

## New Contributions to Theory and Numerics for State-constrained Elliptic Optimal Control Problems

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# New Contributions to Theory and Numerics for State-constrained Elliptic Optimal Control Problems

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#### **Motivation: Fuel Cells**



with non-standard non-linear boundary conditions



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mathematik

Lehrstuhl

Ingenieur-



## Outline

- Introduction
- Split method
- Bryson-Denham-Dreyfus approach (BDD)
- Shape calculus and optimization on vector bundles
- Numerics







#### Elliptic optimal control problem with state constraints

Minimize

$$J(y,u) := \frac{1}{2} \|y - y_d\|_{L^2(\Omega)}^2 + \frac{\lambda}{2} \|u\|_{L^2(\Omega)}^2$$

subject to

$$-\Delta y + y = u$$
 a.e. in  $\Omega$ 

$$\partial_{\nu} y = 0$$
 a.e. on  $\Gamma$ 

 $G(y) := y - y_{\max} \le 0$  a.e. in  $\Omega$ 

#### with

$$\Omega \subset \mathbb{R}^2 \text{ bounded domain, } \Gamma \in C^{1,1},$$
$$u \in U_{ad} := L^2(\Omega), \quad y_d \in L^2(\Omega), \quad \lambda > 0, \quad y_{max} \in H^4(\Omega)$$



## Theorem (Casas 1986): Slater condition $\implies \exists p^{\mathsf{trad}} \in W^{1,s}(\Omega) \text{ and } \mu = \mu_{\Omega} + \mu_{\Gamma} \in C(\bar{\Omega})^*$ such that $-\Delta y + y = u$ a.e. in $\Omega$ $\partial_{\nu} y = 0$ a.e. on $\Gamma$ $-\Delta p^{\text{trad}} + p^{\text{trad}} = y - y_d + \mu_{\Omega}$ a.e. in $\Omega$ $\partial_{\nu} p^{\text{trad}} = \mu_{\Gamma}$ a.e. on $\Gamma$ $\lambda u + p^{\text{trad}} = 0$ a.e. in $\Omega$ $\langle y - y_{\max}, \mu \rangle_{C(\bar{\Omega}), C(\bar{\Omega})^*} = 0, \quad \mu > 0$

#### low regularity causes problems in numerical treatment

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#### Goals and ideas

### Goals

- new necessary conditions with higher regularity of Lagrange multipliers
- formulate efficient numerical algorithms, which don't require any regularization technique, exploit the structure of the multiplier, and are mesh-independent

Ideas

- geometric split
- BDD approach
- shape calculus
- optimization

on vector bundles



- set optimal control problem
- higher regularity
  - necessary conditions
- design of algorithms





#### Goals and ideas

### Goals

- new necessary conditions with higher regularity of Lagrange multipliers
- formulate efficient numerical algorithms, which don't require any regularization technique, exploit the structure of the multiplier, and are mesh-independent

Ideas

- geometric split
- BDD approach
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- set optimal control problem
- higher regularity
  - necessary conditions
- on vector bundles  $\implies$  design of algorithms





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(Analog to the multipoint-boundary-value-problem formulation; Oberle)

#### Minimize

$$J(y_{\mathcal{I}}, y_{\mathcal{A}}, u_{\mathcal{I}}, u_{\mathcal{A}}) := \frac{1}{2} \|y_{\mathcal{I}} - y_d\|_{\mathcal{I}} \|_{L^2(\mathcal{I})}^2 + \frac{1}{2} \|y_{\mathcal{A}} - y_d\|_{\mathcal{A}} \|_{L^2(\mathcal{A})}^2 + \frac{\lambda}{2} \|u_{\mathcal{I}}\|_{L^2(\mathcal{I})}^2 + \frac{\lambda}{2} \|u_{\mathcal{A}}\|_{L^2(\mathcal{A})}^2$$

subject to  $-\Delta y_{\mathcal{T}} + y_{\mathcal{T}} = u_{\mathcal{T}}$ , a.e. in  $\mathcal{I}$ a.e. in  $\mathcal{A}$  $-\Delta y_A + y_A = u_A$ ,  $\partial_{\nu} y_{\mathcal{T}} = 0$ , a.e. on  $\Gamma$ How can we determine a.e. on  $\gamma$  $y_{\mathcal{T}} = y_A$ , the active set?  $\partial_{\nu_{\mathcal{T}}} y_{\mathcal{I}} + \partial_{\nu_{\mathcal{A}}} y_{\mathcal{A}} = 0 \,,$ a.e. on  $\gamma$ a.e. in  $\tilde{\mathcal{A}}$  $y_{\mathcal{A}} = y_{\max}$ , a.e. in  $\mathring{I}$  $y_{\mathcal{T}} < y_{\max}$ , a.e. on  $\gamma$  $y_A = y_{\max}$ ,





