Solving Inverse Problems
without using Forward Operators

Part I: Reduced versus All-At-Once Formulations

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joint work with

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Woudschoten Conference, October 6, 2021

FWF Der Wissenschaftsfonds.

Modeling - Analysis - Optimization
DOC.FUNDS DOCTORAL SCHOOL

UNIVERSITÄT KLAGENFURT

Outline

- inverse problems
- examples of inverse problems for PDEs
- regularization: Tikhonov, Newton type and Landweber in
  - reduced formulation
  - all-at-once formulation
- numerical results
- time dependent problems

Inverse Problems

identification

↗

Determining causes for observed or desired effects.

↘

optimization

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Inverse probleme are often unstable:
Small perturbations in the data can lead to large deviations in the solution.
$\rightarrow$ regularization necessary

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Determining causes for observed (→ identification) or desired (→ optimization) effects.

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Question of identifiability:
Are the searched for quantities uniquely determined by the given data

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Are the searched for quantities uniquely determined
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Mathematical modeling:
Formulate the underlying physical/biological/economic. . . laws in a
mathematical language (usually partial differential equations PDEs)

Inverse Problems

forward problem:

$$\textbf{cause} \quad \Longrightarrow \quad \textbf{effect}$$

Inverse Problems

forward problem:

cause $\Longrightarrow$ **effect**

inverse problem:

cause $\Longrightarrow$ **effect**

PDE coefficients,
initial conditions,
boundary conditions,
source terms,
shapes,
...

data:

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boundary traces
Dirichlet-to-Neumann map
far field
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examples

Parameter Identification in Differential Equations: Some Examples

- Identify spatially varying coefficients/source a, b, c in linear elliptic boundary value problem on $\Omega \subseteq \mathbb{R}^d$, $d \in \{1,2,3\}$

$$-\nabla(a\nabla u) + cu = b \text{ in } \Omega\,, \qquad \frac{\partial u}{\partial n} = j \text{ on } \partial\Omega\,,$$

from boundary or (restricted) interior observations of u.

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- Identify parameter ϑ in initial value problem for ODE / PDE

  $$\dot{u}(t) = f(t, u(t), \vartheta) \; t \in (0,T)\,, \quad u(0) = u_0$$

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  $y_i = g_i(u(t_i))$, $i \in \{1, \dots, m\}$ or $y(t) = g(t, y(t))$, $t \in (0,T)$

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  applications in population dynamics, epidemology, combustion (parabolic); imaging with waves (hyperbolic),...

Abstract Formulation

Identify parameter q in (PDE or ODE) model

$$A(q, u) = 0$$

from observations of the state u

$$C(u) = y\,,$$

where $q \in X$, $u \in V$, $y \in Y$, $X, V, Y \ldots$ Hilbert (Banach) spaces
$A : X \times V \to W^* \ldots$ differential operator
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(a) reduced approach: operator equation for q

$$F(q) = y,$$

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(b) all-at once approach: observations and model as system for (q,u)

$$\begin{array}{rcl} A(q,u) & = & 0 \text{ in } W^* \\ C(u) & = & y \text{ in } Y \end{array} \quad \Leftrightarrow \quad \mathbf{F}(q,u)=\mathbf{y}$$

The Parameter-to-State Map S in some Examples

- Identify spatially varying coefficients/source a, b, c in

$$-\nabla(a\nabla u) + cu = b \text{ in } \Omega\,, \qquad \frac{\partial u}{\partial n} = 0 \text{ on } \partial\Omega\,,$$

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- generally for model $\quad A(q, u) = 0$:

$$S : q \mapsto u \text{ solving } A(q, S(q)) = 0$$

Motivation for All-at-once Formulation

- well-definedness of parameter-to-state map often requires restrictions on ...
  ... parameters (e.g., $a \geq \underline{a} > 0$, $c \geq 0$ in $-\nabla(a\nabla u) + cu = b$)
  ... models (e.g., monotonicity of ξ in $-\Delta u + \xi(u) = q$)

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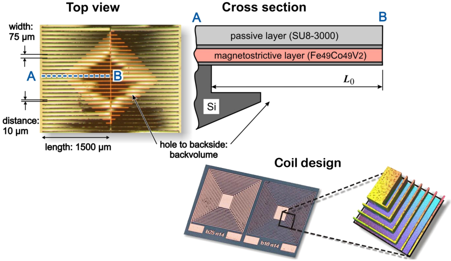
- singular PDEs: parameter-to state map may exist only on a very restricted set

MicroElectroMechanical Systems (MEMS)

acceleration sensors,
microphones, pumps,
loudspeakers, ...

