# Theory and Practice of PDE-Constrained Optimization

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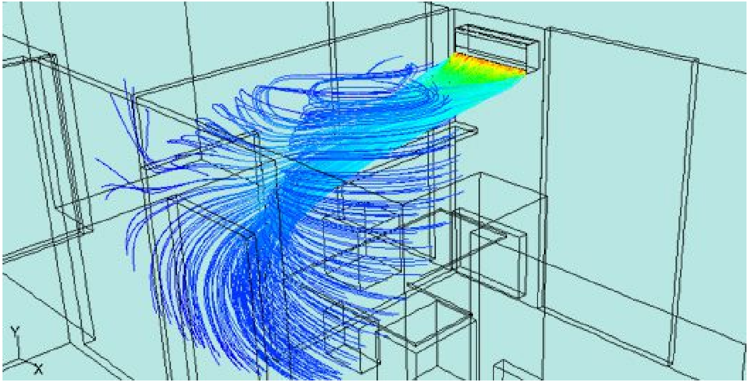
# Outline

# Optimal heating

Let $\Omega$ be a bounded domain in $\mathbb{R}^3$ with boundary $\Gamma$ which represents a body that has to be heated. We may act along the boundary by setting a temperature $u = u(x)$.




The goal of the problem consists in getting as close as possible to a given desired temperature $z_d(x)$ in $\Omega$.

# Optimal heating

$$\min J(y,u) := \frac{1}{2}\int_\Omega (y(x) - z_d(x))^2 dx + \frac{\alpha}{2}\int_\Gamma u(x)^2 \, ds,$$

subject to:

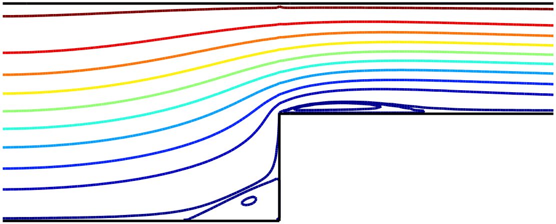
$$\left.\begin{aligned} -\Delta y &= 0 && \text{in } \Omega, \\ \frac{\partial y}{\partial n} &= \lambda(u - y) && \text{in } \Gamma, \end{aligned}\right\} \quad \text{State equation.}$$

$$u_a(x) \le u(x) \le u_b(x). \qquad \text{Control constraints.}$$

The scalar $\alpha > 0$ can be interpreted as a control cost, which also lead to more regular solutions of the optimization problem. The function $\lambda$ represents the heat transfer along the boundary.

# Forward facing step channel

- Uncontrolled Navier-Stokes flow $Re = 1000$.



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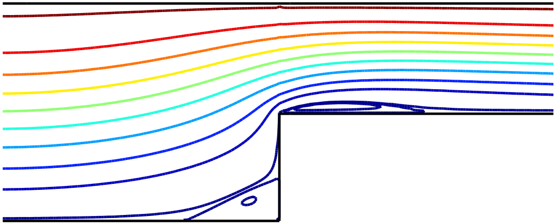

- Goal: reduce recirculatons, delay transition to turbulence

# Problem

$$\min \; J(y,u) = \frac{1}{2}\int_{\Omega} |y - z_d|^2 \, dx + \frac{\alpha}{2}\int_{\Gamma_1} |u|^2 \, ds$$

subject to

$$-\nu\Delta y + (y\cdot\nabla)y + \nabla p = f$$

$$\text{div } y = 0 \qquad (\mathcal{P})$$

$$y|_{\Gamma_1} = u$$

$$y|_{\Gamma\setminus\Gamma_1} = g$$

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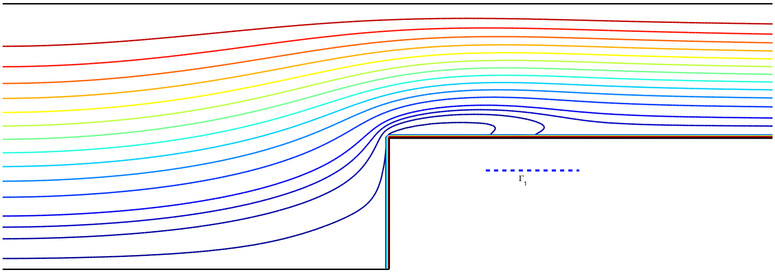
div $y = 0$

$y|_{\Gamma_1} = u$ (boundary control)

$y|_{\Gamma\setminus\Gamma_1} = g$

$(\mathcal{P})$

# Controlled flow



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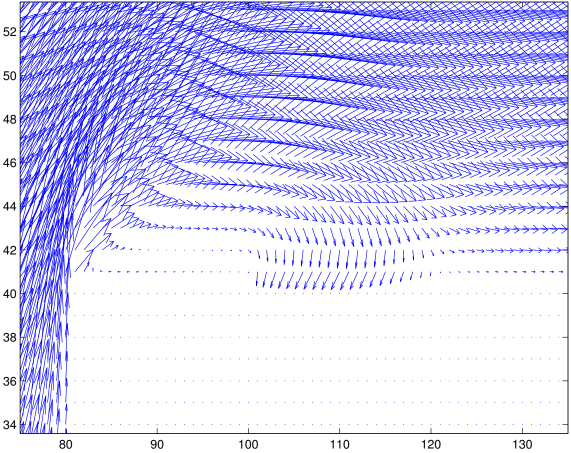
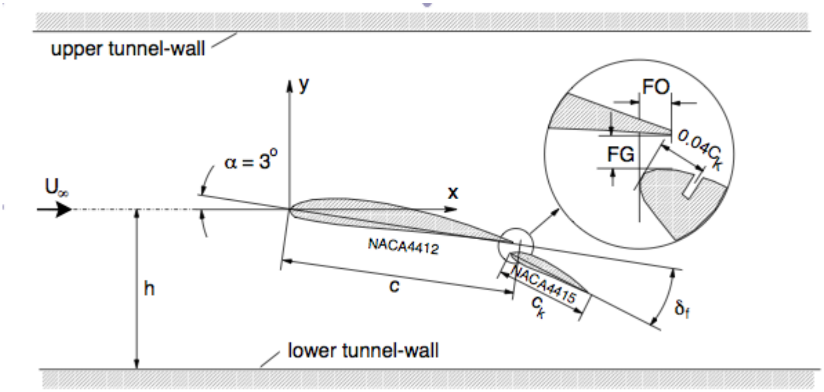
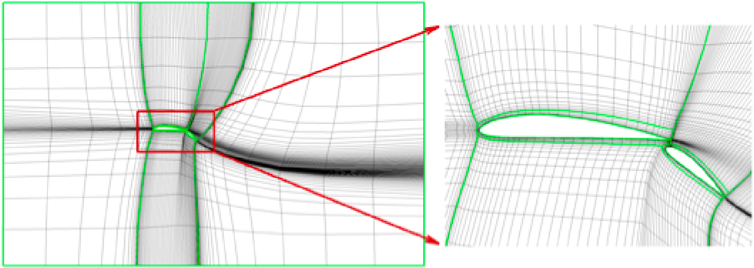


# Wing configuration



# Adapted mesh



# Problem

$$\min \; J(y,u) = \int_{\Gamma_b} (\nu \partial_{\vec{n}} y - p\vec{n})\, \vec{e}_l \, ds$$

sujeto a:

$$\partial_t y - \nu \Delta y + (y \cdot \nabla) y + \nabla p = 0$$

$$\text{div } y = 0 \qquad (\mathcal{P})$$

$$y|_{\Gamma_1} = u = a \sin(2\pi f (t - t_0)) \begin{pmatrix} \cos(\beta - \delta) \\ \sin(\beta - \delta) \end{pmatrix}$$

$$y|_{\Gamma \setminus \Gamma_1} = g,$$

where $\Gamma_b$ is the boundary of the wing, $a$ denotes the amplitude, $f$ the frequence, $\beta$ is the suction angle and $\delta$ is the angle of the valve.

# Problem

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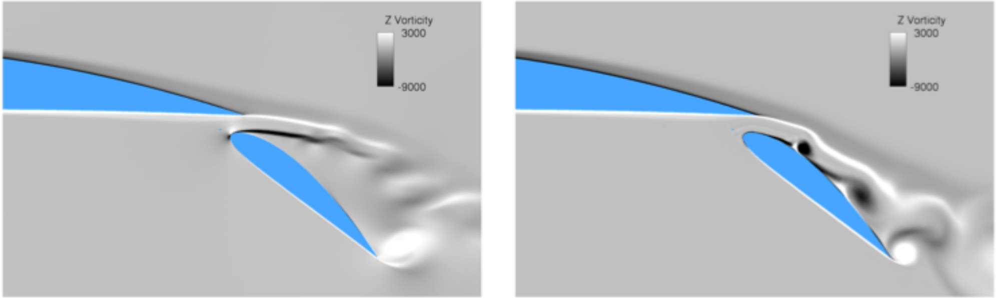
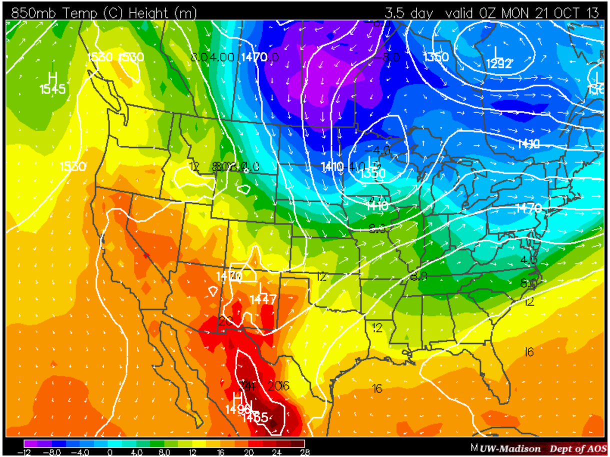
# Results




(a) Base flow (b) Perturbed flow

# Numerical weather prediction




**Problem**

The constitutive model is in general known, but not the initial condition.

