Optimal Control of Coupled Systems

Current Methods and Perspectives

Roland Griesse

CHEMNITZ UNIVERSITY
OF TECHNOLOGY

Numerical Mathematics

MPI Magdeburg
December 1–2, 2008

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Overview

Coupled systems

- systems of (partial) differential equations
- often subsystems with different characteristics

Optimal control

- often driven by application
- tool to understand system dynamics

Goal of this talk

- present a toolbox of methods
- applicable to a broad range of applications

Outline

Motivation for Sensitivity Analysis

Observation

Real-life (optimization) problems usually involve uncertain data.

Modeling uncertainty

Two points of view:

- stochastic (not considered here)
- deterministic

Sources for uncertain data

- model parameters not exactly known
- model parameters have changed since solution was computed

Finite-Dimensional Optimization

Parametric optimization problems

$$\begin{aligned} \text{Minimize} \quad & f(x, p) \quad \text{w.r.t. } x \\ \text{subject to} \quad & g(x, p) = 0 \\ \text{and} \quad & h(x, p) \leq 0 \end{aligned} \qquad (\textbf{NLP}(p))$$

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Finite-Dimensional Optimization

Parametric optimization problems

$$\begin{aligned} \text{Minimize} \quad & f(x,p) \quad \text{w.r.t. } x \\ \text{subject to} \quad & g(x,p) = 0 \\ \text{and} \quad & h(x,p) \le 0 \end{aligned} \qquad (\mathbf{NLP}(p))$$

Purpose of parametric sensitivity analysis

- analyze the dependence of (local) optimal solution $x^*(p)$ on p
- yields both qualitative and quantitative information
- later: $g(x,p) = 0 \;\Leftrightarrow\;$ partial differential equation

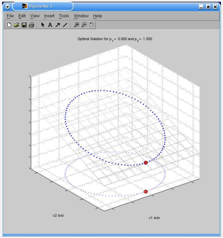
Finite-Dimensional Optimization

A simple example

$$\text{Minimize} \quad p_1\, x_1 + p_2\, x_2 \quad \text{over } x \in \mathbb{R}^2$$

$$\text{s.t.} \quad x_1^2 + x_2^2 = 1$$

$$(\text{and} \quad x_1 \geq 0)$$



Definition

parametric sensitivity derivative $:= D\, x^*(p\,;\delta p)$

Benefits and Effort

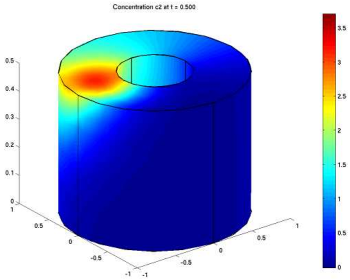
Benefits

- qualitative and quantitative assessment of stability w.r.t. perturbations
- fast update schemes, real-time control

Computational effort

- solve one simple (QP) problem per perturbation direction
- same structure, same algorithm as original problem
- perfectly parallelizable

Reaction Diffusion Model Problem



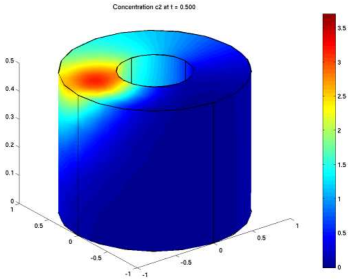
Reaction $E_1 + E_2 \longrightarrow P$

$$\frac{\partial}{\partial t} c_1 = D_1 \Delta c_1 - k\, c_1 c_2$$
$$\frac{\partial}{\partial t} c_2 = D_2 \Delta c_2 - k\, c_1 c_2$$

concentrations c_1, c_2

reaction rate $\sim c_1\, c_2$

Reaction Diffusion Model Problem



Reaction $E_1 + E_2 \longrightarrow P$

$$\frac{\partial}{\partial t} c_1 = D_1 \Delta c_1 - k\, c_1 c_2$$
$$\frac{\partial}{\partial t} c_2 = D_2 \Delta c_2 - k\, c_1 c_2$$

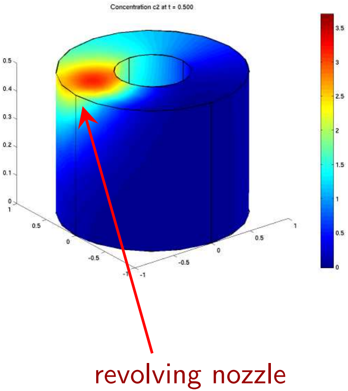
concentrations c_1, c_2

reaction rate $\sim c_1\, c_2$

Boundary conditions

$$\frac{\partial}{\partial n} c_{1,2} = 0$$
$$\frac{\partial}{\partial n} c_2 = u(t)\, \alpha(x,t)\, |_{\Gamma_c}$$

