An introduction to shape and topology optimization

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Part VI

Topological derivatives

Topological derivatives (I)

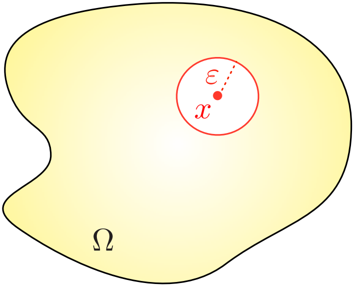
- The algorithms that we have seen during the previous lectures feature an update process of shapes by deformation of their boundary.
- In the mathematical framework, the shapes produced during the process are all homeomorphic to one another; in particular, they must have the same topology.
- With a little abuse of the mathematical theory (depending on the numerical representation), it is possible that holes merge during the process.
- However, holes cannot spring up inside the bulk of the shape.
- This may be enabled by topological derivative, which measure the dependence of a function $J(\Omega)$ with respect to the nucleation of a small hole inside Ω.

Topological derivatives (II)

Topological derivatives appraise variations of a domain Ω of the form:

$$\Omega_{x,\varepsilon} := \Omega \setminus \overline{B(x,\varepsilon)},$$

where $B(x,\varepsilon)$ is the open ball centered at $x \in \Omega$ with radius ε.



Definition 1.

A functional $J(\Omega)$ of the domain has a topological derivative at a point $x \in \Omega$ if there exists $g_\Omega^T(x) \in \mathbb{R}$ such that the following asymptotic expansion holds at $\varepsilon = 0$:

$$J(\Omega_{x,\varepsilon}) = J(\Omega) + \varepsilon^d g_\Omega^T(x) + \mathrm{o}(\varepsilon^d), \text{ where } \frac{|\mathrm{o}(\varepsilon^d)|}{\varepsilon^d} \xrightarrow{\varepsilon \to 0} 0.$$

Topological derivatives (III)

- *Intuition:* The value of $J(\Omega)$ decreases if a "small" hole, centered at some point x where $g_\Omega^T(x) < 0$, is nucleated inside Ω.

- The mathematical calculation of topological derivatives is difficult. Fortunately, explicit formulas have been achieved in many situations; see e.g. [Am, NoSo].

- The information contained in topological derivatives can be employed for shape and topology optimization purposes in at least two ways:

  1. It can be naturally coupled with shape derivative based algorithms: for instance, at every n_{top} iteration, a small hole is nucleated inside the shape Ω^n instead of modifying its boundary.
  2. It can be used as the standalone ingredient of a fixed point algorithm, enforcing the optimality conditions of the optimization problem as expressed in the language of topological derivatives.

Part IV

Topological derivatives

Model setting: the "background" equation (I)

- We analyze *formally* the conductivity equation, in a bounded domain $D \subset \mathbb{R}^d$, whose boundary reads:

$$\partial D = \overline{\Gamma_D} \cup \overline{\Gamma_N}.$$

- The "background" potential u_0 belongs to the space:

$$H^1_{\Gamma_D}(D) := \left\{ u \in H^1(D),\ \ u = 0 \text{ on } D \right\};$$

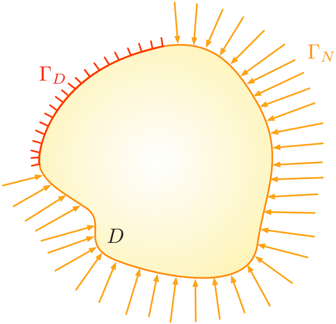
  it is the unique solution to the equation:

$$\begin{cases} -\text{div}(\gamma_0 \nabla u_0) = f & \text{in } D, \\ u_0 = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_0}{\partial n} = g & \text{on } \Gamma_N, \end{cases}$$

  with

  - Smooth data $f : D \to \mathbb{R}$ and $g : \Gamma_N \to \mathbb{R}$;
  - A smooth, elliptic conductivity $\gamma_0 \in \mathcal{C}^\infty(\overline{D})$:

$$\forall x \in D,\ \ 0 < \gamma_- \leq \gamma_0(x) \leq \gamma_+.$$



Model setting: the "background" equation (II)

- The variational formulation for $u_0 \in H^1_{\Gamma_D}(D)$ reads:

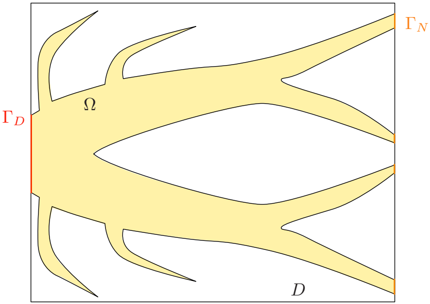
$$\forall v \in H^1_{\Gamma_D}(D), \int_D \gamma_0(x) \nabla u_0 \cdot \nabla v \, \mathrm{d}x = \int_D f v \, \mathrm{d}x + \int_{\Gamma_N} g v \, \mathrm{d}s.$$

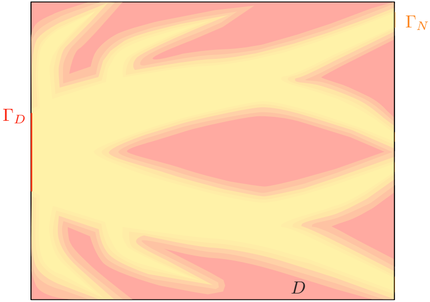
- Owing to elliptic regularity, u_0 is smooth on any open set $V \Subset D$ [Bre].

- Roughly speaking, u_0 is smooth everywhere, except near the region $\overline{\Gamma_D} \cap \overline{\Gamma_N}$ where boundary conditions are changing types.

Model setting: the "background" equation (III)

Up to an adapted choice of γ_0, this framework mimicks the one-phase and void conductivity equation, thanks to the ersatz material approximation.





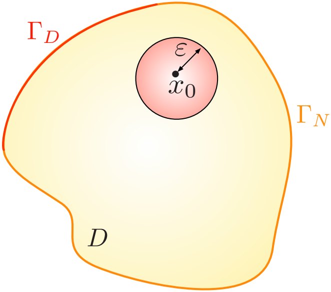
$$\begin{cases} -\mathrm{div}(\gamma \nabla u) = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u}{\partial n} = g & \text{on } \Gamma_N, \\ \gamma \frac{\partial u}{\partial n} = 0 & \text{on } \partial\Omega \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}). \end{cases}$$

$$\begin{cases} -\mathrm{div}(\gamma_\eta \nabla u_\eta) = f & \text{in } D, \\ u_\eta = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_\eta}{\partial n} = g & \text{on } \Gamma_N, \\ \gamma \frac{\partial u_\eta}{\partial n} = 0 & \text{on } \partial D \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}), \end{cases}$$

$$\gamma_\eta(x) = \text{(smoothed)} \begin{cases} \gamma(x) & \text{if } x \in \Omega, \\ \eta\gamma(x) & \text{if } x \in D \setminus \Omega. \end{cases}$$

Model setting: the perturbed equation

In the perturbed situation, a small hole $B(x_0, \varepsilon)$ is filled with another material $\gamma_1(x)$.



- The perturbed conductivity equation is:

$$\begin{cases} -\mathrm{div}(\gamma_\varepsilon \nabla u_\varepsilon) = f & \text{in } D, \\ u_\varepsilon = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_\varepsilon}{\partial n} = g & \text{on } \Gamma_N, \end{cases}$$

where

$$\gamma_\varepsilon(x) = \begin{cases} \gamma_0(x) & \text{if } x \in D \setminus B(x_0, \varepsilon), \\ \gamma_1(x) & \text{if } x \in B(x_0, \varepsilon), \end{cases}$$

and $\gamma_1(x)$ is also smooth and elliptic.

- The variational formulation for the perturbed potential $u_\varepsilon \in H^1_{\Gamma_D}(D)$ reads:

$$\forall v \in H^1_{\Gamma_D}(D), \int_D \gamma_\varepsilon(x) \nabla u_\varepsilon \cdot \nabla v \, \mathrm{d}x = \int_D fv \, \mathrm{d}x + \int_{\Gamma_N} gv \, \mathrm{d}s.$$

Goal and plan of the study (I)

- We consider an objective functional of the form:

$$J(\varepsilon) = \int_D j(u_\varepsilon)\,\mathrm{d}x,$$

for a smooth function $j : \mathbb{R} \to \mathbb{R}$, satisfying adequate growth conditions.

