Dealing with Optimization Problems Constrained by Nonlinear Non-Smooth PDEs

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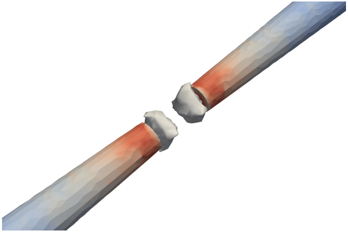
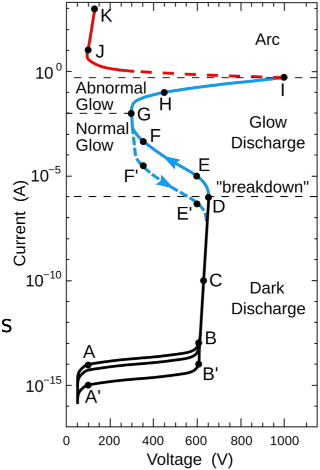
Outline

1. Motivation & Model Problem
2. Optimization Strategy for Non-Smooth Problems
3. Numerical Results
4. Conclusion and Outlook

Motivation





- Aim:
  simulation and optimization of hysteresis
- Challenge:
  - Switches
  - History dependency
- Study model problem: PDE with switches

Model Problem for Switches

$$\min_{(y,u)\in H_0^1\times L^2} \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\alpha}{2}\|u\|_{L^2}^2$$
$$\text{s.t.} \quad -\Delta y + \ell(y) - u = 0 \quad \text{in } \Omega$$

- Lipschitz domain $\Omega \subset \mathbb{R}^n, n \in \mathbb{N}$
- $\ell : H_0^1(\Omega) \to L^2(\Omega)$ non-smooth, locally Lipschitz continuous, bounded and strictly monotone
- Non-differentiablilities are constructed from abs() and smooth elementals. (Also covers min() and max()).

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Challenge: Standard techniques can not be applied.

Observed Properties

- Weakly lower semi-continuous and twice continuously Fréchet-differentiable objective functional
- Well posed simulation problem with unique solution y for any given control u

  Browder-Minty Theorem
- Well defined, Lipschitz continuous and directionally differentiable control-to-state-mapping $S : u \mapsto y$
- Existence of a solution for the optimal control problem

Previous Results for Finite Dimensions

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Theoretical results for

- Lipschitz continuous, piecewise smooth function $f : \mathbb{R}^n \to \mathbb{R}$
- All non-differentiabilities are incorporated by abs()

$\Rightarrow$ First and second order optimality conditions

A. Griewank und A. Walther, First and second order optimality conditions for piecewise smooth objective functions.*Optimization Methods and Software*, 31(5):904-930 (2016), 2013.

Development of minimization algorithm

- Convergence theory & promising numerical results

$\Rightarrow$ LiPsMin - Lipschitzian Piecewise Smooth Minimization

S. Fiege, A. Walther, A. Griewank, An Algorithm for Non-Smooth Optimization by Successive Piecewise Linearization, *Mathematical Programming*, 2018

Handling of abs

Convert max and min to abs via:

$$\max(u,v) = \tfrac{1}{2}(u + v + |v - u|)$$
$$\min(u,v) = \tfrac{1}{2}(u + v - |v - u|)$$

$$\begin{array}{|lcll|}\hline \ell(y) & = & \Psi(y, |y|) & \\ \hline z_i & = & \psi^i(y, \sigma z)_{j \prec i} & \multirow{3}{*}{$\left.\right\}\ i = 1, \dots, s$} \\ \sigma_i & = & \operatorname{sgn}(z_i) & \\ \sigma_i z_i & = & \operatorname{abs}(z_i) & \\ \hline \hat{\ell}(y, \sigma z) & = & \psi^{s+1}(y, \sigma z)_{j \prec s+1}, & \sigma z = (\sigma_1 z_1, \dots, \sigma_s z_s) \\ \hline \end{array}$$

Table: Reduced evaluation procedure

Example

Reduced evaluation procedure for
$\ell(y) = \max(0, y) + \min(0, y + \frac{1}{2}|y|)$

