OPTIMAL DESIGN OF STRUCTURES (MAP 562)

CHAPTER VI

GEOMETRIC OPTIMIZATION (first part)

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Academic year 2019-2020

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Geometric optimization of a membrane

A membrane is occupying a variable domain Ω in $\mathbb{R}^N$ with boundary

$$\partial\Omega = \Gamma \cup \Gamma_N \cup \Gamma_D,$$

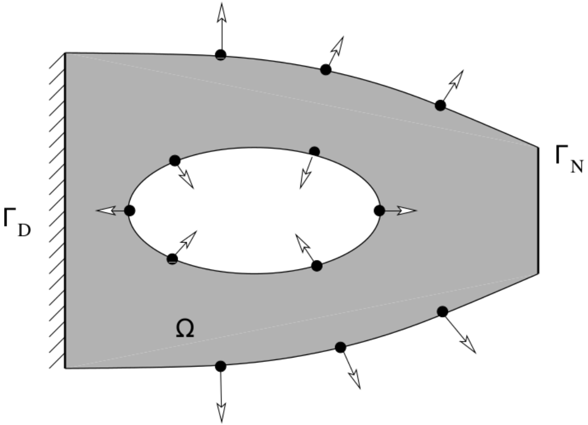
where

- $\Gamma \neq \emptyset$ is the variable part of the boundary,
- $\Gamma_D \neq \emptyset$ is a fixed part of the boundary where the membrane is clamped,
- $\Gamma_N \neq \emptyset$ is another fixed part of the boundary where the loads $g \in L^2(\Gamma_N)$ are applied.

$$\begin{cases} -\Delta u = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} = g & \text{on } \Gamma_N \\ \frac{\partial u}{\partial n} = 0 & \text{on } \Gamma \end{cases}$$

(No surface load for simplicity)

Boundary variation in geometric optimization



Shape optimization of a membrane

Geometric optimization problem:

$$\inf_{\Omega \in \mathcal{U}_{ad}} J(\Omega).$$

We must define the set of admissible shapes $\mathcal{U}_{ad}$. That is a major difficulty.

Examples:

- Compliance or work done by the load (rigidity measure)

$$J(\Omega) = \int_{\Gamma_N} gu \, ds$$

- Least square criterion for a target displacement $u_0 \in L^2(\Omega)$

$$J(\Omega) = \int_{\Omega} |u - u_0|^2 dx$$

where u depends on Ω through the state equation.

Existence results

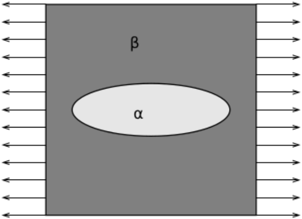
In full generality, there does not exist any optimal shape !

- Existence under a geometric constraint (e.g. uniforme cone property, perimeter constraint).
- Existence under a topological constraint (e.g. number of holes).
- Existence under a regularity constraint (e.g. proximity to a given shape).
- Counter-example in the absence of these conditions.

Related questions:

- How to set the problem ? How to parametrize shapes ?
- Calculus of variations for shapes.
- Mathematical framework for establishing numerical algorithms.

Counter-example of existence



Let $D =]0;1[\times]0;L[$ be a rectangle in $\mathbb{R}^2$. We fill D with a mixture of two materials, homogeneous isotropic, characterized by an elasticity coefficient β for the strong material, and α for the weak material (almost like void) with $\beta >> \alpha > 0$. We denote by $\chi(x) \in \{0,1\}$ the **characteristic function** of the weak phase α, and we define

$$a_\chi(x) = \alpha\chi(x) + \beta(1 - \chi(x)).$$

(Other possible interpretation: variable thickness which can take only two values.)

State equation:

$$\left\{ \begin{array}{ll} -\operatorname{div}\left(a_\chi \nabla u_\chi\right) = 0 & \text{in } D \\ a_\chi \nabla u_\chi \cdot n = e_1 \cdot n & \text{on } \partial D \end{array} \right.$$

The (vertical) load leads to horizontal traction.

Objective function: compliance

$$J(\chi) = \int_{\partial D} (e_1 \cdot n) u_\chi ds$$

Admissible set: **no geometric or smoothness constraint, i.e.** $\chi \in L^\infty(D; \{0,1\})$. There is however a volume constraint

$$\mathcal{U}_{ad} = \left\{ \chi \in L^\infty\left(D; \{0,1\}\right) \text{ such that } \frac{1}{|D|} \int_D \chi(x)\, dx = \theta \right\},$$

otherwise the strong phase would always be preferred !