- We seek an asymptotic expansion of $J(\varepsilon)$:

$$J(\varepsilon) = J(0) + \varepsilon^d J'(0) + \mathrm{o}(\varepsilon^d),$$

where

  - The 0^{th} order term

$$J(0) = \int_D j(u_0)\,\mathrm{d}x$$

is the performance of the background situation;

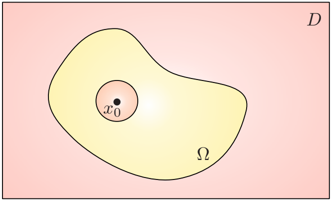
  - The first non trivial term $J'(0)$ indicates whether the background situation is improved if the properties γ_0 are replaced by γ_1 inside the small hole $B(x_0, \varepsilon)$.

Goal and plan of the study (II)

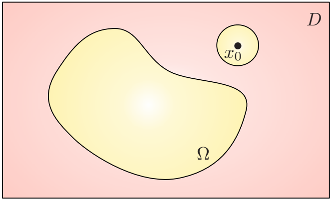
Suppose that the background equation formally approximates a situation featuring one phase Ω and "void" in $D \setminus \Omega$ via the ersatz material approximation, i.e.

$$\gamma_0(x) \text{ is of the form } \gamma_0(x) = \begin{cases} \gamma & \text{if } x \in \Omega, \\ \eta\gamma & \text{if } x \in D \setminus \Omega, \end{cases} \quad \text{for some } \eta \ll 1.$$

- *If $x_0 \in \Omega$ and $\gamma_1(x) = \eta\gamma$*, $J'(0)$ measures the sensitivity of $J(\Omega)$ with respect to the nucleation of a small "hole" inside Ω.



- *If $x_0 \in D \setminus \overline{\Omega}$ and $\gamma_1(x) = \gamma$*, $J'(0)$ measures the sensitivity of $J(\Omega)$ to the addition of a small "bubble" to Ω.



Goal and plan of the study (III)

The desired expansion of $J(\varepsilon)$ is obtained within three steps:

1. We search for the asymptotic expansion of the potential u_ε:

$$u_\varepsilon(x) = u_0(x) + \varepsilon^d u_1(x) + \mathrm{o}(\varepsilon^d), \text{ for } x \in D \setminus \{x_0\},$$

   where

   - $u_0(x)$ is the solution to the background equation;
   - The decay rate ε^d is dictated by the measure of the ball $B(0, \varepsilon)$;
   - $u_1(x)$ measures the sensitivity of the potential to a variation $\gamma_0 \to \gamma_1$ of the conductivity inside a "small" ball around x_0.

2. The Lebesgue dominated convergence theorem then ensures that:

$$\frac{1}{\varepsilon^d}(J(\varepsilon) - J(0)) \xrightarrow{\varepsilon \to 0} \int_D j'(u_0(x))u_1(x)\,\mathrm{d}x.$$

3. Finally, an avatar of the adjoint method allows to transform this expression, making explicit its dependence with respect to x_0.

Goal and plan of the study (IV)

Disclaimer

- We only sketch the main stages of the calculation in a formal way.
- We refer to [Da] for more details about the presented formal argument, and to [CedMosVog] for a rigorous calculation.
- See also [Am, NoSo] for different calculation means of topological expansions or two-phase expansions.

Part IV

Topological derivatives

Let $\mathcal{L}$ be a linear, partial differential operator on $\mathbb{R}^d$, i.e. a mapping of the form:

$$\forall u \in \mathcal{C}^\infty(\mathbb{R}^d),\ \ \mathcal{L}u(x) = \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| \leq k}} a_\alpha \partial^\alpha u(x),$$

with constant coefficients $a_\alpha \in \mathbb{R}$.

Example: The (negative) Laplace operator reads: $\mathcal{L}u = -\sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}$.

Definition 2.

A fundamental solution for $\mathcal{L}$ is a distribution $G \in \mathcal{D}'(\mathbb{R}^d)$ which satisfies:

$$\mathcal{L}G = \delta_0 \text{ in } \mathcal{D}'(\mathbb{R}^d).$$

- The Malgrange-Ehrenpreis theorem states that any linear partial differential operator with constant coefficients has a fundamental solution.
- In "most cases", $G(x)$ is of class $\mathcal{C}^\infty$ in $\mathbb{R}^d \setminus \{0\}$, and blows up at $x = 0$.