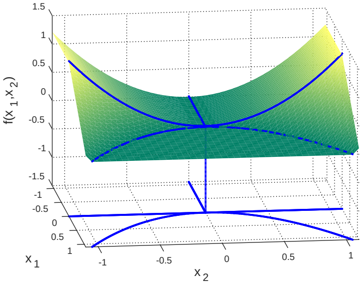
$$\ell(y) = y + \tfrac{3}{4}|y| - \tfrac{1}{2}\left|y + \tfrac{1}{2}|y|\right|$$

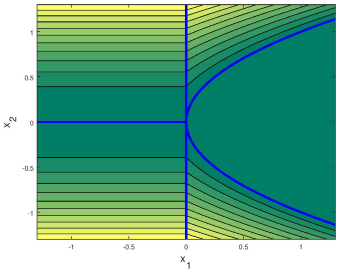
$$\begin{aligned}
z_1 &= \psi^1(y, \sigma z)_{j \prec 1} &&= y \\
\sigma_1 & &&= \mathrm{sgn}(z_1) \\
\sigma_1 z_1 & &&= \mathrm{abs}(z_1) \\
z_2 &= \psi^2(y, \sigma z)_{j \prec 2} &&= y + \tfrac{1}{2}\sigma_1 z_1 \\
\sigma_2 & &&= \mathrm{sgn}(z_2) \\
\sigma_2 z_2 & &&= \mathrm{abs}(z_2)
\end{aligned}$$

$$\hat{\ell}(y, \sigma z) = \psi^3(y, \sigma z)_{j \prec 3} = y + \tfrac{3}{4}\sigma_1 z_1 - \tfrac{1}{2}\sigma_2 z_2$$

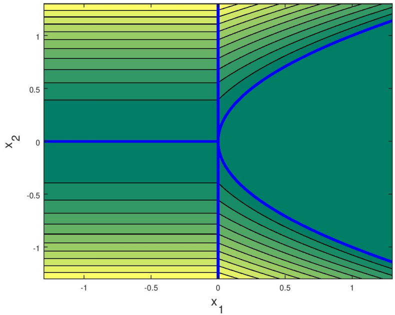
The Idea of Abs-Linearization in Finite Dimensions

$$\min_{x_1, x_2} \max(0, x_2^2 - \max(0, x_1))$$





$$\min_{x_1,x_2} \underbrace{\max(0, x_2^2 - \max(0, x_1))}$$
$$= \tfrac{1}{2}\left[x_2^2 - \tfrac{1}{2}(x_1 + |x_1|)\right]$$
$$+ \tfrac{1}{2}\left[\left|x_2^2 - \tfrac{1}{2}(x_1 + |x_1|)\right|\right]$$



1. Substitute all abs:

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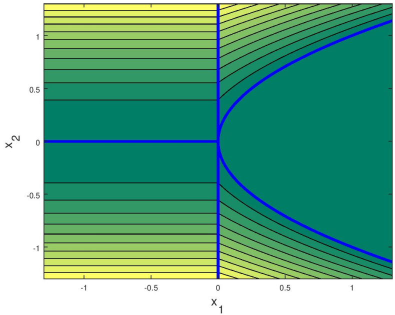
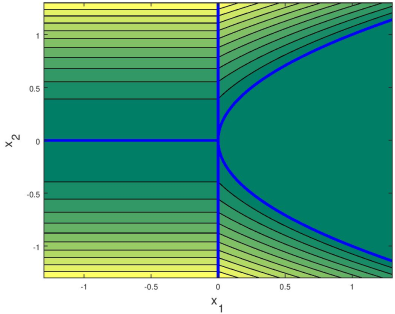