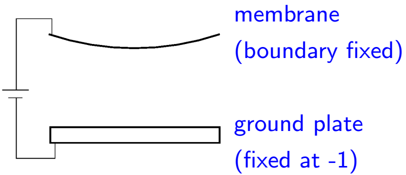


transient MEMS equation

$$u_{tt} + cu_t + du + \rho\Delta^2 u - \eta\Delta u + \frac{b(t)a(x)}{(1+u)^2} = 0$$

u... membrane/beam displacement
$b(t)$... voltage excitation
$a(x)$... dielectric properties

MicroElectroMechanical Systems (MEMS)



$\rightsquigarrow$ control of voltage $b(t)$ and/or design of dielectric properties $a(x)$ to achieve prescribed displacement $y_d(x,t)$;

$$u_{tt} + cu_t + du + \rho\Delta^2 u - \eta\Delta u + \frac{b(t)a(x)}{(1+u)^2} = 0$$

achieve large displacements $|u|$
avoid pull-in instability at $u = -1$!

parameter-to space map exists only on a very restricted set
(too restrictive for certain tracking tasks)

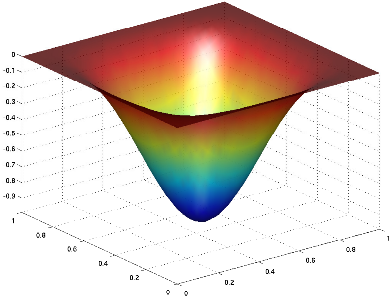
Numerical tests

$$J(a,u) = \frac{1}{2}\,\|u - y_d\|^2_{L^2} + \frac{\alpha}{2}\,\|a\|^2_{L^2}$$

static case

$$-\Delta u + \frac{a(x)}{(1+u)^2} = 0$$

$\Omega = (0,1)^2$, $\alpha = 10^{-6}$, 64×64 grid.

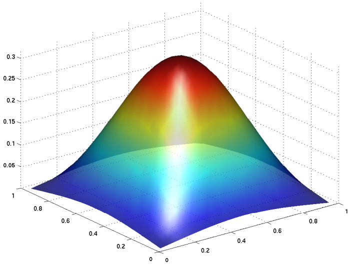


Target y_d (desired maximal deflection: -0.99)

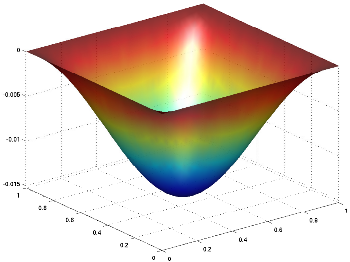
Numerical tests: Using control-to-state map

impose control constraints: $\|a\|_{L^2} \leq \frac{4}{27} = 0.14815\cdots$
to guarantee well-definedness of control-to-state map

optimal control a



optimal state u



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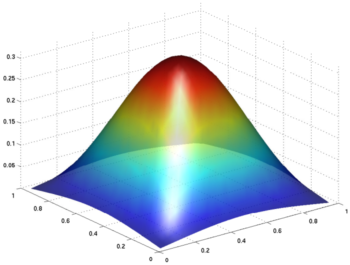

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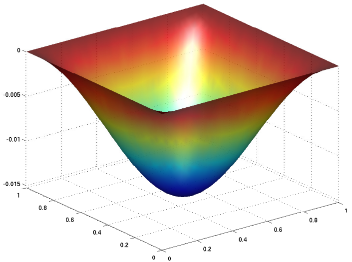
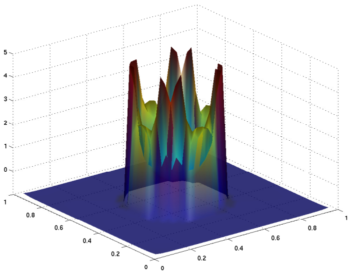


maximal deflection: -0.015!

Numerical tests: Not using control-to-state map

impose pointwise state constraints: $u(x) \geq -0.99$
to avoid singularity

optimal control a



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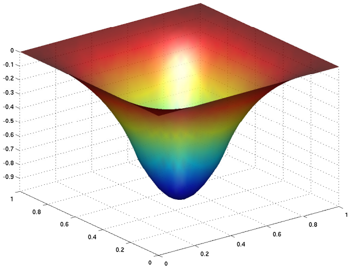
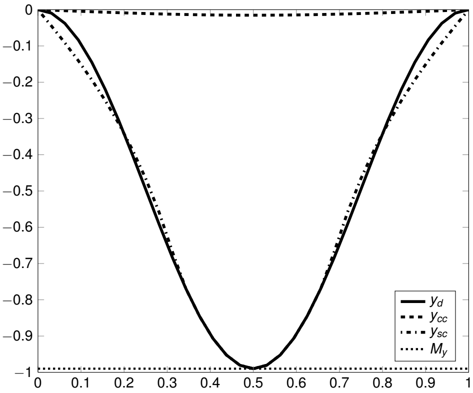


Comparison: with vs without control-to-state map



Cross sections of states for approach with (dashed) and without (dash-dotted) control-to-state map,
as well as target y_d (solid) and bound -0.99 (dotted)

[BK&Clason 2013]

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- it can make a difference in implementation and in the analysis (convergence conditions)
- enables to preserve some causality in parameter identification for time dependent PDEs

reduced formulation

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existence of parameter-to-state map S defined by $A(q,S(q))=0$ requires condition of the Implicit Function Theorem type

$$A_u(q,u)^{-1} \text{ exists and } \|A_u(q,u)^{-1}\|\le C_A$$

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ill-posedness (F not continuously invertible)
only noisy measurements $y^\delta \approx y$ given
$\Rightarrow$ regularization needed

