Adaptive discretization strategies for the identification of distributed parameters in partial differential equations

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joint work with

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Overview

- motivation: parameter identification in PDEs
- ideas on adaptivity for inverse problems
- principles of goal oriented error estimators
- Tikhonov & discrepancy principle
- regularized Newton iterations & discrepancy principle
- outlook

Motivation: Parameter Identification in PDEs

- instability: amplification of numerical errors
- computational effort:
  - large scale: several PDE solves per regularized inversion
  - several reg. inversions to determine regularization parameter

Example $-\Delta u = q$:
refine grid for u and q:
- at jumps or large gradients or
- at locations with large error contribution

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(example $-\nabla q(u)\nabla u) = f$)

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Regularization of Inverse Problems

- unstable operator equation: $F(q) = g$ with $F : q \mapsto u$ or $C(u)$
- solution $q = F^{-1}(g)$ does not depend continuously on g
  i.e., $\left(\forall (g_n), g_n \to g \;\not\Rightarrow\; q_n := F^{-1}(g_n) \to F^{-1}(g)\right)$

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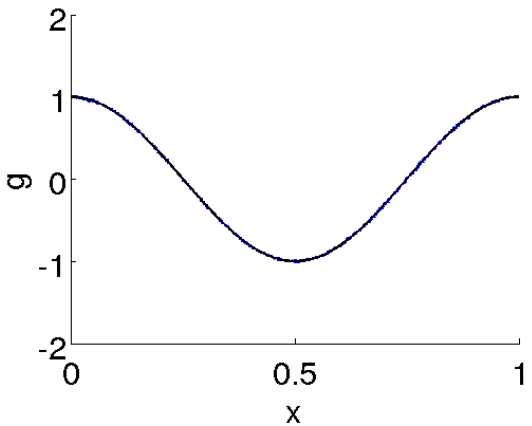
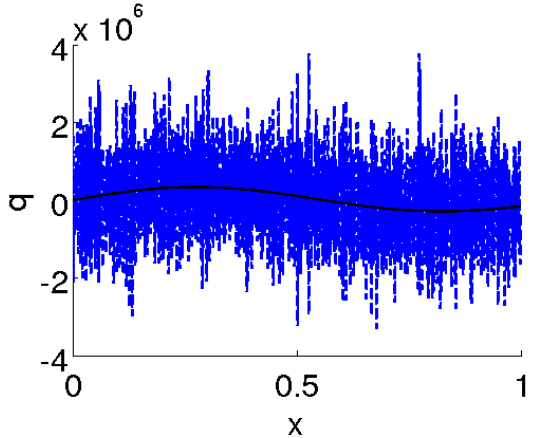
An Example

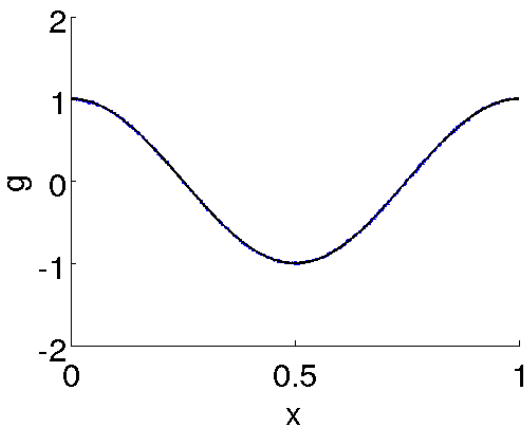
(Identification of a source term in a 1-d differential equation, $\delta = 1\%$)

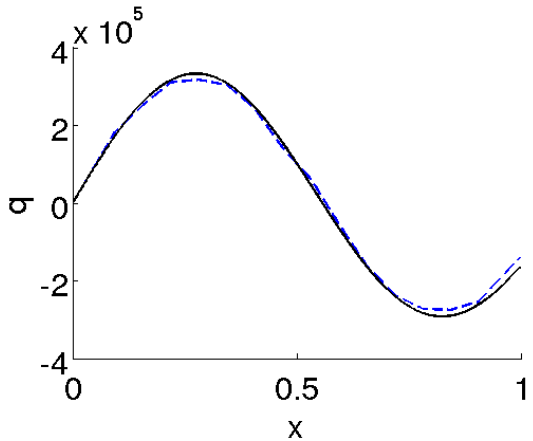
exact and noisy data g, g^δ exact q vs $\tilde{q}$ with $\|F(\tilde{q}) - g^\delta\| = 1.e-14$





exact and noisy data g, g^δ exact q vs $\tilde{q}$ with $\|F(\tilde{q}) - g^\delta\| = 2\delta$





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- *regularization method*:
  family $(R_\alpha)_{\alpha>0}$ with parameter choice $\alpha = \alpha(g^\delta, \delta)$
  such that worst case convergence as $\delta \to 0$:

$$\sup_{\|g^\delta - g\| \leq \delta} \|R_{\alpha(g^\delta,\delta)}(g^\delta) - F^{-1}(g)\| \to 0 \text{ as } \delta \to 0$$