 $y_{\mathcal{B}} = y_{\max}$ ,

**Minimize** 

$$J(y_{\mathcal{J}}, y_{\mathcal{B}}, u_{\mathcal{J}}, u_{\mathcal{B}}, \mathcal{B}) := \frac{1}{2} \|y_{\mathcal{J}} - y_d|_{\mathcal{J}}\|_{L^2(\mathcal{J})}^2 + \frac{1}{2} \|y_{\mathcal{B}} - y_d|_{\mathcal{B}}\|_{L^2(\mathcal{B})}^2 + \frac{\lambda}{2} \|u_{\mathcal{J}}\|_{L^2(\mathcal{J})}^2 + \frac{\lambda}{2} \|u_{\mathcal{B}}\|_{L^2(\mathcal{B})}^2$$

subject to  $-\Delta y_{\mathcal{J}} + y_{\mathcal{J}} = u_{\mathcal{J}}$ , a.e. in  $\mathcal{J}$ a.e. in  $\mathcal{B}$  $-\Delta y_{\mathcal{B}} + y_{\mathcal{B}} = u_{\mathcal{B}},$  $\partial_{\nu} y_{\mathcal{J}} = 0 \,,$ a.e. on  $\Gamma$ a.e. on  $\beta$  $y_{\mathcal{T}} = y_{\mathcal{B}},$  $\partial_{\nu_{\mathcal{T}}} y_{\mathcal{T}} + \partial_{\nu_{\mathcal{B}}} y_{\mathcal{B}} = 0,$ a.e. on  $\beta$ a.e. in  $\mathcal{B}$  $y_{\mathcal{B}} = y_{\max}$ , a.e. in  $\mathring{\mathcal{J}}$  $y_{\mathcal{J}} < y_{\max}$ , a.e. on  $\beta$ 

How to handle the strict inequality?

Theorem: The original problem and the set optimal control problem possess the same unique solution

**Minimize**  $J(y_{\mathcal{J}}, y_{\mathcal{B}}, u_{\mathcal{J}}, u_{\mathcal{B}}, \mathcal{B}) := \frac{1}{2} \|y_{\mathcal{J}} - y_d|_{\mathcal{J}} \|_{L^2(\mathcal{J})}^2 + \frac{1}{2} \|y_{\mathcal{B}} - y_d|_{\mathcal{B}} \|_{L^2(\mathcal{B})}^2$ inner outer +  $\frac{\lambda}{2} \|u_{\mathcal{J}}\|_{L^{2}(\mathcal{J})}^{2} + \frac{\lambda}{2} \|u_{\mathcal{B}}\|_{L^{2}(\mathcal{B})}^{2}$ subject to  $\begin{vmatrix} -\Delta y_{\mathcal{J}} + y_{\mathcal{J}} = u_{\mathcal{J}}, & \text{a.e. in } \mathcal{J} \\ -\Delta y_{\mathcal{B}} + y_{\mathcal{B}} = u_{\mathcal{B}}, & \text{a.e. in } \mathcal{B} \end{vmatrix}$ a.e. in  ${\mathcal J}$  $\partial_{\nu} y_{\mathcal{J}} = 0$ , a.e. on Г 
$$\begin{split} y_{\mathcal{J}} &= y_{\mathcal{B}}, & \text{a.e. on } \beta \\ \partial_{\nu_{\mathcal{J}}} y_{\mathcal{J}} &+ \partial_{\nu_{\mathcal{B}}} y_{\mathcal{B}} &= 0, & \text{a.e. on } \beta \\ y_{\mathcal{B}} &= y_{\text{max}}, & \text{a.e. in } \mathring{\mathcal{B}} \end{split}$$
constraint of a.e. in  $\mathcal{J}$  $y_{\mathcal{T}} < y_{\max}$ outer optimization a.e. on  $\beta$  $y_{\mathcal{B}} = y_{\max}$ ,