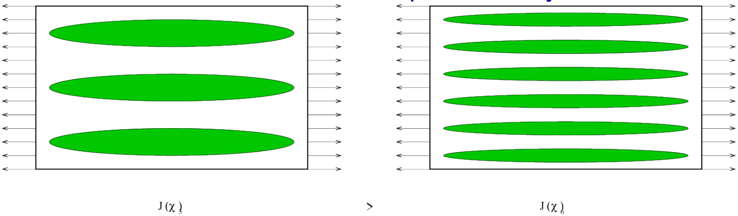
The shape optimization problem is:

$$\inf_{\chi \in \mathcal{U}_{ad}} J(\chi).$$

Non-existence

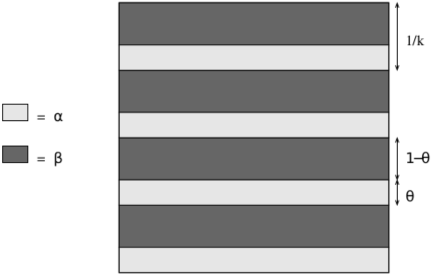
Proposition If $0 < \theta < 1$, there does not exist an optimal shape in the set $\mathcal{U}_{ad}$.

Remark. Cause of non-existence = lack of geometric or smoothness constraint on the shape boundary.



Many small holes are better than just a few bigger holes !

Mechanical intuition



Minimizing sequence $k \to +\infty$: k rigid fibers, aligned in the principal stress e_1, and uniformly distributed. To achieve a uniform deformation, the fibers must be finer and finer and alternate more and more weak and strong ones.
This is the main idea of a minimizing sequence which never achieves the minimum.

Existence under a regularity condition

Mathematical framework for shape deformation based on diffeomorphisms applied to a reference domain Ω_0 (useful to compute a gradient too).

A space of diffeomorphisms (or smooth one-to-one map) in $\mathbb{R}^N$

$$\mathcal{T} = \left\{ T \text{ such that } (T - \mathrm{Id}) \text{ and } (T^{-1} - \mathrm{Id}) \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N) \right\}.$$

(They are perturbations of the identity Id: $x \to x$.)

Definition of $W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Space of Lipschitz vectors fields:

$$\phi : \begin{cases} \mathbb{R}^N & \to & \mathbb{R}^N \\ x & \to & \phi(x) \end{cases}$$

$$\|\phi\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} = \sup_{x \in \mathbb{R}^N} \left(|\phi(x)|_{\mathbb{R}^N} + |\nabla\phi(x)|_{\mathbb{R}^{N\times N}} \right) < \infty$$

Remark: ϕ is continuous but its gradient is jut bounded. Actually, one can replace $W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$ by $C^1_b(\mathbb{R}^N; \mathbb{R}^N)$.

Space of admissible shapes

Let Ω_0 be a reference smooth open set.

$$\mathcal{C}(\Omega_0) = \{\Omega \text{ such that there exists } T \in \mathcal{T}, \Omega = T(\Omega_0)\} .$$

- Each shape Ω is parametrized by a diffeomorphism T (not unique !).
- All admissible shapes have the same topology.
- We define a pseudo-distance on $\mathcal{D}(\Omega_0)$

$$d(\Omega_1, \Omega_2) = \inf_{T \in \mathcal{T} \,|\, T(\Omega_1) = \Omega_2} \left(\| T - \mathrm{Id} \| + \| T^{-1} - \mathrm{Id} \| \right)_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} .$$

- If Ω_0 is bounded, it is possible to use $C^1(\mathbb{R}^N;\mathbb{R}^N)$ instead of $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Existence theory

Space of admissible shapes

$$\mathcal{U}_{ad} = \left\{ \Omega \in \mathcal{C}(\Omega_0) \text{ such that } \Gamma_D \bigcup \Gamma_N \subset \partial\Omega \text{ and } |\Omega| = V_0 \right\}.$$

For a fixed constant $R > 0$, we introduce the smooth subspace

$$\mathcal{U}_{ad}^{reg} = \{ \Omega \in \mathcal{U}_{ad} \text{ such that } d(\Omega, \Omega_0) \leq R, \ \} .$$

Interpretation: in practice, it is a "feasability" constraint.
Theorem. The shape optimization problem

$$\inf_{\Omega \in \mathcal{U}_{ad}^{reg}} J(\Omega)$$

admits at least one optimal solution.
Remark. All shapes share the same topology in $\mathcal{U}_{ad}$. Furthermore, the shape boundaries in $\mathcal{U}_{ad}^{reg}$ cannot oscillate too much.

Shape differentiation

Goal: to compute a derivative of $J(\Omega)$ by using the parametrization based on diffeomorphisms T.
We restrict ourselves to diffeomorphisms of the type

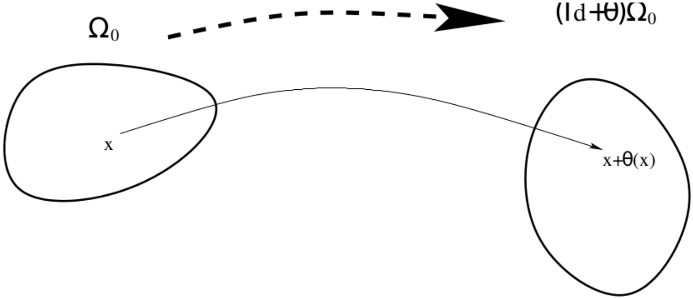
$$T = \mathrm{Id} + \theta \quad \text{with} \quad \theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N).$$

Idea: we differentiate $\theta \to J\big((\mathrm{Id}+\theta)\Omega_0\big)$ at 0.