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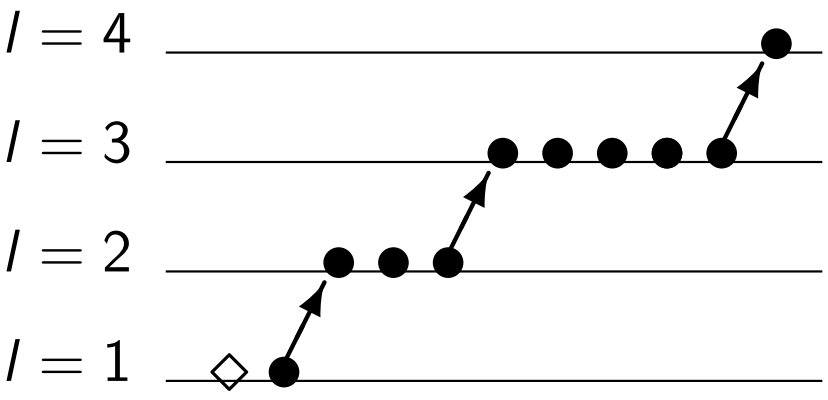
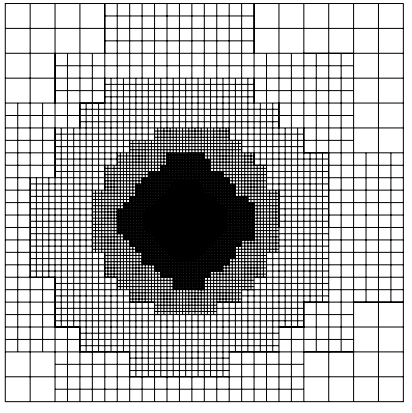
Efficient Methods for PDEs

multilevel iteration:



start with coarse discretization
refine successively

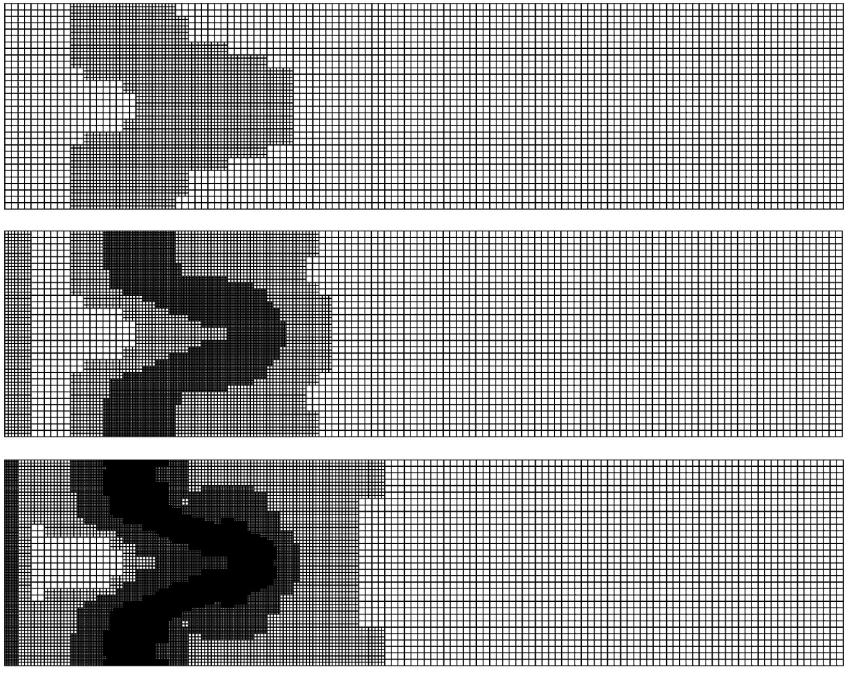
adaptive discretization:



coarse discretization where possible
fine grid only where necessary

Efficient Methods for PDEs

combined multilevel adaptive strategy:



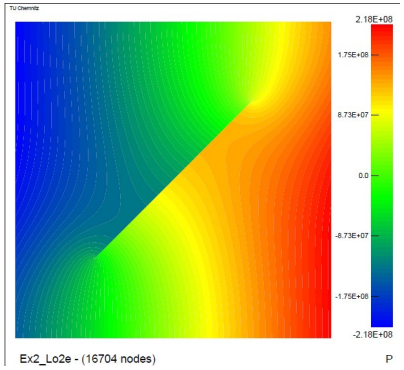
courtesy to [R.Becker&M.Braack&B.Vexler, App.Num.Math., 2005]

start on coarse grid

sucessive adaptive refinement

An Example: Crack Identification in Piezoelectric Ceramics

$$
\begin{aligned}
-DIV\,\vec{\sigma} &= 0 && \text{in } \Omega \\
-\nabla D &= 0 && \text{in } \Omega \\
N^T\vec{\sigma} &= 0 && \text{on } \partial\Omega \cup \Sigma \\
\phi &= \phi^e && \text{on } \Gamma_e = \partial\Omega \\
\vec{n}\cdot D &= 0 && \text{on } \Sigma
\end{aligned}
$$



