Aspects of numerical analysis in the optimal control of nonlinear PDEs
I: problems with semilinear equations and control constraints

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Inverse Problems and Optimal Control for PDEs

Warwick, 23-27 May 2011

Outline

- Motivating industrial applications
- Elliptic problems with linear state equation
- Semilinear elliptic state equation
- State-constrained control problems
- The case of quasilinear elliptic equations
- Error estimates

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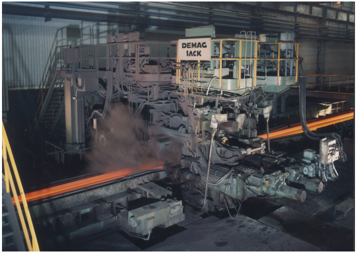
1. Some examples of industrial application
   - Optimal cooling of steel profiles
   - Optimal control of magnetic fields
   - Optimal control of sublimation crystal growth
2. Control of linear elliptic equations
   - Problems without control or state constraints
   - Additional pointwise control constraints
   - The semismooth Newton method
   - An a posteriori estimate – perturbation method
3. Semilinear elliptic equation
   - The optimal control problem
   - First-order necessary conditions
   - On second-order sufficient optimality conditions

Our applied topic in Chemnitz, 1991

Optimal cooling of milled steel profiles

Cooperation with Mannesmann-Demag-Sack GmbH

Cooling line



Cooling segment

Joint work with R. Lezius, A. Unger, and K. Eppler

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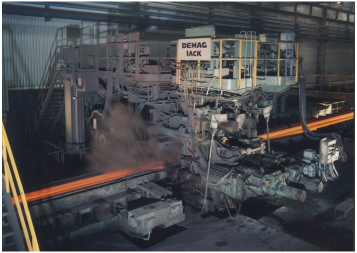

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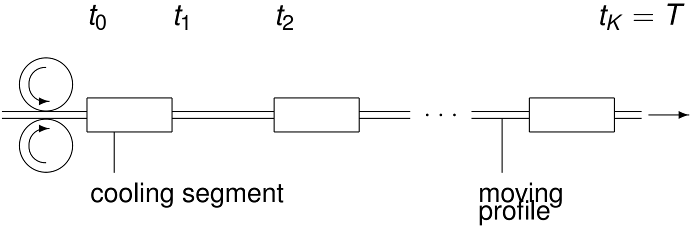
Supported by

DFG-SPP ”Anwendungsbezogene Optimierung und Steuerung” (Coordinator: K.H. Hoffmann)

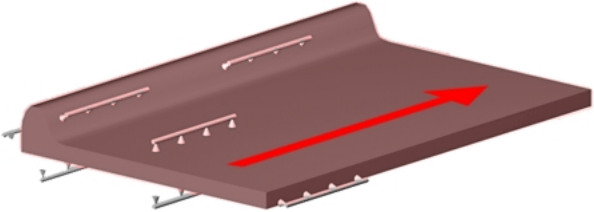
DFG-SPP ”Echtzeitoptimierung großer Systeme” (Coordinator: M. Grötschel)