Remark. This approach generalizes the Hadamard method of boundary shape variations along the normal: $\Omega_0 \to \Omega_t$ for $t \geq 0$

$$\partial\Omega_t = \Big\{ x_t \in \mathbb{R}^N \mid \exists x_0 \in \partial\Omega_0 \mid x_t = x_0 + t\, g(x_0)\, n(x_0) \Big\}$$

with a given incremental function g.



The shape $\Omega = (\mathrm{Id} + \theta)(\Omega_0)$ is defined by

$$\Omega = \{x + \theta(x) \mid x \in \Omega_0\}\,.$$

Thus $\theta(x)$ is a vector field which plays the role of the **displacement** of the reference domain Ω_0.

Lemma. For any $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ satisfying $\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} < 1$, the map $T = \mathrm{Id} + \theta$ is one-to-one into $\mathbb{R}^N$ and belongs to the set $\mathcal{T}$.

Proof. Based on the formula

$$\theta(x) - \theta(y) = \int_0^1 (x-y) \cdot \nabla\theta\big(y + t(x-y)\big)\, dt\,,$$

we deduce that $\mid \theta(x) - \theta(y) \mid \leq \|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} \mid x - y \mid$ and θ is a strict contraction. Thus, $T = \mathrm{Id} + \theta$ is one-to-one into $\mathbb{R}^N$.

Indeed, $\forall b \in \mathbb{R}^N$ the map $K(x) = b - \theta(x)$ is a contraction and thus admits a unique fixed point y, i.e., $b = T(y)$ and T is therefore one-to-one into $\mathbb{R}^N$.

Since $\nabla T(x) = I + \nabla\theta(x)$ and $|\nabla\theta(x)| < 1$, the matrix $\nabla T(x)$ is invertible (Neumann series). We then check that

$$|T^{-1}(b) - b| = |y - b| = |\theta(y)| \leq \|\theta\|_{L^\infty}\,,$$

$$|I-(\nabla T)^{-1}(x)| = |I-(I+\nabla\theta(x))^{-1}| = |\sum_{k=1}^{\infty}(-\nabla\theta(x))^k| \leq \frac{\|\nabla\theta\|_{L_\infty}}{1 - \|\nabla\theta\|_{L_\infty}},$$

hence $(T^{-1} - \mathrm{Id}) \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Definition of the shape derivative

Definition. Let $J(\Omega)$ be a map from the set of admissible shapes $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$. We say that J is shape differentiable at Ω_0 if the function

$$\theta \to J\big((\,\mathrm{Id} + \theta)(\Omega_0)\big)$$

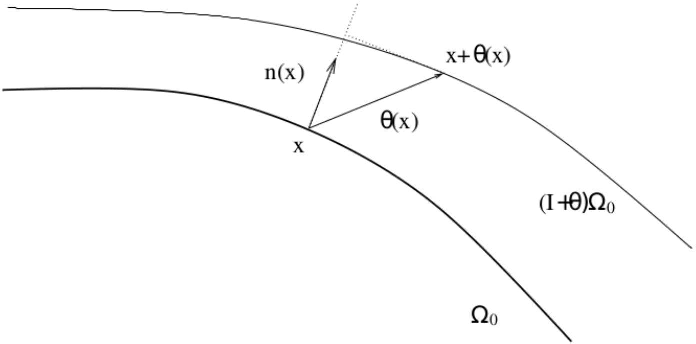
is Fréchet differentiable at 0 in the Banach space $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$, i.e., there exists a linear continuous functional $L = J'(\Omega_0)$ on $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ such that

$$J\big((\,\mathrm{Id}+\theta)(\Omega_0)\big) = J(\Omega_0) + L(\theta) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta\to 0} \frac{|o(\theta)|}{\|\theta\|} = 0\ .$$

$J'(\Omega_0)$ is called the shape derivative and $J'(\Omega_0)(\theta)$ is a directional derivative.