Reaction Diffusion Model Problem



Reaction $E_1 + E_2 \longrightarrow P$

$$\frac{\partial}{\partial t} c_1 = D_1 \Delta c_1 - k\, c_1 c_2$$
$$\frac{\partial}{\partial t} c_2 = D_2 \Delta c_2 - k\, c_1 c_2$$

concentrations c_1, c_2

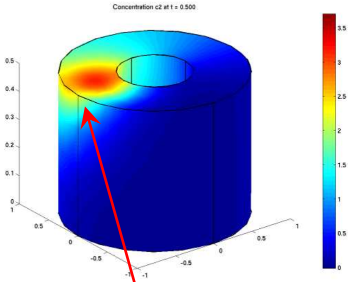
reaction rate $\sim c_1\, c_2$

Boundary conditions

$$\frac{\partial}{\partial n} c_{1,2} = 0$$
$$\frac{\partial}{\partial n} c_2 = u(t)\, \alpha(x,t)\, |_{\Gamma_c}$$

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Reaction Diffusion Model Problem



Reaction $E_1 + E_2 \longrightarrow P$

$$\frac{\partial}{\partial t} c_1 = D_1 \Delta c_1 - k\, c_1 c_2$$

$$\frac{\partial}{\partial t} c_2 = D_2 \Delta c_2 - k\, c_1 c_2$$

concentrations c_1, c_2

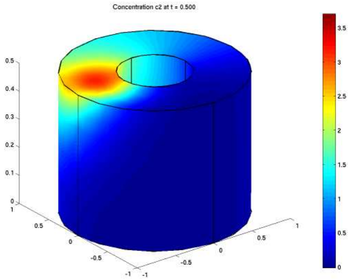
reaction rate $\sim c_1\, c_2$

Boundary conditions

$$\frac{\partial}{\partial n} c_{1,2} = 0$$

$$\frac{\partial}{\partial n} c_2 = u(t)\, \alpha(x,t)\, |_{\Gamma_c}$$

Reaction Diffusion Model Problem



Reaction $E_1 + E_2 \longrightarrow P$

$$\frac{\partial}{\partial t} c_1 = D_1 \Delta c_1 - k\, c_1 c_2$$

$$\frac{\partial}{\partial t} c_2 = D_2 \Delta c_2 - k\, c_1 c_2$$

concentrations c_1, c_2

reaction rate $\sim c_1\, c_2$

Initial conditions

$$c_1(\cdot, 0) = c_{10}$$

$$c_2(\cdot, 0) = c_{20}$$

Boundary conditions

$$\frac{\partial}{\partial n} c_{1,2} = 0$$

$$\frac{\partial}{\partial n} c_2 = u(t)\, \alpha(x, t)\, |_{\Gamma_c}$$

Reaction Diffusion Model Problem

problem statement

Minimize deviation from desired states c_{iT} plus control cost

$$f(c_1, c_2, u) = \sum_{i=1}^{2} \frac{\beta_i}{2} \int_\Omega |c_i(x,T) - c_{iT}(x)|^2 \, dx + \frac{\gamma}{2} \int_0^T |u(t)|^2 \, dt$$

subject to the RD model and control constraints

$$a(t) \le u(t) \le b(t)$$

Reaction Diffusion Model Problem

Perturbed problem statement

Minimize deviation from desired states c_{iT} plus control cost

$$f(c_1, c_2, u, p) = \sum_{i=1}^{2} \frac{\beta_i}{2} \int_\Omega |c_i(x, T) - c_{iT}(x)|^2 \, dx + \frac{\gamma}{2} \int_0^T |u(t)|^2 \, dt$$

subject to the RD model and control constraints

$$a(t) \le u(t) \le b(t)$$

Reaction Diffusion Model Problem

Perturbed problem statement

Minimize deviation from desired states c_{iT} plus control cost

$$f(c_1, c_2, u, p) = \sum_{i=1}^{2} \frac{\beta_i}{2} \int_\Omega |c_i(x, T) - c_{iT}(x)|^2 \, dx + \frac{\gamma}{2} \int_0^T |u(t)|^2 \, dt$$

subject to the perturbed RD model and control constraints

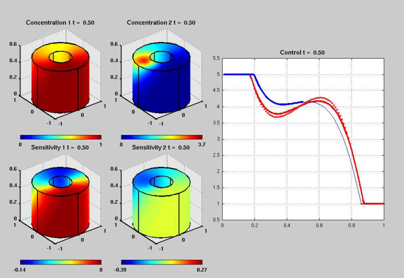
$$a(t) \le u(t) \le b(t)$$

Note

The parameter p may be infinite-dimensional!

Parametric Sensitivity Analysis

Movie: Optimal control and parametric sensitivities



Objective

to consume educt E_1

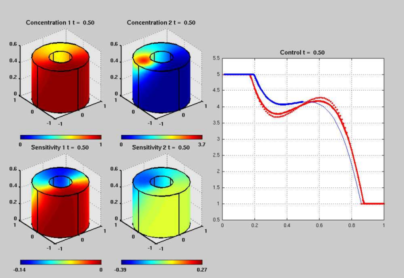
Reaction constant

nominal $k = 1.0$

perturbed $k = 1.5$

Parametric Sensitivity Analysis

Movie: Optimal control and parametric sensitivities



Objective

to consume educt E_1

Reaction constant

nominal $k = 1.0$

perturbed $k = 1.5$

Summary

- qualititative and quantitative sensitivity information
- fast update schemes, real-time control
- efficient computation

References: Parametric Sensitivity Analysis

K. Brandes and R. Griesse.
Quantitative stability analysis of optimal solutions in PDE-constrained optimization.
Journal of Computational and Applied Mathematics, 206(2):908–926, 2007.