Tikhonov Regularization

regularization functional $\mathcal{R} : X \to \overline{\mathbb{R}}$ (proper, convex)
e.g., $\mathcal{R}(q) := \frac{1}{2}\|q - q_*\|^2$ for some a priori guess q_*;
$\partial\mathcal{R}(q) = q - q_*$

regularization parameter $\alpha > 0$

$$\min_q \frac{1}{2}\|F(q) - y^\delta\|^2 + \alpha\mathcal{R}(q)$$

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[Seidman&Vogel '89, Engl&Kunisch&Neubauer '89,. . .] in Hilbert space
[Burger& Osher'04, Resmerita & Scherzer'06, Scherzer et al. '08, Hofmann&Pöschl&BK&Scherzer '07, Pöschl '09, Flemming '11, Werner '12,. . .] in Banach space

Regularized Gauss-Newton Method

q^k fixed, one Gauss-Newton step:

$$\min_q \tfrac{1}{2}\|F(q^k) + F'(q^k)(q - q^k) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q)$$

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$\tilde{u} = S(q_k), \; u = S(q_k) + S'(q_k)(q - q_k)$

equivalent to

$$\min_{q,u,\tilde{u}} \tfrac{1}{2}\|C(\tilde{u}) + C'(\tilde{u})(u - \tilde{u}) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q)$$

$$\text{s.t. } A(q^k, \tilde{u}) + A'_u(q^k, \tilde{u})(u - \tilde{u}) + A'_q(q^k, \tilde{u})(q - q^k) = 0$$

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[Bakushinskii '92, Hohage '97, BK&Neubauer&Scherzer '97,...] in Hilbert space

e.g., [Bakushinskii&Kokurin'04, BK&Schöpfer&Schuster '08, Jin '12, Hohage&Werner '13,...] in Banach space

Gradient Methods

gradient steps for

$$\min_q \frac{1}{2}\|F(q) - y^\delta\|^2$$

$\rightsquigarrow$ Landweber iteration (steepest descent, mimimal error)

$$q^{k+1} = q^k - \mu^k F'(q^k)^*(F(q^k) - y^\delta)$$

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$$\begin{aligned} q^{k+1} &= q^k - \mu^k F'(q^k)^* \left(F(q^k) - y^\delta\right) \\ &= q^k - \mu^k (C'(S(q^k))S'(q^k))^* \left(C(S(q^k)) - y^\delta\right) \end{aligned}$$

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$$\begin{cases} A(q^k, \tilde{u}) = 0 \\ A'_u(q^k, \tilde{u})^* p = -C'(\tilde{u})^*(C(\tilde{u}) - y^\delta) \end{cases}$$

[Hanke&Neubauer&Scherzer '95,. . .] in Hilbert space
[BK&Schöpfer&Schuster '08,. . .] in Banach space

all-at-once formulation

Abstract Formulation

Identify parameter q in (PDE or ODE) model

$$A(q,u) = 0$$

from observations of the state u

$$C(u) = y\,,$$

(b) all-at once approach: observations and model as system for (q, u)

$$\begin{array}{rcl} A(q,u) &=& 0 \text{ in } W^* \\ C(u) &=& y \text{ in } Y \end{array} \quad \Leftrightarrow \quad \mathbf{F}(q,u) = \mathbf{y}$$

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for other all-at-once type approaches see, e.g.,
[Kupfer & Sachs '92, Shenoy & Heinkenschloss & Cliff '98, Haber & Ascher '01, Burger & Mühlhuber '02,. . .]

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for other all-at-once type approaches see, e.g.,
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ill-posedness (**F** not continuously invertible)
only noisy measurements $y^\delta \approx y$ given
$\Rightarrow$ regularization needed

Tikhonov Regularization

$$\min_{q,u} \frac{1}{2}\|C(u) - y^\delta\|^2 + \frac{1}{2}\|A(q,u)\|^2 + \alpha\mathcal{R}(q) + \alpha\tilde{\mathcal{R}}(u)$$

Tikhonov Regularization

$$\min_{q,u} \tfrac{1}{2}\|C(u) - y^\delta\|^2 + \tfrac{1}{2}\|A(q,u)\|^2 + \alpha\mathcal{R}(q) + \alpha\tilde{\mathcal{R}}(u)$$

first order optimality condition:

$$\begin{aligned} A_q'(q,u)^* A(q,u) + \alpha\partial\mathcal{R}(q) &= 0 \\ C'(u)^*(C(u) - y^\delta) + A_u'(q,u)^* A(q,u) + \alpha\partial\tilde{\mathcal{R}}(u) &= 0 \end{aligned}$$

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first order optimality condition:

$$A'_q(q,u)^* A(q,u) + \alpha\partial\mathcal{R}(q) = 0$$
$$C'(u)^*(C(u) - y^\delta) + A'_u(q,u)^* A(q,u) + \alpha\partial\tilde{\mathcal{R}}(u) = 0$$

i.e., with $p = A(q,u)$:

$$\begin{cases} A(q,u) - p = 0 & \text{...state equation} \\ A'_q(q,u)^* p + \alpha\partial\mathcal{R}(q) = 0 & \text{...gradient equation} \\ A'_u(q,u)^* p + C'(u)^*(C(u) - y^\delta) + \alpha\partial\tilde{\mathcal{R}}(u) = 0 & \text{...adjoint equation} \end{cases}$$