# Primitive equations

## Very basic model

$$\frac{\partial u}{\partial t} = -u\frac{\partial u}{\partial x} - v\frac{\partial u}{\partial y} - w\frac{\partial u}{\partial z} + \frac{uv\tan(\phi)}{a} - \frac{uw}{a} - \frac{1}{\rho}\frac{\partial p}{\partial x} - 2\Omega(w\cos(\phi) - v\sin(\phi)) + Fr_x$$

$$\frac{\partial v}{\partial t} = -u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} - w\frac{\partial v}{\partial z} + \frac{u^2\tan(\phi)}{a} - \frac{uw}{a} - \frac{1}{\rho}\frac{\partial p}{\partial y} - 2\Omega u\sin(\phi) + Fr_y$$

$$\frac{\partial w}{\partial t} = -u\frac{\partial w}{\partial x} - v\frac{\partial w}{\partial y} - w\frac{\partial w}{\partial z} + \frac{u^2 + v^2}{a} - \frac{1}{\rho}\frac{\partial p}{\partial z} + 2\Omega u\cos(\phi) - g + Fr_z$$

$$\frac{\partial T}{\partial t} = -u\frac{\partial T}{\partial x} - v\frac{\partial T}{\partial y} + (\gamma - \gamma_d)w + \frac{1}{c_p}\frac{dH}{dt}$$

$$\frac{\partial \rho}{\partial t} = -u\frac{\partial \rho}{\partial x} - v\frac{\partial \rho}{\partial y} - w\frac{\partial \rho}{\partial z} - \rho\left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z}\right)$$

$$\frac{\partial q}{\partial t} = -u\frac{\partial q}{\partial x} - v\frac{\partial q}{\partial y} - w\frac{\partial q}{\partial z} + Q_v$$

+ Boundary conditions

+ Initial conditions

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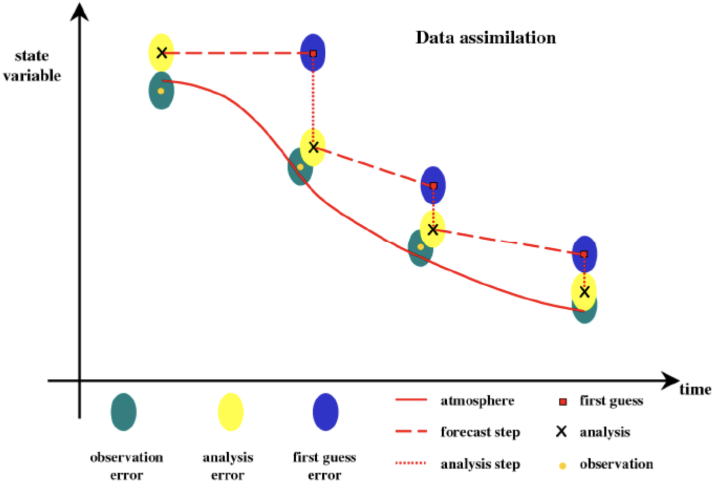
Data assimilation methods aim at finding a good initial condition of the athmospheric system in order to get better weather forecasts

- Information can be obtained mainly from ground stations, radionsonds or satellite images;
- Reconstruction results depend strongly on the number of observations.



## DA approaches

- Optimal interpolation
- 3D-Var
- Ensemble Kalman filter
- Hybrid methods



# Data assimilation

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## 4D-Var

$$\min J(y,u) = \frac{1}{2}\sum_{i=1}^{n}[H(y(t_i)) - z_d(t_i)]^T R_i^{-1}[H(y(t_i)) - z_d(t_i)] + \frac{1}{2}[u - y^b(t_0)]^T B^{-1}[u - y^b(t_0)]$$

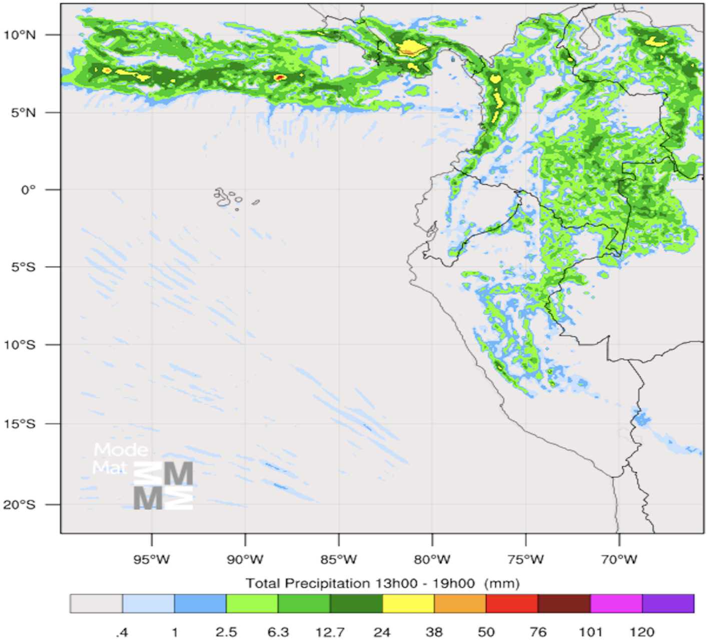
subject to

$y(t_j) = M_j(y(t_0)),$ (system of PDEs)

$y(t_0) = u,$ (initial condition)

where $z_d$ are the observations, $y^b$ is the background vector, and $R_i$ and $B$ are the observation and background error covariances, respectively.

# Operational use of 3D-Var



# An example in finite dimensions

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## Linear quadratic optimization problem

$$\begin{cases} \min\ J(y,u) = \frac{1}{2}\left\|y - z_d\right\|^2 + \frac{\alpha}{2}\left\|u\right\|^2 \\ \text{subject to:} \\ Ay = u \\ u \in U_{\text{ad}}, \end{cases} \tag{QP}$$

where $y, u \in \mathbb{R}^n$ correspond to the state and control variables, $\alpha > 0$, $U_{\text{ad}}$ is a closed convex set and $A \in \mathcal{M}_{n\times n}$ is invertible.
$\|\cdot\|$ and $(\cdot,\cdot)$ stand for the euclidean norm and scalar product, respectively.

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By introducing $S = A^{-1}$ we obtain that $y = Su$ and we may rewrite the cost function in the following reduced form:

$$J(y,u) = J(Su,u) =: f(u).$$

As a consequence we obtain the following **reduced** optimization problem:

$$\min_{u\in U_{\mathrm{ad}}} f(u). \tag{rQP}$$

# Existence of optimal solution

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## Definition

A vector $\bar{u} \in U_{\text{ad}}$ is called (local) **optimal solution** to (rQP) if

$$f(\bar{u}) \leq f(u), \qquad \forall u \in U_{\text{ad}} \quad (\forall u \in U_{\text{ad}} \cap B_r(\bar{u})).$$

Its correspondent state $\bar{y} = S\bar{u}$ is called **optimal state** and the matrix $S : \mathbb{R}^n \to \mathbb{R}^n$ **solution** or **control-to-state** operator.

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## Theorem

Let $U_{\text{ad}}$ be a non empty, closed and bounded set, and $A$ an invertible matrix. Then there exists at least an optimal control for (rQP)

## Proof

Since $J$ is continuous, it follows that the reduced cost $f$ is also continuous. Since $U_{\text{ad}}$ is a closed bounded subset of a finite dimensional space, it is compact and the result follows by Weierstrass theorem.

# First order optimality condition

## Theorem

Let $\bar{u}$ be a local optimal solution for (rQP). Then it satisfies the variational inequality:

$$f'(\bar{u})(v-\bar{u}) \geq 0, \qquad \text{for all } v \in U_{\text{ad}}.$$

## Proof

$f$ is differentiable, $U_{\text{ad}}$ is convex and $\bar{u}$ is a local optimal solution, i.e., $f(\bar{u}) \leq f(w)$, $\forall w \in U_{\text{ad}} \cap B_r(\bar{u})$. Taking $w = \bar{u} + t(v-\bar{u})$, with $0 < t \leq 1$ and $v - \bar{u}$ admissible,

$$0 \leq f(\bar{u} + t(v-\bar{u})) - f(\bar{u}).$$

Dividing by $t$ and taking the limit:

$$0 \leq \frac{f(\bar{u} + t(v-\bar{u})) - f(\bar{u})}{t} \xrightarrow{t \to 0} f'(\bar{u})(v-\bar{u}).$$

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- Thanks to the strong convexity of the reduced cost function and the convexity of $U_{\text{ad}}$, the first order optimality condition is both necessary and sufficient.

# First technique

Replace $y = A^{-1}u$ and consider

$$\min f(u) = \frac{1}{2}\left\|A^{-1}u - z_d\right\|^2 + \frac{\alpha}{2}\left\|u\right\|^2$$

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Necessary condition:

$$(\nabla f(\bar{u}), v - \bar{u}) = (A^{-1}\bar{u} - z_d, A^{-1}(v - \bar{u})) + \alpha(\bar{u}, v - \bar{u})$$

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or, equivalently,

$$A^T p = \bar{y} - z_d \quad \text{(adjoint equation)}$$

$$(\alpha\bar{u} + p, v - \bar{u}) \geq 0, \forall v \in U_{ad} \quad \text{(optimality condition)}$$

# Second technique

Lagrangian:

$$\mathcal{L}(y,u,p) = \frac{1}{2}\left\|y - z_d\right\|^2 + \frac{\alpha}{2}\left\|u\right\|^2 - (p, Ay - u).$$

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- $\mathcal{L}_u(v - u) = (\alpha u, v - u) + (p, v - u) \geq 0, \forall v \in U_{ad}$

$$\Rightarrow (\alpha u + p, v - u) \geq 0, \forall v \in U_{ad} \quad \text{(optimality condition)}$$

# Optimality system

Let $u$ be a local optimal solution to problem (QP). Then it satisfies:

$$Ay = u \qquad \text{(state equation)}$$

$$A^T p = y - z_d \qquad \text{(adjoint equation)}$$

$$(\alpha u + p, v - u) \geq 0, \forall v \in U_{ad} \qquad \text{(optimality condition)}$$

- The optimality condition can also be expressed by means of the projection operator on a convex set:

$$u = P_{U_{ad}}\left(u - c(p + \alpha u)\right), \qquad \forall c > 0.$$

- One frequent choice for $U_{\text{ad}}$ is given by the so-called box constraints

$$U_{\text{ad}} = \{u \in \mathbb{R}^n : u_a \leq u \leq u_b\},$$

where $u_a,\ u_b \in \mathbb{R}^n$ satisfy $u_a \leq u_b$ componentwise.