R. Griesse, T. Grund, and D. Wachsmuth.
Update strategies for perturbed nonsmooth equations.
Optimization Methods and Software, 23(3):321–343, 2008.

R. Griesse and B. Vexler.
Numerical sensitivity analysis for the quantity of interest in PDE-constrained optimization.
SIAM Journal on Scientific Computing, 29(1):22–48, 2007.

R. Griesse and D. Wachsmuth.
Sensitivity analysis and the adjoint update strategy for optimal control problems with mixed control-state constraints.
Computational Optimization and Applications, to appear.

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Outline

1. Parametric Sensitivity Analysis
2. Problems Promoting Sparsity
3. Free Boundary Value Problems

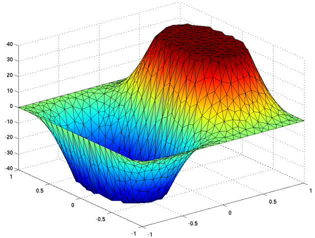
Introducing Sparsity

standard opt. control problem

$$\text{Minimize} \quad \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{\alpha}{2}\,\|u\|_{L^2}^2$$

$$\text{s.t.} \quad \begin{cases} -\triangle y = u & \text{in } \Omega \\ y = 0 & \text{on } \Gamma \end{cases}$$

$$\text{and} \quad u_a \le u \le u_b$$



$$\|u\|_{L^2}^2 = \int_\Omega |u(x)|^2 \, dx$$

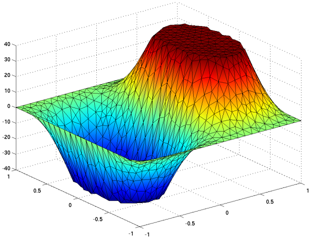
Introducing Sparsity

standard opt. control problem

$$\text{Minimize} \quad \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{\alpha}{2}\|u\|_{L^2}^2$$

$$\text{s.t.} \quad \begin{cases} -\triangle y = u & \text{in } \Omega \\ y = 0 & \text{on } \Gamma \end{cases}$$

$$\text{and} \quad u_a \le u \le u_b$$



$$\|u\|_{L^2}^2 = \int_\Omega |u(x)|^2 \, dx$$

Features

- optimal control u is $\neq 0$ everywhere
- differentiable optimization problem

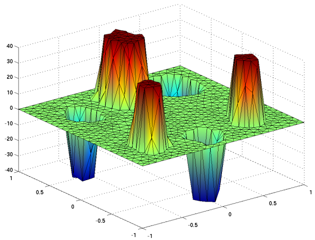
Introducing Sparsity

problem with sparsity term

Minimize $\frac{1}{2}\|y - y_d\|_{L^2}^2 + \beta \, \|u\|_{L^1}$

s.t. $\begin{cases} -\triangle y = u & \text{in } \Omega \\ y = 0 & \text{on } \Gamma \end{cases}$

and $u_a \le u \le u_b$



$$\|u\|_{L^2}^2 = \int_\Omega |u(x)|^2 \, dx, \quad \|u\|_{L^1} = \int_\Omega |u(x)| \, dx$$

Features

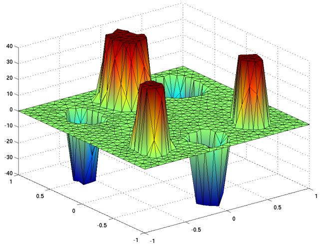
- optimal control u is sparse
- non-differentiable (convex) optimization problem

[Stadler (2008)]

Sparsity in Applications

Examples

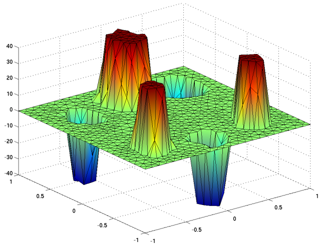
- sparse placement of actuators
- sparse identification of relevant mechanisms
  - in regulatory networks (systems biology)
  - in reaction kinetics (chemical engineering)



Sparsity in Applications

Examples

- sparse placement of actuators
- sparse identification of relevant mechanisms
  - in regulatory networks (systems biology)
  - in reaction kinetics (chemical engineering)

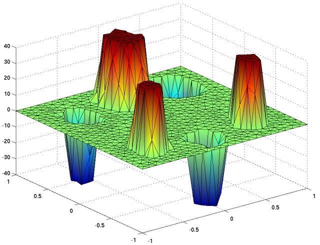


	A	B	C	D	E	F	G	H	I
A	x	x	x	x	x	x	x	x	x
B	x	x	x	x	x	x	x	x	x
C	x	x	x	x	x	x	x	x	x
D	x	x	x	x	x	x	x	x	x
E	x	x	x	x	x	x	x	x	x
F	x	x	x	x	x	x	x	x	x
G	x	x	x	x	x	x	x	x	x
H	x	x	x	x	x	x	x	x	x
I	x	x	x	x	x	x	x	x	x

Sparsity in Applications

Examples

- sparse placement of actuators
- sparse identification of relevant mechanisms
  - in regulatory networks (systems biology)
  - in reaction kinetics (chemical engineering)