1. Substitute all abs:

$$z_1 \leftarrow x_1$$
$$z_2 \leftarrow x_2^2 - \tfrac{1}{2}(x_1 + \operatorname{sgn}(z_1) z_1)$$

$$\min_{x_1,x_2} \underbrace{\max(0, x_2^2 - \max(0, x_1))}_{\begin{aligned} &= \tfrac{1}{2}\left[x_2^2 - \tfrac{1}{2}(x_1 + |x_1|)\right] \\ &\quad + \tfrac{1}{2}\left[\left|x_2^2 - \tfrac{1}{2}(x_1 + |x_1|)\right|\right]\end{aligned}}$$



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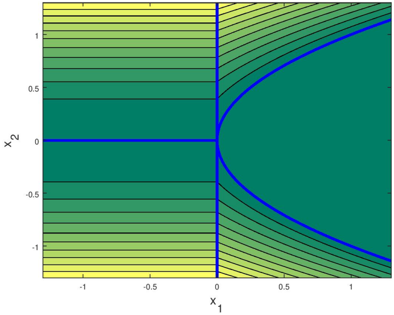

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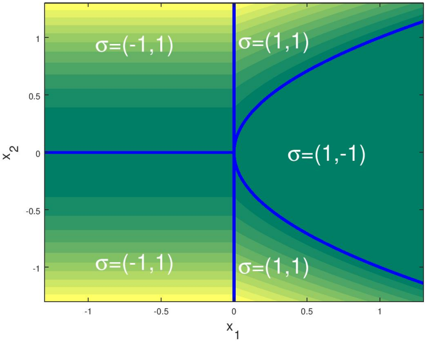
$$\min_{z_1,z_2} \tfrac{1}{2}\left[z_2 + \sigma_2 z_2\right]$$
$$s.t. \quad z_1 - x_1 = 0$$
$$z_2 - x_2^2 + \tfrac{1}{2}(x_1 + \sigma_1 z_1) = 0$$

$$\min_{x_1,x_2} \max(0, x_2^2 - \max(0, y_1))$$



$$\min_{z_1,z_2} \frac{1}{2}\left[z_2 + \sigma_2 z_2\right]$$

$$\begin{aligned} s.t.\ & z_1 - x_1 = 0 \\ & z_2 - x_2^2 + \frac{1}{2}(x_1 + \sigma_1 z_1) = 0 \\ & \sigma_1 z_1 \geq 0 \\ & \sigma_2 z_2 \geq 0 \end{aligned}$$

- New problem is smooth if σ is fixed parameter
- Changing a σ_i, means changing a region

$\mathbb{R}^n$ vs. Function Space Scenario

- $\mathbb{R}^n$
  - $\sigma_i \in \{-1, 0, 1\}$
  - Piecewise linearization
  - Decomposition of the domain

- Function Space

  $\Rightarrow$ Need adopted ideas and new concepts.

Handling of abs in Function Spaces

$$\ell(y) = \Psi(y, |y|)$$

$$\left.\begin{aligned} z_i &= \psi^i(y, \sigma z)_{j \prec i} \\ \sigma_i &= \mathrm{sgn}(z_i) \\ \sigma_i z_i &= \mathrm{abs}(z_i) \end{aligned}\right\} \quad i = 1, \ldots, s$$

$$\hat{\ell}(y, \sigma z) = \psi^{s+1}(y, \sigma z)_{j \prec s+1}, \qquad \sigma z = (\sigma_1 z_1, \ldots, \sigma_s z_s)$$

Nemytskii operator

$$\mathrm{abs} : H_0^1(\Omega) \to L^2(\Omega), \qquad [abs(y)](x) = |y(x)| \quad \text{f.a.a. } x \in \Omega$$

$$\sigma_i : H_0^1(\Omega) \to L^2(\Omega), \qquad [\sigma_i(z)](x) = sgn(z_i(x)) z_i(x) \quad \text{f.a.a. } x \in \Omega$$

$$\Rightarrow \quad \sigma_i(z_i) = abs(z_i) \in L^2(\Omega)$$

Equivalent Problem Reformulation

$$\min_{(y,u)\in H_0^1\times L^2} \frac{1}{2}\|y-y_d\|_{L^2}^2 + \frac{\alpha}{2}\|u\|_{L^2}^2 =: \mathcal{J}(y,u)$$

$$\text{s.t} \quad -\Delta y + \ell(y) - u = 0$$

$$\Updownarrow$$

$$\min_{(y,u)\in H_0^1\times L^2} \mathcal{J}(y,u)$$

$$\text{s.t} \quad -\Delta y + \hat{\ell}(y,\sigma z) - u = 0$$

$$\left.\begin{aligned} \psi^i(y,\sigma z)_{j\prec i} - z_i &= 0 \\ \sigma_i z_i - \text{abs}(z_i) &= 0 \end{aligned}\right\} \quad \forall\ i = 1,\dots,s$$