# Karush-Kuhn-Tucker

**Theorem**

Let $(\bar{y}, \bar{u})$ be an optimal pair and $U_{\text{ad}} = \{u \in \mathbb{R}^n : u_a \leq u \leq u_b\}$. Then there exist multipliers $p \in \mathbb{R}^n$ and $\lambda_a, \lambda_b \in \mathbb{R}^n$ such that:

$$\begin{cases} A\bar{y} = \bar{u}, \\ A^T p = \bar{y} - z_d, \\ \alpha\bar{u} + p - \lambda_a + \lambda_b = 0, \\ \lambda_a \geq 0, \quad \lambda_b \geq 0, \\ \lambda_a^\top (u_a - \bar{u}) = \lambda_b^\top (\bar{u} - u_b) = 0, \\ u_a \leq \bar{u} \leq u_b. \end{cases}$$

## Proof

From the optimality condition we obtain that

$$(p + \alpha\bar{u}, \bar{u}) \leq (p + \alpha\bar{u}, u)\,, \ \forall u \in U_{\mathrm{ad}},$$

which implies that $\bar{u}$ is solution of

$$\min_{u \in U_{\mathrm{ad}}} (p + \alpha\bar{u}, u) = \min_{u \in U_{\mathrm{ad}}} \sum_{i=1}^{n} (p + \alpha\bar{u})_i \, u_i.$$

Thanks to the special structure of $U_{\mathrm{ad}}$ and the independence of the $u_i$'s, it then follows that

$$(p + \alpha\bar{u})_i \cdot \bar{u}_i = \min_{u_{a,i} \leq u_i \leq u_{b,i}} (p + \alpha\bar{u})_i \cdot u_i$$

for $i = 1, \ldots, l$. Consequently,

$$\bar{u}_i = \begin{cases} u_{b,i} & \text{if} \quad (p + \alpha\bar{u})_i < 0, \\ u_{a,i} & \text{if} \quad (p + \alpha\bar{u})_i > 0. \end{cases} \tag{1}$$

Otherwise $(p + \alpha\bar{u})_i = 0$.

Let us now define the multipliers:

$$\lambda_a := \max\left(\vec{0}, p + \alpha\bar{u}\right), \\ \lambda_b := \left|\min\left(\vec{0}, p + \alpha\bar{u}\right)\right|, \tag{2}$$

where $\max,\ \min$ and $|\cdot|$ are considered componentwise. Then, it follows that

$$\lambda_a \geq 0, \qquad u_a - \bar{u} \leq 0, \qquad (\lambda_a, u_a - \bar{u}) = 0,$$

$$\lambda_b \geq 0, \qquad \bar{u} - u_b \leq 0, \qquad (\lambda_b, \bar{u} - u_b) = 0,$$

which is called a *complementary system.* From (2) we then obtain that

$$\lambda_a - \lambda_b = p + \alpha\bar{u}.$$

# Complementarity function

The last three relations of the optimality system, namely,

$$\lambda_a \geq 0, \quad \lambda_b \geq 0,$$
$$\lambda_a^\top (u_a - \bar{u}) = \lambda_b^\top (\bar{u} - u_b) = 0,$$
$$u_a \leq \bar{u} \leq u_b.$$

can be rewritten as

$$\lambda_a = -\min(0, \lambda_a + c(u - a)), \qquad \forall c > 0$$
$$\lambda_b = \max(0, \lambda_b + c(u - b)), \qquad \forall c > 0,$$

and the optimality system to be solved

$$A\bar{y} = \bar{u},$$
$$A^T p = \bar{y} - z_d,$$
$$\alpha\bar{u} + p - \lambda_a + \lambda_b = 0,$$
$$\lambda_a = -\min(0, \lambda_a + c(u - a))$$
$$\lambda_b = \max(0, \lambda_b + c(u - b))$$

# Integration by parts

Let $\Omega \in \mathbb{R}^N$ be a bounded Lipschitz domain with boundary $\Gamma$. By applying Green's formula, with $y, v \in C^1(\overline{\Omega})$, we obtain that

$$\int_\Omega v(x) D_i y(x) \, dx = \int_\Gamma v(x) y(x) n_i(x) \, ds - \int_\Omega y(x) D_i v(x) \, dx,$$

where $n_i(x)$ denotes the $i$-th component of the exterior normal vector to $\Omega$ at the point $x \in \Gamma$ and $ds$ the Lebesgue surface measure at the boundary $\Gamma$.

If in addition $v = 0$ on $\Gamma$ then

$$\int_\Omega y(x) D_i v(x) dx = - \int_\Omega v(x) D_i y(x) dx.$$

More generally, we obtain the following formula

$$\int_\Omega y(x) D^\alpha v(x) \, dx = (-1)^{|\alpha|} \int_\Omega v(x) D^\alpha y(x) dx, \quad \text{with } |\alpha| \leq k,$$

where $\alpha = (\alpha_1, \ldots, \alpha_N)$ is a multi-index and $D^\alpha$ the corresponding diferentiation operator.

# Weak derivatives

Let $L^1_{\mathrm{loc}}(\Omega)$ denote the set of locally integrable functions on $\Omega$, *i.e.*, integrable on any compact subset of $\Omega$.

## Definition

Let $y \in L^1_{\mathrm{loc}}(\Omega)$ and $\alpha$ a given multi-index. If there exists a function $w \in L^1_{\mathrm{loc}}(\Omega)$ such that

$$\int_\Omega y(x) D^\alpha v(x)\, dx = (-1)^{|\alpha|} \int_\Omega w(x) v(x) dx,$$

for all $v \in C_0^\infty(\Omega)$, then w is called the derivative of order $k$ of $y$ in the weak sense or **weak derivative**, and is denoted by $w = D^\alpha y$.

# Example

$y(x) = |x|$ in $\Omega = (-1, 1)$. The weak derivative of $y(x)$ is given by

$$y'(x) = w(x) = \begin{cases} -1 & \text{if } x \in (-1, 0), \\ 1 & \text{if } x \in [0, 1). \end{cases}$$

Indeed, for $v \in C_0^\infty(-1, 1)$,

$$\begin{aligned} \int_{-1}^{1} |x| v'(x) dx &= \int_{-1}^{0} (-x) v'(x) dx + \int_{0}^{1} x v'(x) dx \\ &= -x.v(x)\Big|_{-1}^{0} - \int_{-1}^{0} (-1) v(x) + x.v(x)\Big|_{0}^{1} - \int_{0}^{1} 1 v(x) dx \\ &= -\int_{-1}^{1} w(x) v(x) dx. \end{aligned}$$

Note that the value of $y'$ at the point $x = 0$ is not important since the set $\{x = 0\}$ has zero measure.

# Sobolev spaces

## Definition

Let $1 \leq p < \infty$ and $k \in \mathbb{N}$. The space of functions $y \in L^p(\Omega)$ whose weak derivatives $D^\alpha y$, $\forall \alpha : |\alpha| \leq k$ exist and belong to $L^p(\Omega)$ is denoted by $W^{k,p}(\Omega)$ and is called Sobolev space. This space is endowed with the norm

$$\|y\|_{W^{k,p}(\Omega)} = \left( \sum_{|\alpha| \leq k} \int_\Omega |D^\alpha y|^p \, dx \right)^{1/p}.$$

If $p = \infty$ the space $W^{k,p}(\Omega)$ is defined in a similar way and endowed with the norm

$$\|y\|_{W^{k,p}(\Omega)} = \max_{|\alpha| \leq k} \|D^\alpha y\|_{L^\infty(\Omega)}.$$

The spaces $W^{k,p}(\Omega)$ constitute Banach spaces.

In the special case $p = 2$ the Sobolev spaces are denoted by

$$H^k(\Omega) := W^{k,2}(\Omega).$$

A frequently used space is

$$H^1(\Omega) = \{y \in L^2(\Omega) : D_i y \in L^2(\Omega),\ i = 1, \dots, N\}$$

endowed with the norm

$$\|y\|_{H^1(\Omega)} = \left( \int_\Omega (y^2 + |\nabla y|^2) dx \right)^{1/2}$$

with $|\nabla y|^2 = (D_1 y)^2 + \cdots + (D_N y)^2$, and the scalar product

$$(u, v)_{H^1(\Omega)} = \int_\Omega u \cdot v \, dx + \int_\Omega \nabla u \cdot \nabla v \, dx.$$

The space $H^1(\Omega)$ constitutes a Hilbert space with the provided scalar product.

### Definition

The closure of $C_0^\infty(\Omega)$ in $W^{k,p}(\Omega)$ is denoted by $W_0^{k,p}(\Omega)$. The resulting space is endowed with the $W^{k,p}$ norm and constitutes a closed subspace of $W^{k,p}(\Omega)$.

### Theorem

Let $\Omega \in \mathbb{R}^N$ be a bounded Lipschitz domain. There exist a bounded linear mapping $\tau : W^{1,p}(\Omega) \to L^p(\Gamma)$ such that

$$(\tau y)(x) = y(x) \qquad \text{a.e. on } \Gamma,$$

for each $y \in C(\overline{\Omega})$.

### Definition

The function $\tau y$ is called the trace of $y$ on $\Gamma$ and $\tau$ is called the **trace operator**.