The directional derivative $J'(\Omega_0)(\theta)$ depends only on the **normal component of θ on the boundary** of Ω_0.
This property is linked to the fact that the internal variations of the field θ do not change the shape Ω, i.e.,

$$\theta \in C_c^1(\Omega)^N \text{ and } \|\theta\| << 1 \ \Rightarrow (\mathrm{Id} + \theta)\Omega = \Omega.$$



Proposition. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$. Let J be a differentiable map at Ω_0 from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$. Its directional derivative $J'(\Omega_0)(\theta)$ depends only on the normal trace on the boundary of θ, i.e.

$$J'(\Omega_0)(\theta_1) = J'(\Omega_0)(\theta_2)$$

whenever $\theta_1, \theta_2 \in C^1(\mathbb{R}^N; \mathbb{R}^N)$ satisfy

$$\theta_1 \cdot n = \theta_2 \cdot n \quad \text{on } \partial\Omega_0.$$

Proof. Take $\theta = \theta_2 - \theta_1$ and, for fixed x, introduce the solution $t \mapsto \phi(t, x, \theta)$ of

$$\begin{cases} \frac{dy}{dt}(t) = \theta\big(y(t)\big) \\ y(0) = x \end{cases}$$

which satisfies

$$\phi(t + t', x, \theta) = \phi(t, \phi(t', x, \theta), \theta) \quad \text{for any } t, t' \in \mathbb{R} \qquad (a)$$
$$\phi(\lambda t, x, \theta) = \phi(t, x, \lambda\theta) \quad \text{for any } \lambda \in \mathbb{R}. \qquad (b)$$

Then we define the one-to-one map from $\mathbb{R}^N$ into $\mathbb{R}^N$, $x \;\rightarrow\; e^{\theta}(x) := \phi(1, x, \theta)$, the inverse of which is $e^{-\theta}$ by (a). Moreover $e^0 = \mathrm{Id}$ and $t \rightarrow e^{t\theta}(x)$ is the solution of the o.d.e. by (b).

Lemma. Let $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ be such that $\theta \cdot n = 0$ on $\partial\Omega_0$. Then $e^{t\theta}(\Omega_0) = \Omega_0$ for all $t \in \mathbb{R}$.

Proof (by contradiction). Assume $\exists x \in \Omega_0$ such that the trajectory $\phi(t,x,\theta)$ escapes from Ω_0 (or conversely). Thus $\exists t_0 > 0$ such that $x_0 = \phi(t_0,x,\theta) \in \partial\Omega_0$.
Locally the boundary $\partial\Omega_0$ is parametrized by an equation $\psi(x) = 0$ and the normal is $n = n_0/|n_0|$ with $n_0 = \nabla\psi$ (defined around $\partial\Omega_0$).
In the vicinity of $\partial\Omega_0$, we modify the vector field as $\tilde{\theta} = \theta - (\theta \cdot n)n$ to obtain a trajectory $\phi(t,x_0,\tilde{\theta})$ such that, for any $t \geq t_0$,

$$\frac{d}{dt}\Big(\psi(\phi(t,x_0,\tilde{\theta}))\Big) = (\nabla\psi \cdot \tilde{\theta})(\phi(t,x_0,\tilde{\theta}) = (\tilde{\theta} \cdot n|n_0|)(\phi(t,x_0,\tilde{\theta})) = 0.$$

Since $\psi(\phi(t_0,x_0,\tilde{\theta})) = 0$, we deduce $\psi(\phi(t,x_0,\tilde{\theta})) = 0$, i.e., the trajectory stays on $\partial\Omega_0$. Since $\theta \cdot n = 0$ on $\partial\Omega_0$, $\phi(.,x_0,\tilde{\theta})$ is **also** a trajectory for the vector field θ. Uniqueness of the o.d.e. solution yields $\phi(t,x_0,\tilde{\theta}) = \phi(t,x_0,\theta) \in \partial\Omega_0$ for any t which is a contradiction with $x \in \Omega_0$.

Remark. The crucial point is that θ is tangent to the boundary $\partial\Omega_0$.

Proof of the proposition

Since $e^{t\theta}(\Omega_0) = \Omega_0$ for any $t \in \mathbb{R}$, the function J is constant along this path and

$$\frac{d}{dt} J\big(e^{t\theta}(\Omega_0)\big)(0) = 0.$$

By the chain rule we deduce

$$0 = \frac{d}{dt} J\big(e^{t\theta}(\Omega_0)\big)(0) = J'(\Omega_0)\left(\frac{de^{t\theta}}{dt}\right)(0) = J'(\Omega_0)\,(\theta)\,,$$

because the path $e^{t\theta}(x)$ satisfies

$$\frac{de^{t\theta}(x)}{dt}(0) = \theta(x).$$

Review of known formulas

To compute shape derivatives we need to recall how to change variables in integrals.

Lemma. Let Ω_0 be an open set of $\mathbb{R}^N$. Let $T \in \mathcal{T}$ be a diffeomorphism and $1 \leq p \leq +\infty$. Then $f \in L^p\big(T(\Omega_0)\big)$ if and only if $f \circ T \in L^p(\Omega_0)$, and

$$\int_{T(\Omega_0)} f \, dx = \int_{\Omega_0} f \circ T \mid \det \nabla T \mid dx$$

$$\int_{T(\Omega_0)} f \mid \det(\nabla T)^{-1} \mid dx = \int_{\Omega_0} f \circ T \, dx.$$

Moreover, $f \in W^{1,p}\big(T(\Omega_0)\big)$ if and only if $f \circ T \in W^{1,p}(\Omega_0)$, and

$$\big(\nabla f\big) \circ T = \big((\nabla T)^{-1}\big)^t \, \nabla(f \circ T).$$

(^{t} = adjoint or transposed matrix)

Remark. This latter formula stems from

$$\nabla(f \circ T)(x) \cdot h = \nabla f\big(T(x)\big) \cdot \big(\nabla T(x) h\big).$$

Change of variables in a boundary integral.

