Adaptive discretization of parameter identification problems in PDEs for variational and iterative regularization

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joint work with

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Overview

- motivation: parameter identification in PDE
- ideas on adaptivity for inverse problems
- principles of goal oriented error estimators
- variational regularization
- iterative regularization
- conclusions and outlook

Motivation: Parameter Identification in PDE

Some Model problems:

- *a*-example: identify the diffusivity $a = a(x)$ in

  $$-\nabla (a(x) \nabla u) = f \quad \text{in } \Omega$$

  from measurements of the state u
  $\rightsquigarrow$ nonlinear inverse problem

- *c*-example: identify the potential $c = c(x)$ in

  $$-\Delta u + c(x) u = f \quad \text{in } \Omega$$

  from measurements of the state u.
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- inverse source problem: identify the source $f = f(x)$ in

  $$-\Delta u = f(x) \quad \text{in } \Omega$$

  from measurements of the state u.
  $\rightsquigarrow$ linear inverse problem
- nonlinearity identification: identify the heat conductivity $q = q(u)$ in

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

  from measurements of the state u.
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$$-\Delta u + cu = f \qquad -\nabla(q(u)\nabla u) = f$$

- The majority of parameter identification problems in PDEs leads to nonlinear inverse problems

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Abstract formulation:

$$A(q,u)(v) = (f,v) \quad \forall v \in V \qquad \dots \text{ PDE in weak form}$$
$$Cu = g \qquad \dots \text{ measurements}$$

or equivalently

$$F(q) = g$$

$F \dots$ forward operator: $F(q) = (C \circ S)(q) = Cu$
where $u = S(q)$ solves PDE; $S \dots$ coefficient-to-state-map

Hilbert spaces Q, V, G: $q \in Q \stackrel{S}{\to} u \in V \stackrel{C}{\to} g \in G$

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$$\min_{q,u} \ \|Cu - g^\delta\|^2$$
$$\text{s.t.} \ \ A(q,u)(v) = (f,v) \quad \forall v \in V$$

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e.g. **Tikhonov regularization:**[1]

Minimize $J_\alpha(q,u) = \|Cu - g^\delta\|^2 + \alpha\|q\|^2$ over $q \in Q$, $u \in V$
under the constraint $A(q,u)(v) = (f,v) \quad \forall v \in V$

or equivalently

Minimize $j_\alpha(q) = \|F(q) - g^\delta\|^2 + \alpha\|q\|^2$ over $q \in Q$,

$\rightsquigarrow$ PDE constrained optimization

additional issue: choice of α!

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e.g., **Discrepancy Principle**[2]

assume noise level $\delta \geq \|g - g^\delta\|$ to be known;
fix constant $\tau \geq 1$ independent of δ;
determine $\alpha = \alpha_*$ such that

$$\|F(q^\delta_{\alpha_*}) - g^\delta\| = \tau\delta$$

(relaxed version $\underline{\tau}^2\delta^2 \leq \|F(q^\delta_{\alpha_*}) - g^\delta\|^2 \leq \overline{\tau}^2\delta^2$)
where q^δ_α is the Tikhonov minimizer

$\rightsquigarrow$ nonlinear 1-d equation $\phi(\alpha) = 0$ for α;

each evaluation of ϕ requires minimization of Tikhonov functional!

[2] There exist many other regularization parameter choice strategies!

Motivation: Coefficient Identification in PDE

computational issues:

- instability:
  amplification of numerical errors
- computational effort:
  several reg. inversions to determine regularization parameter

Motivation: Coefficient Identification in PDE

adaptive discretization:

- examples $-\nabla(q\nabla u) = f$; $-\Delta u + qu = f$; $-\Delta u = q$: refine grid for u and q
  - at jumps or large gradients
  - close to measurements
  - at locations with large error contribution

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Some Ideas on Adaptivity for Inverse Problems

- Haber&Heldmann&Ascher'07: Tikhonov with BV type reg.:
  Refine for u to compute residual term sufficiently precisely;
  Refine for q to compute regularization term sufficiently precisely
- Neubauer'03, '06, '07: moving mesh reg., adaptive grid reg.:
  Refine where q has jumps or large gradients
- Borcea&Druskin'02: optimal finite difference grids (a priori):
  Refine close to measurements
- Chavent&Bissell'98, Ben Ameur&Chavent&Jaffré'02, BK&Ben Ameur'02:
  Refine to reduce data misfit and coarsen to reduce number of dofs
  (refinement and coarsening indicators)
- Becker&Vexler'04, Griesbaum&BK&Vexler'07, Bangerth&Joshi'08,
  Beilina et. al.'05,'06,'09,'10,'11,'12, BK&Kirchner&Vexler'11,
  BK&Kirchner&Veljovic&Vexler'13:
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Variational Regularization

Coefficient Identification in PDE as Operator Equation

$$\begin{aligned} A(q,u)(v) &= (f,v) \quad \forall v \in V && \ldots \text{ PDE in weak form} \\ Cu &= g && \ldots \text{ measurements} \end{aligned}$$

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Tikhonov Regularization

Minimize $j_\alpha(q) = \|F(q) - g^\delta\|^2 + \alpha\|q\|^2$ over $q \in Q$,

or equivalently

Minimize $J_\alpha(q,u) = \|Cu - g^\delta\|^2 + \alpha\|q\|^2$ over $q \in Q$, $u \in V$
under the constraint $A(q,u)(v) = (f,v) \quad \forall v \in V$