Consider the following problem:

$$\begin{cases} -\Delta y = f & \text{in } \Omega, \\ y = 0 & \text{on } \Gamma. \end{cases} \tag{3}$$

Assuming $y$ is a classical solution, multiplying (3) with a test function $v \in C_0^\infty(\Omega)$ and integrating over $\Omega$ we obtain

$$-\int_\Omega v \Delta y \, dx = \int_\Omega f v \, dx,$$

which using integration by parts yields

$$-\int_\Omega v \partial_{\vec{n}} y \, ds + \int_\Omega \nabla y \cdot \nabla v \, dx = \int_\Omega f v \, dx,$$

where $\partial_{\vec{n}} y = \nabla y \cdot \vec{n}$. Since $v = 0$ on $\Gamma$, it follows that

$$\int_\Omega \nabla y \cdot \nabla v \, dx = \int_\Omega f v \, dx.$$

Since $C_0^\infty(\Omega)$ is dense into $H_0^1(\Omega)$ and both terms in the previous equation are continuos with respect to $v \in H_0^1(\Omega)$ then the equation holds for all $v \in H_0^1(\Omega)$.

### Definition

A function $y \in H_0^1(\Omega)$ is called a **weak solution** for problem (3) if it satisfies the following variational formulation:

$$\int_\Omega \nabla y \cdot \nabla v \, dx = \int_\Omega f \, v \, dx, \qquad \forall v \in H_0^1(\Omega).$$

## Definition

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## Theorem (Minty-Browder)

Let $V$ be a reflexive Banach space, $\ell \in V'$ and $A : V \to V'$ be an operator satisfying

i) $A$ is *monotone*, i.e., for all $u, v \in V$, $\langle A(u) - A(v), u - v \rangle_{V',V} \geq 0$.

ii) $A$ is *hemicontinuous*, i.e., the function $t \to \langle A(u + tv), w \rangle_{V',V}$ is continuous on the interval $[0, 1]$, for all $u, v, w \in V$.

iii) $A$ is *coercive*, i.e., $\lim_{\|u\|_V \to \infty} \frac{\langle A(u), u \rangle_{V',V}}{\|u\|_V} = +\infty$.

Then there exists a solution to the variational equation

$$\langle A(y), v \rangle_{V',V} = \langle \ell, v \rangle_{V',V}, \qquad \text{for all } v \in V.$$

If $A$ is strictly monotone, then the solution is unique.

# Problem statement

Consider the following general PDE-constrained optimization problem:

$$\begin{cases} \min \ J(y,u), \\ \text{subject to:} \\ \qquad e(y,u) = 0, \end{cases} \tag{$\mathcal{P}$}$$

where $J\colon\ Y \times U \longrightarrow \mathbb{R}$ and $e\colon\ Y \times U \longrightarrow W$, and $Y$, $U$ and $W$ are reflexive Banach spaces. We assume that there exists a unique solution $y(u)$ to $e(y,u) = 0$ and refer to the operator

$$\begin{aligned} G\colon\ U &\longrightarrow Y \\ u &\longmapsto y(u) = G(u), \end{aligned}$$

which assigns to each $u \in U$ the solution $y(u)$ to

$$e(y(u), u) = 0 \tag{4}$$

as **control-to-state operator**.

# Reduced problem

Using the control-to-state operator we can write the optimal control problem in reduced form as

$$\min_{u \in U} f(u) := J(y(u), u). \qquad (\mathcal{R})$$

Hereafter we assume that $f : U \longrightarrow \mathbb{R}$ is bounded from below.

**Definition**

An element $\bar{u} \in U$ is called a global solution to $(\mathcal{R})$ if $f(\bar{u}) \leq f(u), \forall u \in U$. Further, $\bar{u}$ is called a local solution if there exists a neighborhood $V(\bar{u})$ of $\bar{u}$ in $U$ such that

$$f(\bar{u}) \leq f(u), \qquad \forall u \in U \cap V(\bar{u}).$$

A functional $h\colon U \longrightarrow \mathbb{R}$ is called weakly lower semicontinuous (w.l.s.c) if for every weakly convergent sequence $u_n \rightharpoonup u$ in $U$ it follows that

$$h(u) \leq \liminf_{n\to\infty} h(u_n).$$

## Theorem

If $f\colon U \longrightarrow \mathbb{R}$ is w.l.s.c and

$$\lim_{\|u\|_U\to\infty} f(u) = +\infty \tag{5}$$

then $f$ has a global minimum.

## Proof

Let $\{u_n\}_{n\in\mathbb{N}}$ be a minimizing sequence, *i.e.* $\{u_n\} \subset U$ and $\lim_{n\to\infty} f(u_n) = \inf_{u\in U} f(u)$. Thanks to (5) it follows that the sequence $\{u_n\}$ is bounded. Since $U$ is reflexive, there exists a subsequence $\{u_{n_k}\}_{k\in\mathbb{N}}$ which converges weakly to a limit $\bar{u}$ as $k \to \infty$. Due to the weakly lower semi continuity of $f$ it follows that

$$f(\bar{u}) \leq \liminf_{k\to\infty} f(u_{n_k}) = \inf_{u\in U} f(u).$$

Consequently, $\bar{u}$ is a global minimum.

# Example

$$\min J(y,u) = \frac{1}{2}\|y - z_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)}, \tag{6a}$$

subject to:

$$-\Delta y = u \qquad \text{in } \Omega, \tag{6b}$$

$$y = 0 \qquad \text{on } \Gamma, \tag{6c}$$

where $\Omega \subset \mathbb{R}^N$ is a bounded Lipschitz domain, $\alpha > 0$, $z_d \in L^2(\Omega)$.

Control space: $U = L^2(\Omega)$ and, there exists for each $u \in U$ a unique weak solution for (6b) -- (6c). The reduced functional $f : U \longrightarrow \mathbb{R}$ satisfies

$$f(u) = J(y(u), u) \geq \frac{\alpha}{2}\|u\|^2_{L^2}$$

and, consequently, is bounded from below and satisfies (5). Moreover $f$ is convex and continuous, and, therefore, w.l.s.c. Consequently, there exists an optimal solution for (6).

# Differentiability in Banach spaces

Let $U, V$ be two real Banach spaces and $F\colon U \longrightarrow V$ a mapping from $U$ to $V$.

## Directional derivative

If for given elements $u \in U$, $h \in U$ the limit

$$F'(u;h) := \lim_{t \to 0} \frac{1}{t}(F(u+th) - F(u))$$

exists, then $F'(u;h)$ is called the *directional derivative* of $F$ at $u$ in direction $h$. If this limit exists for all $h \in U$, then $F$ is called directionally differentiable at $u$.

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## Gâteaux derivative

If for some $u \in U$ and all $h \in U$ the limit

$$F'(u;h) = \lim_{t \to 0} \frac{1}{t}(F(u+th) - F(u))$$

exists and if $F'(u;h)$ is a continuous linear mapping from $U$ to $V$ with respect to $h$, then $F'(u)$ and is called the Gâteaux derivative of $F$ at $u$, and $F$ is called Gâteaux differentiable at $u$.

# Example 1

Let $U = C[0,1]$ and $f\colon U \longrightarrow \mathbb{R}$ given through

$$f(u(\cdot)) = \sin(u(1)).$$

Let also $h = h(x)$ be a function from $C[0,1]$. The directional derivative of $f$ at $u$ in direction $h$ is then given by

$$\begin{aligned}
\lim_{t\to 0} \frac{1}{t}(f(u+th) - f(u)) &= \lim_{t\to 0} \frac{1}{t}(\sin(u(1)+th(1)) - \sin(u(1))) \\
&= \frac{d}{dt} \sin(u(1)+th(1))\Big|_{t=0} \\
&= \cos(u(1)+th(1))h(1)\Big|_{t=0} \\
&= \cos(u(1))h(1).
\end{aligned}$$

Therefore, $f'(u;h) = \cos(u(1))h(1)$ and since $f'(u)$ is linear and continuous with respect to $h$, $f$ is Gâteaux differentiable with its derivative given by

$$f'(u)h = \cos(u(1))h(1).$$

# Example 2

Let $H$ be a Hilbert space with scalar product $(\cdot,\cdot)_H$ and norm $\|\cdot\|_H$. Let $f: H \longrightarrow \mathbb{R}$ be defined by

$$f(u) = \|u\|_H^2 .$$

The directional derivative of $f$ at $h$ in derivation $h$ is given by

$$\begin{aligned}\lim_{t\to 0}\frac{1}{t}(f(u+th)-f(u)) &= \lim_{t\to 0}\frac{1}{t}(\|u+th\|_H^2 - \|u\|_H^2)\\ &= \lim_{t\to 0}\frac{1}{t}(2t(u,h)_H + t^2\left\|h_H^2\right\|\\ &= 2(u,h)_H.\end{aligned}$$

Therefore $f'(u;h) = 2(u,h)_H$, which is linear and continuous whit respect to $h$. Consequently, $f$ is Gâteaux differentiable with

$$f'(u)h = 2u,$$

(upon identification of $H$ and $H'$).

## Fréchet derivative

If $F$ is Gâteaux differentiable at $u \in U$ and satisfies in addition that

$$\lim_{\|u\|_H \to 0} \frac{\|F(u+h) - F(u) - F'(u)h\|_V}{\|h\|_H} = 0,$$

then $F'(h)$ is called the Fréchet derivative if $F$ at $u$ and $F$ is called Fréchet differentiable at $u$.

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then $F'(h)$ is called the Fréchet derivative if $F$ at $u$ and $F$ is called Fréchet differentiable at $u$.

1. If $F$ is Fréchet differentiable at some $u \in U$, then it is continuous at $u$.
2. *Chain Rule*: Let $F\colon U \longrightarrow V$ and $G\colon V \longrightarrow Z$ be Fréchet differentiable at $u$ and $F(u)$, respectively. Then

   $$E(u) = G(F(u))$$

   is also Fréchet differentiable and its derivative is given by

   $$E'(u) = G'(F(u)) \circ F'(u).$$

3. If $F\colon U \longrightarrow V$ is Fréchet differentiable and $F'\colon U \longrightarrow \mathcal{L}(U, V)$ is also F-differentiable, then $F$ is called twice F-differentiable and we write

   $$F''(u) \in \mathcal{L}(U, \mathcal{L}(U, V))$$

   for the second derivative of $F$ at $u$.