Lemma. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$. Let $T \in \mathcal{T} \cap C^1(\mathbb{R}^N; \mathbb{R}^N)$ be a diffeomorphism and $f \in L^1\big(\partial T(\Omega_0)\big)$. Then $f \circ T \in L^1(\partial\Omega_0)$, and we have

$$\int_{\partial T(\Omega_0)} f \, ds = \int_{\partial\Omega_0} f \circ T \mid \det \nabla T \mid \; \left| \left((\nabla T)^{-1}\right)^t n \right|_{\mathbb{R}^N} ds,$$

where n is the exterior unit normal to $\partial\Omega_0$ and $|\cdot|_{\mathbb{R}^N}$ is the Euclidean norm.

Examples of shape derivatives

Proposition. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$, $f(x) \in W^{1,1}(\mathbb{R}^N)$ and J the map from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$ defined by

$$J(\Omega) = \int_\Omega f(x)\,dx.$$

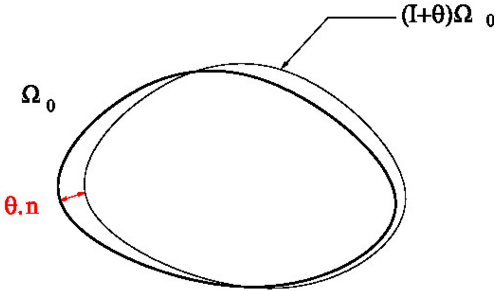
Then J is shape differentiable at Ω_0 and

$$\boxed{J'(\Omega_0)(\theta) = \int_{\Omega_0} \operatorname{div}\big(\theta(x)\,f(x)\big)\,dx = \int_{\partial\Omega_0} \theta(x)\cdot n(x)\,f(x)\,ds}$$

for any $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$.

Remark. To make sure the result is right, the safest way (but not the easiest) is to make a change of variables to get back to the reference domain Ω_0.

Intuitive proof



Surface shifted by the transformation: the difference between $(\mathrm{Id} + \theta)\Omega_0$ and Ω_0 is close to $\partial\Omega_0$ thickened by $\theta \cdot n$. Thus

$$\int_{(\mathrm{Id}+\theta)\Omega_0} f(x)\, dx \approx \int_{\Omega_0} f(x)\, dx + \int_{\partial\Omega_0} f(x)\theta \cdot n\, ds.$$

Proof. We rewrite $J(\Omega)$ as an integral on the reference domain Ω_0

$$J\big((\,\mathrm{Id}+\theta)\Omega_0\big) = \int_{\Omega_0} f \circ (\,\mathrm{Id}+\theta) \mid \det(I+\nabla\theta) \mid dx.$$

The functional $\theta \to \det(I+\nabla\theta)$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^\infty(\mathbb{R}^N)$ because

$$\det(I+\nabla\theta) = \det I + \mathrm{div}\theta + o(\theta) \quad \text{with} \quad \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^\infty(\mathbb{R}^N;\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

On the other hand, if $f(x) \in W^{1,1}(\mathbb{R}^N)$, the functional $\theta \to f \circ (\,\mathrm{Id}+\theta)$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^1(\mathbb{R}^N)$ because

$$f \circ (\,\mathrm{Id}+\theta)(x) = f(x) + \nabla f(x)\cdot\theta(x) + o(\theta) \quad \text{with} \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^1(\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

By product of these two expansions we obtain the result.

Proposition. Let Ω_0 be a smooth bounded open set of $\mathbb{R}^N$, $f(x) \in W^{2,1}(\mathbb{R}^N)$ and J the map from $\mathcal{C}(\Omega_0)$ into $\mathbb{R}$ defined by

$$J(\Omega) = \int_{\partial\Omega} f(x)\, ds.$$

Then J is shape differentiable at Ω_0 and

$$\boxed{J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \big(\nabla f \cdot \theta + f\big(\,\mathrm{div}\theta - \nabla\theta n \cdot n\big)\big)\, ds}$$

for any $\theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. By a (boundary) integration by parts this formula is equivalent to

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \left(\frac{\partial f}{\partial n} + Hf\right) ds,$$

where H is the mean curvature of $\partial\Omega_0$ defined by $H = \,\mathrm{div} n$.

Interpretation

Two simple examples:

- If $\partial\Omega_0$ is an hyperplane, then $H = 0$ and the variation of the boundary integral is proportional to the normal derivative of f.
- If $f \equiv 1$, then $J(\Omega)$ is the perimeter (in 2-D) or the surface (in 3-D) of the domain Ω and its variation is proportional to the mean curvature.