Scheme of a cooling line

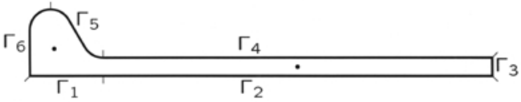


Water cooling segments are followed by air cooling segments

Moving profile and spray nozzles

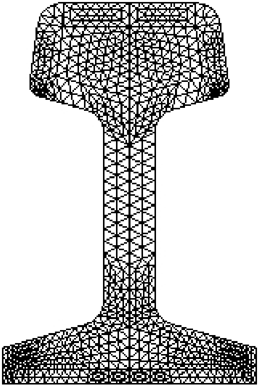


Ship profile passing a cooling line



Cross section and partitioning of the boundary

Rail profile and FEM grid



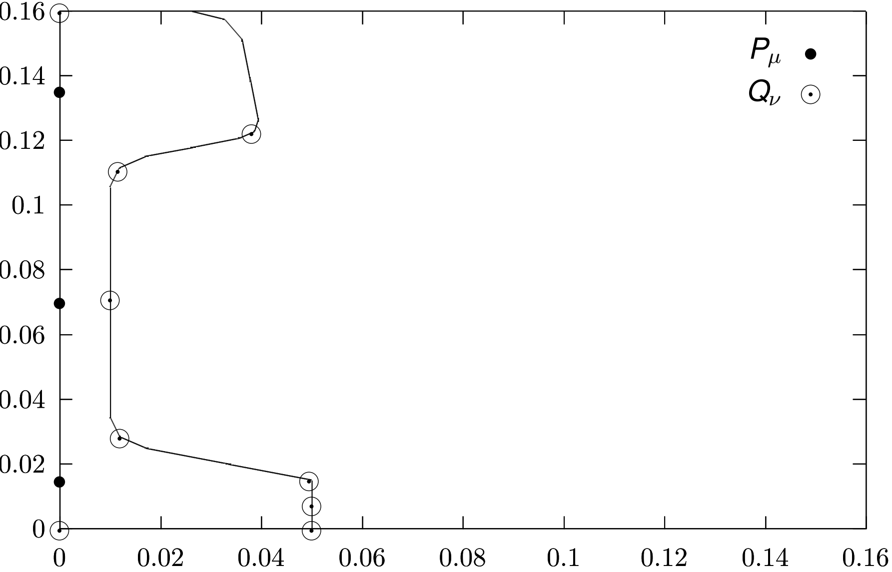
Rail profile

Heat equation of the model

State equation

$$\begin{aligned} c(\vartheta)\rho(\vartheta)\,\vartheta_t &= \operatorname{div}\,(\lambda(\vartheta)\,\operatorname{grad}\vartheta) && \text{in } Q,\\ \lambda(\vartheta)\,\partial_n\vartheta &= \sum_{i,k} u_{ki}\,\chi(\Sigma_{ki})\,\alpha(\cdot,\vartheta)(\vartheta_{fl}-\vartheta) && \text{in } \Sigma,\\ \vartheta(x,0) &= \vartheta_0(x) && \text{in } \Omega, \end{aligned}$$

Location of minimization and observation points



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and subject to the constraints on control and state

$$|\vartheta(R_\mu, t) - \vartheta(Q_\nu, t)| \le c_{\mu\nu},$$
$$0 \le u_{ki} \le 1.$$

With markers of theoretical difficulties

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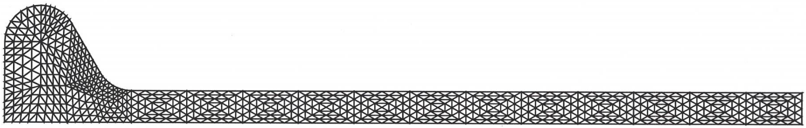
semilinear term, state constraints, quasilinear parts

Computational example

In view of the theoretical difficulties, we just solved the problem numerically. Thanks to model predictive control techniques, we were able to reduce the computing time from some days to 5 minutes. This was our contribution to real time optimization.



Finite element method – the grid

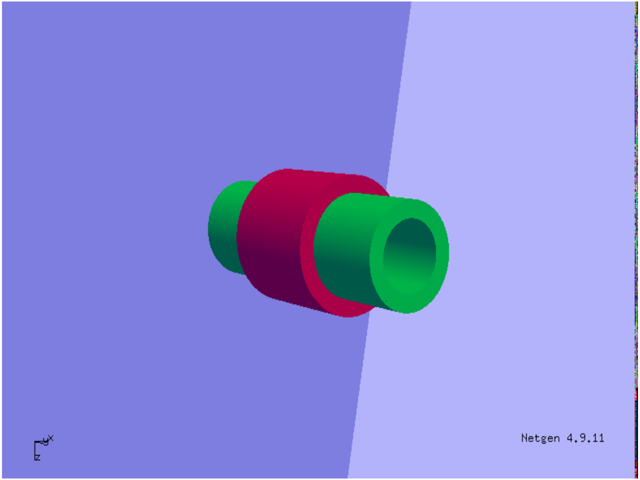
It took quite a long time to resolve the theoretical difficulties to some level of completeness.
We shall discuss this briefly for simpler elliptic model problems.