	A	B	C	D	E	F	G	H	I
A					X				
B								X	X
C									
D				X					
E							X		
F					X				
G	X								
H		X	X						
I					X				

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Structural Properties

Adjoint equation for example problem

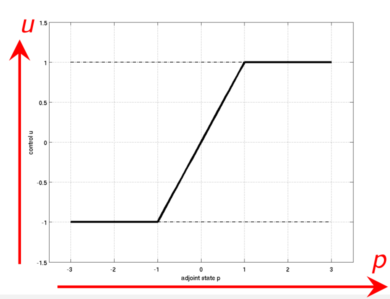
$$\begin{aligned} -\triangle p &= y - y_d \quad \text{in } \Omega \\ p &= 0 \quad \text{on } \Gamma \end{aligned}$$

Structural Properties

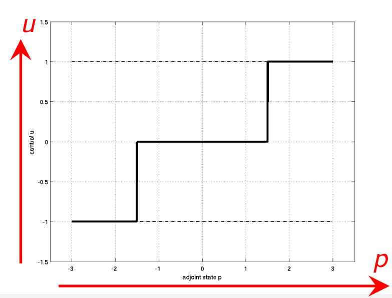
Adjoint equation for example problem

$$\begin{aligned} -\triangle p &= y - y_d \quad \text{in } \Omega \\ p &= 0 \quad \text{on } \Gamma \end{aligned}$$

Problem with $\frac{\alpha}{2} \|u\|_{L^2}^2$



Problem with $\beta \|u\|_{L^2}$

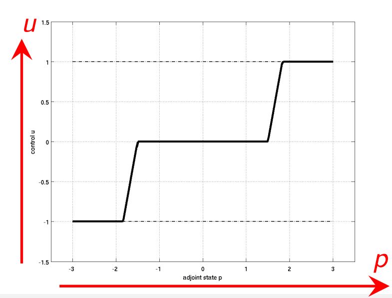


Numerical Solution of Problems with Sparsity

Regularized formulation

$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{\alpha}{2}\|u\|_{L^2}^2 + \beta\|u\|_{L^1} \\ \text{s.t.} \quad & \text{PDE and } u_a \le u \le u_b. \end{aligned}$$

Sparsity is maintained



Numerical Solution of Problems with Sparsity

Regularized formulation

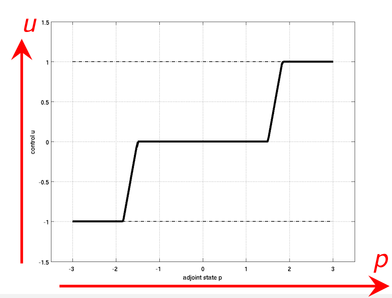
$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\alpha}{2}\,\|u\|_{L^2}^2 + \beta\,\|u\|_{L^1} \\ \text{s.t.} \quad & \text{PDE and } u_a \le u \le u_b. \end{aligned}$$

Optimality conditions

$$\mu = p - \alpha\, u$$

$$\begin{aligned} u = {} & \max\{0, u + c\,(\mu-\beta)\} \\ & + \min\{0, u + c\,(\mu+\beta)\} \\ & - \max\{0, u - u_b + c\,(\mu-\beta)\} \\ & - \min\{0, u - u_a + c\,(\mu+\beta)\} \end{aligned}$$

Sparsity is maintained



Numerical Solution of Problems with Sparsity

Regularized formulation

$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{\alpha}{2}\|u\|_{L^2}^2 + \beta\,\|u\|_{L^1} \\ \text{s.t.} \quad & \text{PDE and } u_a \le u \le u_b. \end{aligned}$$

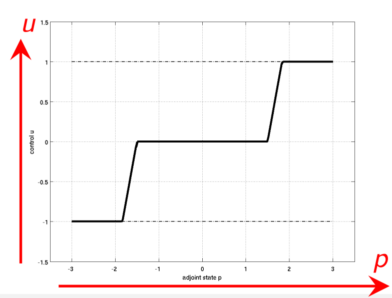
Optimality conditions

$$\mu = p - \alpha\, u$$

$$\begin{aligned} u = {} & \max\{0, u + c\,(\mu - \beta)\} \\ & + \min\{0, u + c\,(\mu + \beta)\} \\ & - \max\{0, u - u_b + c\,(\mu - \beta)\} \\ & - \min\{0, u - u_a + c\,(\mu + \beta)\} \end{aligned}$$

Newton differentiable for $\alpha > 0$

Sparsity is maintained



Numerical Solution of Problems with Sparsity

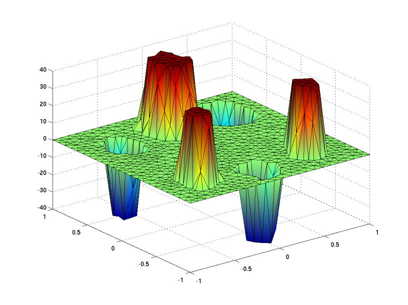
Solution of regularized problems ($\alpha > 0$)

- sparsity is maintained for regularized problems
- efficient solution using semi-smooth Newton method for $\alpha > 0$
- continuation method as $\alpha \searrow 0$
- convergence rates up to $\alpha^{1/3}$

[Hintermüller, Ito, Kunisch (2002)]   [Ulbrich (2003)]