# Optimality condition

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Let $S \subset U$ be a nonempty subset of a real normed space $U$ and $f : S \subset U \longrightarrow \mathbb{R}$ a given functional, bounded from below. Consider the following problem:

$$\min_{u \in S} f(u). \tag{7}$$

## Definition

For $u \in S$ the direction $v - u \in U$ is called admissible if there exists a sequence $\{\varepsilon_n\}_{n \in \mathbb{N}}$ with $0 < \varepsilon_n \to 0$ as $n \to \infty$ and $u + \varepsilon_n(v - u) \in S$ for every $n \in \mathbb{N}$.

## Theorem

Suppose that $\bar{u} \in S$ is a local solution of (7) and that $v - \bar{u}$ is an admissible direction. If $f$ is directionally differentiable at $\bar{u}$ in direction $v - \bar{u}$, then

$$f'(\bar{u}, v - \bar{u}) \geq 0.$$

## Corollary

Let $S = U$ and $\bar{u}$ a local optimal solution for 7. If $f$ is Gâteaux differentiable at $\bar{u}$, then

$$f'(\bar{u})h = 0, \qquad \text{for all } h \in U.$$

# Standing assumptions

Let us now turn to PDE constrained optimization problems and recall problem $(\mathcal{P})$:

$$\begin{cases} \min J(y,u), \\ \text{subject to:} \\ \qquad e(y,u) = 0, \end{cases}$$

or, in reduced form $(\mathcal{R})$,

$$\min_{u \in U} f(u) := J(y(u), u).$$

We assume that $J\colon Y \times U \longrightarrow \mathbb{R}$ and $e\colon Y \times U \longrightarrow W$ are continuously Fréchet differentiable. We further assume that the partial derivative of $e$ with respect to $y$ at $(\bar{y}, \bar{u}) = (y(\bar{u}), \bar{u})$ satisfies the following condition:

$$e_y(\bar{y}, \bar{u}) \text{ is invertible.} \tag{8}$$

## Definition

An element $p \in W'$ is called the **adjoint state** related to $\bar{u}$ if it solves the following **adjoint equation**:

$$e_y\left(y(\bar{u}), \bar{u}\right)^* p = J_y\left(y(\bar{u}), \bar{u}\right), \tag{9}$$

where $e_y\left(y(\bar{u}), \bar{u}\right)^*$ denotes the adjoint operator of $e_y\left(y(\bar{u}), \bar{u}\right)$.

## Theorem (Optimality System)

Let $\bar{u}$ be a local optimal solution for $(\mathcal{R})$ and $y(\bar{u})$ its associated state. If (8) holds, then there exists an adjoint state $p \in W'$ such that the following system of equations is satisfied.

$$e\left(y(\bar{u}), \bar{u}\right) = 0 \tag{10a}$$

$$e_y\left(y(\bar{u}), \bar{u}\right)^* p = J_y\left(y(\bar{u}), \bar{u}\right) \tag{10b}$$

$$e_u\left(y(\bar{u}), \bar{u}\right)^* p = J_u\left(y(\bar{u}), \bar{u}\right) \tag{10c}$$

## Proof

By taking the derivative, with respect to $u$ in direction $h$, on both sides of the state equation $e\left(y(u), u\right) = 0$, we obtain that

$$e_y\left(y(u), u\right) y'(u) + e_u\left(y(u), u\right) h = 0. \tag{11}$$

If $\bar{u} \in U$ is a local optimal solution for $(\mathcal{R})$ we obtain the following necessary condition

$$f'(\bar{u})h = \langle J_y(\bar{y}(\bar{u}), \bar{u}), y'(\bar{u})h\rangle_{Y',Y} + J_u\left(y(\bar{u}, \bar{u})\right) h = 0, \quad \forall h \in U. \tag{12}$$

Using the adjoint equation,

$$\begin{aligned} f'(\bar{u})h &= \langle e_y(\bar{y}(\bar{u})^* p, y'(\bar{u})h\rangle_{Y',Y} + J_u\left(y(\bar{u}, \bar{u})\right) h \\ &= \langle p, e_y(\bar{y}(\bar{u})y'(\bar{u})h\rangle_{W',W} + J_u\left(y(\bar{u}, \bar{u})\right) h \end{aligned}$$

and using the linearized equation (11)

$$\begin{aligned} f'(\bar{u})h &= \langle p, -e_u(\bar{y}(\bar{u})h\rangle_{W',W} + J_u\left(y(\bar{u}, \bar{u})\right) h \\ &= -\langle e_u(\bar{y}(\bar{u})p, h\rangle_{U',U} + J_u\left(y(\bar{u}, \bar{u})\right) h = 0 \end{aligned}$$

Consequently,

$$e_u(\bar{y}(\bar{u})p = J_u(y(\bar{u}, \bar{u}).$$

# Example

Consider the heating problem given by

$$\begin{cases} \min J(y,u) = \frac{1}{2}\left\| y - z_d \right\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\left\| u \right\|^2_{L^2(\Omega)}, \\ \text{subject to:} \\ \qquad -\Delta y = u \qquad \text{in } \Omega, \\ \qquad\quad y = 0 \qquad \text{on } \Gamma. \end{cases}$$

The variational formulation of the state equation is given by

$$\int_\Omega \nabla y \cdot \nabla v \, dx = \int_\Omega u \cdot v \, dx, \qquad \forall v \in H_0^1(\Omega).$$

Consequently, $e\colon H_0^1(\Omega)\times L^2(\Omega)\longrightarrow H^{-1}(\Omega)=(H_0^1(\Omega))'$ is defined by

$$\langle e(y,u),v\rangle_{H^{-1},H_0^1}=\int_\Omega \nabla y\cdot\nabla v\,dx-\int_\Omega uv\,dx$$

and its partial derivative with respect to $y$ is given by

$$\langle e_y(y,u)w,v\rangle=\int_\Omega \nabla w\cdot\nabla v\,dx.$$

For a given function $\varphi\in H^{-1}(\Omega)$, equation

$$\langle e_y(y,u)w,v\rangle_{H^{-1},H_0^1}=\int_\Omega \nabla w\cdot\nabla v\,dx=\langle\varphi,v\rangle_{H^{-1},H_0^1}$$

has a unique solution and $\|w\|_{H_0^1}\le C\,\|\varphi\|_{H^{-1}}$ for some constant $C>0$ (*Lax-Milgram Theorem*). Consequently, (8) is satisfied.

In order to apply the Theorem we compute the remaining derivatives:

$$\begin{aligned} e_u(y,u)h &= h, \\ J_y(y,u)w &= y - z_d, \\ J_u(y,u) &= \alpha u. \end{aligned}$$

The optimality system is then given through:

$$\int_\Omega \nabla y \cdot \nabla v dx = \int_\Omega uv \, dx, \quad \forall v \in H_0^1(\Omega),$$

$$\int_\Omega \nabla p \cdot \nabla v dx = \int_\Omega (y - z_d) v dx, \quad \forall v \in H_0^1(\Omega),$$

$$\alpha u + p = 0, \qquad \text{a.e. in } \Omega,$$

where we used that

$$\langle e_y(y(\bar{u}))w, v \rangle = \int_\Omega \nabla w \cdot \nabla v \, dx = \int_\Omega \nabla v \cdot \nabla w \, dx = \langle w, e_y(\bar{y},\bar{u})^* v \rangle_{H_0^1, H^{-1}}$$

and, similarly,

$$(e_u(\bar{y},\bar{u})h, \phi)_{L^2(\Omega)} = \int_\Omega h\phi \, dx = (h, e_u(\bar{y},\bar{u})^* \phi) \, .$$

# Lagrangian derivation

Consider again problem $(\mathcal{P})$ with $J\colon Y \times U \longrightarrow \mathbb{R}$ and $e\colon Y \times U \longrightarrow W$. The Lagrangian functional is given by

$$\begin{aligned} \mathcal{L}\colon Y \times U \times W' &\longrightarrow \mathbb{R} \\ (y,u,p) &\longmapsto \mathcal{L}(y,u,p) = J(y,u) - \langle p, e(y,u)\rangle_{W',W}. \end{aligned}$$

By differentiating $\mathcal{L}(y,u,p)$ with respect to $y$ in direction $w$ we obtain that

$$\begin{aligned} \mathcal{L}_y(y,u,p) &= J_y(y,u)w - \langle p, e_y(y,u)w\rangle_{W',W} \\ &= J_y(y,u)w - \langle e_y(y,u)^* p, w\rangle_{Y',Y}. \end{aligned}$$

Consequently, equation (10b) can also be expressed as

$$\mathcal{L}_y(\bar{y},\bar{u},p) = 0.$$

In a similar manner, by taking the derivative of $\mathcal{L}(y,u,p)$ with respect to $u$, in direction h, we obtain

$$\begin{aligned}\mathcal{L}_y(y,u,p)h &= J_u(y,u)h - \langle p, e_u(y,u)h\rangle_{W',W} \\ &= J_u(y,u)h - \langle e_u(y,u)^* p, h\rangle_{U',U}\end{aligned}$$

and, therefore equation (10c) can be written as

$$\mathcal{L}_u(\bar{y},\bar{u},p) = 0.$$

Summarizing, the optimality system (10) can be written in the following way:

$$e\left(y(\bar{u}),\bar{u}\right) = 0, \tag{13a}$$
$$\mathcal{L}_y\left(\bar{y},\bar{u},p\right) = 0, \tag{13b}$$
$$\mathcal{L}_u\left(\bar{y},\bar{u},p\right) = 0. \tag{13c}$$