Theorem: The inner optimization problem possesses a unique solution for  $\mathcal{B} \in \mathcal{B}_{ad}$ 

**Consequences: existence of a geometry to solution operator** 



**Consequences: existence of a geometry to solution operator** 

Reduced functional: 
$$\exists G: \mathcal{B} 
ightarrow (y_{\mathcal{J}}, y_{\mathcal{B}}, u_{\mathcal{J}}, u_{\mathcal{B}})$$
  
 $\mathcal{F}(\mathcal{B}) = J(G(\mathcal{B}), \mathcal{B})$ 

is well-defined on  $\mathcal{B}_{ad}$  :

$$\min_{\mathcal{B}} \mathcal{F}(\mathcal{B})$$
 subject to  $\left\{egin{array}{c} \mathcal{B} \in \mathcal{B}_{ ext{ad}} \ y_{\mathcal{J}} < y_{ ext{max}} ext{ in } \mathcal{J} \end{array}
ight.$ 

Set optimal control problem (shape-/topology-optimization)





#### Geometry to solution operator



#### Theorem:

For any  $\mathcal{B} \in \mathcal{B}_{ad}$  there exist Lagrange multipliers associated with the equality constraints of the inner optimization problem

Inner optimization problem is strictly convex



Necessary conditions are sufficient

# Replace inner optimization problem by its necessary conditions





#### Set optimal control problem

T	$\min_{\mathcal{B}\in\mathcal{B}_{ad}}\mathcal{F}($	$\mathcal{B})$ subject	t to	$y_{\mathcal{J}} < g$	/max	in ${\cal J}$
	and –	$\Delta y_{\mathcal{J}} + y_{\mathcal{J}} = -$	$-\frac{1}{\lambda}p_{\mathcal{J}},$	a.e.	in ${\cal J}$	
		$\partial_{\nu} y_{\mathcal{J}} = 0 ,$		a.e.	on Г	no measures
	—2	$y_d - y_d$ ,	a.e.	in ${\mathcal J}$	involved	
	$\partial_{\nu} p_{\mathcal{J}} = 0,$ $y_{\mathcal{J}} = y_{\max},$			a.e.	on Г	unusual boundary
				a.e.	on $\beta$	conditions
		$\partial_{\nu_{\mathcal{J}}} y_{\mathcal{J}} = \partial_{\nu_{\mathcal{J}}} y_{fr}$	nax,	a.e.	on $\beta$	
		everything else car	n be comp	outed a poster	riori —	
	$y_{\mathcal{B}} = y_{\max}$ ,	a.e. in ${\cal B}$		$u_{\mathcal{J}} = -\frac{1}{\lambda} p_{\zeta}$	$\mathcal J$ ,	a.e. in ${\cal J}$
$u_{\mathcal{B}}$ =	$= -\Delta y_{\max} + y_{\max}$ ,	a.e. in ${\cal B}$	$\mu_eta$	$= \partial_{\nu_{\mathcal{J}}} p_{\mathcal{J}} + c$	a.e. on $\beta$	
	$p_{\mathcal{B}} = -\lambda  u_{\mathcal{B}} ,$	a.e. in ${\cal B}$	$\mu_{\mathcal{B}} = -2$	$\Delta p_{\mathcal{B}} + p_{\mathcal{B}} -$	$y_{\mathcal{B}} + y_{m}$	$_{ax},$ a.e. in $\mathcal B$





Shape calculus for the optimal active set



determines the interface

We omit  $y_{\mathcal{J}} < y_{\max}$  in the outer optimization and determine the interface  $\beta$  by

$$d\mathcal{F}(\mathcal{B};V) = 0 \quad \forall \quad V \in C^{1,1}(\bar{\Omega})$$
$$\implies \quad p_{\mathcal{J}} = p_{\max} \quad \text{on} \quad \beta$$
$$\implies \quad u_{\mathcal{J}} = u_{\mathcal{B}} \quad \text{on} \quad \beta$$

Needs an a posteriori-check on feasability:  $y_{\mathcal{J}} < y_{\max}$ 





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- Bryson-Denham-Dreyfus<sup>\*</sup> approach (BDD)
- Shape calculus and optimization on vector bundles
- Numerics
- \* A.E. Bryson, Jr, W.F. Denham, S.E. Dreyfus: Optimal programming problems with inequality constraints I, AIAA Journal 1(11):2544-2550, 1963.