Decomposition into Smooth Branch Problems

$$\min_{(y,u)\in H_0^1\times L^2} \frac{1}{2}\|y-y_d\|_{L^2}^2+\frac{\alpha}{2}\|u\|_{L^2}^2 =: \mathcal{J}(y,u)$$

$$\text{s.t} \quad -\Delta y+\ell(y)-u=0$$

$$\Downarrow$$

$$\min_{(y,u)\in H_0^1\times L^2} \mathcal{J}(y,u)$$

$$\text{s.t} \quad -\Delta y+\hat{\ell}(y,\sigma z)-u=0$$

$$\left.\begin{aligned} \psi^i(y,\sigma z)_{j\prec i}-z_i &= 0 \\ \sigma_i z_i &\geq 0 \\ \sigma_i:\Omega\to\{-1,&\ +1\} \end{aligned}\right\} \forall\ i=1,\dots,s$$

Optimization Strategy - Lagrangian with Penalty

$$\min_{(y,u)\in H_0^1\times L^2} \quad \mathcal{J}(y,u)$$

$$\text{s.t} \quad -\Delta y + \hat{\ell}(y,\sigma z) - u = 0$$

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$$\mathcal{L}(y,u,\sigma z,\lambda_{PDE},\lambda_1,\dots,\lambda_s)$$

$$= \mathcal{J}(y,u) + (\nabla\lambda_{PDE},\nabla y)_{L^2(\Omega)} + (\lambda_{PDE},\hat{\ell}(y,\sigma z) - u)_{L^2(\Omega)}$$

$$+ \sum_{i=1,j\prec i}^{s} (\lambda_i,\psi^i(y,\sigma z)_{j\prec i} - z_i)_{L^2(\Omega)} + \mu\int_\Omega \sum_{i=1}^{s}\Big(\max(-\sigma_i z_i,0)\Big)^4\, d\Omega$$

with $\mu > 0$ sufficiently large.

Necessary Optimality Conditions

$$0 \stackrel{!}{=} \frac{\partial \mathcal{J}}{\partial y}\tilde{y} + (\Delta\lambda_{PDE}, \Delta\tilde{y}) + (\lambda_{PDE}, \frac{\partial \hat{\ell}}{\partial y}\tilde{y}) + \sum_{i=1}^{s} (\lambda_i, \frac{\partial \psi^i(y,\sigma_j z_j)}{\partial y}\tilde{y}) \quad \forall \tilde{y}$$

$$0 \stackrel{!}{=} \frac{\partial \mathcal{J}}{\partial u}\tilde{u} - (\lambda_{PDE}, \tilde{u}) \quad \forall \tilde{u}$$

$$0 \stackrel{!}{=} (\Delta\tilde{\lambda}_{PDE}, \Delta y) + (\tilde{\lambda}_{PDE}, \hat{\ell}) - (\tilde{\lambda}_{PDE}, u) \quad \forall \tilde{\lambda}_{PDE}$$

$$0 \stackrel{!}{=} (\tilde{\lambda}_i, \psi^i(y, \sigma z)_{j\prec i} - z_i)_{L^2(\Omega)} \quad \forall \tilde{\lambda}_i,\ \forall i = 1, \dots, s$$

$$0 \stackrel{!}{=} (\lambda_{PDE}, \frac{\partial \hat{\ell}(y,\sigma z)}{\partial z_k}\tilde{z}_k) + (\lambda_k, \frac{\partial \psi^i(y,\sigma_j z_j)}{\partial z_k}\tilde{z}_k) - (\lambda_k, \tilde{z}_k)$$
$$+ \sum_{i=k+1,\ j\prec i}^{s} (\lambda_i, \frac{\partial \psi^i(y,\sigma z)_{j\prec i}}{\partial z_k}\tilde{z}_k) + \mu \int_\Omega -4\sigma_k \max(-\sigma_k z_k, 0)^3\ \tilde{z}_k\ d\Omega$$
$$\forall \tilde{z}_k,\ \forall k = 1, \dots, s$$