# Semilinear example

## Rigorous derivation

$$\begin{cases} \min \ J(y,u) = \dfrac{1}{2} \|y - z_d\|^2_{L^2(\Omega)} + \dfrac{\alpha}{2} \|u\|^2_{L^2(\Omega)}, \\ \text{subject to:} \\ \qquad -\Delta y + y^3 = u \quad \text{in } \Omega, \\ \qquad\qquad\quad y = 0 \quad \text{on } \Gamma. \end{cases}$$

*Weak formulation of the PDE.* Multiplying the state equation by a test function $v \in C_0^\infty(\Omega)$ and integrating yields

$$\int_\Omega -\Delta y \, v dx + \int_\Omega y^3 v dx = \int_\Omega uv \, dx.$$

Using integration by parts,

$$\int_\Omega \nabla y \cdot \nabla v \, dx + \int_\Omega y^3 v \, dx = \int_\Omega uv \, dx.$$

Since $C_0^\infty$ is dense in $H_0^1(\Omega)$ and all terms are continuous with respect to $v$ in the $H_0^1(\Omega)$ norm, we obtain the following variational formulation: Find $y \in H_0^1(\Omega)$ such that

$$\int_\Omega \nabla y \cdot \nabla v \, dx + \int_\Omega y^3 v \, dx = \int_\Omega uv \, dx, \quad \forall v \in H_0^1(\Omega).$$

Consequently, $e \colon H_0^1(\Omega) \times L^2(\Omega) \longrightarrow H^{-1}(\Omega)$ is defined by

$$\langle e(y,u), v \rangle_{H^{-1},H_0^1} = \int_\Omega \nabla y \cdot \nabla v \, dx + \int_\Omega y^3 v \, dx - \int_\Omega uv \, dx,$$

for all $v \in H_0^1(\Omega)$. By monotone operator theory, there exists a unique solution.

*Derivatives.* The partial derivatives of $e(y,u)$ are given by

$$
\begin{aligned}
\langle e_y(y,u)w, v\rangle_{H^{-1},H_0^1} &= \int_\Omega \nabla w \cdot \nabla v \, dx + 3\int_\Omega y^2 w v \, dx, \\
\langle e_u(y,u)h, v\rangle_{H^{-1},H_0^1} &= -\int_\Omega h v \, dx.
\end{aligned}
$$

*Differentiability.* Since $y \in H_0^1(\Omega) \hookrightarrow L^6(\Omega)$, we consider the operator

$$
\begin{aligned}
N\colon L^6(\Omega) &\longrightarrow L^2(\Omega) \\
y &\longmapsto y^3.
\end{aligned}
$$

The derivative of $N$ is given by

$$N'(y)w = 3y^2 w.$$

Indeed,

$$
\begin{aligned}
\left\|(y+w)^3 - y^3 - 3y^2 w\right\|_{L^2} &= \left\|3yw^2 + w^3\right\|_{L^2} \\
&\le 3\left\|y\right\|_{L^6}\left\|w\right\|_{L^6}^2 + \left\|w\right\|_{L^6}^3 = O\left(\left\|w\right\|_{L^6}^2\right) \\
&= o\left(\left\|w\right\|_{L^6}\right).
\end{aligned}
$$

*Lagrangian.* The Lagrangian is defined by:

$$\mathcal{L}(y,u,p) = \frac{1}{2}\|y - z_d\|^2_{L^2(\Omega)} + \frac{\alpha}{2}\|u\|^2_{L^2(\Omega)} \\ - \int_\Omega \nabla y \cdot \nabla p \, dx + \int_\Omega y^3 p \, dx + \int_\Omega up \, dx$$

Taking the partial derivative with respect to the state:

$$\mathcal{L}_y(y,u,p)w = (y - z_d, w) - \int_\Omega \nabla w \cdot \nabla p \, dx - 3\int_\Omega y^2 wp \, dx \\ = \int_\Omega (y - z_d) w \, dx - \int_\Omega \nabla p \cdot \nabla w \, dx - 3\int_\Omega y^2 pw \, dx = 0$$

$$\Rightarrow \int_\Omega \nabla p \cdot \nabla w \, dx + 3\int_\Omega y^2 pw \, dx = \int_\Omega (y - z_d) w \, dx$$

On the other hand, taking the partial derivative with respect to $u$ we get that:

$$\mathcal{L}_u(y,u,p)h = \alpha(u,h)_{L^2(\Omega)} + \int_\Omega hp \, dx = 0$$

$$\Rightarrow \quad \alpha u + p = 0 \quad \text{a.e. in } \Omega.$$

*Optimality system.*

$$\int_\Omega \nabla y \cdot \nabla v \, dx + \int_\Omega y^3 v \, dx = \int_\Omega uv \, dx, \qquad \forall v \in H_0^1(\Omega),$$

$$\int_\Omega \nabla p \cdot \nabla w \, dx + 3 \int_\Omega y^2 pw \, dx = \int_\Omega (y - z_d) w \, dx, \qquad \forall w \in H_0^1(\Omega),$$

$$\alpha u + p = 0 \qquad \text{a.e. in } \Omega.$$

or, in strong form,

$$\begin{cases} -\Delta y + y^3 = u & \text{in } \Omega, \\ y = 0 & \text{on } \Gamma, \\ -\Delta p + 3y^2 p = y - z_d & \text{in } \Omega, \\ p = 0 & \text{on } \Gamma, \\ \alpha u + p = 0 & \text{a.e. in } \Omega. \end{cases}$$

# Elliptic control problem

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## Optimal control problem

$$\min \ J(y,u) = \frac{1}{2}\int_\Omega |y - z_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx$$

subject to:

$$-\Delta y = u$$

$$y|_\Gamma = g$$

# Elliptic control problem

**Optimal control problem**

$$\min \; J(y,u) = \frac{1}{2}\int_\Omega |y - z_d|^2 dx + \frac{\alpha}{2}\int_\Omega |u|^2 dx$$

subject to:

$$-\Delta y = u \quad \text{(distributed control)}$$

$$y|_\Gamma = g$$

# Elliptic control problem

Mode Mat

## Optimal control problem

$$\min \ J(y,u) = \frac{1}{2}\int_{\Omega} |y - z_d|^2 dx + \frac{\alpha}{2}\int_{\Omega} |u|^2 dx$$

subject to:

$$-\Delta y = u$$

$$y|_{\Gamma} = g$$

## Lagrangian:

$$\mathcal{L}(y,u,p,\psi) = J(y,u) - \int_{\Omega} p(-\Delta y - u) - \int_{\Gamma} \xi(y-g)$$

# Necessary condition I

$$\mathcal{L}_y(w) = \int_\Omega (y - z_d)w - \int_\Omega p(-\Delta w) - \int_\Gamma \xi w$$

# Necessary condition I

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\begin{aligned}
\mathcal{L}_y(w) &= \int_\Omega (y - z_d)w - \int_\Omega p(-\Delta w) - \int_\Gamma \xi w \\
&= \int_\Omega (y - z_d)w - \int_\Omega \nabla p \cdot \nabla w + \int_\Gamma p \frac{\partial w}{\partial n} - \int_\Gamma \xi w
\end{aligned}
$$

$$\Rightarrow \qquad -\Delta p = y - z_d \tag{14}$$

$$\frac{\partial p}{\partial n} + \xi = 0 \qquad \text{on } \Gamma \tag{15}$$

$$p|_\Gamma = 0. \tag{16}$$

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&= \int_\Omega (y - z_d + \Delta p)w - \int_\Gamma (\frac{\partial p}{\partial n} + \xi)w + \int_\Gamma p \frac{\partial w}{\partial n} = 0
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$$
\mathcal{L}_u(v) = \alpha \int_\Omega u\, v + \int_\Omega p\, v = \int_\Omega (\alpha u + p)\, v = 0.
$$

$$
\Rightarrow \qquad \alpha u + p = 0. \tag{17}
$$

# Optimality system:

$$\begin{cases} -\Delta y = u \\ y|_{\Gamma} = g \end{cases} \qquad \text{(state equation)}$$

$$\begin{cases} -\Delta p = y - z_d \\ p|_{\Gamma} = 0 \end{cases} \qquad \text{(adjoint equation)}$$

$$\alpha u + p = 0 \qquad \text{(optimality condition)}$$

# Parabolic control problem

## Problem

$$
\begin{cases}
\min\ J(y,u) = \frac{1}{2}\int\limits_0^T\int\limits_\Omega |y - z_d|^2 + \frac{\alpha}{2}\int\limits_0^T\int\limits_\Omega |u|^2 \\
\text{subject to:} \\
\frac{\partial y}{\partial t} - \Delta y = f \\
y|_\Gamma = u \\
y(0) = y_0,
\end{cases}
$$

where $y$ is the state and $u$ the control.

# Parabolic control problem

## Problem

$$\begin{cases} \min \ J(y,u) = \frac{1}{2}\int\limits_0^T\int\limits_\Omega |y - z_d|^2 + \frac{\alpha}{2}\int\limits_0^T\int\limits_\Omega |u|^2 \\ \text{subject to:} \\ \frac{\partial y}{\partial t} - \Delta y = f \\ y|_\Gamma = u \\ y(0) = y_0, \end{cases}$$

where $y$ is the state and $u$ the control.