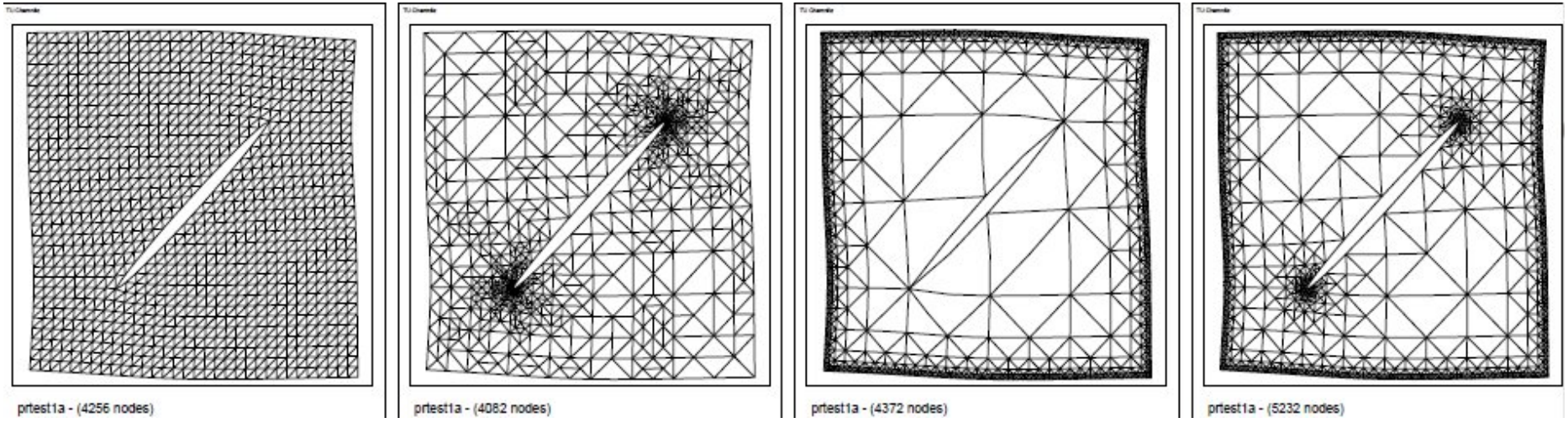
electric potential distribution

$$
\begin{aligned}
\vec{\sigma} &= \mathbf{c}^E DIV^T\vec{d} + \mathbf{e}^T\nabla\phi \ldots \text{stress} \\
\vec{D} &= \mathbf{e}DIV^T\vec{d} - \varepsilon^S\nabla\phi \ldots \text{dielectr. displacement} \\
DIV^T &= \tfrac{1}{2}(\nabla + \nabla^T), \quad \mathbf{c}^E, \mathbf{e}, \varepsilon^S \ldots \text{ material tensors} \\
\vec{d} &= (d_x, d_y, d_z) \ldots \text{mech. displacement} \\
\phi &\quad \ldots \text{electr. potential}
\end{aligned}
$$

Given additional boundary measurements $q^e = \vec{n}\cdot D$ and/or $\vec{d}$ on $\partial\Omega$, determine Σ. [Steinhorst&BK 2011]

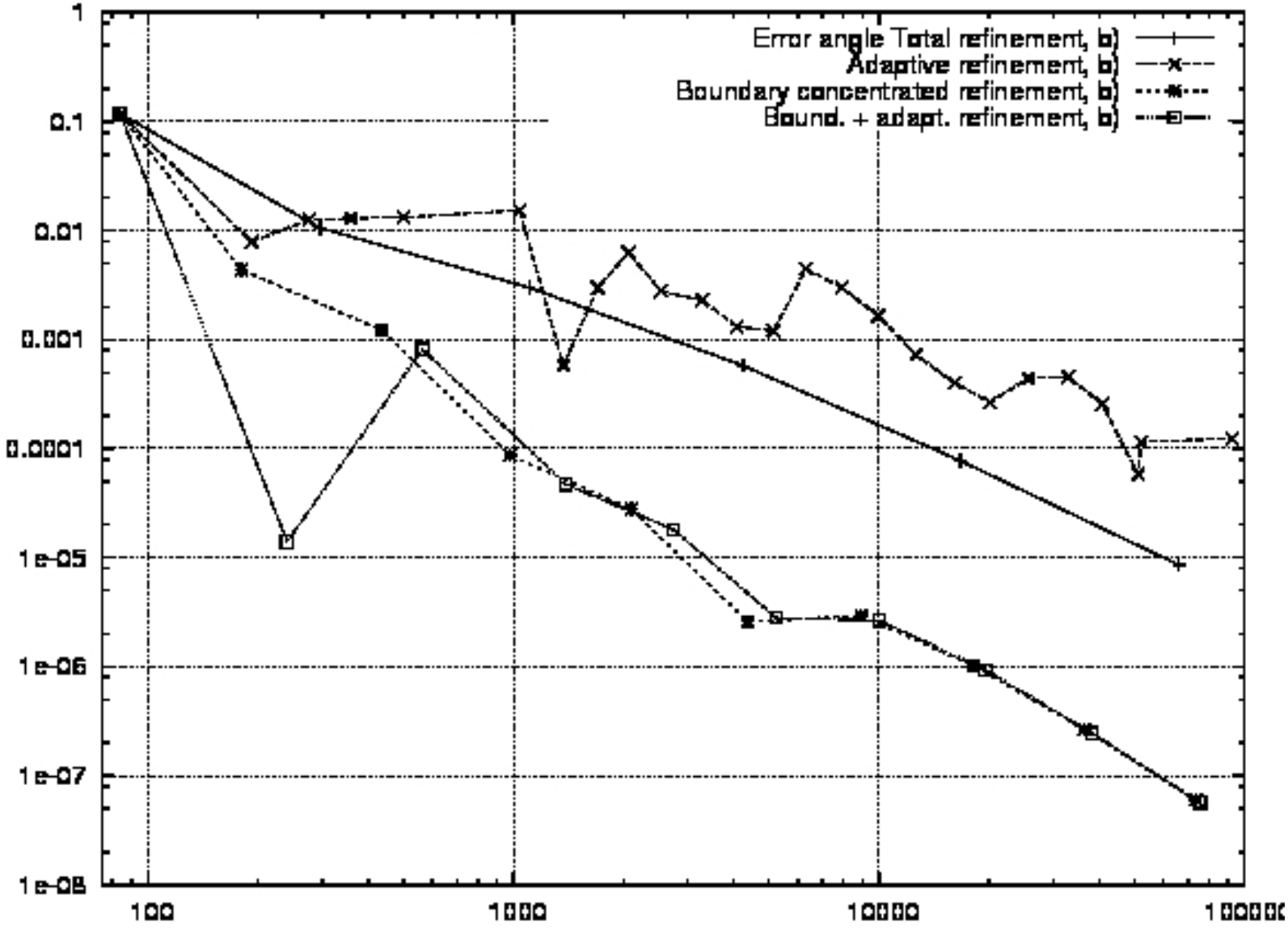
Different Refinement Strategies

$\sim$ 4000 nodes with ...