Tikhonov Regularization and the Discrepancy Principle

$$\text{Minimize} \quad j_\alpha(q) = \|F(q) - g^\delta\|^2 + \alpha\|q\|^2 \text{ over } q \in Q\,,$$

Choice of α: discrepancy principle (fixed constant $\tau \geq 1$)

$$\|F(q^\delta_{\alpha_*}) - g^\delta\| = \tau\delta$$

$\leadsto$ nonlinear 1-d equation $\phi(\alpha) = 0$ for α;
evaluation of ϕ requires minimization of Tikhonov functional

Convergence analysis as $\delta \to 0$:
[Engl& Hanke& Neubauer 1996] and the references therein

Goal Oriented Error Estimators in PDE Constrained Optimization

[Becker&Kapp&Rannacher'00], [Becker&Rannacher'01], [Becker&Vexler '04, '05]

Minimize $J(q, u)$ over $q \in Q$, $u \in V$
under the constraint $A(q, u)(v) = f(v) \quad \forall v \in V$

Lagrange functional:

$$\mathcal{L}(q, u, z) = J(q, u) + f(z) - A(q, u)(z)\,.$$

First order optimality conditions:

$$\mathcal{L}'(q, u, z)[(p, v, y)] = 0 \quad \forall (p, v, y) \in Q \times V \times V \qquad (1)$$

Discretization $Q_h \subseteq Q$, $V_h \subseteq V$ $\rightsquigarrow$ discretized version of (1).

Estimate the error due to discretization in some quantity of interest I:

$$I(q, u) - I(q_h, u_h) \leq \eta$$

Goal Oriented Error Estimators (II)

Auxiliary functional:

$$\mathcal{M}(q,u,z,p,v,y) = I(q,u) + \mathcal{L}'(q,u,z)[(p,v,y)]$$

Consider additional equations:

$$\mathcal{M}'(x_h)(dx_h) = 0 \quad \forall dx_h \in X_h = (Q_h \times V_h \times V_h)^2 \quad (*)$$

Theorem (Becker&Vexler, J. Comp. Phys., 2005):

$$I(q,u) - I(q_h,u_h) = \underbrace{\frac{1}{2}\mathcal{M}'(x_h)(x-\tilde{x}_h)}_{=:\eta} + O(\|x-x_h\|^3) \quad \forall \tilde{x}_h \in X_h\,.$$

After computing a stationary point (q_h, u_h, z_h), computation of $x_h = (q_h, u_h, z_h, p_h, v_h, y_h)$ from $(*)$ only requires one more Newton step:

$$0 \stackrel{!}{=} \mathcal{M}'_{(q,u,z)}(x_h) \quad = \quad I'_{(q,u,z)}(q_h,u_h) + \mathcal{L}''_{(q,u,z)}(q_h,u_h,z_h)[(p_h,v_h,y_h)]$$

$$0 = \mathcal{M}'_{(p,v,y)}(x_h) \quad = \quad \mathcal{L}'(q_h,u_h,z_h)[(p_h,v_h,y_h)] \text{ since } (q_h,u_h,z_h) \text{ stat. point}$$

Goal Oriented Error Estimators (III)

$$I(q,u) - I(q_h,u_h) = \underbrace{\frac{1}{2}\mathcal{M}'(x_h)(x-\tilde{x}_h)}_{=:\eta} + O(\|x-x_h\|^3) \quad \forall \tilde{x}_h \in X_h\,.$$

Error estimator η is a sum of local contributions due to either q, u, z, . . .

$$\eta = \sum_{i=1}^{N_q} \eta_i^q + \sum_{i=1}^{N_u} \eta_i^u + \sum_{i=1}^{N_z} \eta_i^z + \sum_{i=1}^{N_p} \eta_i^p + \sum_{i=1}^{N_v} \eta_i^v + \sum_{i=1}^{N_y} \eta_i^y$$

$\rightsquigarrow$ local refinement at large error contributions η_i^j
separately for $q \in Q_h$, $u \in V_h$, $z \in V_h$, . . .

Choice of Quantity of Interest $I(q,u)$?

First guess:
Since we wish to reconstruct the coefficient $q = q(x)$,
all $I_x(q,u) := q(x), \;\; x \in \Omega$ are quantities of interest.

These are by far too many!

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Idea of proof for Tikhonov & Discrepancy Principle [3]

- minimality in Q of Tikhonov minimizer $q^\delta_{\alpha_*}$ and $q^\dagger \in Q$

$$\Rightarrow \quad J_{\alpha_*}(q^\delta_{\alpha_*}, u^\delta_{\alpha_*}) \leq \|F(q^\dagger) - g^\delta\|^2 + \alpha_*\|q^\dagger\|^2 \leq \delta^2 + \alpha_*\|q^\dagger\|^2$$

[3] $q^\dagger \ldots$ exact solution of inverse problem $F(q^\dagger) = Cu^\dagger = g$

q^δ_α Tikhonov minimizer, $\quad u^\delta_\alpha = S(q^\delta_\alpha) \ldots$ corresponding state

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with $|J_{\alpha_*}(q^\delta_{\alpha_*}, u^\delta_{\alpha_*}) - |J_{\alpha_*}(q^\delta_{\alpha_* h}, u^\delta_{\alpha_* h})| \leq \eta_1 \leq (\underline{\underline{\tau}}^2 - 1)\delta^2$

$\Rightarrow\ J_{\alpha_*}(q^\delta_{\alpha_* h}, u^\delta_{\alpha_* h}) \leq \|F(q^\dagger) - g^\delta\|^2 + \alpha_*\|q^\dagger\|^2 + \eta_1 \leq \delta^2 + \alpha_*\|q^\dagger\|^2 + \eta_1$