Algorithmic Idea

Solving non-smooth optimal control problems:

0. Reformulate non-smoothness in terms of abs.
1. Choose corresponding branch problem,
   i.e. choose $\sigma_i : \Omega \to \{-1, +1\}$.
2. Solve smooth branch problem
   (e.g. with FEM & Newton) for (y, u, z, λ).
3. If $\lambda_i = 0, \ \forall i$: STOP
   Else: Determine new σ_i according to λ_i & go to 1.

How to Switch Branch Problems?

$$0 \stackrel{!}{=} \frac{\partial \mathcal{J}}{\partial y}\tilde{y} + (\Delta\lambda_{PDE}, \Delta\tilde{y}) + (\lambda_{PDE}, \frac{\partial \hat{\ell}}{\partial y}\tilde{y}) + \sum_{i=1}^{s} (\lambda_i, \frac{\partial \psi^i(y,\sigma_j z_j)}{\partial y}\tilde{y}) \quad \forall \tilde{y}$$

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$$0 \stackrel{!}{=} (\tilde{\lambda}_i, \psi^i(y, \sigma z)_{j \prec i} - z_i)_{L^2(\Omega)} \quad \forall \tilde{\lambda}_i, \ \forall i = 1, \dots, s$$

$$0 \stackrel{!}{=} (\lambda_{PDE}, \frac{\partial \hat{\ell}(y,\sigma z)}{\partial z_k}\tilde{z}_k) + (\lambda_k, \frac{\partial \psi^i(y,\sigma z)_{j \prec i}}{\partial z_k}\tilde{z}_k) - (\lambda_k, \tilde{z}_k)$$
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$$\forall \tilde{z}_k, \ \forall k = 1, \dots, s$$

How to Switch Branch Problems?

$$0 \leq \mu \int_\Omega 4 \max(-\sigma_k z_k, 0)^3 \; \tilde{z}_k \; d\Omega = (\lambda_{PDE}, \frac{\partial \hat{\ell}(y,\sigma z)}{\partial z_k} \tilde{z}_k) + (\lambda_k, \frac{\partial \psi^i(y,\sigma z)}{\partial z_k} \tilde{z}_k) - (\lambda_k \sigma_k, \tilde{z}_k) + \sum_{i=k+1}^{s} (\lambda_i, \frac{\partial \psi^i(y,\sigma_j z_j)}{\partial z_k} \tilde{z}_k) \quad \forall k = 1, \dots, s$$

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This optimality condition is violated iff $\exists k \in \{1, \dots, s\}$ such that $\sigma_k = sgn(\lambda_k)$ with

$$0 > (\lambda_{PDE}, \frac{\partial \hat{\ell}(y,\sigma z)}{\partial z_k} \tilde{z}_k) + (|\lambda_k|, \frac{\partial \tilde{\psi}^i(y,\sigma z)}{\partial z_k} \tilde{z}_k - \tilde{z}_k) + \sum_{i=k+1}^{s} (\lambda_i, \frac{\partial \psi^i(y,\sigma_j z_j)}{\partial z_k} \tilde{z}_k)$$

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⇒ Natural strategy: choose k for which RHS is minimal.

⇒ Swap σ_k where discretized λ_k^h is pointwise largest.
⇒ Explore branch with highest importance first.

⇒ Use λ_k^h as indicator to swap sign.