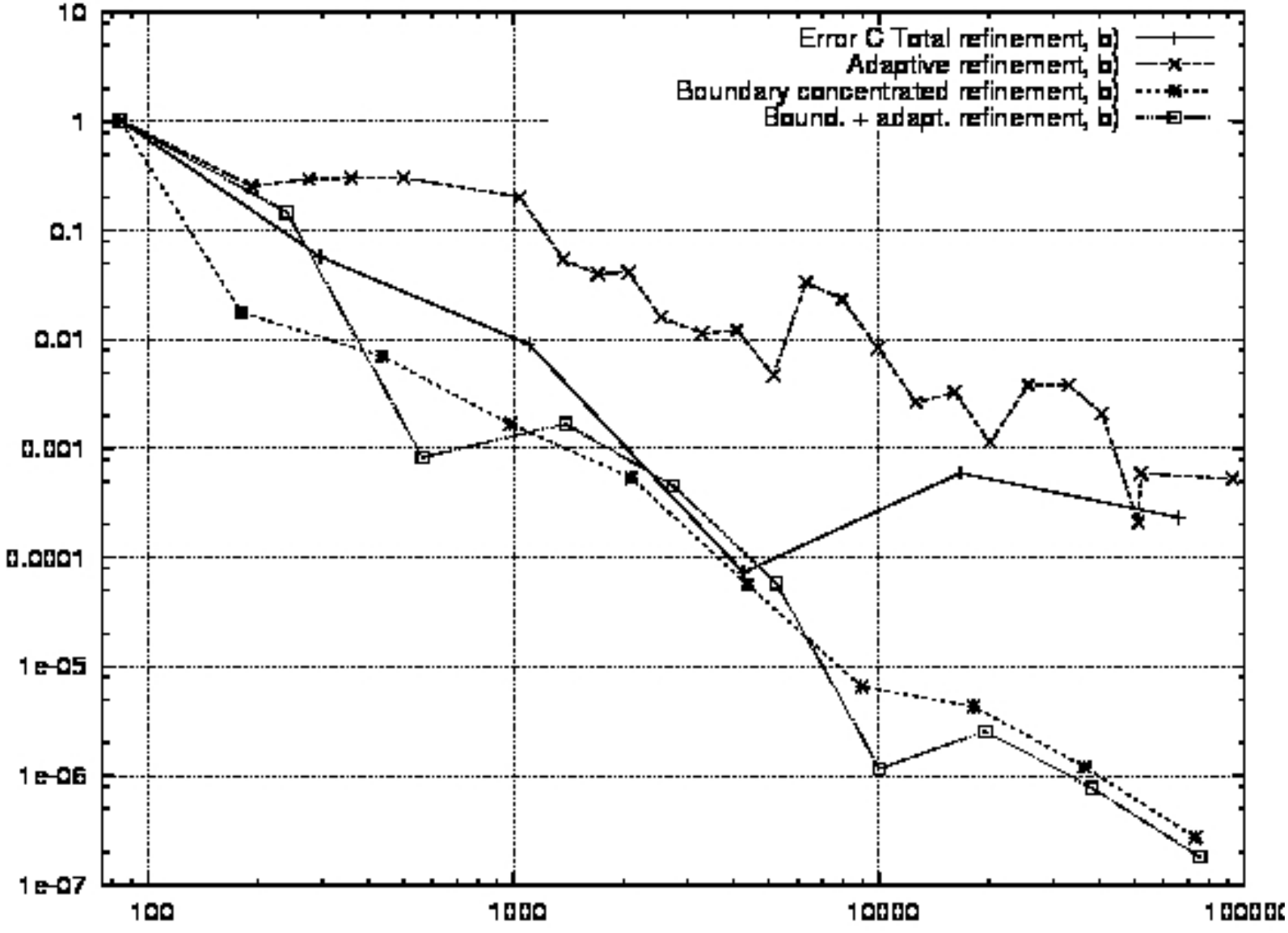


uniform | adaptive (residual based) | boundary concentrated | adaptive & bndy conc.

Error in crack plane angle with different refinement strategies:



Error in crack plane offset with different refinement strategies:



Errors with Different Refinement Strategies

$\sim$ 20.000 nodes:

	uniform	adaptive (residual based)	boundary concentrated	adaptive & bndy conc.
error angle	0.8 e-4	0.3 e-3	1.e-6	1.e-6
error offset	0.7 e-3	0.3 e-2	0.5e-5	0.3e-5

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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.:
  Tikhonov with BV type regularization:
  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:
  refinement and coarsening indicators
- Becker&Vexler'04, Griesbaum&BK&Vexler'07, Bangerth'08, BK&Kirchner&Vexler'11, BK&Kirchner&Veljovic&Vexler'11:
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Parameter identification as nonlinear operator equation

$$F(q) = g$$

$g^\delta \approx g \ldots$ given data; noise level $\delta \geq \|g^\delta - g\|$