Tikhonov Regularization

$$\min_{q,u} \frac{1}{2}\|C(u) - y^\delta\|^2 + \rho\|A(q,u)\| + \alpha\mathcal{R}(q) + \alpha\tilde{\mathcal{R}}(u)$$

Tikhonov Regularization

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i.e., (exact penalization) with ρ sufficiently large

$$\min_{q,u} \tfrac{1}{2}\|C(u) - y^\delta\|^2 + \alpha\mathcal{R}(q) + \alpha\tilde{\mathcal{R}}(u) \text{ s.t. } A(q,u) = 0$$

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Lagrange function

$$\mathcal{L}(q,u,p) = \frac{1}{2}\|C(u) - y^\delta\|^2 + \alpha\mathcal{R}(q) + \alpha\tilde{\mathcal{R}}(u) + \langle A(q,u), p\rangle$$

first order optimality condition:

$$\begin{cases} A(q,u) = 0 & \ldots \text{state equation} \\ A'_q(q,u)^* p + \alpha\partial\mathcal{R}(q) = 0 & \ldots \text{gradient equation} \\ A'_u(q,u)^* p + C'(u)^*(C(u) - y^\delta) + \alpha\partial\tilde{\mathcal{R}}(u) = 0 & \ldots \text{adjoint equation} \end{cases}$$

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first order optimality condition:

$$\begin{cases} A(q,u) = 0 \quad \ldots\text{state equation} \\ A_q'(q,u)^* p + \alpha\partial\mathcal{R}(q) = 0 \quad \ldots\text{gradient equation} \\ A_u'(q,u)^* p + C'(u)^*(C(u) - y^\delta) + \alpha\partial\tilde{\mathcal{R}}(u) = 0 \quad \ldots\text{adjoint equation} \end{cases}$$

i.e., reduced and all-at-once Tikhonov regularization are basically the same.

Regularized Gauss-Newton Method

(q^k, u^k) fixed, one Gauss-Newton step:

$$\min_{q,u} \frac{1}{2}\|C(u^k) + C'(u^k)(u - u^k) - y^\delta\|^2 + \alpha_k \mathcal{R}(q) + \alpha_k \tilde{\mathcal{R}}(u)$$
$$+ \frac{1}{2}\|A(q^k, u^k) + A'_u(q^k, u^k)(u - u^k) + A'_q(q^k, u^k)(q - q^k)\|^2$$

$\rightsquigarrow (q^{k+1}, u^{k+1})$

Regularized Gauss-Newton Method

(q^k, u^k) fixed, one Gauss-Newton step:

$$\min_{q,u} \frac{1}{2}\|C(u^k) + C'(u^k)(u-u^k) - y^\delta\|^2 + \alpha_k \mathcal{R}(q) + \alpha_k \tilde{\mathcal{R}}(u)$$
$$+ \frac{1}{2}\|A(q^k,u^k) + A'_u(q^k,u^k)(u-u^k) + A'_q(q^k,u^k)(q-q^k)\|^2$$

$\rightsquigarrow (q^{k+1}, u^{k+1})$

first order optimality condition:
with $p = A(q^k,u^k) + A'_u(q^k,u^k)(u-u^k) + A'_q(q^k,u^k)(q-q^k)$:

$$\begin{cases} A'_u(q^k,u^k)(u-u^k) + A(q^k,u^k) + A'_q(q^k,u^k)(q-q^k) - p = 0 \\ \qquad \text{... linear state equation} \\ A'_q(q^k,u^k)^* p + \alpha\partial\mathcal{R}(q) = 0 \qquad \text{... gradient equation} \\ A'_u(q^k,u^k)^* p + C'(u^k)^*(C(u^k) + C'(u_k)(u-u_k) - y^\delta) + \alpha\partial\tilde{\mathcal{R}}(u) = 0 \\ \qquad \text{... adjoint equation} \end{cases}$$

Regularized Gauss-Newton Method

(q^k, u^k) fixed, one Gauss-Newton step:

$$\min_{q,u} \tfrac{1}{2}\|C(u^k) + C'(u^k)(u - u^k) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q) + \alpha_k \tilde{\mathcal{R}}(u)$$
$$+ \rho\|A(q^k, u^k) + A'_u(q^k, u^k)(u - u^k) + A'_q(q^k, u^k)(q - q^k)\|$$

i.e. (exact penalization) with ρ sufficiently large

$$\min_{q,u} \tfrac{1}{2}\|C(u^k) + C'(u^k)(u - u^k) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q) + \alpha_k \tilde{\mathcal{R}}(u)$$
$$\text{s.t. } A(q^k, u^k) + A'_u(q^k, u^k)(u - u^k) + A'_q(q^k, u^k)(q - q^k) = 0$$

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(q^k, u^k) fixed, one Gauss-Newton step:

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$$\text{s.t. } A(q^k,u^k) + A'_u(q^k,u^k)(u-u^k) + A'_q(q^k,u^k)(q-q^k) = 0$$

first order optimality condition:

$$\begin{cases} A'_u(q^k,u^k)(u-u^k) + A(q^k,u^k) + A'_q(q^k,u^k)(q-q^k) = 0 & \ldots \text{linear state eq.} \\ A'_q(q^k,u^k)^* p + \alpha \partial \mathcal{R}(q) = 0 & \ldots \text{gradient eq.} \\ A'_u(q^k,u^k)^* p + C'(u^k)^*(C(u^k) + C'(u_k)(u-u_k) - y^\delta) + \alpha \partial \tilde{\mathcal{R}}(u) = 0 & \text{adj.eq.} \end{cases}$$

Regularized Gauss-Newton Method

The latter is **not** reduced regularized Gauss-Newton!