Fundamental solutions of partial differential operators (II)

- The datum of a fundamental solution G for a partial differential operator $\mathcal{L}$ allows to produce one solution to an equation of the form:

$$\mathcal{L}u = f \text{ for a given source } f \in \mathcal{C}_c^\infty(\mathbb{R}^d).$$

- Indeed, it is enough to take

$$u(x) = (G * f)(x) = \int_{\mathbb{R}^d} G(x-y) f(y)\, \mathrm{d}y,$$

since then:

$$\mathcal{L}u = \left(\mathcal{L}G\right) * f = \delta_0 * f = f.$$

- This is often rewritten by introducing the convolution kernel $G(x,y) = G(x-y)$:

$$u(x) = \int_{\mathbb{R}^d} G(x,y) f(y)\, \mathrm{d}y.$$

- This calculation can often be generalized to more general right-hand sides than $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$, depending on the decay of $G(x)$ as $|x| \to \infty$.

Fundamental solutions of partial differential operators (III)

- The concept of fundamental solutions can be generalized to the case where $\mathcal{L}$ has non constant coefficients $a_\alpha(x) \in \mathcal{C}^\infty(\mathbb{R}^d)$:

$$\forall u \in \mathcal{C}^\infty(\mathbb{R}^d), \;\; \mathcal{L}u(x) = \sum_{\substack{\alpha \in \mathbb{N}^d \\ |\alpha| \leq k}} a_\alpha(x) \partial^\alpha u(x).$$

- The solution to an equation of the form $\mathcal{L}u = f$ is now expressed as:

$$u(x) = \int_{\mathbb{R}^d} G(x, y) f(y) \, \mathrm{d}y.$$

- The kernel $G(x, y)$ is no longer of convolution type (i.e. of the form $G(x - y)$).
- For a fixed point $y \in \mathbb{R}^d$, the function $x \mapsto G(x, y)$ is a distributional solution to

$$\mathcal{L}_x G(x, y) = \delta_{x=y},$$

where $\delta_{x=y}$ is the Dirac distribution at y.

The fundamental solution to the "background" equation (I)

- The Green's function for the Laplace equation in the free space is the solution to:

$$\text{For fixed } x \in \mathbb{R}^d, \;\; -\Delta_y G(x,y) = \delta_{y=x} \text{ in } \mathbb{R}^d.$$

- The function $G(x,y)$ reads:

$$G(x,y) = \begin{cases} -\frac{1}{2\pi}\log|x-y| & \text{if } d = 2, \\ \frac{1}{(d-2)\omega_d}|x-y|^{2-d} & \text{if } d \geq 3, \end{cases}$$

where ω_d is the surface of the $(d-1)$ dimensional sphere in $\mathbb{R}^d$ *.

- Equivalently, for any point $x \in \mathbb{R}^d$, and any test function $\varphi \in \mathcal{C}_c^\infty(\mathbb{R}^d)$,

$$\varphi(x) = \int_{\mathbb{R}^d} \nabla\varphi(y) \cdot \nabla_y G(x,y)\,\mathrm{d}y.$$

* Warning: Depending on authors, different conventions are used as for the sign of the Green's function.

The fundamental solution to the "background" equation (II)

- The fundamental solution $N(x,y)$ to the "background" equation
$$\begin{cases} -\mathrm{div}(\gamma_0 \nabla u_0) = f & \text{in } D, \\ u_0 = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_0}{\partial n} = g & \text{on } \Gamma_N, \end{cases}$$
is defined by: for $x \in D$, $y \mapsto N(x,y)$ is the solution to:
$$\begin{cases} -\mathrm{div}_y(\gamma_0(y)\nabla_y N(x,y)) = \delta_{y=x} & \text{in } D, \\ N(x,y) = 0 & \text{for } y \in \Gamma_D, \\ \gamma_0(y)\frac{\partial N}{\partial n_y}(x,y) = 0 & \text{for } y \in \Gamma_N. \end{cases}$$

- It is constructed from the Green's function of the Laplace equation in the free space $G(x,y)$ as:
$$N(x,y) = G(x,y) + R(x,y),$$
where the difference $y \mapsto R(x,y)$ satisfies the equation:
$$\begin{cases} -\mathrm{div}_y(\gamma_0(y)\nabla_y R(x,y)) = \frac{1}{\gamma_0(x)}\nabla\gamma(y)\cdot\nabla_y G(x,y) & \text{in } \Omega, \\ R(x,y) = -\frac{1}{G(x,y)} & \text{for } y \in \Gamma_D, \\ \gamma_0(y)\frac{\partial R}{\partial n_y}(x,y) = -\frac{\gamma_0(y)}{\gamma_0(x)}\frac{\partial G}{\partial n_y}(x,y) & \text{for } y \in \Gamma_N. \end{cases}$$

The fundamental solution to the "background" equation (III)

Proposition 1.