- discrepancy principle $\underline{\underline{\tau}}^2\delta^2 \leq \|F_h(q^\delta_{\alpha_* h}) - g^\delta\|^2$

$\Rightarrow J_{\alpha_*}(q^\delta_{\alpha_* h}, u^\delta_{\alpha_* h}) = \|F_h(q^\delta_{\alpha_* h}) - g^\delta\|^2 + \alpha_*\|q^\delta_{\alpha_* h}\|^2 \geq \underline{\underline{\tau}}^2\delta^2 + \alpha_*\|q^\delta_{\alpha_* h}\|^2$

- sum up, use $\underline{\underline{\tau}}^2\delta^2 > \delta^2 + \eta_1$, divide by α_* $\Rightarrow$ $\|q^\delta_{\alpha_* h}\|^2 \leq \|q^\dagger\|^2$

$\Rightarrow\ \exists$ weakly convergent subsequence $q^\delta_{\alpha_* h} \rightharpoonup \bar{q}$ as $\delta \to 0$.

- discrepancy principle $\|F_h(q^\delta_{\alpha_* h}) - g^\delta\|^2 \leq \overline{\overline{\tau}}\delta^2$ $\delta \to 0$

with $|\|F(q^\delta_{\alpha_* h}) - g^\delta\|^2 - \|F_h(q^\delta_{\alpha_* h}) - g^\delta\|^2| \leq \eta_2 \to 0$ as $\delta \to 0$

$\Rightarrow\ F(\bar{q}) = g$

Convergence Analysis $\rightsquigarrow$ Choice of Quantities of Interest

Theorem [Griesbaum&BK& Vexler'07], [BK&Kirchner&Vexler'11]:

$\alpha_* = \alpha_*(\delta, g^\delta)$ and $Q_h \times V_h \times V_h$ such that

$\underline{\underline{\tau}}^2\delta^2 \leq \|F_h(q^\delta_{h,\alpha_*}) - g^\delta\|^2_G = \|Cu^\delta_{h,\alpha_*} - g^\delta\|^2_G \leq \overline{\overline{\tau}}\delta^2$

$I_1(q,u,\alpha) = J_\alpha(q,u) = \|Cu - g^\delta\|^2_G + \alpha\|q\|^2$

satisfies $|I_1(q^\delta_{\alpha_*}, u^\delta_{\alpha_*}, \alpha_*) - I_1(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}, \alpha_*)| \leq (\underline{\underline{\tau}}^2 - 1)\delta^2$

$I_2(u,\alpha) := \|F(q_{h,\alpha_*}) - g^\delta\|^2_G = \|Cu - g^\delta\|^2_G$

satisfies $|I_2(u^\delta_{\alpha_*}, \alpha_*) - I_2(u^\delta_{h,\alpha_*}, \alpha_*)| \leq cI_2(u^\delta_{h,\alpha_*}, \alpha_*)$

Then $q^\delta_{\alpha_*} \to q^\dagger$ as $\delta \to 0$.

(Optimal rates under source conditions of logarithmic/Hölder type.)

Remarks

- Also works for stationary points q^{δ}_{h,α_*} instead of global minimizers if F is not too nonlinear
- Also works in Banach spaces with general data misfit and (convex) regularization term [4]
  $J_\alpha(q,u) = \mathcal{S}(Cu, g^\delta) + \alpha\mathcal{R}(q)$

[4] see, e.g., the PhD theses of Christiane Pöschl 2008 (Otmar Scherzer), Jens Flemming 2011 (Bernd Hofmann), Frank Werner 2012 (Thorsten Hohage) for the continuous setting.

Efficient Computation of α $\rightsquigarrow$ Choice of QoI

Choice of α: discrepancy principle (fixed constant $\tau \geq 1$)

$$\|F(q^{\delta}_{\alpha_*}) - g^{\delta}\| \approx \tau\delta$$

$\rightsquigarrow$ 1-d nonlinear equation $\phi(\alpha) = 0$ for α
"less nonlinear" version $\psi(\beta) = \phi(\frac{1}{\beta}) = 0$ for β

$\rightsquigarrow$ solve by Newton's method

$$\beta^{k+1} = \beta^k - \frac{\psi(\beta^k)}{\psi'(\beta^k)}$$

Efficient Computation of $\alpha \rightsquigarrow$ Choice of QoI

Theorem [Griesbaum&BK&Vexler'07], [BK& Kirchner&Vexler'11]:

$I_1(q,u) := \psi(\beta) = \psi(\frac{1}{\alpha}) = \|F(q) - g^\delta\|_G^2 - \tau^2\delta^2 = \|Cu - g^\delta\|_G^2 - \tau^2\delta^2$

$I_2(q,u) := \psi'(\beta)$

$\beta^{k+1} = \beta^k - \frac{\psi_h^k}{{\psi'}_h^k}$ (approximate Newton method)

for $k \leq k_* - 1$ with $k_* = \min\{k \in \mathbb{N} \mid i_h^k - \tau^2\delta^2 \leq 0\}$ with

$|\psi(\beta^k) - \psi_h^k| \leq \varepsilon^k\,,\qquad |\psi'(\beta^k) - {\psi'}_h^k| \leq {\varepsilon'}^k\,,\quad \varepsilon^k, {\varepsilon'}^k$ sufficiently small.