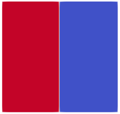
Finite dimensional approach in: A. Griewank, A. Walther: An algorithm for piecewise linear optimization of objective functions in abs-normal form. Submitted 2017, available at Optimization Online.

Numerical Results

$$\ell(y) = \max(0, y) + \min(0, y + \frac{1}{2}|y|), \qquad \bar{\Omega} = [0,1] \times [0,1]$$

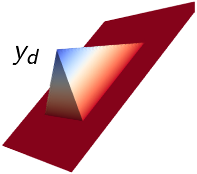
$$y_d(x_1, x_2) = \min\left(\max\left(\left|x_1 - \tfrac{1}{2}\right|, \left|x_2 - \tfrac{1}{2}\right| \right) - \tfrac{1}{4},\ 0 \right)$$

σ_1

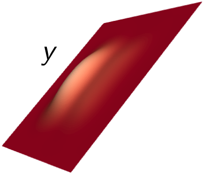


σ_2

y_d



y



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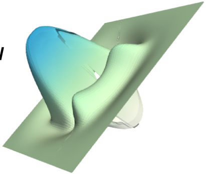

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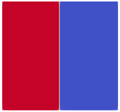
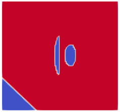
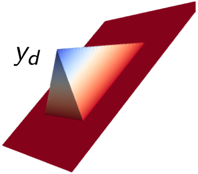


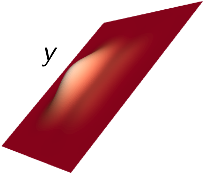
σ_2



y_d



y



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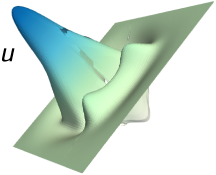

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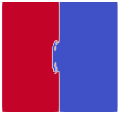
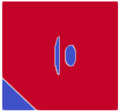
$$y_d(x_1, x_2) = \min\left(\max\left(|x_1 - \tfrac{1}{2}|, |x_2 - \tfrac{1}{2}| \right) - \tfrac{1}{4},\ 0 \right)$$

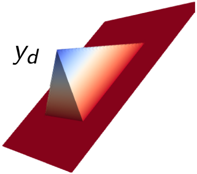
σ_1



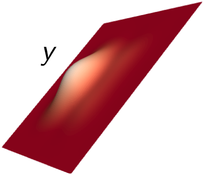
σ_2



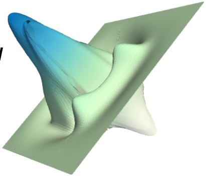
y_d



y



u



Numerical Results

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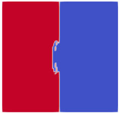
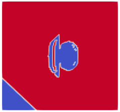
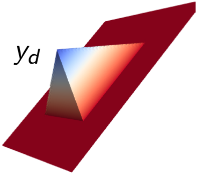


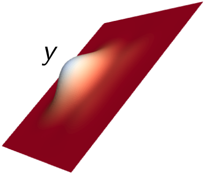
σ_2



y_d



y



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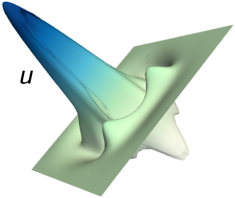

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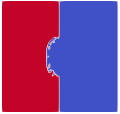
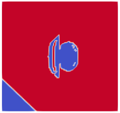
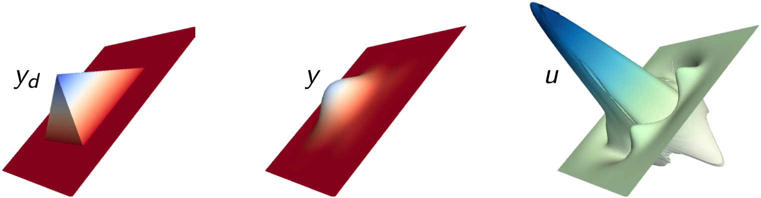


σ_2





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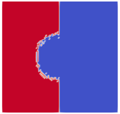
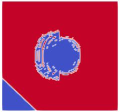
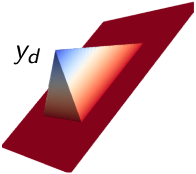