Regularized Gauss-Newton Method

The latter is **not** reduced regularized Gauss-Newton!
So what would then reduced regularized Gauss-Newton mean?

Regularized Gauss-Newton Method (reduced)

q^k fixed, one reduced Gauss-Newton step:

$$\min_{q,u,\tilde{u}} \frac{1}{2}\|C(\tilde{u}) + C'(\tilde{u})(u - \tilde{u}) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q)$$

$$\text{s.t. } A(q^k, \tilde{u}) + A'_u(q^k, \tilde{u})(u - \tilde{u}) + A'_q(q^k, \tilde{u})(q - q^k) = 0$$

$$\text{and } A(q^k, \tilde{u}) = 0$$

Regularized Gauss-Newton Method (reduced)

q^k fixed, one reduced Gauss-Newton step:

$$\min_{q,u,\tilde{u}} \tfrac{1}{2}\|C(\tilde{u}) + C'(\tilde{u})(u-\tilde{u}) - y^\delta\|^2 + \alpha_k \mathcal{R}_k(q)$$
$$\text{s.t. } A(q^k,\tilde{u}) + A'_u(q^k,\tilde{u})(u-\tilde{u}) + A'_q(q^k,\tilde{u})(q-q^k) = 0$$
$$\text{and } A(q^k,\tilde{u}) = 0$$

first order optimality condition:

$$\begin{cases} A(q^k,\tilde{u}) = 0 & \ldots \text{nonlinear decoupled state equation} \\ A'_u(q^k,\tilde{u})(u-\tilde{u}) + A(q^k,\tilde{u}) + A'_q(q^k,\tilde{u})(q-q^k) = 0 & \ldots \text{linear state equation} \\ A'_q(q^k,\tilde{u})^* p + \alpha \partial \mathcal{R}(q) = 0 & \ldots \text{gradient equation} \\ A'_u(q^k,\tilde{u})^* p + C'(\tilde{u})^*(C(\tilde{u}) + C'(\tilde{u})(u-\tilde{u}) - y^\delta) = 0 & \ldots \text{adjoint equation} \end{cases}$$

Comparison of optimality conditions for reduced and all-at-once Newton

reduced:

$$\begin{cases} A(q^k,\tilde{u})=0 & \text{(nonlinear decoupled state equation)} \\ A'_u(q^k,\tilde{u})(u-\tilde{u})+A(q^k,\tilde{u})+A'_q(q^k,\tilde{u})(q-q^k)=0 & \text{(linear state eq.)} \\ A'_q(q^k,\tilde{u})^*p+\alpha\partial\mathcal{R}(q)=0 & \ldots\text{gradient equation} \\ A'_u(q^k,\tilde{u})^*p+C'(\tilde{u})^*(C(\tilde{u})+C'(\tilde{u})(u-\tilde{u})-y^\delta)=0 & \ldots\text{adjoint equation} \end{cases}$$

all-at-once:

$$\begin{cases} A'_u(q^k,u^k)(u-u^k)+A(q^k,u^k)-A'_q(q^k,u^k)(q-q^k)=0 & \ldots\text{linear state eq.} \\ A'_q(q^k,u^k)^*p+\alpha\partial\mathcal{R}(q)=0 & \ldots\text{gradient eq.} \\ A'_u(q^k,u^k)^*p+C'(u^k)^*(C(u^k)+C'(u_k)(u-u_k)-y^\delta)+\alpha\partial\tilde{\mathcal{R}}(u)=0 & \text{adj.eq.} \end{cases}$$

Gradient Methods (reduced)

q^k fixed, one Landweber step

$$
\begin{aligned}
q^{k+1} &= q^k - \mu^k F'(q^k)^* \Big(F(q^k) - y^\delta \Big) \\
&= q^k - \mu^k (C'(S(q^k))S'(q^k))^* \Big(C(S(q^k)) - y^\delta \Big) \\
&= q^k + \mu^k A'_q(q^k, \tilde{u})^* p
\end{aligned}
$$

where

$$
\begin{cases}
A(q^k, \tilde{u}) = 0 & \ldots \text{nonlinear decoupled state equation} \\
A'_u(q^k, \tilde{u})^* p + C'(\tilde{u})^*(C(\tilde{u}) - y^\delta) = 0 & \ldots \text{adjoint equation}
\end{cases}
$$

Gradient Methods (all-at-once)