Proof. A change of variable yields

$$J\big((\mathrm{Id}+\theta)\Omega_0\big) = \int_{\partial\Omega_0} f\circ(\mathrm{Id}+\theta)|\det(I+\nabla\theta)|\ \left|\ (I+\nabla\theta)^{-t}\, n\ \right|_{\mathbb{R}^N} ds.$$

We already proved that $\theta \to \det(I+\nabla\theta)$ and $\theta \to f\circ(\mathrm{Id}+\theta)$ are differentiable.
Moreover, $\theta \to \big((I+\nabla\theta)^{-1}\big)^t\, n$ is differentiable from $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ into $L^\infty(\partial\Omega_0;\mathbb{R}^N)$ because

$$(I+\nabla\theta)^{-t}\, n = n-(\nabla\theta)^t n+o(\theta) \quad \text{with} \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^\infty(\partial\Omega_0;\mathbb{R}^N)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

By composition with $|y+h|_{\mathbb{R}^N} = |y|_{\mathbb{R}^N} + \frac{y\cdot h}{|y|_{\mathbb{R}^N}} + o(h)$ we infer

$$\left|\ (I+\nabla\theta)^{-t}\, n\ \right|_{\mathbb{R}^N} = 1-(\nabla\theta)^t n\cdot n+o(\theta) \text{ with} \lim_{\theta\to 0} \frac{\|o(\theta)\|_{L^\infty(\partial\Omega_0)}}{\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)}} = 0.$$

Multiplying these three expansions leads to the result.
The formula including the mean curvature is obtained by an integration by parts on the surface $\partial\Omega_0$ (delicate).

Derivation of a function depending on the shape

Let $u(\Omega, x)$ be a function depending (and defined) on the domain Ω.
For example $u(\Omega, x)$ could be the solution of a p.d.e. defined in Ω.
Computing the shape derivative of $u(\Omega, x)$ is difficult !

- The function $u(\Omega, x)$ may belong to a Sobolev space, $H^1(\Omega)$, $H^1_0(\Omega)$, which varies with Ω.
- How can we differentiate a boundary condition with respect to the domain ?
- The use of a variational formulation is crucial.

Two notions of derivative

1) Eulerian (or shape) derivative U

$$u((\mathrm{Id}+\theta)\Omega_0, x) = u(\Omega_0, x)+U(\theta, x)+o(\theta), \quad \text{with} \quad \lim_{\theta\to 0} \frac{\|o(\theta)\|}{\|\theta\|} = 0$$

OK if $x \in \Omega_0 \cap (\mathrm{Id}+\theta)\Omega_0$ (local definition, makes no sense on the boundary).

2) Lagrangian (or material) derivative Y

We define the **transported** function $\overline{u}$ by

$$\overline{u}(\theta, x) = u\Big((\mathrm{Id}+\theta)\Omega_0, x+\theta(x)\Big) \quad \forall\, x \in \Omega_0.$$

The Lagrangian derivative Y is obtained by differentiating $\overline{u}(\theta, x)$

$$\overline{u}(\theta, x) = \overline{u}(0, x) + Y(\theta, x) + o(\theta) \quad , \quad \text{with} \quad \lim_{\theta\to 0} \frac{\|o(\theta)\|}{\|\theta\|} = 0.$$

If we assume that both derivatives exist, then the chain rule yields

$$Y(\theta, x) = U(\theta, x) + \theta(x) \cdot \nabla u(\Omega_0, x).$$

The Eulerian derivative, although being simpler, is **very delicate to use** and often not rigorous. For example, if $u \in H_0^1(\Omega)$, the space of definition varies with Ω... Equivalently what boundary condition should the derivative satisfy ?

For the moment, we assume that the shape derivative $U = u'(\Omega)(\theta)$ exists. We use the Lagrangian method which does not require a precise formula for U !
Later on, we shall rigorously justify the existence of U and find its formula.

Fast derivation: the Lagrangian method

- One can avoid the computations of U or Y by a simple and fast (albeit formal) method, called the Lagrangian method (proposed in this context by J. Céa).
- The Lagrangian allows us to find the correct definition of the adjoint state too.
- It is easy for Neumann boundary conditions, a little more involved for Dirichlet ones.
- That is the method to be known !

Fast derivation for Neumann boundary conditions

If the objective function is

$$J(\Omega) = \int_\Omega j(u(\Omega))\,dx, \qquad \left\{ \begin{array}{l} -\Delta u + u = f \text{ in } \Omega \\ \partial_n u = g \text{ on } \partial\Omega \end{array} \right.$$

the Lagrangian is defined as the sum of J and of the variational formulation of the state equation

$$\mathcal{L}(\Omega, v, q) = \int_\Omega j(v)\,dx + \int_\Omega \Big(\nabla v \cdot \nabla q + vq - fq\Big)dx - \int_{\partial\Omega} gq\,ds,$$

with v and $q \in H^1(\mathbb{R}^N)$. It is important to notice that the space $H^1(\mathbb{R}^N)$ does not depend on Ω and thus the three variables in $\mathcal{L}$ are clearly independent.