Numerical example – Ship profile

Initial temperature field

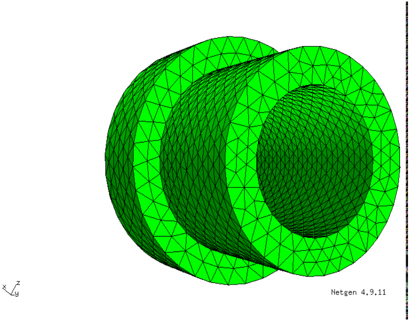
Final temperature fields with and without equilibration

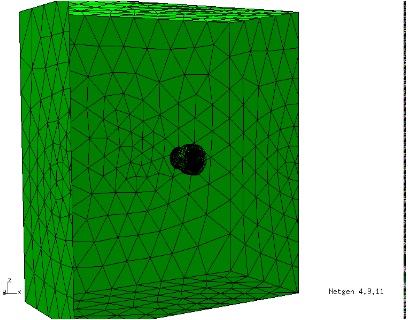
The geometry



Metal tube with induction coil

Finite element mesh





Tube and holdall domain

State equation

Control: Electrical current or voltage

Ansatz: $j_c = e(x)i(t)$ with fixed vector field e.

State equation:

$$
\begin{aligned}
\sigma \frac{\partial \mathbf{A}}{\partial t}(t) + \operatorname{curl} \mu^{-1} \operatorname{curl} \mathbf{A}(t) &= \mathbf{e}\, i(t) && \text{in } Q = \Omega \times (0, T) \\
\mathbf{n} \times \mathbf{A}(t) &= 0 && \text{on } \Sigma = \Gamma \times (0, T) \\
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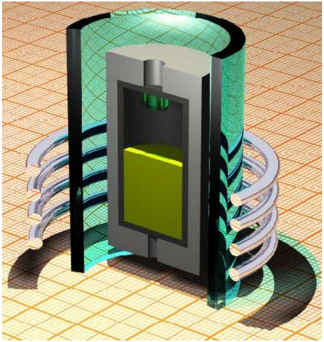
Aim: Changing A_0 to $-A_0$ in shortest time

Main difficulties: σ vanishes in the nonconducting parts, $\mu = \mu(B)$, hence the system is quasilinear elliptic-parabolic.

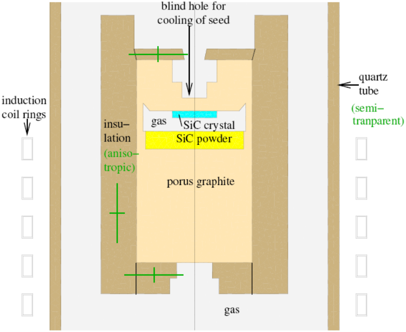
Production of SiC bulk single crystals by sublimation

J. Sprekels, O. Klein (WIAS), F. T. (TUB)

Cooperation of WIAS with IKZ in Berlin-Adlershof



Graphite crucible



Scheme of the crucible

Heat equation

The following equations model the problem:

Heat equation:

$$
\begin{aligned}
-\mathrm{div}(\kappa(x,\theta)\,\nabla\theta) &= \frac{1}{2\mathfrak{s}}|\mathrm{curl}\, H|^2 && \text{in } \Omega\,,\\
[-\kappa(x,\theta)\frac{\partial\theta}{\partial\nu_{\mathrm{r}}}] &= G(\sigma\,|\theta|^3\theta) && \text{on } \Gamma_r\,,\\
\kappa(x,\theta)\frac{\partial\theta}{\partial\nu_0} + \varepsilon\sigma\,|\theta|^3\theta &= \varepsilon\sigma\,\theta_0^4 && \text{on } \Gamma_0.
\end{aligned}
$$

Here, G is an integral operator accounting for radiation; [...] denotes the jump of normal derivatives of θ at Γ_r.
This equation is quasilinear.

Maxwell's equations for H

Maxwell's equations (time harmonic setting, resistivity r):

$$\begin{aligned} i\,\omega\mu H(x) + \operatorname{curl}\,(r\,\operatorname{curl}\,H(x)) &= j_g \quad \text{in } O \\ \nu \cdot (\mu H) &= 0 \quad \text{on } \partial O. \end{aligned}$$

Form of the control function j_g:

$$j_g(x) = \sum_{j=1}^{n} u_j\, v_j(x)$$

where $u \in \mathbb{R}^n$ is the control and $v_j : R_j \to \mathbb{R}^3$, $j = 1, \ldots, n$, are fixed functions defined in the coils R_j and extended by zero to $O \setminus R_j$.