(q^k, u^k) fixed, one Landweber step for $\mathbf{F}\begin{pmatrix} q \\ u \end{pmatrix} = \begin{pmatrix} A(q,u) \\ C(u) \end{pmatrix}$:

$$\begin{pmatrix} q^{k+1} \\ u^{k+1} \end{pmatrix} = \begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mu_k \mathbf{F}'\begin{pmatrix} q^k \\ u^k \end{pmatrix}^* \left(\mathbf{F}\begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mathbf{y}^\delta \right)$$

$$= \begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mu_k \begin{pmatrix} A'_q(q^k, u^k) & A'_u(q^k, u^k) \\ 0 & C'(u^k) \end{pmatrix}^* \begin{pmatrix} A(q^k, u^k) \\ C(u^k) - y^\delta \end{pmatrix}$$

Gradient Methods (all-at-once)

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$$\begin{pmatrix} q^{k+1} \\ u^{k+1} \end{pmatrix} = \begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mu_k \mathbf{F}' \begin{pmatrix} q^k \\ u^k \end{pmatrix}^* \left(\mathbf{F} \begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mathbf{y}^\delta \right)$$
$$= \begin{pmatrix} q^k \\ u^k \end{pmatrix} - \mu_k \begin{pmatrix} A'_q(q^k,u^k) & A'_u(q^k,u^k) \\ 0 & C'(u^k) \end{pmatrix}^* \begin{pmatrix} A(q^k,u^k) \\ C(u^k) - y^\delta \end{pmatrix}$$

i.e.

$$\begin{cases} q^{k+1} = q^k - \mu_k A'_q(q^k,u^k)^* A(q^k,u^k) \\ u^{k+1} = u^k - \mu_k C'(u^k)^*(C(u^k) - y^\delta) + A'_u(q^k,u^k)^* A(q^k,u^k) \end{cases}$$

completely explicit, no model to solve!

Convergence Analysis

- Existence of minimizers, stability, convergence, rates under (variational, approximate) source conditions follow as corollaries of existing results for Tikhonov, IRGNM, Landweber, when regularizing with respect to q and u
- Case of regularization $\alpha\mathcal{R}(q)$ of q only:
  Recover bounds on u via solvability condition $\|A_u(q,u)^{-1}\| \leq C_A$

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  solvability condition $\|A_u(q,u)^{-1}\| \leq C_A$ not needed!

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- Case of additional regularization $\beta\tilde{\mathcal{R}}(u)$ of u:
  solvability condition $\|A_u(q,u)^{-1}\| \leq C_A$ not needed!
- Getting rid of solvability condition allows to skip constraints on parameters (e.g. $a \geq \underline{a} > 0$ in a-problem $-\nabla(a\nabla u) = b$)!

numerical results

Numerical Tests

nonlinear inverse source problem:

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

Identify q from distributed measurements of u in Ω

Comparison of reduced and all-at-once Landweber

ζ	$\mathrm{it}_{\mathrm{aao}}$	$\mathrm{it}_{\mathrm{red}}$	$\mathrm{cpu}_{\mathrm{aao}}$	$\mathrm{cpu}_{\mathrm{red}}$	$\frac{\|q^\delta_{k_*(\delta),\mathrm{aao}}-q^\dagger\|_X}{\|q^\dagger\|_X}$	$\frac{\|q^\delta_{k_*(\delta),\mathrm{red}}-q^\dagger\|_X}{\|q^\dagger\|_X}$
0.5	5178	2697	2.97	18.07	0.0724	0.1047
5	$> 2 \cdot 10^6$	48510	1293.60	482.19	0.7837	0.1633
10	$> 2 \cdot 10^6$	$> 10^5$	1257.50	639.87	0.9621	0.1632
-0.5	10895	2016	8.85	14.55	0.1406	0.2295
-1	18954	-	11.42	-	0.2313	-

(1% Gaussian noise)

Comparison of reduced and all-at-once IRGNM

ζ	it_{aao}	it_{red}	cpu_{aao}	cpu_{red}	$\frac{\Vert q^{\delta}_{k_*(\delta),\text{aao}} - q^{\dagger} \Vert_X}{\Vert q^{\dagger} \Vert_X}$	$\frac{\Vert q^{\delta}_{k_*(\delta),\text{red}} - q^{\dagger} \Vert_X}{\Vert q^{\dagger} \Vert_X}$
0	34	32	0.14	0.10	0.0149	0.0151
10	43	43	0.20	0.55	0.0996	0.1505
100	55	56	0.28	0.82	0.0721	0.0770
1000	68	68	0.42	1.07	0.0543	0.0588
-0.5	33	32	0.13	0.35	0.1174	0.2165
-1.	35	-	0.23	-	0.2023	-
-10	44	-	0.23	-	0.0768	-
-100	77	-	0.59	-	0.2246	-
-1000	70	-	0.49	-	0.0321	-

(1% Gaussian noise)

Numerical Tests in 2-d with Adaptive Discretization

nonlinear inverse source problem:

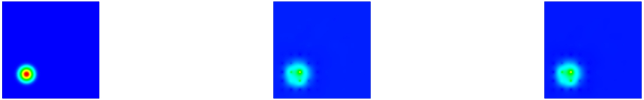
$$-\Delta u + \zeta u^3 = q \text{ in } \Omega = (0,1)^2 \quad \text{\& homogeneous Dirichlet BC}$$