A new Type of Sparsity

Sparsity

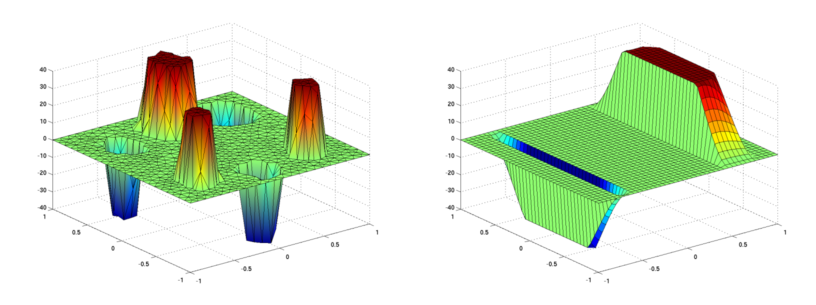


Objective function

$$\frac{1}{2}\|y - y_d\|_{L^2}^2 + \beta \|u\|_{L^1}$$

A new Type of Sparsity

Sparsity vs. directional sparsity

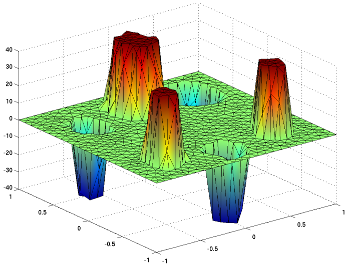


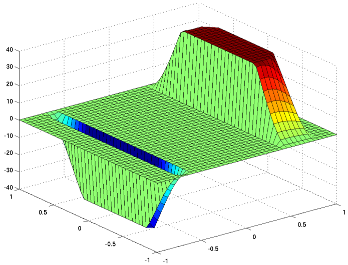
Objective function

$$\frac{1}{2}\|y - y_d\|_{L^2}^2 + \beta\,\|u\|_{L^1}$$

A new Type of Sparsity

Sparsity vs. directional sparsity





Objective function

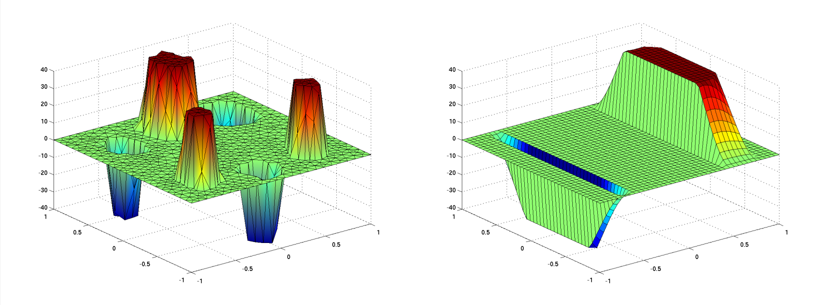
$$\frac{1}{2}\|y - y_d\|_{L^2}^2 + \beta\,\|u\|_{L^1}$$

Objective function

$$\frac{1}{2}\|y - y_d\|_{L^2}^2 + \beta\,\|u\|_{L^1(L^2)}$$

A new Type of Sparsity

Sparsity vs. directional sparsity



Properties

- no structural assumptions made

Properties

- exploits known or desired group sparsity structure

Optimality for Directional Sparsity Problems

Fixed point property

$\overline{u}$ is optimal $\quad\Leftrightarrow\quad$ $\overline{u}$ solves

$$\text{Minimize} \quad \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{1}{2}\int_{\Omega^+} \left(\alpha + \frac{\beta}{\|\overline{u}(x_1,\cdot)\|_{L^2}}\right) u(x)^2 \, dx$$
$$\text{s.t.} \quad \text{PDE and } u_a \le u \le u_b$$

and if it satisfies the complementarity property

$$\|p(x_1,\cdot)\|_{L^2} \le \beta \quad \text{where } \overline{u}(x_1,\cdot) = 0.$$

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Optimality for Directional Sparsity Problems

Fixed point property

$\overline{u}$ is optimal $\quad\Leftrightarrow\quad$ $\overline{u}$ solves

$$\begin{aligned} \text{Minimize} \quad & \frac{1}{2}\|y - y_d\|_{L^2}^2 + \frac{1}{2}\int_{\Omega^+} \left(\alpha + \frac{\beta}{\|\overline{u}(x_1,\cdot)\|_{L^2}}\right) u(x)^2 \, dx \\ \text{s.t.} \quad & \text{PDE and } u_a \le u \le u_b \end{aligned}$$

and if it satisfies the complementarity property

$$\|p(x_1,\cdot)\|_{L^2} \le \beta \quad \text{where } \overline{u}(x_1,\cdot) = 0.$$

Numerical solution

- fixed-point iteration for $\|\overline{u}(x_1,\cdot)\|_{L^2}$, semi-smooth Newton method inside
- alternative: complementarity formulation, semi-smooth Newton method

Summary: Problems Promoting Sparsity

Applications

- sparse placement of actuators
- sparse identification of relevant mechanisms
- directional sparsity as a new device

Algorithmics

- regularized problems for $\alpha > 0$
- efficient semi-smooth Newton algorithm
- directional sparsity: fixed-point formulation (globalization)

References: Problems Promoting Sparsity

R. Griesse and D. Lorenz.
A semismooth Newton method for Tikhonov functionals with sparsity constraints.
Inverse Problems, 24(3):035007 (19pp), 2008.