Then β^k satisfies quadratic convergence estimate and

$\underline{\underline{\tau}}^2\delta^2 \leq \|F_h(q_h, \frac{1}{\beta_{k_*}}) - g^\delta\|_G^2 \leq \overline{\overline{\tau}}^2\delta^2$

Remarks

- computation of error estimators for $\psi(\beta)$:
  just one more SQP type step after $\mathcal{L}'(q,u,z)[(p,v,y)] = 0$;
- evaluation of $\psi'(\beta)$:
  can be directly extracted from quantities computed for error estimators for $\psi(\beta)$
- error estimators for $\psi'(\beta)$:
  stationary point of another auxiliary functional
  by another SQP step

Numerical Tests

nonlinear inverse source problem:

$$-\Delta u + 1000u^3 = q \text{ in } \Omega = (0,1)^2 \quad + \text{ homogeneous Dirichlet BC}$$

Identify q from distributed measurements of u at 10×10 points in Ω

$$(a) \quad q^\dagger(x,y) = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{(x-\frac{5}{11})^2+(y-\frac{5}{11})^2}{2\sigma^2}\right), \ \sigma = 0.01$$

$$(b) \quad q^\dagger(x,y) = q_1(x,y) + q_2(x,y)$$

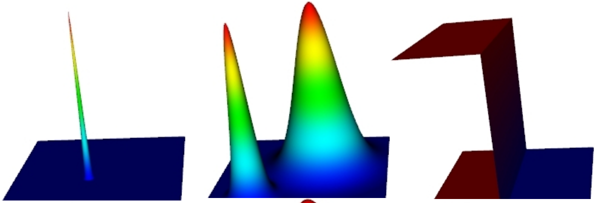
$$q_i = \frac{1}{2\pi\sigma^2} \exp\left(-\frac{1}{2}\left(\left(\frac{s_i x - \frac{1}{2}}{\sigma}\right)^2 + \left(\frac{s_i y - \frac{1}{2}}{\sigma}\right)^2\right)\right), \quad \begin{array}{l} \sigma = 0.1 \\ s_1 = 2, \\ s_2 = 0.8 \end{array}$$

$$(c) \quad q^\dagger(x,y) = \begin{cases} 1 & x \leq \frac{1}{2} \\ 0 & x > \frac{1}{2} \end{cases}$$

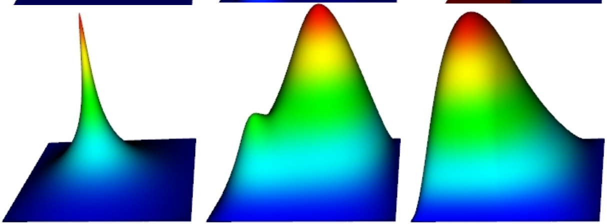
Computations with *Gascoigne* and *RoDoBo*.

Numerical Tests

exact par. q:
(a), (b), (c)



exact state u:
(a), (b), (c)



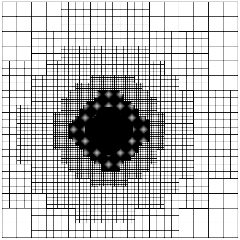
Numerical Results (I)

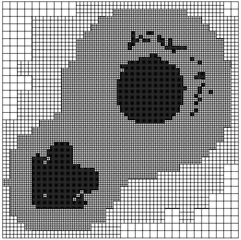
Computations with 1% random noise:

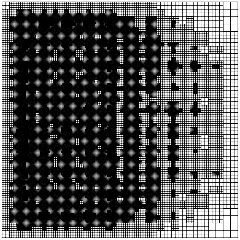
number of nodes on finest grid:

	(a)	(b)	(c)
uniform	263169	66049	66049
adaptive	14157	18035	56409
reduction of CPU time	92%	53%	10%

adaptive grids:







wrong regularization term

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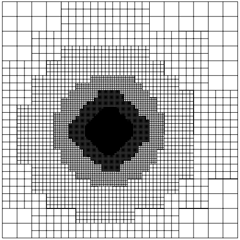
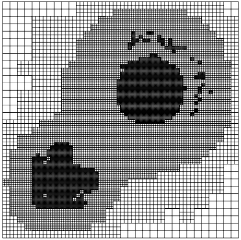
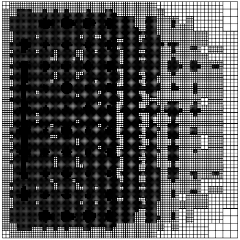




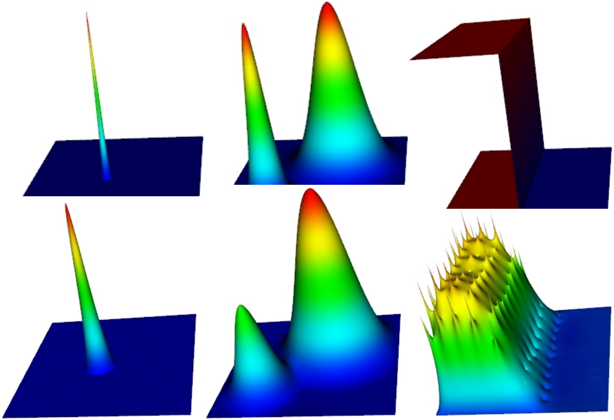


wrong regularization term

Numerical Results (II)

exact par. q:
(a), (b), (c)

computed par.
(a), (b), (c)



Numerical Results (III)