Later extended by Maurer, 1979.



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Transfering the Bryson-Denham-Dreyfus approach  $G(\bar{y}_{\mathcal{A}}) \equiv 0 \text{ a. e. in } \mathcal{A} \iff$   $-\Delta G(\bar{y}_{\mathcal{A}}) + G(\bar{y}_{\mathcal{A}}) = 0, \qquad \text{ a. e. in } \mathcal{A}$  $G(\bar{y}_{\mathcal{A}}) = 0, \qquad \text{ a. e. on } \gamma$ 

Using the state equation

$$\begin{aligned} \Delta y_{\max} - y_{\max} + \bar{u}_{\mathcal{A}} &= 0, & \text{a.e. in } \mathcal{A} \\ \bar{y}_{\mathcal{A}} &= y_{\max}, & \text{a.e. on } \gamma \end{aligned}$$

Optimal solution on  $\mathcal{A}$  given by data, but  $\mathcal{A}$  optimization variable





#### First-order necessary condition of set-OCP (split method)



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#### First-order necessary condition of set-OCP (BDD method)



#### First-order necessary condition of set-OCP (BDD method)

(new adjoint state and multpliers with higher regularity)

$$\begin{split} -\Delta q + q &= \mu_{\mathcal{A}}, \text{ a.e. in } \mathcal{A} \\ \partial_{\nu_{\mathcal{A}}} q + \sigma &= \mu_{\gamma}, \text{ a.e. on } \gamma \end{split}$$

#### BDD approach reveals control law, i.e. "hidden" condition (as for PDAE)

$$u_{\mathcal{A}} = -\Delta y_{\max} + y_{\max}$$





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#### **Basic considerations with respect to shape calculus**



$$\lim_{t \to 0} \frac{1}{t} \left( J(x+tw) - J(x) \right) \lim_{\substack{t \to 0 \\ \dot{\alpha}(0) = w}} \frac{1}{t} \left( J(\alpha(t)) - J(x) \right)$$



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#### Basic considerations with respect to shape calculus

set  $\mathcal{B} \in \mathcal{B}_{\mathsf{ad}} \subset \mathcal{M}$ 

(no linear structure, infinite dimensional manifold)

vector field  $\,V\,$ image

 $\mathcal{A} := (\mathrm{Id} + V)(\mathcal{B})$  holdall  $\Omega$ 

Delfour, Zolésio, 2011

perturbation of identity defines curves  $\,\mathcal{B}_{ad}\,$ 

$$\mathcal{B} \to T_t(\mathcal{B}) := (\mathrm{Id} + t \, V)(\mathcal{B})$$



)  $dJ(\mathcal{B}; V) := \lim_{t \to 0} \frac{J(\mathcal{B}_t) - J(\mathcal{B})}{t}$ 



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- Hadamard directional derivative is suitable for nonlinear spaces
- Deformation of sets yields "perturbation of identity"
- Metric of function spaces induces metric in  $\mathcal{B}_{ad}$

 $\mathcal{B}_{ad}~$  has no linear structure

 $\mathcal{B}_{ad}$  is similar to an infinite dimensional manifold

- $t\mapsto \mathcal{B}_t\,$  defines curves in  $\,\mathcal{B}_{\mathrm{ad}}\,$
- suitable difference quotient

$$\lim_{t \to 0} \frac{J(\mathcal{B}_t) - J(\mathcal{B})}{t}$$



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#### **Exemplary derivation of directional shape derivative**