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Linear-quadratic control problem

$$(P) \qquad \min J(y,u) := \frac{1}{2}\int_\Omega \big(y(x) - y_d(x)\big)^2\,dx + \frac{\lambda}{2}\int_\Omega u(x)^2\,dx$$

subject to the state equation

$$\begin{aligned} -\Delta y + c(x)y &= u \quad \text{in } \Omega \\ y &= 0 \quad \text{on } \Gamma \end{aligned}$$

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- $\Omega \subset \mathbb{R}^n$, $n \in \{2,3\}$ for simplicity, bounded domain with Lipschitz boundary Γ
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To find:

- Control $u \in L^2(\Omega)$ with state $y \in H_0^1(\Omega)$.

Well-posedness

Theorem

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The mapping $G : u \mapsto y_u$ is continuous from $L^2(\Omega)$ to $H_0^1(\Omega)$ and from $L^p(\Omega)$ to $H_0^1(\Omega) \cap C(\bar{\Omega})$.

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Theorem

The optimal control problem (P) admits a unique optimal control $\bar{u}$ with associated optimal state $\bar{y} := y_{\bar{u}}$. A control u is optimal if and only if

$$f'(u) = 0.$$

Parabolic case

$$\min J(y,u) := \frac{1}{2}\int_0^T\int_\Omega \big(y(x,t)-y_d(x,t)\big)^2\,dxdt + \frac{\lambda}{2}\int_0^T\int_\Omega u(x,t)^2\,dxdt$$

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Optimality system

$$\begin{aligned} y_t - \Delta y &= -\lambda^{-1}\varphi, \quad y(0) = 0 \\ -\varphi_t - \Delta \varphi &= y - y_d, \quad \varphi(T) = 0. \end{aligned}$$

with homogeneous boundary conditions.

This forward-backward system is difficult to solve, if $n \geq 2$.

Numerical options

Option 1: Multigrid methods

A. Borzi and V. Schulz, *Multigrid methods for PDE optimization*, SIAM Review 2009.

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3. If $\|v_k\|_{L^2(\Omega)} < \varepsilon$, then STOP.
4. $u_{k+1} = u_k + s_k v_k$ with exact stepsize s_k
   $k := k + 1$, goto 1.

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A control $\bar{u} \in U_{ad}$ is optimal if and only if it obeys the projection formula

$$\bar{u}(x) = \mathbb{P}_{[\alpha,\beta]}\left(-\frac{\bar{\varphi}(x)}{\lambda}\right).$$

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Current iterate: (y_k, φ_k), $I_{k+1} = \{x \in \Omega : \alpha \le -\varphi_k(x)/\lambda \le \beta\},.$

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Fix the next control on A_{k+1} by

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The next iterate (y_{k+1}, φ_{k+1}) is obtained by the Newton step

$$\begin{aligned} -\Delta y + cy &= \mathbb{P}\big(-\varphi_k/\lambda\big) + \mathbb{P}'\big(-\varphi_k/\lambda\big)(-1/\lambda)(\varphi - \varphi_k) \\ -\Delta \varphi + c\varphi &= y - y_d \end{aligned}$$

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$$\mathbb{P}\big(-\varphi_k/\lambda\big) + \mathbb{P}'\big(-\varphi_k/\lambda\big)\big(-1/\lambda\big)(\varphi - \varphi_k) =$$

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Semismooth Newton method / PDAS

Therefore, the next iterate is obtained from

$$\begin{aligned} -\Delta y + cy &= \chi_{I_{k+1}} \cdot (-\lambda^{-1}\varphi) + \chi_{A_{k+1}}\, u_{k+1} \\ -\Delta \varphi + c\varphi &= y - y_d \end{aligned}$$

$\rightarrow (y_{k+1}, \varphi_{k+1});$

$$u_{k+1} := \begin{cases} -\lambda^{-1}\varphi_{k+1} & \text{on } I_{k+1} \\ \tilde{u}_{k+1} & \text{on } A_{k+1}. \end{cases}$$

This is one step of a primal-dual active set strategy. A rigorous mathematical discussion needs the concept of Newton differentiability. The mapping

$$u \mapsto \mathbb{P}_{[\alpha,\beta]}(S^*(Su - y_d))$$

is Newton differentiable in the right spaces.