The partial derivative of $\mathcal{L}$ with respect to q in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial q}(\Omega, v, q), \phi \rangle = \int_\Omega \Big(\nabla v \cdot \nabla \phi + v\phi - f\phi \Big) dx - \int_{\partial\Omega} g\phi \, ds,$$

which, upon equating to 0, gives the variational formulation of the state.

The partial derivative of $\mathcal{L}$ with respect to v in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial v}(\Omega, v, q), \phi \rangle = \int_\Omega j'(v)\phi \, dx + \int_\Omega \Big(\nabla \phi \cdot \nabla q + \phi q \Big) dx,$$

which, upon equating to 0, gives the variational formulation of the adjoint.

The partial derivative of $\mathcal{L}$ with respect to Ω in the direction θ is

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega, v, q)(\theta) = \int_{\partial\Omega} \theta \cdot n \Big(j(v) + \nabla v \cdot \nabla q + vq - fq - \frac{\partial (gq)}{\partial n} - Hgq \Big) ds.$$

When evaluating this derivative with the state $u(\Omega_0)$ and the adjoint $p(\Omega_0)$, we precisely find the derivative of the objective function:

$$\boxed{\frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, u(\Omega_0), p(\Omega_0)\Big)(\theta) = J'(\Omega_0)(\theta)}$$

Indeed, if we differentiate the equality

$$\mathcal{L}(\Omega, u(\Omega), q) = J(\Omega) \quad \forall\, q \in H^1(\mathbb{R}^N),$$

the chain rule yields

$$J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u(\Omega_0), q)(\theta) + \langle \frac{\partial \mathcal{L}}{\partial v}(\Omega_0, u(\Omega_0), q), u'(\Omega_0)(\theta)\rangle.$$

Taking $q = p(\Omega_0)$, the last term cancels since $p(\Omega_0)$ is the solution of the adjoint equation.
Thanks to this computation, the "correct" result can be guessed for $J'(\Omega_0)$ without using the notions of shape or material derivatives.
Nevertheless, in full rigor, this "fast" computation of the shape derivative $J'(\Omega_0)$ is valid only if we know that u is shape differentiable.

The compliance case (self-adjoint)

Theorem. The functional $J(\Omega) = \int_\Omega fu\,dx + \int_{\partial\Omega} gu\,ds$ is shape-differentiable

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \left(-|\nabla u(\Omega_0)|^2 - |u(\Omega_0)|^2 + 2u(\Omega_0)f\right) ds$$

$$+ \int_{\partial\Omega_0} \theta \cdot n \left(2\frac{\partial(gu(\Omega_0))}{\partial n} + 2Hgu(\Omega_0)\right) ds,$$

Interpretation: assume $f = 0$ and $g = 0$ where $\theta \cdot n \neq 0$. The formula simplifies as

$$J'(\Omega_0)(\theta) = -\int_{\partial\Omega_0} \theta \cdot n \left(|\nabla u|^2 + u^2\right) ds.$$

It is always advantageous to increase the domain (i.e., $\theta \cdot n > 0$) for decreasing the compliance.

Fast derivation for Dirichlet boundary conditions

It is more involved ! Let $u \in H_0^1(\Omega)$ be the solution of

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \phi \in H_0^1(\Omega).$$

The "usual" Lagrangian is

$$\mathcal{L}(\Omega, v, q) = \int_\Omega j(v) \, dx + \int_\Omega \Big(\nabla v \cdot \nabla q - fq \Big) dx,$$

for $v, q \in H_0^1(\Omega)$. The variables (Ω, v, q) are not independent !

Indeed, the functions v and q satisfy

$$v \;=\; q \;=\; 0 \quad \text{on } \partial\Omega.$$

Another Lagrangian has to be introduced.

Lagrangian for Dirichlet boundary conditions

The Dirichlet boundary condition is penalized

$$\mathcal{L}(\Omega, v, q, \lambda) = \int_\Omega j(v)\,dx - \int_\Omega (\Delta v + f) q\,dx + \int_{\partial\Omega} \lambda v\,ds$$

where λ is the Lagrange multiplier for the boundary condition. It is now possible to differentiate since the 4 variables v, q, λ defined on $\mathbb{R}^N$ are independent.