Convergence as $\delta \to 0$ for example (a),
linear inverse source problem

with $\sigma = 0.05$

δ	$\frac{\|q^\delta_{\alpha_*} - q^\dagger\|}{\|q^\dagger\|}$	$1/\alpha_*$
8%	0.761	156.390
4%	0.592	660.930
2%	0.414	2426.109
1%	0.288	7047.472
0.5%	0.229	17042.825

with $\sigma = 0.01$

δ	$\frac{\|q^\delta_{\alpha_*} - q^\dagger\|}{\|q^\dagger\|}$	$1/\alpha_*$
8%	0.869	2396.281
4%	0.776	9044.374
2%	0.744	24364.894
1%	0.734	55017.364
0.5%	0.731	117560.866

Iterative Regularization

Coefficient Identification in PDE as Operator Equation

$$\begin{aligned} A(q,u)(v) = & \quad (f,v) \quad \forall v \in V & \quad \ldots \text{ PDE in weak form} \\ Cu = & \quad g & \quad \ldots \text{ measurements} \end{aligned}$$

or equivalently

$$F(q) = g$$

$F \ldots$ forward operator: $F(q) = (C \circ S)(q) = Cu$
where $u = S(q)$ solves PDE; $\quad S \ldots$ coefficient-to-state-map

Hilbert spaces Q, V, G: $\quad q \in Q \stackrel{S}{\to} u \in V \stackrel{C}{\to} g \in G$

inverse problem: identify q from measurements g^δ of g

Newton type Regularization

Newton step as least squares problem:

$$q_{k+1}^{\delta} = \arg\min_q \|F'(q_k^{\delta})(q - q_k^{\delta}) + F(q_k^{\delta}) - g^{\delta}\|^2,$$

Iteratively Regularized Gauss-Newton Method IRGNM

$$q_{k+1}^{\delta} = \arg\min_q \|\underbrace{F'(q_k^{\delta})(q - q_k^{\delta})}_{Cw} + \underbrace{F(q_k^{\delta})}_{Cu} - g^{\delta}\|^2 + \alpha_k \|q - q_0\|^2,$$

or equivalently

Minimize

$$J_k(q,u,w) = \|C(w+u) - g^{\delta}\|_G^2 + \alpha_k \|q - q_0\|^2 \text{ over } \begin{array}{c} q \in Q \\ u \in V \\ w \in V \end{array}$$

under the constraints

$$A'_u(q_k^{\delta}, u)[w](v) + A'_q(q_k^{\delta}, u)[q - q_k^{\delta}](v) = 0 \quad \forall v \in V\,,$$

$$A(q_k^{\delta}, u)(v) = f(v) \quad \forall v \in V\,,$$

Newton type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

$$q_{k+1}^{\delta} = \arg\min_q \|F'(q_k^{\delta})(q - q_k^{\delta}) + F(q_k^{\delta}) - g^{\delta}\|^2 + \alpha_k \|q - q_0\|^2,$$

a posteriori selection of α_k (inexact Newton)

$$\underline{\tilde{\theta}} \|F(q_k) - g^{\delta}\| \leq \|F'(q_k)(q_{k+1} - q_k) + F(q_k) - g^{\delta}\| \leq \tilde{\overline{\theta}} \|F(q_k) - g^{\delta}\|$$

Newton type Regularization and the Discrepancy Principle

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a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \ : \ \|F(q_k) - g^{\delta}\| \leq \tau\delta\}$$

Newton type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

$$q_{k+1}^\delta = \arg\min_q \|F'(q_k^\delta)(q - q_k^\delta) + F(q_k^\delta) - g^\delta\|^2 + \alpha_k \|q - q_0\|^2,$$

a posteriori selection of α_k (inexact Newton)

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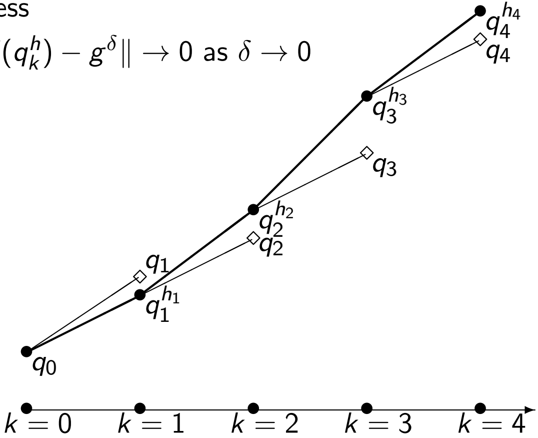
a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \ : \ \|F(q_k) - g^\delta\| \leq \tau\delta\}$$

Idea of Proof

- minimality of q_k in Q, compare with $q^\dagger$
  $\rightsquigarrow$ boundedness
- show that $\|F(q_k^h) - g^\delta\| \to 0$ as $\delta \to 0$



Convergence Analysis $\rightsquigarrow$ Choice of QoI

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3,4\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$\begin{aligned}
I_{1,h}^{k+1} &= \|\overbrace{F_h'(q_k^H)(q_{k+1}^h - q_k^H)}^{Cw_k^h} + \overbrace{F_h(q_k^H)}^{Cu_k^h} - g^\delta\|^2 + \alpha_k \|q_{k+1}^h - q_0\|^2 \\
I_{2,h}^{k+1} &= \|F_h'(q_k^H)(q_{k+1}^h - q_k^H) + F_h(q_k^H) - g^\delta\|^2 \\
I_{3,h}^{k+1} &= \|F_h(q_k^H) - g^\delta\|^2 \\
I_{4,h}^{k+1} &= \|\underbrace{F_h(q_{k+1}^h)}_{Cu_{k+1}^h} - g^\delta\|^2,
\end{aligned}$$

Theorem [BK&Kirchner&Veljovic&Vexler'12]:
Let $(*)$ hold with η_i^{k+1} sufficiently small. Then $q_{h,k_*}^\delta \to q^\dagger$ as $\delta \to 0$.
(Optimal rates under source conditions of logarithmic/Hölder type).