Let $N(x,y)$ be the fundamental solution to the "background" equation; then:

1. *$N(x,y)$ is symmetric with respect to its arguments: $N(x,y) = N(y,x)$;*
2. *For given $x \in \overline{D}$, the fundamental solution $y \mapsto N(x,y)$ is smooth on any open subset U far from x and the transition region $\overline{\Gamma_D} \cap \overline{\Gamma_N}$.*
3. *"Variational formulation": For any point $x \in D$, the function $y \mapsto N(x,y)$ is the unique solution to:*

$$\forall \varphi \in \mathcal{C}^\infty(\mathbb{R}^d) \text{ s.t. } \varphi = 0 \text{ on } \Gamma_N, \;\; \varphi(x) = \int_D \gamma_0(y) \nabla_y N(x,y) \cdot \nabla \varphi(y) \, \mathrm{d}y.$$

Comments:

1. is a consequence of the self-adjoint character of the "background" operator.
2. follows from elliptic regularity applied to the system for $R(x,y)$.
3. is the definition of the equation for $y \mapsto N(x,y)$ in the sense of distributions.

The fundamental solution to the "background" equation (IV)

The fundamental solution $N(x,y)$ allows for a convenient representation of the solution u_0 to the "background" equation:

$$\begin{cases} -\mathrm{div}(\gamma_0 \nabla u_0) = f & \text{in } D, \\ u_0 = 0 & \text{for } y \in \Gamma_D, \\ \gamma \frac{\partial u_0}{\partial n_y} = g & \text{for } y \in \Gamma_N. \end{cases}$$

Indeed, repeated integration by parts (which can be justified) yield:

$$\begin{aligned} u_0(x) &= \int_D -\mathrm{div}_y(\gamma_0(y)\nabla_y N(x,y))u_0(y)\,\mathrm{d}y \\ &= -\int_{\partial D} \underbrace{\gamma_0(y)\frac{\partial N}{\partial n_y}(x,y)}_{=0 \text{ for } y\in\Gamma_N} \underbrace{u_0(y)}_{=0 \text{ for } y\in\Gamma_D} \,\mathrm{d}s(y) + \int_D \gamma_0(y)\nabla_y N(x,y)\cdot\nabla u_0\,\mathrm{d}y \\ &= \int_{\partial D} \underbrace{\gamma_0(y)\frac{\partial u_0}{\partial n}(y)}_{=g(y) \text{ on } \Gamma_N} \underbrace{N(x,y)}_{=0 \text{ on } \Gamma_D} \,\mathrm{d}s(y) + \int_D \underbrace{(-\mathrm{div}(\gamma_0\nabla u_0))}_{=f(y) \text{ on } D} N(x,y)\,\mathrm{d}y. \end{aligned}$$

Finally, we have the representation formula:

$$u_0(x) = \int_D f(y)N(x,y)\,\mathrm{d}y + \int_{\Gamma_N} g(y)N(x,y)\,\mathrm{d}s(y).$$

Part IV

Topological derivatives

Asymptotic expansion of the field u_ε

- Without loss of generality, we assume that $x_0 = 0$.
- The main result about the behavior of the potential u_ε as $\varepsilon \to 0$ is the following:

Theorem 2.

The following expansion holds, at any point $x \in D \setminus \{0\}$:

$$u_\varepsilon(x) = u_0(x) + \varepsilon^d u_1(x) + \mathrm{o}(\varepsilon^d), \text{ where } u_1(x) := -\mathcal{M}\nabla u_0(0) \cdot \nabla_y N(x,0).$$

In here, the polarization tensor $\mathcal{M} = (\mathcal{M}_{ij})_{i,j=1,\dots,d}$ is defined by:

$$\forall \xi \in \mathbb{R}^d, \ \mathcal{M}\xi = (\gamma_1(0) - \gamma_0(0)) \int_\omega (\xi + \nabla\phi_\xi(y))\,\mathrm{d}y,$$

where for any $\xi \in \mathbb{R}^d$, ϕ_ξ is the unique solution in $W_0^{1,-1}(\mathbb{R}^d)$ to the exterior problem:

$$\begin{cases} -\Delta\phi_\xi = 0 & \text{in } \omega \cup (\mathbb{R}^d \setminus \overline{\omega}), \\ \gamma_0(0)\frac{\partial\phi_\xi^+}{\partial n} - \gamma_1(0)\frac{\partial\phi_\xi^-}{\partial n} = -(\gamma_0(0) - \gamma_1(0))\xi \cdot n & \text{on } \partial\omega, \\ |\phi_\xi(y)| \to 0 & \text{when } y \to \infty. \end{cases}$$

Proposition 3.

