{u}), (q, u))\| &\leq c_Q \|\mathbf{F}'(q^\dagger, u^\dagger)((\tilde{q}, \tilde{u}) - (q, u))\| \end{aligned}$$

for all $(q, u), (\tilde{q}, \tilde{u}) \in \mathcal{B}_\rho(q_0, u_0)$ and that $\|(q^\dagger, u^\dagger) - (q_0, u_0)\|$, $\|(s, v)\|$, η, ρ, c_R are sufficiently small.

(ii) If (84) holds with $\kappa(\lambda) = \lambda^\nu$, $1/2 \leq \nu \leq 1$, we assume that

$$\|\mathbf{F}'((\tilde{q}, \tilde{u})) - \mathbf{F}'(q, u)\| \leq L \|(\tilde{q}, \tilde{u}) - (q, u)\|$$

for all $(q, u), (\tilde{q}, \tilde{u}) \in \mathcal{B}_\rho(q_0, u_0)$ and $\|(q^\dagger, u^\dagger) - (q_0, u_0)\|$, $\|(s, v)\|$, η, ρ are sufficiently small.

Then for $(q^{k_*,\delta}, u^{k_*,\delta})$ *defined by* (23) *(i.e.,* (24)*), we obtain convergence* $(q^{k_*,\delta}, u^{k_*,\delta}) \to (q^\dagger, u^\dagger)$ *as* $\delta \to 0$ *and convergence rates*

$$\|q_h^{k_*} - q^\dagger\|^2 + \|u_h^{k_*} - u^\dagger\|^2 \leq \frac{\bar{C}^2\delta^2}{\Theta^{-1}\left(\frac{\bar{C}}{2\|(s,v)\|}\delta\right)} = 4\|(s,v)\|^2\kappa^2(\Theta^{-1}(\tfrac{\bar{C}}{2\|(s,v)\|}\delta)) \tag{87}$$

where $\Theta(\lambda) \coloneqq \kappa(\lambda)\sqrt{\lambda}$*.*