Some References

- Bergounioux, M., Ito, K., Kunisch, K., *Primal-dual active set strategy for constrained optimal control problems,* SICON 1999.
- Ito, K., Kunisch, K., *The Lagrange multiplier approach to variational problems and applications*, SIAM 2008.
- Herzog, R., Kunisch, K., *Algorithms for PDE-constrained optimization*, GAMM-Mitteilungen 2010.

The perturbation method

The control $\tilde{u}$ solves the perturbed control problem

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$$\Rightarrow \lambda \|\bar{u} - \tilde{u}\|^2 \leq \|\zeta\| \|\bar{u} - \tilde{u}\| \Rightarrow$$

The a posteriori estimate

$$\boxed{\|\bar{u} - \tilde{u}\|_{L^2(\Omega)} \le \frac{1}{\lambda}\|\zeta\|_{L^2(\Omega)}}$$

Notice that ζ is available with the adjoint state for the approximated control $\tilde{u}$. Therefore, this is some type of a posteriori error estimate.

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An application to the estimation of suboptimal controls computed by POD:

- F.T., S. Volkwein, *POD a-posteriori error estimates for linear-quadratic optimal control problems*, Computational Optimization and Applications 2009.

Outline

1. Some examples of industrial application
   - Optimal cooling of steel profiles
   - Optimal control of magnetic fields
   - Optimal control of sublimation crystal growth
2. Control of linear elliptic equations
   - Problems without control or state constraints
   - Additional pointwise control constraints
   - The semismooth Newton method
   - An a posteriori estimate – perturbation method
3. Semilinear elliptic equation
   - The optimal control problem
   - First-order necessary conditions
   - On second-order sufficient optimality conditions

The control problem

$$(P) \qquad \min J(y,u) := \frac{1}{2}\int\limits_{\Omega} \big(y(x) - y_d(x)\big)^2\,dx + \frac{\lambda}{2}\int\limits_{\Omega} u(x)^2\,dx$$

subject to the state equation

$$\begin{aligned} -\Delta y + d(y) &= u \quad \text{in } \Omega \\ y &= 0 \quad \text{on } \Gamma \end{aligned}$$

$$\alpha \le u(x) \le \beta \quad \text{a.e. in } \Omega.$$

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Additionally given:

$d \in C^1(\mathbb{R}), \quad d'(y) \ge 0 \; \forall y \in \mathbb{R}$

Control-to-state mapping

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The mapping $G : u \mapsto y_u$ is continuous from $L^2(\Omega)$ to $H_0^1(\Omega)$ and from $L^p(\Omega)$ to $H_0^1(\Omega) \cap C(\bar{\Omega})$.

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Proof: Monotone operators; Stampacchia truncation method; see later part on quasilinear equations

Control-to-state operator

Conclusion:

For $n = 2, 3$, to each $u \in L^2(\Omega)$ there exists a unique weak solution $y_u \in H_0^1(\Omega) \cap C(\bar{\Omega})$ and
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Theorem

For all u, $v \in L^2(\Omega)$, the derivative $y = G'(u)\, v$ is given by the solution y of the linearized equation

$$\begin{aligned} -\Delta y + \underbrace{d'(y_u)}_{c \geq 0}\, y &= v \quad \text{in } \Omega \\ y &= 0 \quad \text{on } \Gamma. \end{aligned}$$

Existence of an optimal control

Theorem

(P) has at least one optimal control $\bar{u}$.

- (P) is not convex, although the functional J is convex. Several global or local solutions might exist.
- Necessary conditions are no longer sufficient for optimality.
- Can we have accumulation points of infinitely many different local optima?
- Are locally optimal solutions stable with respect to small perturbations (say error in the data, approximation by finite elements)?

We shall invoke second-order sufficient optimality conditions to deal with some of these questions.

Adjoint equation

Let $u \in L^2(\Omega)$ be given, $y_u = G(u)$. Then the adjoint state $\varphi_u \in H_0^1(\Omega)$ is defined as the solution to the

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$$\begin{aligned} -\Delta\varphi + d'(y_u)\,\varphi &= y_u - y_d \quad \text{in } \Omega \\ \varphi &= 0 \quad \text{on } \Gamma. \end{aligned}$$

We have $\varphi_u \in H_0^1(\Omega) \cap C(\bar{\Omega})$ if $n \leq 3$ and also $\varphi \in H^2(\Omega)$, if Ω is convex or $\Gamma \in C^{1,1}$.