$F \ldots$ forward operator: $F(q) = (C \circ S)(q) = C(u)$

where $C \ldots$ observation operator

where $S \ldots$ parameter-to-solution operator, i.e., $u = S(q)$ solves

$$A(q, u)(v) = (f, v) \quad \forall v \in V \quad \ldots \text{ PDE in weak form}$$

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

Tikhonov Regularization and the Discrepancy Principle

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

$$\Leftrightarrow$$

$$\begin{aligned} &\text{Minimize} \quad J_\alpha(q,u) = \|C(u) - g^\delta\|^2 + \alpha\|q\|^2 \text{ over } q \in Q\,,\ u \in V \\ &\text{under the constraint} \quad A(q,u)(v) = (f,v) \quad \forall v \in V \end{aligned}$$

Tikhonov Regularization and the Discrepancy Principle

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

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

Convergence analysis: [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]

$$\begin{aligned} &\text{Minimize} \quad J(q,u) \quad \text{over } q \in Q\,,\ u \in V \\ &\text{under the constraints} \quad A(q,u)(v) = f(v) \quad \forall v \in V\,, \end{aligned}$$

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:

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

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

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

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 separately for $q \in Q_h$, $u \in V_h$, $z \in V_h$, ...

Choice of Quantity of Interest ?

aim: recover infinite dimensional convergence results
for Tikhonov + discrepancy principle
in the adaptively discretized setting

challenge: carrying over infinite dimensional results is

. . . straightforward if we can guarantee smallness of operator norm $\|F_h - F\|$

$\rightsquigarrow$ huge number of quantities of interest!

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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 for

$$I(q,u) := \|C(u) - g^\delta\|_G^2 = \|F(q) - g^\delta\|_G^2$$

$$\underline{\tau}^2\delta^2 \leq I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) \leq \overline{\tau}\delta^2$$

(i) If additionally

$$|I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) - I(q^\delta_{\alpha_*}, u^\delta_{\alpha_*})| \leq cI(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*})$$

for some sufficiently small constant $c > 0$ then $q^\delta_{\alpha_*} \to q^\dagger$ as $\delta \to 0$.

Optimal rates under source conditions (logarithic/Hölder).

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$$\underline{\tau}^2\delta^2 \leq I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) \leq \overline{\tau}\delta^2$$

(ii) If additionally for

$$I_2(q,u) := J_\alpha(q,u)$$

$$|I_2(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) - I_2(q^\delta_{\alpha_*}, u^\delta_{\alpha_*})| \leq \sigma\delta^2$$

for some constant $C > 0$ with $\underline{\tau}^2 \geq 1 + \sigma$, then $q^\delta_{h,\alpha_*} \to q^\dagger$ as $\delta \to 0$.
Optimal rates under source conditions (logarithic/Hölder).

see also [Neubauer&Scherzer 1990]

J as quantity of interest $\rightsquigarrow$ [Becker&Kapp&Rannacher'00], [Becker&Rannacher'01]

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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 for

$$I(q,u) := \|C(u) - g^\delta\|_G^2 = \|F(q) - g^\delta\|_G^2$$

$$\underline{\tau}^2\delta^2 \leq I(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) \leq \overline{\tau}\delta^2$$

(ii) If additionally for

$$I_2(q,u) := J_\alpha(q,u)$$

$$|I_2(q^\delta_{h,\alpha_*}, u^\delta_{h,\alpha_*}) - I_2(q^\delta_{\alpha_*}, u^\delta_{\alpha_*})| \leq \sigma\delta^2$$

for some constant $C > 0$ with $\underline{\tau}^2 \geq 1 + \sigma$, then $q^\delta_{h,\alpha_*} \to q^\dagger$ as $\delta \to 0$.
Optimal rates under source conditions (logarithic/Hölder).

see also [Neubauer&Scherzer 1990]

J as quantity of interest $\rightsquigarrow$ [Becker&Kapp&Rannacher'00], [Becker&Rannacher'01]

Efficient Computation of α $\rightsquigarrow$ Choice of QoI

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

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

$\rightsquigarrow$ 1-d nonlinear equation

$\rightsquigarrow$ solve by Newton's method

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

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

Define

$$i(\tfrac{1}{\alpha}) := I(q,u) := \|C(u) - g^\delta\|_G^2 = \|F(q) - g^\delta\|_G^2$$

$$I_2(q,u) := i'(\tfrac{1}{\alpha})$$

β_* sol. to $i(\beta_*) = \tau^2\delta^2$ (discr.princ.) $\quad \beta^{k+1} = \beta^k - \dfrac{i_h^k - \tau^2\delta^2}{i'^k_h}$ (Newton)

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

$$|i(\beta^k) - i_h^k| \le \varepsilon^k\,, \qquad |i'(\beta^k) - i'^k_h| \le \varepsilon'^k\,,$$

$\varepsilon^k, \varepsilon'^k$ sufficiently small.
Then β^k satisfies quadratic convergence estimate and

$$(\tau^2 - \tilde{\tau}^2)\delta^2 \le i(\beta^{k_*}) \le (\tau^2 + \tilde{\tau}^2)\delta^2$$

Remarks

- computation of error estimators for $i(\beta)$:
  just one more SQP type step;
- evaluation of $i'(\beta)$:
  can be extracted from quantities computed for error estimators for $i(\beta)$
- error estimators for $i'(\beta)$:
  stationary point of another auxiliary functional

Newton type Regularization and the Discrepancy Principle

Newton's method for $F(q) = g$:

$$q_{k+1} = q_k - F'(q_k)^{-1}(F(q_k) - g)$$

Iteratively Regularized Gauss-Newton Method IRGNM

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

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or equivalently

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

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Newton type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

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

or equivalently

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

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

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

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Newton type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

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

a posteriori selection of α_k (inexact Newton)

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

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Iteratively Regularized Gauss-Newton Method IRGNM

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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

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

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Convergence Analysis $\rightsquigarrow$ Choice of QoI

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

by goal oriented adaptivity, where

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

Theorem [BK&Kirchner&Veljovic&Vexler'11]:
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 (logarithic/Hölder).