R. Griesse, G. Stadler, and G. Wachsmuth.
Elliptic optimal control problems with directional sparsity terms.
in preparation.

G. Stadler.
Elliptic optimal control problems with L^1-control cost and applications for the placement of control devices.
Computational Optimization and Applications, to appear.

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Outline

1. Parametric Sensitivity Analysis
2. Problems Promoting Sparsity
3. Free Boundary Value Problems

Free Boundary Value Problems

Examples

- phase transitions in solidification and melting processes
- Stefan problem
- multi-phase fluid flow, fluid-structure interaction

Features

- domain of definition of the underlying equation is a priori unknown
- it is determined along with the solution
- coupled system with differing characteristics:
  - heat equation (temperature)
  - geometric evolution equation (free boundary)

The Stefan Problem

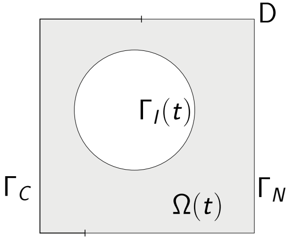
The Stefan Problem

Heat equation

$$
\begin{aligned}
\varrho\, c_p\, y_t - k\Delta y &= f \quad \text{in } \Omega(t)\\
y &= 0 \quad \text{auf } \Gamma_I(t)
\end{aligned}
$$

[Stefan 1889]

The Stefan Problem

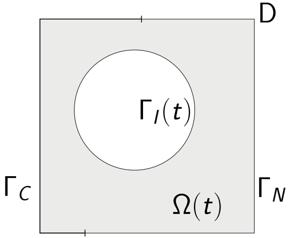


Heat equation

$$
\begin{aligned}
\varrho\, c_p\, y_t - k\Delta y &= f \quad \text{in } \Omega(t)\\
y &= 0 \quad \text{auf } \Gamma_I(t)\\
k\frac{\partial y}{\partial n} &= u \quad \text{auf } \Gamma_C\\
k\frac{\partial y}{\partial n} &= g \quad \text{auf } \Gamma_N\\
y(0) &= y_0 \quad \text{in } \Omega(0)
\end{aligned}
$$

[Stefan 1889]

The Stefan Problem



[Stefan 1889]

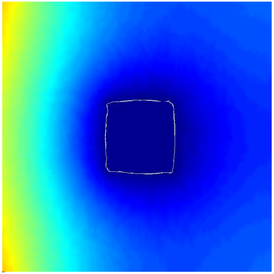
Heat equation

$$\begin{aligned} \varrho\, c_p\, y_t - k\Delta y &= f && \text{in } \Omega(t) \\ y &= 0 && \text{auf } \Gamma_I(t) \\ k\frac{\partial y}{\partial n} &= u && \text{auf } \Gamma_C \\ k\frac{\partial y}{\partial n} &= g && \text{auf } \Gamma_N \\ y(0) &= y_0 && \text{in } \Omega(0) \end{aligned}$$

Stefan condition

$$\varrho\, L\, F \cdot n = k\frac{\partial y}{\partial n} \quad \text{auf } \Gamma_I(t)$$

The Stefan Problem



Heat equation

$$
\begin{aligned}
\varrho\, c_p\, y_t - k\Delta y &= f \quad \text{in } \Omega(t) \\
y &= 0 \quad \text{auf } \Gamma_I(t) \\
k\frac{\partial y}{\partial n} &= u \quad \text{auf } \Gamma_C \\
k\frac{\partial y}{\partial n} &= g \quad \text{auf } \Gamma_N \\
y(0) &= y_0 \quad \text{in } \Omega(0)
\end{aligned}
$$

Stefan condition

$$
\varrho\, L\, F \cdot n = k\frac{\partial y}{\partial n} \quad \text{auf } \Gamma_I(t)
$$

[Stefan 1889]

Level-Set Description

- Signed distance function:

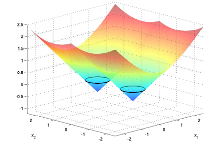
$$\phi(x,t) \begin{cases} < 0 & \text{in } \Omega(t) \\ = 0 & \text{on } \Gamma_I(t) \\ > 0 & \text{in } D \setminus \Omega(t) \end{cases}$$

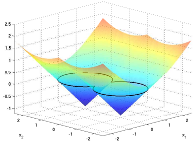
- Linear transport equation:

$$0 = \phi_t + F \cdot \nabla \phi.$$

- Level-set equation:

$$n = \frac{\nabla \phi}{|\nabla \phi|} \Rightarrow 0 = \phi_t + F_n \, |\nabla \phi|.$$





CHEMNITZ UNIVERSITY OF TECHNOLOGY

Level-Set Description

- Signed distance function:

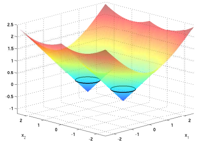
$$\phi(x,t) \begin{cases} < 0 & \text{in } \Omega(t) \\ = 0 & \text{on } \Gamma_I(t) \\ > 0 & \text{in } D \setminus \Omega(t) \end{cases}$$

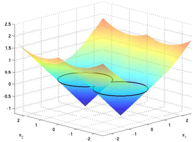
- Linear transport equation:

$$0 = \phi_t + F \cdot \nabla \phi.$$

- Level-set equation:

$$n = \frac{\nabla \phi}{|\nabla \phi|} \Rightarrow 0 = \phi_t + F_n \, |\nabla \phi|.$$





- Flexible.
- Suitable for 2D, 3D.
- Solver for PDE $\Rightarrow$ Effort!
- F is known on $\Gamma_I(t)$ only.