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The reduced gradient is given by

$$
f'(u)v = \int_\Omega (\varphi_u + \lambda u)\, v\, dx
$$

Necessary optimality condition

Definition: $\bar{u} \in U_{ad}$ is said to be locally optimal (in the sense of $L^2(\Omega)$), if there exists $\varepsilon > 0$ such that

$$f(u) \geq f(\bar{u}) \quad \forall u \in U_{ad} \text{ with } \|u - \bar{u}\|_{L^2(\Omega)} \leq \varepsilon.$$

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If $\bar{u}$ is locally optimal for (P), then the variational inequality

$$\int_\Omega (\bar{\varphi} + \lambda \bar{u})(u - \bar{u})\, dx \quad \forall u \in U_{ad}$$

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Conclusion: As in the linear-quadratic case, it holds

$$\bar{u}(x) = \mathbb{P}_{[\alpha,\beta]}\Big(- \frac{\bar{\varphi}(x)}{\lambda} \Big).$$

Numerical application

The projection formula can be used again numerically:

- Direct numerical solution of the nonsmooth optimality system

$$
\begin{aligned}
-\Delta y + d(y) &= \mathbb{P}_{[\alpha,\beta]}\big(-\varphi/\lambda\big), & y_{|\Gamma} &= 0\\
-\Delta\varphi + d'(y)\,\varphi &= y - y_d, & \varphi_{|\Gamma} &= 0.
\end{aligned}
$$

  We did this by COMSOL Multiphysics.

Semismooth Newton method

- Semismooth Newton method

  If (y_k, φ_k) is given, define $\quad I_{k+1} = \{x \in \Omega : \alpha \le -\frac{\varphi_k(x)}{\lambda} \le \beta\}$,

$$A_{k+1}^- = \{x \in \Omega : -\frac{\varphi_k(x)}{\lambda} < \alpha\}, \qquad A_{k+1}^+ = \{x \in \Omega : -\frac{\varphi_k(x)}{\lambda} > \beta\}$$

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$$\begin{aligned} -\Delta y + d(y_k) + d'(y_k)(y - y_k) &= \chi_{I_{k+1}} \cdot (-\varphi/\lambda) + \chi_{A_{k+1}} \tilde{u}_{k+1} \\ -\Delta \varphi + d'(y_k)\,\varphi + d''(y_k)(\varphi - \varphi_k) &= y - y_d \end{aligned}$$

subject to homogeneous boundary conditions. The solution is (y_{k+1}, φ_{k+1}).

Semismooth Newton method

Then

$$u_{k+1}(x) := \begin{cases} -\varphi_{k+1}(x)/\lambda & \text{if } x \in I_{k+1} \\ \tilde{u}_{k+1}(x) & \text{if } x \in \chi_{A_{k+1}}. \end{cases}$$

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Under natural assumptions, local superlinear convergence of the semismooth Newton method can be proved (cf. book by K. Ito and K. Kunisch, Thm. 8.16).

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However, this obstacle does not cause troubles, provided we do not need second-order sufficient optimality conditions. Notice that $U_{ad} \in L^\infty$.

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The use of $L^\infty(\Omega)$ avoids the discussion of growth conditions for the nonlinearities.

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Notice: $d'(y_k)\varphi \approx d'(y_k)\varphi_k + d'(y_k)(\varphi - \varphi_k) + d''(y_k)\varphi_k(y - y_k)$

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$$+2\frac{\partial^2 J}{\partial y \partial u}(y_u, u)[G'(u)v, v] + \frac{\partial^2 J}{\partial u^2}(y_u, u)v^2$$

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$$+2\frac{\partial^2 J}{\partial y \partial u}(y_u, u)[G'(u)v, v] + \frac{\partial^2 J}{\partial u^2}(y_u, u)v^2$$
$$= J''(y_u, u)(y, u)^2 + \frac{\partial J}{\partial y}(y_u, u)G''(u)v^2$$

We need $G''(u)$...

Equation for G''

Lemma

The element $z := G''(u)v_1v_2$ is the unique solution to

$$-\Delta z + d'(y_u)z = -d''(y_u)y_1y_2, \quad z_{|\Gamma} = 0,$$

where $y_i = G'(u)v_i$ solve the linearized state equation associated with u.