However...
need to solve

$$
\begin{aligned}
2\alpha_k(q_{k+1}-q_0)+A'_q(q_k^H,u_{old})^*v^1 &= 0\\
2C^*(C(w+u_{old})-g^\delta)+A''_{uu}(q_k^H,u_{old})[w,\cdot](v^1)&\\
+A''_{qu}(q_k^H,u_{old})[q-q_k^H,\cdot](v^1)+A'_u(q_k^H,u_{old})^*v^2 &= 0\\
2C^*(C(w+u_{old})-g^\delta)+A'_u(q_k^H,u_{old})^*v^1 &= 0\\
A'_u(q_k^H,u_{old})[w]+A'_q(q_k^H,u_{old})[q-q_k^H] &= 0\\
A(q_k^H,u_{old})-f &= 0\\
A(q,u)-f &= 0
\end{aligned}
$$

- second order derivatives of PDEs appear
- nonlinear PDEs have to be solved

An all-at once Formulation (I)

$$\begin{array}{lrcl} \text{measurements:} & C(u) & = & g \text{ in } G \\ \text{PDE:} & A(q,u) & = & f \text{ in } V^* \end{array} \quad \text{i.e., } \mathbf{F}(u,q) = \mathbf{g}$$

$\rightsquigarrow$ Iteratively Regularized Gauss-Newton Method IRGNM

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

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

or equivalently: unconstrained quadratic minimization

$$(q_{k+1}^\delta, u_{k+1}^\delta)$$
$$= \arg\min_{q,u} \quad \|A_q'(q_k,u_k)(q-q_k) + A_u'(q_k,u_k)(u-u_k) + A(q_k,u_k) - f\|_{V^*}^2$$
$$+ \|Cu - g^\delta\|_G^2 + \alpha_k \|q - q_0\|_Q^2 \,.$$

An all-at once Formulation (I)

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$$+ \|Cu - g^\delta\|_G^2 + \alpha_k \|q - q_0\|_Q^2 .$$

see also [Burger&Mühlhuber'02]: SQP type approach

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

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$$(q_{k+1}^\delta, u_{k+1}^\delta)$$
$$= \arg\min_{q,u} \quad \|A_q'(q_k,u_k)(q-q_k) + A_u'(q_k,u_k)(u-u_k) + A(q_k,u_k) - f\|_{V^*}^2$$
$$+ \|Cu - g^\delta\|_G^2 + \alpha_k \|q - q_0\|_Q^2 \,.$$

see also [Burger&Mühlhuber'02]: SQP type approach

An all-at once Formulation (II)

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

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

K regular $\Rightarrow$ Hessian $\begin{pmatrix} L^*L + \alpha_k I & L^*K \\ K^*L & C^*C + K^*K \end{pmatrix}$ positive definite.

An all-at once 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 \,.
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K regular $\Rightarrow$ Hessian $\begin{pmatrix} L^*L + \alpha_k I & L^*K \\ K^*L & C^*C + K^*K \end{pmatrix}$ positive definite.

First order optimality system:

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

An all-at once Formulation (II)

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

$$
K \text{ regular} \quad \Rightarrow \quad \text{Hessian} \begin{pmatrix} L^*L + \alpha_k I & L^*K \\ K^*L & C^*C + K^*K \end{pmatrix} \text{ positive definite.}
$$

First order optimality system:

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

All-At-Once-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)

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

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Iteratively Regularized Gauss-Newton Method IRGNM

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a posteriori selection of k_* (discrepancy principle)

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

All-At-Once-Newton type Regularization and the Discrepancy Principle

Iteratively Regularized Gauss-Newton Method IRGNM

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

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Convergence Analysis $\rightsquigarrow$ Choice of QoI

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

by goal oriented adaptivity, where

$$\begin{aligned}
I_{1,h}^{k+1} &= \|\mathbf{F}_h'(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\| + \alpha_k\|q_{k+1}^h - q_0\|^2 \\
I_{2,h}^{k+1} &= \|\mathbf{F}_h'(q_k^H,u_k^H)\begin{pmatrix} q_{k+1}^h - q_k^H \\ u_{k+1}^h - u_k^H \end{pmatrix} + \mathbf{F}_h(q_k^H,u_k^H) - \mathbf{g}^\delta\| \\
I_{3,h}^{k+1} &= \|\mathbf{F}_h(q_k^H, u_k^H) - \mathbf{g}^\delta\|^2 \\
I_{4,h}^{k+1} &= \|\mathbf{F}_h(q_{k+1}^h, u_{k+1}^h) - \mathbf{g}^\delta\|^2,
\end{aligned}$$

Theorem [BK&Kirchner&Veljovic&Vexler'11]:
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 (logarithic/Hölder).