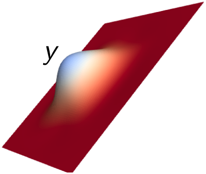
σ_2



y_d



y



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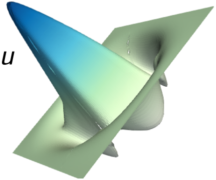

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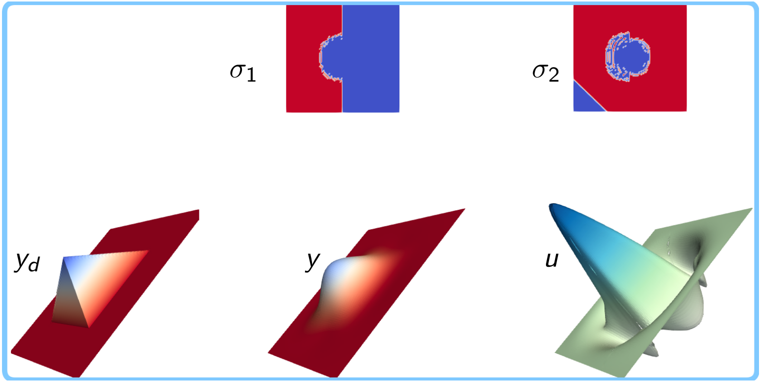
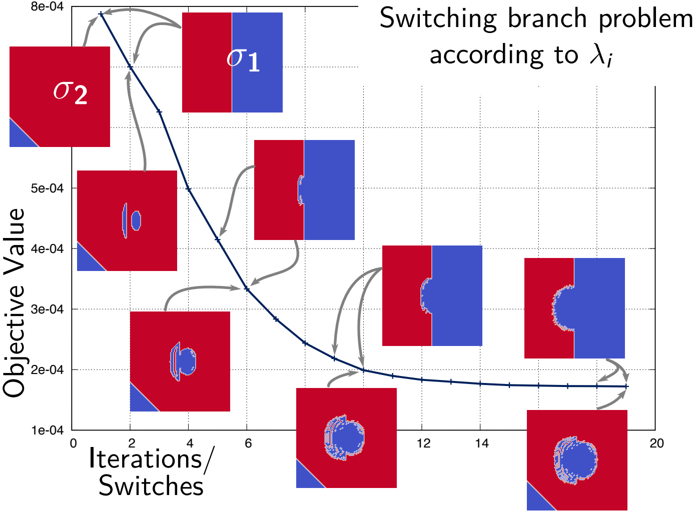
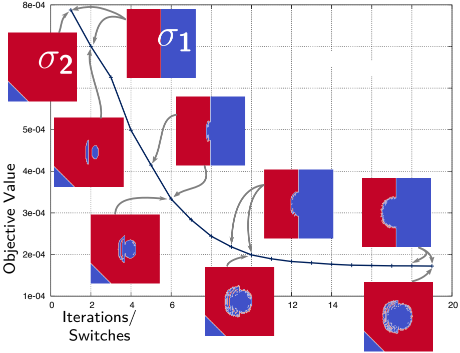


Numerical Results



Conclusion



- Optimization of non-smooth Lipschitz-continuous problems
- Extension to function space setting
- Handling and solving without regularizations for the non-smoothness
- Each branch problem is smooth, Newton/SQP allows quick solution
- Stopping criterion: sufficient reduction in adjoint, thus no more switching

Ongoing and Future Work

- Two publications in preparation
  - O. Ebel, S. Schmidt, A. Walther, A. Griewank, Optimization by Successive Abs-Linearization in Function Spaces, 2018
  - O. Ebel, S. Schmidt, A. Walther, Solving Non-Smooth Semi-Linear Elliptic Optimal Control Problems with Abs-Linearization, 2018
- Extension to non-smooth parabolic and hyperbolic PDE constraints
- Extension to general switches and hysteresis
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Thank you for your attention!