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$I_{1,h}^{k+1} = \|F_h'(q_k^H)(q_{k+1}^h - q_k^H) + F_h(q_k^H) - g^\delta\|^2 + \alpha_k \|q_{k+1}^h - q_0\|^2$$

$$I_{2,h}^{k+1} = \|F_h'(q_k^H)(q_{k+1}^h - q_k^H) + F_h(q_k^H) - g^\delta\|^2$$

⇝ solution of a linear PDE

$$I_{3,h}^{k+1} = \|F_h(q_k^H) - g^\delta\|^2$$

⇝ solution of a nonlinear PDE

⇝ all-at once formulations

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$I_{1,h}^{k+1} = \|F_h'(q_k^H)(q_{k+1}^h - q_k^H) + F_h(q_k^H) - g^\delta\|^2 + \alpha_k \|q_{k+1}^h - q_0\|^2$$

$$I_{2,h}^{k+1} = \|F_h'(q_k^H)(q_{k+1}^h - q_k^H) + F_h(q_k^H) - g^\delta\|^2$$

⇝ solution of a linear PDE

$$I_{3,h}^{k+1} = \|F_h(q_k^H) - g^\delta\|^2$$

⇝ solution of a nonlinear PDE

⇝ all-at once formulations

A Least Squares Formulation (I)

$$\left.\begin{array}{llcl} \text{measurements:} & Cu & = & g \text{ in } G \\ \text{PDE:} & A(q,u) & = & f \text{ in } V^* \end{array}\right\} \Leftrightarrow: \ \mathbf{F}(u,q) = \mathbf{g}$$

$\rightsquigarrow$ Iteratively Regularized Gauss-Newton Method IRGNM

$$\begin{pmatrix} q^\delta_{k+1} \\ u^\delta_{k+1} \end{pmatrix} = \begin{pmatrix} q^\delta_k \\ u^\delta_k \end{pmatrix} - \left(\mathbf{F}'(q^\delta_k, u^\delta_k)^* \mathbf{F}'(q^\delta_k, u^\delta_k) + \alpha_k \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix}\right)^{-1} \times \left(\mathbf{F}'(q^\delta_k, u^\delta_k)^* (\mathbf{F}(q^\delta_k, u^\delta_k) - \mathbf{g}^\delta) + \alpha_k \begin{pmatrix} q^\delta_k - q_0 \\ 0 \end{pmatrix}\right)$$

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or equivalently: unconstrained quadratic minimization

$$\begin{pmatrix} q^\delta_{k+1} \\ u^\delta_{k+1} \end{pmatrix} = \arg\min_{q,u} \|A'_q(q_k,u_k)(q-q_k) + A'_u(q_k,u_k)(u-u_k) + A(q_k,u_k) - f\|^2_{V^*} + \|Cu - g^\delta\|^2_G + \alpha_k\|q-q_0\|^2_Q$$

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A Least Squares Formulation (II)

$$
\begin{aligned}
&(q_{k+1}^\delta, u_{k+1}^\delta) \\
&\quad = \arg\min_{q,u} \quad \|L(q-q_k) + K(u-u_k) + A(q_k,u_k) - f\|_{V^*}^2 \\
&\qquad\qquad\qquad + \|Cu - g^\delta\|_G^2 + \alpha_k \|q - q_0\|_Q^2 \,.
\end{aligned}
$$

with $K = A'_u(q_k,u_k),\ L = A'_q(q_k,u_k)$.

$$
\left.\begin{array}{l} K \text{ regular} \\ \alpha > 0 \end{array}\right\} \Rightarrow \text{ Hessian } \begin{pmatrix} L^*L + \alpha I & L^*K \\ K^*L & C^*C + K^*K \end{pmatrix} \text{ positive definite.}
$$

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&(q^\delta_{k+1}, u^\delta_{k+1}) \\
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&\qquad\qquad\qquad\quad + \|Cu - g^\delta\|^2_G + \alpha_k \|q - q_0\|^2_Q \,.
\end{aligned}
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with $K = A'_u(q_k, u_k)$, $L = A'_q(q_k, u_k)$.

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Least Squares Newton Type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \begin{pmatrix} q_k^\delta \\ u_k^\delta \end{pmatrix} - \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* \mathbf{F}'(q_k^\delta, u_k^\delta) + \alpha_k \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \right)^{-1} \times \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* (\mathbf{F}(q_k^\delta, u_k^\delta) - \mathbf{g}^\delta) + \alpha_k \begin{pmatrix} q_k^\delta - q_0 \\ 0 \end{pmatrix} \right)$$

a posteriori selection of α_k (inexact Newton)

$$\underline{\tilde{\theta}} \| \mathbf{F}(q_k, u_k) - \mathbf{g}^\delta \| \leq \| \mathbf{F}'(q_k, u_k) \begin{pmatrix} q_{k+1} - q_k \\ u_{k+1} - u_k \end{pmatrix} + \mathbf{F}(q_k, u_k) - \mathbf{g}^\delta \| \leq \overline{\tilde{\theta}} \| \mathbf{F}(q_k, u_k) - \mathbf{g}^\delta \|$$