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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,
\end{aligned}$$

- only first order derivatives of PDEs appear
- only residuals of nonlinear PDEs have to be evaluated

Numerical Tests (Tikhonov & Discrepancy Principle)

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

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

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

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

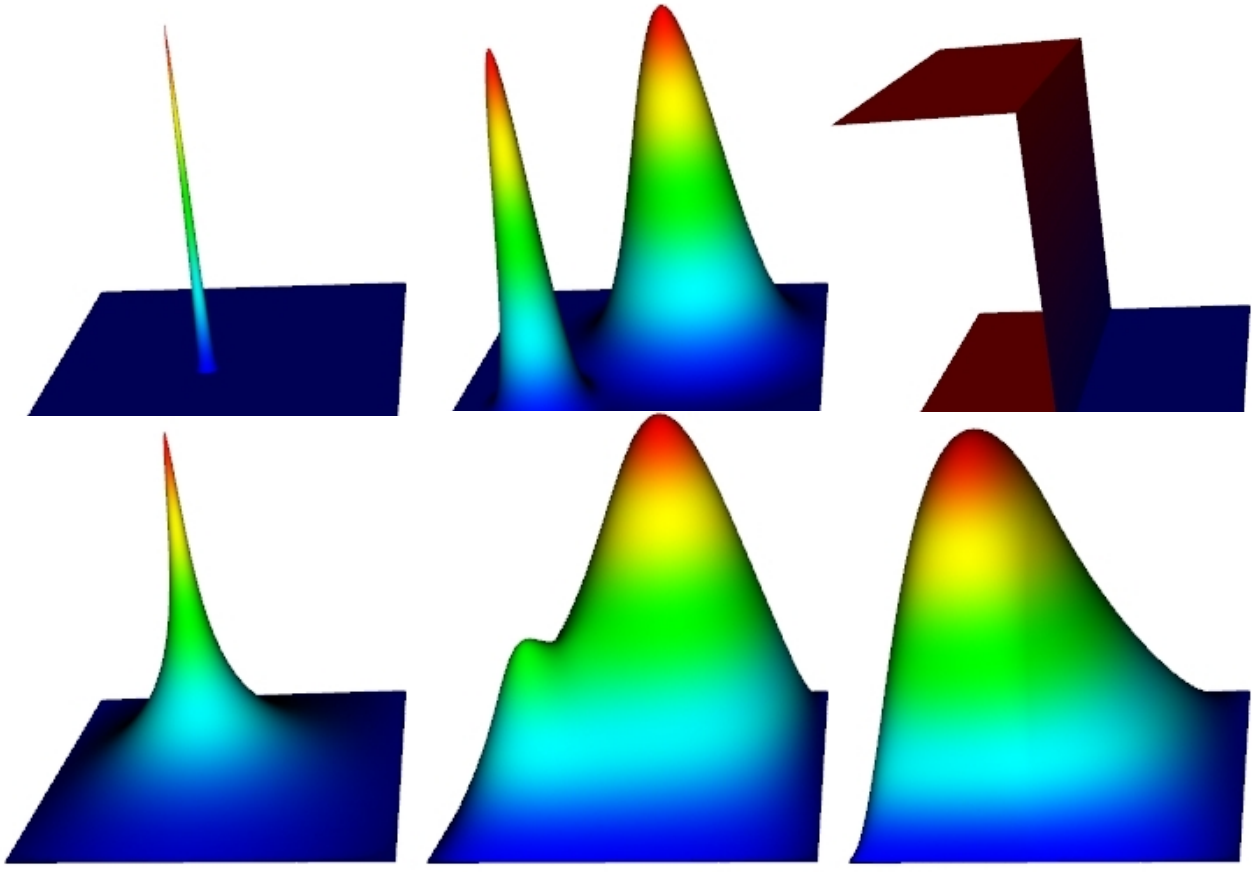
$$(c) \qquad q^\dagger(x,y) = \begin{cases} 1 & x \le \frac{1}{2} \\ 0 & x > \frac{1}{2} \end{cases}$$

Computations with *Gascoigne* and *RoDoBo*.