Let  $\mathcal{F}(\mathcal{B}) = \int_{\mathcal{B}} f(\mathcal{B}, X) \, \mathrm{d}X$ implicit set dependence explicit  $d\mathcal{F}(\mathcal{B}, V) = \lim_{t \to 0} \frac{1}{t} \left( \int_{\mathcal{B}_t} f(\mathcal{B}_t, X) \, dX - \int_{\mathcal{B}} f(\mathcal{B}, X) \, dX \right)$  $= \lim_{t \to 0} \frac{1}{t} \left( \int_{\mathcal{B}} f(\mathcal{B}_t, T_t(X)) \det DT_t(X) \, \mathrm{d}X - f(\mathcal{B}, X) \, \mathrm{d}X \right)$  $= \int_{\partial \mathcal{B}} f(\mathcal{B}, X) \left( V(X) \cdot \nu(X) \right) dS(X) + \int_{\mathcal{B}} \frac{\partial}{\partial t} f(\mathcal{B}_t, X)|_{t=0} dX$ 

explicit derivative

#### implicit derivative



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shape calculus is similar to calculus on manifolds



intrinsic nonlinear behaviour

shape (directional) derivative

concentrated on boundary and

on the normal component of the vector field only





#### **Vector bundles**



#### **Optimization on vector bundles: shape optimization**

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## Optimization on vector bundles: set optimal control problem









## **Optimization on vector bundles: set optimal control problem**



Minimize  $\mathcal{F}(\mathcal{B}) = J(\mathcal{B}, G(\mathcal{B}))$ 

**s.t.** 
$$\mathcal{B} \in \mathcal{B}_{ad} \subset \mathcal{M}$$

$$y_{\mathcal{J}} < y_{\max}$$





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#### Analysis of necessary conditions



#### Basic considerations w.r.t. the algorithm

•  $\mathcal{A} \in \mathcal{M}$  is no (local) minimum of the (unconstrained)  $\mathcal{F}$ , second semi-derivative is not definite at critical points. Hence, steepest decent algorithms not applicable, higher order methods are required.







## **Towards Newton 's method on manifolds**



2. loop on k

stoping criterion

Hessian and gradient require Hilbert spaces

Newton equation Hess 
$$J(x_k)[\delta_k] = -\operatorname{grad} J(x_k)$$

ipdate 
$$x_{k+1} = x_k + \delta_k$$

3. end of loop





### **Towards Newton 's method on manifolds**



2. loop on k

stoping criterion

# directional derivatives suitable for linear structure $D^2 J(x_k)[\delta_k, v] = -DJ(x_k)[v] \ \forall v \in \mathcal{V}$

Newton equation

n D- $J(x_k)[\delta_k, v] = -DJ(x_k)$  $x_{k+1} = x_k + \delta_k$ 

3. end of loop

update



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#### Second directional derivative / second covariant derivative



## **Towards Newton 's method on manifolds**

- 1. Initial guess  $k := 1, x_1$
- 2. loop on k
  - stoping criterion

Newton equation 
$$\nabla^2 J(x_k)[\delta_k, v] = -DJ(x_k)[v] \ \forall v \in \mathcal{V}$$
  
update  $x_{k+1} = x_k + \delta_k$ 

3. end of loop

sum requires linear structure





#### Newton update by retraction

 $T_{x_k}\mathcal{M}$ **Retraction:**  $R:T\mathcal{M}\longrightarrow \mathcal{M}$  $\hat{\delta}_{k}$  $x_k$  $x_{k+1} = R(\delta_k)$  $x_{k+1} = R(\delta_k)$  $R: T\mathcal{M} \longrightarrow \mathcal{M}$  is a retraction  $: \iff$  $R_x(\mathbf{0}_x) = x \,\,\forall x \in \mathcal{M}$ with  $0_x$  is zero in  $T_x\mathcal{M}$  and  $DR_x(0_x) = \mathrm{Id}_{T_x\mathcal{M}}$ 





## Newton's method on manifolds

- 1. Initial guess  $k := 1, x_1$
- 2. loop on k
  - stoping criterion

Newton equation 
$$abla^2 J(x_k)[\delta_k,v] = -DJ(x_k)[v] \ \forall v \in \mathcal{V}$$
  
update  $x_{k+1} = R(\delta_k)$ 

3. end of loop





#### Newton 's method on manifolds





2. loop on k

stoping criterion

Newton equation
$$\nabla^2 J(x_k)[\delta_k, v] = -DJ(x_k)[v] \quad \forall v \in \mathcal{V}$$
update $x_{k+1} = R(\delta_k)$ 