Extension Velocity

Stefan condition

$$F = (F_1, F_2)^\top : \quad \rho \, L \, F \cdot n = k \frac{\partial y}{\partial n} \qquad \text{on } \Gamma_I(t)$$

Extension Velocity

Stefan condition

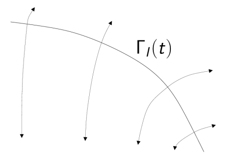
$$F = (F_1, F_2)^\top : \quad \rho\, L\, F \cdot n = k \frac{\partial y}{\partial n} \qquad \text{on } \Gamma_I(t)$$

Constant extension in normal direction

Find F_i, $i = 1, 2$, such that:

$$\operatorname{sign}(\phi)\, \nabla F_i \cdot \nabla \phi = 0 \qquad \text{in } \mathbb{R}^2$$

$$\rho\, L\, F_i = k \frac{\partial y}{\partial x_i} \qquad \text{on } \Gamma_I(t)$$



- maintains signed-distance property
- fast marching schemes
- same technique is used to re-initialize level-set function

[Adalsteinsson, Sethian 1999]

Extended Finite Elements

Moving mesh approach

- mesh conforms to interface
- FEM on moving mesh

Extended Finite Elements

Moving mesh approach

- mesh conforms to interface
- FEM on moving mesh

X-FEM approach

- keep mesh
- modify trial functions

[Chessa et al. 2002]

Extended Finite Elements

Moving mesh approach

- mesh conforms to interface
- FEM on moving mesh

X-FEM approach

- keep mesh
- modify trial functions

$$y_h(x,t) = \sum_{i=1}^{n} v_i(x)\, y_i(t) + \sum_{j=1}^{n_{e,t}} w_j(x,t)\, a_j(t),$$

[Chessa et al. 2002]

Extended Finite Elements

Moving mesh approach

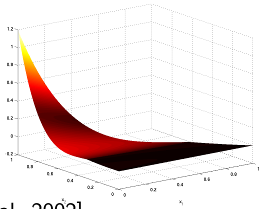
- mesh conforms to interface
- FEM on moving mesh

X-FEM approach

- keep mesh
- modify trial functions

$$y_h(x,t) = \sum_{i=1}^{n} v_i(x)\, y_i(t) + \sum_{j=1}^{n_{e,t}} w_j(x,t)\, a_j(t),$$

$$w_j(x,t) = v_j(x)\, \big(\big|\phi(x,t)\big| - \big|\phi_j(t)\big| \big)$$



[Chessa et al. 2002]

Extended Finite Elements

Moving mesh approach

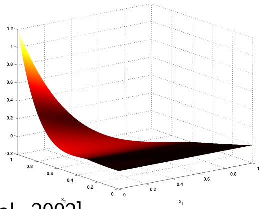
- mesh conforms to interface
- FEM on moving mesh

X-FEM approach

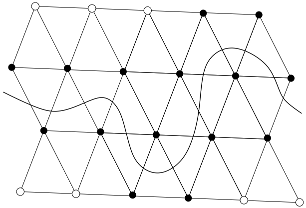
- keep mesh
- modify trial functions

$$y_h(x,t) = \sum_{i=1}^{n} v_i(x)\, y_i(t) + \sum_{j=1}^{n_{e,t}} w_j(x,t)\, a_j(t),$$

$w_j(x,t) = v_j(x)\,\big(\big|\phi(x,t)\big| - \big|\phi_j(t)\big|\big)$ at enriched nodes:



[Chessa et al. 2002]



Optimization of Phase Transitions

Goal: Influence the phase boundary

Optimization of Phase Transitions

Goal: Influence the phase boundary

Optimal control problem

Minimize $\displaystyle \frac{\gamma_1}{2} \int_0^T \int_{\Gamma_I(t)} |\phi_d|^2$

$\displaystyle + \frac{\gamma_2}{2} \int_0^T \int_{\Omega_1(t)} |y - y_d|^2 + \frac{\gamma_3}{2} \int_0^T \int_{\Gamma_C} |u|^2$

s.t. Stefan problem

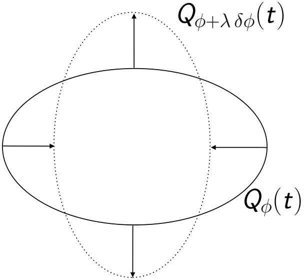
Elements of Shape Calculus

$$E(\phi) = \int_0^T \int_{Q_\phi(t)} f \, dx \, dt, \quad Q_\phi(t) = \{\phi < 0\}$$

$$E'(\phi)\,\delta\phi = \lim_{\lambda \to 0} \frac{E(\phi+\lambda\,\delta\phi) - E(\phi)}{\lambda} = ?$$