Numerical Tests

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

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

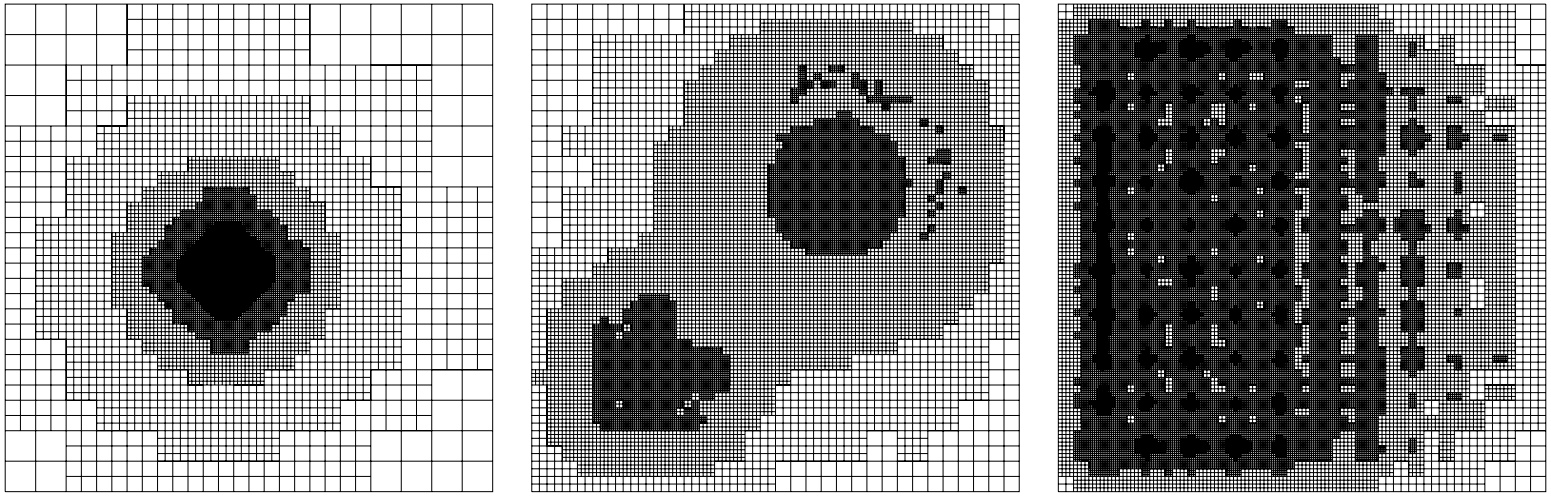


Numerical Results (I)

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%

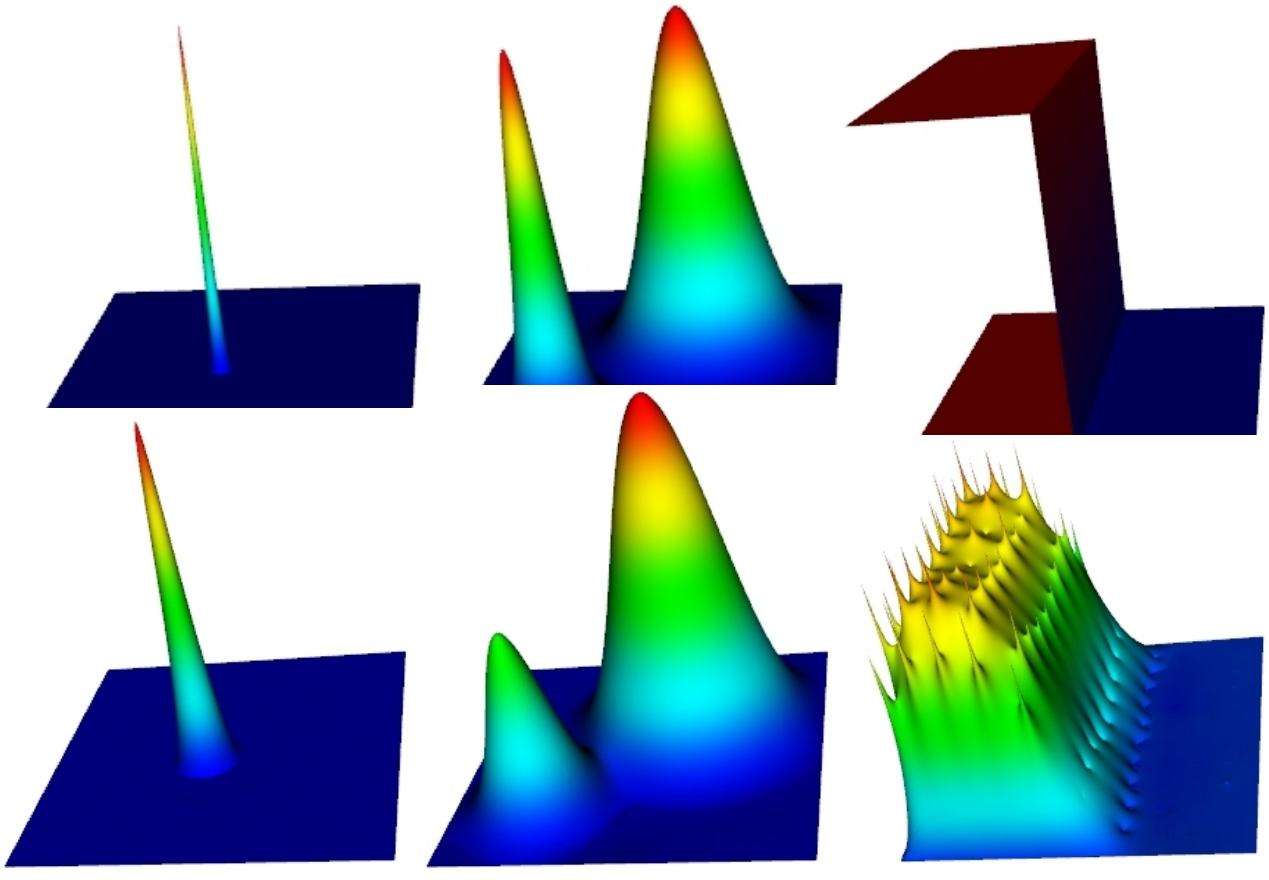
adaptive grids:



Numerical Results (II)

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

computed par. q
(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

Summary and Outlook

- goal oriented error estimators allow to control the error in some quantity of interest
- Tikhonov& discrepancy principle:
  - sufficiently small error in residual norm and Tikh. func.
    $\Rightarrow$ convergence and rates
  - sufficiently small error in residual norm $i(\frac{1}{\alpha})$ and in $i'(\frac{1}{\alpha})$
    $\Rightarrow$ fast convergence of Newton's method for finding α_* (discr.princ.)
    $\rightsquigarrow$ coarse grids at the beginning of Newton's method
    $\rightarrow$ save computational effort
- regularized Newton iterations& discrepancy principle:
  - sufficiently small error in nonlinear residual norm, linearized residual norm, and linearized Tikhonov functional
    $\Rightarrow$ convergence and rates
  - all-at-once-approach

$\rightarrow$ other regularization methods

$\rightarrow$ other parameter choice strategies: e.g., balancing principle

Thank you for your attention!