## Lagrangian:

$$\mathcal{L}(y,u,p,\xi,\theta) = J(y,u) - \int\limits_0^T\int\limits_\Omega p(\frac{\partial y}{\partial t} - \Delta y - f) + \int\limits_0^T\int\limits_\Gamma \xi(y-u) + \int\limits_\Omega \theta(y(0) - y_0)$$

# Adjoint equation I

$$\mathcal{L}_y(w) = \int_0^T \int_\Omega (y - z_d) \cdot w - \int_0^T \int_\Omega p \cdot \frac{\partial w}{\partial t} + \int_0^T \int_\Omega p \cdot (\Delta w) + \int_0^T \int_\Gamma \xi \cdot w + \int\limits_\Omega \theta \cdot w(0)$$

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$$\mathcal{L}_y(w) = \int_0^T \int_\Omega (y - z_d) \cdot w - \int_0^T \int_\Omega p \cdot \frac{\partial w}{\partial t} + \int_0^T \int_\Omega p \cdot (\Delta w) + \int_0^T \int_\Gamma \xi \cdot w + \int_\Omega \theta \cdot w(0)$$

$$= \int_0^T \int_\Omega (y - z_d) \cdot w - \int_\Omega \left[ p(T) \cdot w(T) - p(0) \cdot w(0) - \int_0^T \frac{\partial p}{\partial t} \cdot w \right]$$

$$- \int_0^T \int_\Omega \nabla p \cdot \nabla w + \int_0^T \int_\Gamma p \cdot \frac{\partial w}{\partial n} + \int_0^T \int_\Gamma \xi \cdot w + \int_\Omega \theta \cdot w(0)$$

# Adjoint equation I

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$$
\begin{aligned}
\mathcal{L}_y(w) &= \int_0^T \int_\Omega (y - z_d) \cdot w - \int_0^T \int_\Omega p \cdot \frac{\partial w}{\partial t} + \int_0^T \int_\Omega p \cdot (\Delta w) + \int_0^T \int_\Gamma \xi \cdot w + \int_\Omega \theta \cdot w(0) \\
&= \int_0^T \int_\Omega (y - z_d) \cdot w - \int_\Omega \left[ p(T) \cdot w(T) - p(0) \cdot w(0) - \int_0^T \frac{\partial p}{\partial t} \cdot w \right] \\
&\quad - \int_0^T \int_\Omega \nabla p \cdot \nabla w + \int_0^T \int_\Gamma p \cdot \frac{\partial w}{\partial n} + \int_0^T \int_\Gamma \xi \cdot w + \int_\Omega \theta \cdot w(0) \\
&= \int_0^T \int_\Omega \left( y - z_d + \frac{\partial p}{\partial t} + \Delta p \right) \cdot w - \int_0^T \int_\Gamma \left( \frac{\partial p}{\partial n} - \xi \right) \cdot w \\
&\quad + \int_0^T \int_\Gamma p \cdot \frac{\partial w}{\partial n} - \int_\Omega p(T) \cdot w(T) + \int_\Omega (p(0) + \theta) \cdot w(0).
\end{aligned}
$$

# Adjoint equation II

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$$\Rightarrow \qquad -\frac{\partial p}{\partial t} - \Delta p = y - z_d \tag{18}$$

$$\frac{\partial p}{\partial n} = \xi \ \text{ en } \Gamma \tag{19}$$

$$p|_\Gamma = 0 \tag{20}$$

$$p(T) = 0 \tag{21}$$

$$p(0) + \theta = 0 \tag{22}$$

$$\mathcal{L}_u(v) = \alpha \int_0^T \int_\Gamma u\, v - \int_0^T \int_\Gamma \xi\, v = \int_\Omega (\alpha u - \xi)\, v = 0.$$

$$\Rightarrow \qquad \alpha u - \xi = 0 \quad \text{on } \Gamma. \tag{23}$$

# Optimality system:

$$\begin{cases} \partial_t y - \Delta y = f \\ y|_\Gamma = u \\ y(0) = y_0 \end{cases} \qquad \text{(state equation)}$$

$$\begin{cases} -\partial_t p - \Delta p = y - z_d \\ p|_\Gamma = 0 \\ p(T) = 0 \end{cases} \qquad \text{(adjoint equation)}$$

$$\alpha u - \frac{\partial p}{\partial n} = 0 \qquad \text{(optimality condition)}$$

### Theorem

Let $U$ be a Banach space and $S \subset U$ a convex set. Let $f : U \longrightarrow \mathbb{R}$ be twice continuously F-differentiable in a neighborhood of $\bar{u} \in U$. If $\bar{u}$ satisfies the necessary condition

$$f'(u)(u - \bar{u}) \geq 0, \quad \forall u \in S, \tag{24}$$

and there exists some $\delta > 0$ such that

$$f''(u)[u - \bar{u}] \geq \delta \|u\|_U^2, \quad \forall u \in U, \tag{25}$$

then there exist contstants $\epsilon > 0$ and $\sigma > 0$ such that

$$f(u) \geq f(\bar{u}) + \sigma \|u - \bar{u}\|_U^2$$

for all $u \in S : \|u - \bar{u}\|_U \leq \epsilon$. Therefore, $\bar{u}$ is a local minimun of $f$ on $S$.

Since $f$ is twice Fréchet differentiable, a Taylor expansion can be used. Consequently, for some $\theta \in [0, 1]$

$$\begin{aligned} f(u) &= f(\bar{u}) + f'(\bar{u})(u - \bar{u}) + \frac{1}{2} f''(\bar{u} + \theta(u - \bar{u}))[u - \bar{u}]^2 \\ &\geq f(\bar{u}) + \frac{1}{2} f''(\bar{u} + \theta(u - \bar{u}))[u - \bar{u}]^2 \qquad \text{by (24)} \\ &= f(\bar{u}) + \frac{1}{2} f''(\bar{u})[u - \bar{u}]^2 + \frac{1}{2} \left[ f''(\bar{u} + \theta(u - \bar{u})) - f''(\bar{u}) \right] [u - \bar{u}]^2. \end{aligned}$$

Since $f$ is twice continuously Fréchet differentiable, there exists some $\epsilon > 0$ such that

$$\|u - \bar{u}\| \leq \epsilon \Rightarrow \left| \left[ f''(\bar{u} + \theta(u - \bar{u})) - f''(u) \right] [u - \bar{u}]^2 \right| \leq \frac{\delta}{2} \|u - \bar{u}\|_U^2 .$$

Consequently,

$$\begin{aligned} f(u) &\geq f(\bar{u}) + \frac{1}{2} f''(\bar{u})[u - \bar{u}]^2 - \frac{\delta}{4} \|u - \bar{u}\|_U^2 \\ &\geq f(\bar{u}) + \frac{\delta}{4} \|u - \bar{u}\|_U^2 , \qquad \text{by (25).} \end{aligned}$$

The result follows by choosing $\sigma = \frac{\delta}{4}$.

## Theorem

Let $J\colon Y \times U \longrightarrow \mathbb{R}$ and $e\colon Y \times U \longrightarrow W$ be twice continuously F-differentible. Let $(\bar{y}, \bar{u}, p)$ be a solution to the optimality system (10). If there exists some constant $\delta > 0$ such that

$$\mathcal{L}''_{(y,u)}[(w, h)]^2 \geq \delta \left\| h \right\|_U^2 , \tag{SSC}$$

for all $(w, h) \in Y \times U$ that satisfy the equation

$$e_y(\bar{y}, \bar{u})w + e_u(\bar{y}, \bar{u})h = 0,$$

then there exist constants $\epsilon > 0$ and $\sigma > 0$ such that

$$J(y, u) \geq J(\bar{y}, \bar{u}) + \sigma \left\| u - \bar{u} \right\|_U^2$$

for all $u \in U : \left\| u - \bar{u} \right\|_U \leq \epsilon$.

# Equivalence of (SSC)

The (SSC) condition can be equivalently expressed as,

$$(w,h)\begin{pmatrix} J_{yy}(\bar{y},\bar{u}) & J_{yu}(\bar{y},\bar{u}) \\ J_{uy}(\bar{y},\bar{u}) & J_{uu}(\bar{y},\bar{u}) \end{pmatrix}\begin{pmatrix} w \\ h \end{pmatrix} - \left\langle p, (w,h)\begin{pmatrix} e_{yy}(\bar{y},\bar{u}) & e_{yu}(\bar{y},\bar{u}) \\ e_{uy}(\bar{y},\bar{u}) & e_{uu}(\bar{y},\bar{u}) \end{pmatrix}\begin{pmatrix} w \\ h \end{pmatrix}\right\rangle_{W',W} \geq \delta \left\| h \right\|_U^2$$

for all $(w,h) \in Y \times U$ that satisfy the equation

$$e_y(\bar{y},\bar{u})w + e_u(\bar{y},\bar{u})h = 0,$$

# Example

Consider again the optimal control problem

$$\begin{cases} \min\ J(y,u) = \dfrac{1}{2}\,\|y - z_d\|^2_{L^2(\Omega)} + \dfrac{\alpha}{2}\,\|u\|^2_{L^2(\Omega)}\,, \\ \text{subject to:} \\ \qquad \displaystyle\int_\Omega \nabla y \cdot \nabla u\, dx + \int_\Omega y^3 v\, dx = \int_\Omega u v\, dx, \qquad \forall v \in H_0^1(\Omega). \end{cases}$$

Recall that the first derivatives are given by

$$\langle e_y(y,u)w, v\rangle_{H^{-1},H_0^1} = \int_\Omega \nabla w \cdot \nabla v\, dx + 3\int_\Omega y^2 w v,$$

$$\langle e_y(y,u)h, v\rangle_{H^{-1},H_0^1} = -\int_\Omega h v\, dx$$

and the second derivatives are given by

$$\left\langle e_{yy}(y,u)[w]^2, v\right\rangle_{H^{-1},H_0^1} = 6\int_\Omega y w^2 v\, dx,$$

$$e_{yu}(y,u) = 0, \quad e_{uy}(y,u) = 0, \quad e_{uu}(y,u) = 0.$$

For the quadratic cost functional we get:

$$J_{yy}(\bar{y}, \bar{u})[w]^2 = \|w\|^2_{L^2(\Omega)}, \qquad J_{yu}(y, u) = 0,$$
$$J_{uy}(y, u) = 0, \qquad J_{uu}(y, u)[h]^2 = \alpha \|h\|^2_{L^2(\Omega)}.$$

Condition (SSC) is therefore equivalent to

$$\|w\|_{L^2(\Omega)} + \alpha \|h\|_{L^2(\Omega)} - 6 \int_\Omega y w^2 p \, dx \geq \delta \|h\|^2_{L^2(\Omega)}.$$

This holds in particular if

$$\int_\Omega (1 - 6yp) w^2 \, dx \geq 0.$$

# Sequential quadratic programming

## Semilinear example

Starting point is the optimality system, which in absence of control constraints is given by

$$0 = F(y,p,u) = \begin{cases} -\Delta y + y^3 - u \\ y|_\Gamma \\ -\Delta p + 3y^2\,\lambda - y + z_d \\ p|_\Gamma \\ \alpha u + p \end{cases}$$

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Using a Newton iteration for the coupled system $F(y, p, u) = 0$ yields

$$\begin{cases} -\Delta\delta_y + 3y^2\delta_y - \delta_u = \Delta y - y^3 + u \\ \delta_y|_\Gamma = 0 \\ -\Delta\delta_p + 3y^2\delta_p + 6p\delta_y - \delta_y = \Delta p - 3y^2\,p + y - z_d \\ \delta_p|_\Gamma = 0 \\ \alpha\delta_u + \delta_p = -\alpha u - p \end{cases}$$

and, hence, the Newton update $y_{n+1} = y_n + \delta_y,\ p_{n+1} = p_n + \delta_p,\ u_{n+1} = u_n + \delta_u$.