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$$-\Delta \underbrace{G''(u)v_1 v_2}_{z} + d''(y_u)(\underbrace{G'(u)v_1}_{y_1})(\underbrace{G'(u)v_2}_{y_2}) + d'(y_u)\underbrace{G''(u)v_1 v_2}_{z} = 0$$

$\square$

Second-order sufficient optimality condition

We deduce

$$f''(u)v^2 = J''(u)v^2 - \int_\Omega \varphi_u d''(y_u)y^2\,dx$$

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Theorem (Strong second-order sufficient condition)

Let $\bar{u} \in U_{ad}$ satisfy the first-order necessary optimality condition and the following strong second-order condition: There exists $\delta > 0$ such that

$$f''(u)v^2 \geq \delta \|v\|^2_{L^2(\Omega)} \qquad \forall v \in L^2(\Omega).$$

Then there exist $\varepsilon > 0$ and $\sigma > 0$ such that

$$f(u) \geq f(\bar{u}) + \sigma\|u - \bar{u}\|^2_{L^2(\Omega)} \quad \forall u \in U_{ad} \text{ with } \|u - \bar{u}\|_{L^2(\Omega)} \leq \varepsilon.$$

Therefore, $\bar{u}$ is locally optimal in the sense of $L^2(\Omega)$.

Discouraging example

My favorite example

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In our elliptic distributed case, $f : L^2(\Omega) \to \mathbb{R}$ is C^2.

Second-order condition

The coercivity condition means that

$$J''(u)v^2 - \int_\Omega \varphi_u \, d''(y_u)\, y^2 \, dx \geq \delta \|v\|^2_{L^2(\Omega)}$$

for all $v \in L^2(\Omega)$ and the corresponding solution y of the linearized equation with right-hand side v.

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This is too strong compared with associated necessary conditions. The following weaker condition is already sufficient for local optimality: There exists some threshold $\tau > 0$ such that the coercivity condition is satisfied for all v with

$$v(x) = \begin{cases} \leq 0 & \text{if } \bar{u}(x) = \beta \\ \geq 0 & \text{if } \bar{u}(x) = \alpha \\ 0 & \text{if } |\bar{\varphi}(x) + \lambda \bar{u}(x)| \geq \tau. \end{cases}$$

Second-order conditions

References:

- E. Casas, A. Unger, F. T., *Second order sufficient optimality conditions for a nonlinear elliptic control problem*,
  J. for Analysis and its Applications (ZAA) 1996.
- E. Casas, J.C. de los Reyes, F.T., *Sufficient second-order optimality conditions for semilinear control problems with pointwise state constraints*,
  SIAM J. on Optimization 2008.

Implications of SSC

If the second-order sufficient optimality condition is satisfied at $\bar{u} \in U_{ad}$ that obeys the first-order necessary conditions, then

- $\bar{u}$ is locally optimal
- $\bar{u}$ is locally unique ($\bar{u}$ cannot be an accumulation point of local minima)
- $\bar{u}$ is stable with respect to certain perturbations
- Local convergence of numerical optimization methods can be expected.

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Let (y_k, u_k, φ_k) be the current iterate. Solve

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If $\bar{u}$ satisfies SSC, then the method converges locally quadratic. We prefer now the semismooth Newton method.

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Let $\tilde{u} \in U_{ad}$ some approximate solution of (P) "close" to $\bar{u}$. How far is $\tilde{u}$ from $\bar{u}$?

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- $\|\tilde{u} - \bar{u}\|_{L^2(\Omega)} \leq \rho$
- We have an estimate of δ such that the inequality above is true.

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Insert $\bar{u}$, $\tilde{u}$ in the right variational inequality,

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$$\underbrace{f''(u_\vartheta)(\bar{u} - \tilde{u})^2}_{\geq \frac{\delta}{2}\|u - \bar{u}\|^2} \leq \|\zeta\|_{L^2(\Omega)} \|\tilde{u} - \bar{u}\|_{L^2(\Omega)}$$

Estimate

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- computed the smallest eigenvalue of the Hessian matrix associated with $f''(\tilde{u})$, (after discretization),
- computed the adjoint state associated with $\tilde{u}$,
- determined ζ.

The estimation turned out to be very reliable.