3. end of loop





#### Newton's method on manifolds



 $k := 1, x_1$ 

2. loop on

k

Newton equation

update

3. end of loop

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 $\nabla^2 J(x_k)[\delta_k, v] = -\mathsf{D} J(x_k)[v] \ \forall v \in \mathcal{V}$  $x_{k+1} = R(\delta_k) \delta_k$ 

second covariant derivative: it does not contain full information of second directional derivative, but full second order information on functional

directional derivative. since Hessian and gradient require **Hilbert spaces** 





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 $x_{k+1} = R(\delta_k)$ 

 $T_{x_k}\mathcal{M}$ 

 $\delta_k$ 

 $x_k$ 

#### Newton's method for set optimal control problems

1. provide initial guess  $\mathcal{B}_1$ (by formula on data: candidate active set)  $-\Delta y_{\mathcal{A}} + y_{\mathcal{A}} = u_{\mathcal{A}} \quad \lambda \, u_{\mathcal{A}} + p_{\mathcal{A}} = 0 \qquad y_{\mathcal{A}} = 0$ ymax  $-\Delta p_{\mathcal{A}} + p_{\mathcal{A}} = y_{\mathcal{A}} - y_d + \mu$  $\mu(x) := -\lambda \Delta^2 y_{\max}(x) + 2\lambda \Delta y_{\max}(x) - (1+\lambda) y_{\max}(x) + y_d(x) \ge 0$ 

due to strict complementarity:

$$\mathcal{A} \subset \{x \in \Omega: \mu(x) \ge 0\}$$



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- 3. end of loop
- 4. check a posteriori criteria and eventually restart with other initial guess





#### Newton method on manifold and topology changes



Michael Frey 's dissertation, University of Bayreuth, 2012: Shape calculus applied to state-constrained elliptic optimal control problems

http://opus.ub.uni-bayreuth.de/opus4-ubbayreuth/frontdoor/index/index/docld/996







#### pro

- formulation in infinite dimen. setting  $\implies$  mesh independency
- no regularization loops is better performance than PDAS
- feasible approximations of solutions

## contra

changes of topology heuristically

- no convergence analysis
- only local convergence (with adaptive smooting for stability)
- assumptions on active set





#### The Smiley: construction



algorithm can cope with topology changes

Construction: Prescribe  $y_d$ , choose  $\lambda$  small, press down  $y_{\text{max}}$ .

Initial guess: automatically from unconstrained problem





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#### The Smiley example: rational initial guess





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#### The Smiley example: bad initial guess

Algorithm can cope with topology changes to some extent





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#### The Smiley example: bad initial guess

Adjoint multiplier: continuous on interface, but normal derivatives jump







# Split method

- new problem type: set optimal control problem
- bilevel formulation is geometry-to-solution operator
- split of constraint ⇒ exploitation of structure of multiplier

# **Extended BDD approach for PDEs**

- differentiation of state constraint  $\implies$  control law
- higher regularity of multiplier
- connection with optimal control and PDAE: index reduction





## Shape calculus

- set of admissible active sets has manifold character and thus is intrinsicly nonlinear
- deformation of sets: perturbation of identity
- calculation requires transformation formula

# **Optimization on vector bundles**

- vector bundles: structure depends upon manifolds
- general basis for shape optimization / set optimal control problems
- new challenging class of optimization problems





# **Newton method**

- several approaches towards solution of new necessary conditions
- adaption of Newton method on manifolds
- algorithm in function space without regularization
- comparable performance to sophisticated PDAS
- pays off in case of nonlinear elliptic optimal control problems

# **Open questions**

- active sets of measure zero
- generalization to parabolic problems (first results already obtained)





## Constantin Carathéodory on the Bicentennial of Harvard University (1937)



I will be glad if I have succeeded in impressing the idea that it is not only pleasant and entertaining to read at times the works of the old mathematicial authors, but that this may occasionally be of use for the actual advancement of science.

Besides this there is a great lesson we can derive from the facts which I have just referred to. We have seen that even under conditions which seem most favorable very important results can be discarded for a long time and whirled away from the main stream which is carrying the vessel science. ...

If their ideas are too far in advance of their time, and if the general public is not prepared to accept them, these ideas may sleep for centuries on the shelves of our libraries ... awaiting the arrival of the prince charming who will take them home.

**Constantin Carathéodory** (Κωνσταντίνος Καραθεοδωρή) \* Sept. 13, 1873 in Berlin; † Feb. 2, 1950, Munich





# Thank you for your attention – There 's still much to do





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# Simultaneously I want to say GOOD BYE, friends





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