# General formulation

In general, an optimality system is given by:

$$\begin{cases} \mathcal{L}'_{(y,u)}(\bar{y}, \bar{u}, p) = 0, \\ -e(\bar{y}, \bar{u}) = 0. \end{cases}$$

By applying Newton's method, we obtain the following linearized system:

$$\begin{pmatrix} \mathcal{L}''_{(y,u)}(y_k, u_k, p_k) & -e'(y_k, u_k)^* \\ -e'(y_k, u_k) & 0 \end{pmatrix} \begin{pmatrix} \begin{pmatrix} \delta_y \\ \delta_u \end{pmatrix} \\ \delta_p \end{pmatrix} = \begin{pmatrix} e_y(y_k, u_k)^* p_k - J_y(y_k, u_k) \\ e_u(y_k, u_k)^* p_k - J_u(y_k, u_k) \\ e(y_k, u_k) \end{pmatrix}$$

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$$y_{k+1} = y_k + \delta_y, \qquad u_{k+1} = u_k + \delta_u, \qquad p_{k+1} = p_k + \delta_p.$$

The latter corresponds to the necessary and sufficient optimality condition of the following linear-quadratic problem:

$$\begin{cases} \min\limits_{(\delta_y,\delta_u)} \frac{1}{2}\mathcal{L}''_{(y,u)}(y_k,u_k,p_k)[(\delta_y,\delta_u)]^2 + \mathcal{L}'_{(y,u)}(y_k,u_k,p_k)(\delta_y,\delta_u), \\ \text{subject to:} \\ \qquad e_y(y_k,u_k)\delta_y + e_u(y_k,u_k)\delta_u + e(y_k,u_k) = 0. \end{cases}$$

# SQP properties

- If $(y_k, u_k) \in V(\bar{y}, \bar{u})$, where $(\bar{y}, \bar{u})$ is an optimal solution to the PDE constrained optimization problem such that $e'(\bar{y}, \bar{u})$ is surjective and

$$\mathcal{L}''_{(y,u)}(\bar{y}, \bar{u}, p)[(w, h)]^2 \geq \kappa \|h\|_U^2 ,$$

for some $\kappa > 0$, and the second derivatives of $J$ and $e$ are Lipschitz continuous, then there exists $\delta_p \in W'$ such that the update system is well-posed.

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- Since the SQP corresponds to the Newton method applied to the optimality system, it is also known as *Lagrange-Newton approach*. Local quadratic convergence of this approach can be proved similarly as for Newton's method.

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- Since the SQP corresponds to the Newton method applied to the optimality system, it is also known as *Lagrange-Newton approach*. Local quadratic convergence of this approach can be proved similarly as for Newton's method.
- Control constraints may be included within this framework as well. In that case each linear quadratic subproblem also contains control constraints for the increments.
- A mesh independence principle can also be proved in this case if the discretization satisfies some technical assumptions.

# Nonsmooth optimality system

## Unilateral control constraint

A nonsmooth approach for the solution of the optimality system consists in considering it as an operator equation

$$0 = F(y,p,u) = \begin{cases} -\Delta y + y^3 - u \\ y|_\Gamma \\ -\Delta p + 3y^2\, p - y + z_d \\ p|_\Gamma = 0 \\ \alpha \bar{u} + p + \lambda_b = 0 \\ \lambda_b - \max(0, \lambda_b + c(u-b)) \end{cases}$$

Due to the $\max$ function, $F$ is not Fréchet differentiable.

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Due to the $\max$ function, $F$ is not Fréchet differentiable.

Is it possible to define a weaker differentiability notion for such a function such that a Newton type iterative scheme can be stated?

# Semismoothness

**Definition**

Let $D$ be an open subset of a Banach space $X$. The mapping $F : D \subset X \to Z$ is called Newton differentiable (semismooth) on the open subset $V \subset D$ if there exists a generalized derivative $G : V \to \mathcal{L}(X, Z)$ such that

$$\lim_{h \to 0} \frac{1}{\|h\|_X} \|F(x+h) - F(x) - G(x+h)h\|_Z = 0, \tag{26}$$

for every $x \in V$.

# Example

Consider the absolute value function

$$f = |\cdot| : \mathbb{R} \longrightarrow \mathbb{R}$$
$$x \longmapsto |x|.$$

The function is not differentiable at 0. However, by using the generalized derivative

$$g(x) = \begin{cases} -1 & \text{if } x < 0, \\ 1 & \text{if } x \geq 0. \end{cases}$$

we obtain for the case $x = 0$ :

1. if $h > 0$ : $\quad \big||x+h| - |x| - |h|\big| = 0,$
2. if $h < 0$ : $\quad \big||x+h| - |x| + |h|\big| = |-x-h-x+h| = 0.$

Consequently,

$$\lim_{h \to 0} \frac{1}{|h|} |f(x+h) - f(x) - g(x+h)h| = 0$$

and $|\cdot|$ is Newton differentiable.

# Semismooth Newton method

**Theorem**

Let $\bar{x}$ be a solution to $F(x) = 0$, with $F$ Newton differentiable (semismooth) in an open neighborhood $V$ containing $\bar{x}$. If

$$\left\|G(x)^{-1}\right\|_{\mathcal{L}(Z,X)} \leq C, \tag{27}$$

for some constant $C > 0$ and all $x \in V$, then the Newton iteration

$$x_{k+1} = x_k - G(x_k)^{-1} F(x_k) \tag{28}$$

converges superlinearly to $\bar{x}$ provided that $\|x_0 - \bar{x}\|_X$ is sufficiently small. If $F$ is strongly semismooth the convergence rate is quadratic.

## Proof

Considering that $F(\bar{x}) = 0$ and the iterates given by (28) it follows that

$$\begin{aligned}
\|x_{k+1} - \bar{x}\|_X &= \left\|x_k - G(x_k)^{-1}F(x_k) - \bar{x}\right\|_X \\
&= \left\|G(x_k)^{-1}(F(\bar{x}) - F(x_k) - G(x_k)(\bar{x} - x_k))\right\|_X \\
&\leq C\,\|F(x_k) - F(\bar{x}) - G(x_k)(x_k - \bar{x})\|_Z \,. 
\end{aligned} \tag{29}$$

Thanks to the Newton differentiability it then follows, for $\rho = \frac{1}{2C}$, that there exists a ball $B_\delta(\bar{x})$ such that if $x_k \in B_\delta(\bar{x})$, then

$$\|x_{k+1} - \bar{x}\|_X \leq C\rho\,\|x_k - \bar{x}\|_X = \frac{1}{2}\,\|x_k - \bar{x}\|_X \,.$$

Consequently, if $\|x_0 - \bar{x}\|_X < \delta$ then $x_k \in B_\delta(\bar{x})$, $\forall k \geq 1$, and

$$\lim_{k\to\infty} \|x_k - \bar{x}\|_X = 0.$$

Moreover, from (29) and the Newton differentiability, we get that

$$\lim_{k\to\infty} \frac{\|x_{k+1} - \bar{x}\|_X}{\|x_k - \bar{x}\|_X} \leq \lim_{k\to\infty} C\frac{\|F(x_k) - F(\bar{x}) - G(x_k)(x_k - \bar{x})\|_Z}{\|x_k - \bar{x}\|_X} = 0.$$

# SSN update

In the case of our semilinear optimality system, the semismooth Newton update looks as follows:

$$
\begin{aligned}
-\Delta\delta_y + 3y^2\delta_y - \delta_u &= \Delta y - y^3 + u \\
\delta_y|_\Gamma &= 0 \\
-\Delta\delta_p + 3y^2\,\delta_p + 6y\,p\,\delta_y - \delta_y &= \Delta p - 3y^2\,p + y - z_d \\
\delta_p|_\Gamma &= 0 \\
\alpha\delta_u + \delta_p + \delta_{\lambda_b} &= -\alpha u - p - \lambda_b \\
\delta_\lambda - \chi_{\mathcal{A}}(\delta_\lambda + \alpha\delta_u) &= -\lambda_b + \max(0, \lambda_b + \alpha(u-b))
\end{aligned}
$$

where $\chi_{\mathcal{A}}$ stand for the indicator function of the active set $\mathcal{A} := \{x : \lambda_b + \alpha(u-b) \geq 0\}$.

**Semismooth Newton update**

$y_{n+1} = y_n + \delta_y, \quad p_{n+1} = p_n + \delta_p, \quad u_{n+1} = u_n + \delta_u, \quad \lambda_{n+1} = \lambda_n + \delta_\lambda.$

# Further topics



## Theory

- Problems with pointwise state or pointwise mixed control-state constraints
- Problems constrained by partical differential inclusions (variational inequalities)
- Problems involving sparsity inducing terms in the cost functional

## Numerics

- Discretization methods and error estimates for the numerical approximation of PDE-constrained optimization problems and/or optimality systems
- Efficient solution of sparse PDE-constrained optimization problems
- Reduced space methods for solving PDE-constrained optimization problems Lecture by Todd Munson

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