Set $\tilde{\phi} := \phi + \lambda\,\delta\phi$ and write

$$\int_{Q_{\phi(t)}} f = \int_{Q_\phi(t) \cap Q_{\tilde{\phi}}(t)} f + \int_{Q_\phi(t) \setminus Q_{\tilde{\phi}}(t)} f$$



[Pironneau 1984, Santosa 1995]

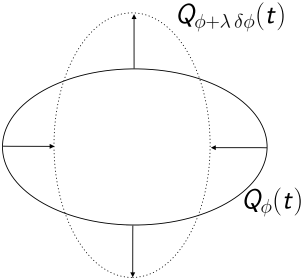
Elements of Shape Calculus

$$E(\phi) = \int_0^T \int_{Q_\phi(t)} f \, dx \, dt, \quad Q_\phi(t) = \{\phi < 0\}$$

$$E'(\phi)\,\delta\phi = \lim_{\lambda \to 0} \frac{E(\phi+\lambda\,\delta\phi) - E(\phi)}{\lambda} = ?$$

Set $\tilde\phi := \phi + \lambda\,\delta\phi$ and write

$$\int_{Q_{\phi(t)}} f = \int_{Q_\phi(t) \cap Q_{\tilde\phi}(t)} f + \int_{Q_\phi(t) \setminus Q_{\tilde\phi}(t)} f$$



$$\frac{E(\phi+\lambda\,\delta\phi) - E(\phi)}{\lambda} = \frac{1}{\lambda} \int_0^T \left(\int_{Q_{\tilde\phi}(t) \setminus Q_\phi(t)} f - \int_{Q_\phi(t) \setminus Q_{\tilde\phi}(t)} f \right)$$

$$= \frac{1}{\lambda} \int_0^T \left(\int_{\partial Q_\phi(t)} \lambda \frac{-\delta\phi}{|\nabla\phi|} f + \mathbf{o}(\lambda) \right) \xrightarrow{\lambda \to 0} \int_0^T \int_{\partial Q_\phi(t)} \frac{-\delta\phi}{|\nabla\phi|} f \, ds \, dt$$

[Pironneau 1984, Santosa 1995]

Optimality System for Motion Planning

$\mathcal{L}_y\,\delta y = 0$:

$$\begin{aligned} -\rho\, c\, p_t - k\,\Delta p &= \gamma_2\, q && \Omega(t) \\ p(T,x) &= 0 && \Omega(T) \\ k\,\tfrac{\partial p}{\partial n} &= 0 && \Gamma_C \cup \Gamma_N \end{aligned}$$

$$\begin{aligned} p_I &= \rho\, c\, p\, k\,\tfrac{\partial y}{\partial n} - k\,\tfrac{\partial p}{\partial n} && \Gamma_I(t) \\ S_i &= -p\, n_i, \quad i = 1,2 && \Gamma_I(t) \end{aligned}$$

$\mathcal{L}_{F_i}\,\delta F_i = 0$:

$$\begin{aligned} \psi\,\phi_{x_i} &= \operatorname{sign}(\phi)\operatorname{div}(G_i\,\nabla\phi) && \mathbb{R}^2 \\ 2\,|\nabla\phi|\,G_i &= -\rho\, L\, p\, n_i && \Gamma_I(t) \end{aligned}$$

$\mathcal{L}_u\,\delta u = 0$:

$$\gamma_3\, u + p = 0 \qquad \Gamma_C$$

$\mathcal{L}_\phi\,\delta\phi = 0$:

$$\begin{aligned} \psi_t + \operatorname{div}(\psi\, F) &= \operatorname{sign}(\phi)\,\operatorname{div}(G_1\,\nabla F_1) + \operatorname{sign}(\phi)\,\operatorname{div}(G_2\,\nabla F_2) && \mathbb{R}^2 \\ \psi(T) &= 0 && \mathbb{R}^2 \end{aligned}$$

$$\begin{aligned} \gamma_1\,\operatorname{div}\left(\frac{|\phi_d|^2}{2}\, n\right) &= \rho\, c\, p\, y_t + k\nabla y\nabla p - f\, p \\ &\quad + \operatorname{div}\left(\left((c\, y - L)\,\rho\, p\, k\,\frac{\partial y}{\partial n} - y\, k\,\frac{\partial p}{\partial n} - p_I\, y_M\right) n\right) && \Gamma_I(t) \end{aligned}$$

$q = \chi_{\Omega_1(t)}(y - y_d), \quad n = \frac{\nabla\phi}{|\nabla\phi|}$

Summary: Free Boundary Value Problems

Challenges and outlook

- optimality conditions
- in particular for problems with constrained interfaces
- gradient based and higher-order numerical solution techniques

Summary: Free Boundary Value Problems

Challenges and outlook

- optimality conditions
- in particular for problems with constrained interfaces
- gradient based and higher-order numerical solution techniques

- developed techniques applicable to other free boundary problems
- for instance, multi-phase fluid flow problems

CHEMNITZ UNIVERSITY OF TECHNOLOGY

Concluding Remarks

Optimal control

- often driven by application
- tool to understand system dynamics

Toolbox of methods applicable to a broad range of applications

- parametric sensitivity analysis
- problems with sparse solutions
- free boundary value problems