Least Squares Newton Type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \begin{pmatrix} q_k^\delta \\ u_k^\delta \end{pmatrix} - \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* \mathbf{F}'(q_k^\delta, u_k^\delta) + \alpha_k \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \right)^{-1} \times \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* (\mathbf{F}(q_k^\delta, u_k^\delta) - \mathbf{g}^\delta) + \alpha_k \begin{pmatrix} q_k^\delta - q_0 \\ 0 \end{pmatrix} \right)$$

a posteriori selection of α_k (inexact Newton)

$$\underline{\tilde{\theta}} \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\| \leq \left\|\mathbf{F}'(q_k, u_k) \begin{pmatrix} q_{k+1} - q_k \\ u_{k+1} - u_k \end{pmatrix} + \mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\right\| \leq \overline{\tilde{\theta}} \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\|$$

a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \ : \ \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\| \leq \tau\delta\}$$

Least Squares Newton Type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \begin{pmatrix} q_k^\delta \\ u_k^\delta \end{pmatrix} - \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* \mathbf{F}'(q_k^\delta, u_k^\delta) + \alpha_k \begin{pmatrix} I & 0 \\ 0 & 0 \end{pmatrix} \right)^{-1}$$

$$\times \left(\mathbf{F}'(q_k^\delta, u_k^\delta)^* (\mathbf{F}(q_k^\delta, u_k^\delta) - \mathbf{g}^\delta) + \alpha_k \begin{pmatrix} q_k^\delta - q_0 \\ 0 \end{pmatrix} \right)$$

a posteriori selection of α_k (inexact Newton)

$$\underline{\tilde{\theta}} \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\| \leq \left\|\mathbf{F}'(q_k, u_k) \begin{pmatrix} q_{k+1} - q_k \\ u_{k+1} - u_k \end{pmatrix} + \mathbf{F}(q_k, u_k) - \mathbf{g}^\delta \right\| \leq \bar{\tilde{\theta}} \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\|$$

a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \; : \; \|\mathbf{F}(q_k, u_k) - \mathbf{g}^\delta\| \leq \tau\delta\}$$

Convergence Analysis $\rightsquigarrow$ Choice of QoI

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3,4\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$I_{1,h}^{k+1} = \|\mathbf{F}_h'(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\| + \alpha_k \|q_{k+1}^h - q_0\|^2$$

$$I_{2,h}^{k+1} = \|\mathbf{F}_h'(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\|$$

$$I_{3,h}^{k+1} = \|\mathbf{F}_h(q_k^H, u_k^H) - \mathbf{g}^\delta\|^2$$

$$I_{4,h}^{k+1} = \|\mathbf{F}_h(q_{k+1}^h, u_{k+1}^h) - \mathbf{g}^\delta\|^2$$

Theorem [BK&Kirchner&Veljovic&Vexler'12]:
Let $(*)$ hold with η_i^{k+1} sufficiently small. Then $q_{h,k_*}^\delta \to q^\dagger$ as $\delta \to 0$.
(Optimal rates under source conditions of logarithmic/Hölder type).

Convergence Analysis ⇝ Choice of QoI

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$I_{1,h}^{k+1} = \|\mathbf{F}'_h(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\| + \alpha_k \|q_{k+1}^h - q_0\|^2$$

$$I_{2,h}^{k+1} = \|\mathbf{F}'_h(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\|$$

⇝ evaluate residual of a linear PDE

$$I_{3,h}^{k+1} = \|\mathbf{F}_h(q_k^H, u_k^H) - \mathbf{g}^\delta\|^2$$

⇝ evaluate residual of a nonlinear PDE

Remarks

- Also works in Banach spaces with general data misfit and (convex) regularization term [5]

$$J_k(q,u) = \mathcal{S}_1(Cu, g^\delta) + \mathcal{S}_2(L_k(q-q_k) + K_k(u-u_k) + A(q_k,u_k), f) + \alpha_k \mathcal{R}(q,u)$$

- Use this to avoid equal treatment of both equations in

$$\left.\begin{array}{llcl} \text{measurements:} & Cu & = & g \text{ in } G \\ \text{PDE:} & A(q,u) & = & f \text{ in } V^* \end{array}\right\}$$

by least-squares approach.
("more confidence in PDE than in measurements $g^\delta \approx g$")

[5] see, e.g., the PhD thesis of Frank Werner 2012 (Thorsten Hohage) for the continuous setting.

A Generalized Newton Method (I)

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|_G^2 + \frac{\alpha_k}{2}\|q - q_0\|_Q^2$$
$$\text{s.t.} \quad A'_q(q_k^\delta, u_k^\delta)(q - q_k^\delta) + A'_u(q_k^\delta, u_k^\delta)(u - u_k^\delta) + A(q_k^\delta, u_k^\delta) = f$$

or equivalently (by exactness of l^1 penalty):

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|_G^2 + \frac{\alpha_k}{2}\|q - q_0\|_Q^2$$
$$+\rho\|A'_q(q_k, u_k)(q - q_k) + A'_u(q_k, u_k)(u - u_k) + A(q_k, u_k) - f\|_{V^*}$$

with ρ sufficiently large (but finite).

A Generalized Newton Method (II)

$$
\begin{aligned}
(q_{k+1}^\delta, u_{k+1}^\delta) = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|_G^2 + \frac{\alpha_k}{2}\|q - q_0\|_Q^2 \\
\text{s.t. } L(q - q_k) + K(u - u_k) + A(q_k, u_k) - f = 0
\end{aligned}
$$

with $K = A'_u(q_k, u_k)$, $L = A'_q(q_k, u_k)$.