Of course, we recover

$$\sup_{q,\lambda} \mathcal{L}(\Omega, v, q, \lambda) = \begin{cases} \int_\Omega j(u)\,dx = J(\Omega) & \text{if } v \equiv u, \\ +\infty & \text{otherwise.} \end{cases}$$

By definition of the Lagrangian:
the partial derivative of $\mathcal{L}$ with respect to q in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial q}(\Omega, v, q, \lambda), \phi \rangle = - \int_\Omega \phi \Big(\Delta v + f \Big) dx,$$

which, upon equating to 0, gives the state equation,
the partial derivative of $\mathcal{L}$ with respect to λ in the direction $\phi \in H^1(\mathbb{R}^N)$ is

$$\langle \frac{\partial \mathcal{L}}{\partial \lambda}(\Omega, v, q, \lambda), \phi \rangle = \int_{\partial\Omega} \phi v \, dx,$$

which, upon equating to 0, gives the Dirichlet boundary condition for the state equation.

To compute the partial derivative of $\mathcal{L}$ with respect to v, we perform a first integration by parts

$$\mathcal{L}(\Omega, v, q, \lambda) = \int_\Omega j(v)\, dx + \int_\Omega (\nabla v \cdot \nabla q - fq)\, dx + \int_{\partial\Omega} \left(\lambda v - \frac{\partial v}{\partial n} q \right) ds,$$

then a second integration by parts

$$\mathcal{L}(\Omega, v, q, \lambda) = \int_\Omega j(v)\, dx - \int_\Omega (v\Delta q - fq)\, dx + \int_{\partial\Omega} \left(\lambda v - \frac{\partial v}{\partial n} q + \frac{\partial q}{\partial n} v \right) ds.$$

We now differentiate in the direction $\phi \in H^1(\mathbb{R}^N)$

$$\langle \frac{\partial \mathcal{L}}{\partial v}(\Omega, v, q), \phi \rangle = \int_\Omega j'(v)\phi\, dx - \int_\Omega \phi \Delta q\, dx + \int_{\partial\Omega} \left(-q \frac{\partial \phi}{\partial n} + \phi \left(\lambda + \frac{\partial q}{\partial n} \right) \right) ds$$

which, upon equating to 0, gives three relationships, the first two ones being the adjoint problem.

1. If ϕ has compact support in Ω_0, we get

$$-\Delta p = -j'(u) \quad \text{in} \quad \Omega_0.$$

2. If $\phi = 0$ on $\partial\Omega_0$ with any value of $\frac{\partial \phi}{\partial n}$ in $L^2(\partial\Omega_0)$, we deduce

$$p = 0 \quad \text{on} \quad \partial\Omega_0.$$

3. If ϕ is now varying in the full $H^1(\Omega_0)$, we find

$$\frac{\partial p}{\partial n} + \lambda = 0 \quad \text{on} \quad \partial\Omega_0.$$

The adjoint problem has actually been recovered but furthermore the optimal Lagrange multiplier λ has been characterized.

Eventually, the partial shape derivative is

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u, p, \lambda)(\theta) = \int_{\partial \Omega_0} \theta \cdot n \Big(j(u) - (\Delta u + f) p + \frac{\partial (u\lambda)}{\partial n} + H u \lambda \Big) ds.$$

Knowing that $u = p = 0$ on $\partial \Omega_0$ and $\lambda = -\frac{\partial p}{\partial n}$ we deduce

$$\frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u, p, \lambda)(\theta) = \int_{\partial \Omega_0} \theta \cdot n \Big(j(0) - \frac{\partial u}{\partial n} \frac{\partial p}{\partial n} \Big) ds = J'(\Omega_0)(\theta).$$

$$\boxed{J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}\Big(\Omega_0, u(\Omega_0), p(\Omega_0)\Big)(\theta)}$$

Indeed, differentiating

$$\mathcal{L}(\Omega, u(\Omega), q, \lambda) = J(\Omega) \quad \forall q, \lambda$$

yields

$$J'(\Omega_0)(\theta) = \frac{\partial \mathcal{L}}{\partial \Omega}(\Omega_0, u(\Omega_0), q, \lambda)(\theta) + \langle \frac{\partial \mathcal{L}}{\partial v}(\Omega_0, u(\Omega_0), q, \lambda), u'(\Omega_0)(\theta)\rangle.$$

Then, taking $q = p(\Omega_0)$ (the adjoint state) and $\lambda = -\frac{\partial p}{\partial n}(\Omega_0)$, the last term cancels and we obtain the desired formula.

Application to compliance minimization

We minimize $J(\Omega) = \int_\Omega f u \, dx$ with $u \in H^1_0(\Omega)$ solution of

$$\int_\Omega \nabla u \cdot \nabla \phi \, dx = \int_\Omega f \phi \, dx \quad \forall \phi \in H^1_0(\Omega).$$

The adjoint state is just $p = -u$. The shape derivative is

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta \cdot n \Big(f u - \frac{\partial u}{\partial n} \frac{\partial p}{\partial n} \Big) ds = \int_{\partial\Omega_0} \theta \cdot n \left(\frac{\partial u}{\partial n} \right)^2 ds.$$

It is always advantageous to shrink the domain (i.e., $\theta \cdot n < 0$) to decrease the compliance.

This is the opposite conclusion compared to Neumann b.c., but it is logical !