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

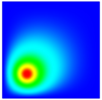
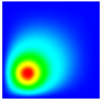
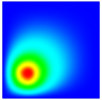
$$q^\dagger = \frac{c}{2\pi\sigma^2} \exp\left(-\frac{1}{2}\left(\left(\frac{sx-\mu}{\sigma}\right)^2 + \left(\frac{sy-\mu}{\sigma}\right)^2\right)\right)$$

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

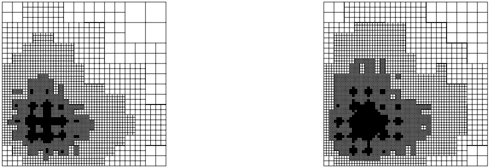
- goal-oriented, dual weighted residual estimators
- computations with *Gascoigne* and *RoDoBo*
- joint work with Alana Kirchner and Boris Vexler (TU Munich)



left: exact source $q^\dagger$,
middle: reconstruction by reduced Tikhonov (RT),
right: reconstruction by all-at-once Gauss-Newton (AGN),
with $\zeta = 100$, 1% noise

left: exact state $u^\dagger$,
middle: reconstruction by reduced Tikhonov (RT),
right: reconstruction by all-at-once Gauss-Newton (AGN),
with $\zeta = 100$, 1% noise



adaptively refined meshes,
left: by reduced Tikhonov (RT),
right: by all-at-once Gauss-Newton (AGN),
with $\zeta = 100$, 1% noise

Table: all-at-once Gauss-Newton (AGN) versus reduced Tikhonov (RT) for different choices of ζ with 1% noise. .
ctr: Computation time reduction using (AGN) in comparison to (RT)

ζ	RT			AGN			ctr
	error	$1/\alpha$	# nodes	error	$1/\alpha$	# nodes	
1	0.418	2985	2499	0.412	4600	3873	-65%
10	0.417	3194	2473	0.411	4918	3965	-59%
100	0.408	5014	6653	0.417	6773	9813	39%
500	0.418	9421	11851	0.404	13756	821	97%
1000	0.439	11486	44391	0.426	16355	793	99%

Conclusions and Outlook

- Tikhonov:
  reduced $\sim$ all-at-once
- Newton:
  reduced: solve nonlinear and linear models in each step
  all-at-once: only solve linearized models
- Landweber:
  reduced: solve nonlinear and linear models in each step
  all-at-once: never solve models!

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$\rightarrow$ time dependent problems

$\rightarrow$ regularization parameter choice

$\rightarrow$ restrictions on nonlinearity of F / $\mathbf{F}$

$\rightarrow$ convergence rates under source conditions

$\rightarrow$ minimization based inverse problems formulations and regularizations

time dependent problems

Parameter identification in time dependent systems

perturbed state space system

$$\begin{aligned} \dot{\mathbf{u}}(t) &= f(t, \mathbf{u}(t), \theta) + \mathbf{w}^\delta(t) \quad t \in (0, T), \quad \mathbf{u}(0) = u_0(\theta) \\ \text{and } \mathbf{y}^\delta(t) &= g(t, \mathbf{u}(t), \theta) + \mathbf{z}^\delta(t) \quad t \in (0, T) \qquad (c^\delta) \\ \text{or } \quad \underline{y}_i^\delta &= g_i(\mathbf{u}(t_i), \theta) + \mathbf{z}_i^\delta \quad i \in \{1, \ldots, n\} \qquad (d^\delta) \end{aligned}$$

Identify parameter θ from continuous (c^δ) or discrete (d^δ) partial observations of the state $\mathbf{u}$.

Parameter identification in time dependent systems

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$$\mathbf{y}^\delta - \mathbf{y} = \mathbf{z}^\delta + g(\cdot,\mathbf{u}^\delta,\theta^\dagger) - g(\cdot,\mathbf{u}^\dagger,\theta^\dagger)$$

where $\dot{\mathbf{u}}^\delta(t) = f(t,\mathbf{u}^\delta(t),\theta^\dagger) + \mathbf{w}^\delta(t) \quad t \in (0,T)\,, \quad \mathbf{u}^\delta(0) = u_0(\theta)$

Observations are caused by the true parameters and perturbed by $\mathbf{w}^\delta$, $\mathbf{z}^\delta$

Parameter identification in time dependent systems

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Conventional formulation as an inverse problem

$$F(\theta) = \mathbf{y}^\delta$$

with forward operator $F : \theta \mapsto g(\cdot, S(\theta), \theta)$

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Conventional formulation as an inverse problem

$$F(\theta) = \mathbf{y}^\delta$$

with forward operator $F : \theta \mapsto g(\cdot, S(\theta), \theta)$

- treats the system as a black box, thus neglecting its causal structure
- requires existence and numerical evaluation of a parameter-to-state map $S : \theta \mapsto \mathbf{u}$

$\rightsquigarrow$ all-at-once formulation?