First order optimality system:

$$
\begin{pmatrix} \alpha_k I & 0 & L^* \\ 0 & C^*C & K^* \\ L & K & 0 \end{pmatrix}
\begin{pmatrix} q_{k+1} \\ u_{k+1} \\ z_{k+1} \end{pmatrix}
=
\begin{pmatrix} \alpha_k q_0 \\ C^* g^\delta \\ Lq_k + Ku_k - A(q_k, u_k) + f \end{pmatrix}
$$

A Generalized Newton Method (II)

$$(q^\delta_{k+1}, u^\delta_{k+1}) = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|^2_G + \frac{\alpha_k}{2}\|q - q_0\|^2_Q$$
$$\text{s.t. } L(q - q_k) + K(u - u_k) + A(q_k, u_k) - f = 0$$

with $K = A'_u(q_k, u_k)$, $L = A'_q(q_k, u_k)$.

First order optimality system:

$$\begin{pmatrix} \alpha_k I & 0 & L^* \\ 0 & C^*C & K^* \\ L & K & 0 \end{pmatrix} \begin{pmatrix} q_{k+1} \\ u_{k+1} \\ z_{k+1} \end{pmatrix} = \begin{pmatrix} \alpha_k q_0 \\ C^* g^\delta \\ Lq_k + Ku_k - A(q_k, u_k) + f \end{pmatrix}$$

Generalized Newton Type Regularization and the Discrepancy Principle

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|_G^2 + \frac{\alpha_k}{2}\|q - q_0\|_Q^2$$

s.t. $A'_q(q_k^\delta, u_k^\delta)(q - q_k^\delta) + A'_u(q_k^\delta, u_k^\delta)(u - u_k^\delta) + A(q_k^\delta, u_k^\delta) = f$

a posteriori selection of α_k

$$\underline{\tilde{\theta}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|) \leq \|C(u_{k+1}) - g^\delta\|_G^2$$
$$\leq \tilde{\tilde{\overline{\theta}}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|)$$

Generalized Newton Type Regularization and the Discrepancy Principle

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \arg\min_{q,u} \tfrac{1}{2}\|Cu - g^\delta\|_G^2 + \tfrac{\alpha_k}{2}\|q - q_0\|_Q^2$$

$$\text{s.t.} \quad A'_q(q_k^\delta, u_k^\delta)(q - q_k^\delta) + A'_u(q_k^\delta, u_k^\delta)(u - u_k^\delta) + A(q_k^\delta, u_k^\delta) = f$$

a posteriori selection of α_k

$$\underline{\tilde{\theta}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|) \le \|C(u_{k+1}) - g^\delta\|_G^2 \le \bar{\tilde{\theta}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|)$$

a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \;:\; \|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_{k+1}) - f\| \le \tau^2\delta^2\}$$

Generalized Newton Type Regularization and the Discrepancy Principle

$$\begin{pmatrix} q_{k+1}^\delta \\ u_{k+1}^\delta \end{pmatrix} = \arg\min_{q,u} \frac{1}{2}\|Cu - g^\delta\|_G^2 + \frac{\alpha_k}{2}\|q - q_0\|_Q^2$$

$$\text{s.t.} \quad A'_q(q_k^\delta, u_k^\delta)(q - q_k^\delta) + A'_u(q_k^\delta, u_k^\delta)(u - u_k^\delta) + A(q_k^\delta, u_k^\delta) = f$$

a posteriori selection of α_k

$$\underline{\tilde{\theta}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|) \leq \|C(u_{k+1}) - g^\delta\|_G^2 \leq \bar{\tilde{\theta}}(\|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_k) - f\|)$$

a posteriori selection of k_* (discrepancy principle)

$$k^* = \min\{k \in \mathbb{N} \ : \ \|C(u_k) - g^\delta\|^2 + \rho\|A(q_k, u_{k+1}) - f\| \leq \tau^2\delta^2\}$$

Convergence Analysis ⇝ Choice of QoI

$$|I_{i,h}^{k+1} - I_i^{k+1}| \leq \eta_i^{k+1}\,, \quad i \in \{1,2,3\} \qquad (*)$$

where for fixed q_k^H and variable q_{k+1}^h, w_k^h, u_k^h, u_{k+1}^h

$$\begin{aligned}
I_{1,h}^{k+1} &= \|C(u_{k+1}^h) - g^\delta\|_G^2 + \alpha_k \|q_{k+1}^h - q_0\|_Q^2 \\
I_{2,h}^{k+1} &= \|C(u_{k+1}^h) - g^\delta\|_G^2 \\
I_{3,h}^{k+1} &= \|C(u_k^h) - g^\delta\|^2 + \rho \|A(q_k^H, u_k^H) - f\| \\
I_{4,h}^{k+1} &= \|C(u_{k+1}^h) - g^\delta\|_G^2 + \rho \|A(q_{k+1}^H, u_{k+1}^h) - f\|_{V^*}
\end{aligned}$$

Theorem [BK&Kirchner&Veljovic&Vexler'12]:
Let $(*)$ hold with η_i^{k+1} sufficiently small. Then $q_{h,k_*}^\delta \to q^\dagger$ as $\delta \to 0$.
(Optimal rates under source conditions of logarithmic/Hölder type).

Idea of proof: equivalence to exact l^1 penalty formulation

Outlook

- $\rightarrow$ other regularization methods: e.g., regularization by discretization
- $\rightarrow$ other parameter choice strategies: e.g., balancing principle
- $\rightarrow$ other noise models: e.g., Poisson noise
- $\rightarrow$ other PDEs: e.g., time adaptivity
- $\rightarrow$ other error estimators: e.g., functional estimators $\rightsquigarrow$ residuals
- $\rightarrow$ ...

Thank you for your attention!