All-at-once formulation

$$\mathbb{F}(\mathbf{u}, \theta) = \mathbb{Y}$$

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$$\mathbb{F} : \mathcal{U} \times \mathcal{X} \to \mathcal{W} \times H \times \mathcal{Y}\,, \quad (\mathbf{u}, \theta) \mapsto \begin{pmatrix} \dot{\mathbf{u}} - f(\cdot, \mathbf{u}, \theta) \\ \mathbf{u}(0) - u_0(\theta) \\ g(\cdot, \mathbf{u}, \theta) \end{pmatrix}$$

$$\mathbb{Y}^\delta = (0, 0, \mathbf{y}^\delta) \approx (0, 0, \mathbf{y}) = \mathbb{Y}$$

All-at-once formulation

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$$\mathcal{U} := \{\mathbf{v} \in L_2(0,T;V) \,:\, \dot{\mathbf{v}} \in L_2(0,T;V^*)\} \subseteq C(0,T;H)\,,\;\; V \subseteq H \subseteq V^*$$
$$\mathbf{w}^\delta \in \mathcal{W} := L_2(0,T;V^*), \quad \mathbf{z}^\delta \in \mathcal{Y} = L_2(0,T;Z)\,.$$
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$$\mathbf{y}^\delta=g(\cdot,\mathbf{u}^\delta,\theta^\dagger)+\mathbf{z}^\delta\,,\quad \mathbf{y}=g(\cdot,\mathbf{u}^\dagger,\theta^\dagger)$$

$f:(0,T)\times V\times\mathcal{X}\to V^*\,,\quad g:(0,T)\times V\times\mathcal{X}\to Z$

are Caratheodory mappings for fixed $\theta\in\mathcal{X}$

and satisfy growth conditions

All-at-once system formulation $[0, T] = \bigcup_{j \in \{1,\dots,m\}} [\tau_{j-1}, \tau_j]$

$$\forall j \in \{0, \dots, m-1\} \ : \ \mathbb{F}_j(\mathbf{u}, \theta) = \mathbb{Y}_j$$

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$$\mathcal{W}_j = L_2(\tau_j, \tau_{j+1}; V^*) \,, \quad \mathcal{Y}_j = L_2(\tau_j, \tau_{j+1}; Z) \,, \quad \mathbb{Y}_j^\delta = (0, (0,)\mathbf{y}_j^\delta)$$

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Continuity of $\mathbf{u}$ over breakpoints τ_j guaranteed by embedding $\mathcal{U} \subseteq C(0,T;H)$.

State space stills goes over whole time interval!

Reduced system formulation $[0, T] = \bigcup_{j \in \{1,\dots,m\}} [\tau_{j-1}, \tau_j]$

$$\forall j \in \{0, \dots, m-1\} \; : \; F_j(\theta) = y_j$$

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where $\mathbf{u} = S(\theta)$ solves

$$\dot{\mathbf{u}}(t) = f(t, \mathbf{u}(t), \theta) \quad t \in (0,T)\,, \quad \mathbf{u}(0) = u_0(\theta)$$

Parameter identification methods to be compared

- reduced Landweber (rLW)
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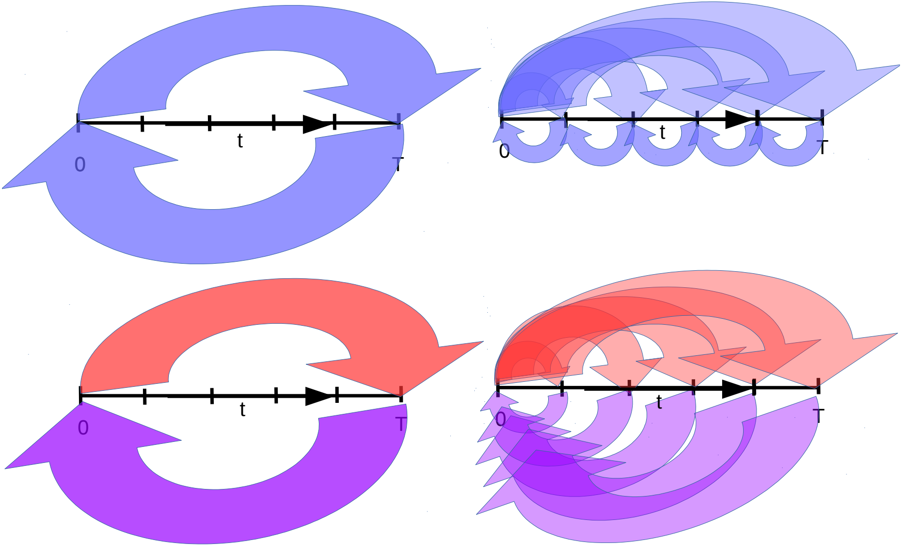
adjoints of $F'(\theta), F'_j(\theta), \mathbb{F}'(\mathbf{u}, \theta), \mathbb{F}_j(\mathbf{u}, \theta)$
$\rightsquigarrow$ adjoint PDEs, to be solved backwards in time

Comparison of all-at-once and reduced Landweber methods

one all-at-once Landweber step

one all-at-once Landweber-Kaczmarz-cycle



one reduced Landweber step

one reduced Landweber-Kaczmarz cycle

Thank you for your attention!

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