There exists a constant $C > 0$ depending only on the domain D and the data f and g such that, for $\varepsilon > 0$ small enough:

$$||u_\varepsilon - u_0||_{H^1(D)} \leq C\varepsilon^{\frac{d}{2}}.$$

<u>*Proof:*</u> The error $r_\varepsilon := u_\varepsilon - u_0 \in H^1_{\Gamma_D}(D)$ solves the variational problem:

$$\forall v \in H^1_{\Gamma_D}(D), \ \int_D \gamma_\varepsilon(x)\nabla r_\varepsilon \cdot \nabla v \, \mathrm{d}x = -\int_{\omega_\varepsilon} (\gamma_1 - \gamma_0)\nabla u_0 \cdot \nabla v \, \mathrm{d}x.$$

Since u_0 is smooth, it follows:

$$\begin{aligned} \gamma_- ||\nabla r_\varepsilon||^2_{L^2(D)^d} \leq \int_D \gamma_\varepsilon |\nabla r_\varepsilon|^2 \, \mathrm{d}x &\leq C\left(\int_{\omega_\varepsilon} |\nabla u_0|^2 \, \mathrm{d}x\right)^{\frac{1}{2}} ||\nabla r_\varepsilon||_{L^2(D)^d}, \\ &\leq C \sup_{x \in D} |\nabla u_0(x)| \left(\int_{\omega_\varepsilon} \mathrm{d}x\right)^{\frac{1}{2}} ||\nabla r_\varepsilon||_{L^2(D)^d}, \\ &\leq C\varepsilon^{\frac{d}{2}} ||\nabla r_\varepsilon||_{L^2(D)^d}, \end{aligned}$$

and so (an adapted version of) the Poincaré inequality yields:

$$||r_\varepsilon||_{H^1(D)} \leq C||\nabla r_\varepsilon||_{L^2(D)^d} \leq C\varepsilon^{\frac{d}{2}}.$$

Asymptotic expansion of u_ε: a formal calculation (I)

Defining the (new version of the) error $r_\varepsilon = \frac{1}{\varepsilon^d}(u_\varepsilon - u_0)$, we aim to prove that:

$$r_\varepsilon(x) \xrightarrow{\varepsilon \to 0} u_1(x), \text{ for } x \in \overline{D} \setminus \{0\}.$$

Step 1: *We represent* $r_\varepsilon(x)$ *at a point* $x \in \overline{D} \setminus \{0\}$, *in terms of* $N(x,y)$, *and the values of* r_ε *inside* ω_ε.

From the definition of $N(x,y)$, it holds:

$$r_\varepsilon(x) = \int_D (-\mathrm{div}_y(\gamma_0(y)\nabla_y N(x,y))) r_\varepsilon(y)\, \mathrm{d}y.$$

An integration by parts then yields:

$$\begin{aligned} r_\varepsilon(x) &= -\int_{\partial D} \underbrace{\gamma_0(y)\frac{\partial N}{\partial n_y}(x,y)}_{=0 \text{ for } y \in \Gamma_N} \underbrace{r_\varepsilon(y)}_{=0 \text{ for } y \in \Gamma_D} \mathrm{d}s(y) + \int_D \gamma_0(y)\nabla_y N(x,y)\cdot \nabla r_\varepsilon(y)\, \mathrm{d}y, \\ &= \int_D \gamma_\varepsilon(y)\nabla_y N(x,y)\cdot\nabla r_\varepsilon(y)\,\mathrm{d}y + \int_{\omega_\varepsilon} (\gamma_0(y)-\gamma_1(y))\nabla_y N(x,y)\cdot\nabla r_\varepsilon(y)\,\mathrm{d}y. \end{aligned}$$

Asymptotic expansion of u_ε: a formal calculation (II)

In order to simplify the first integral

$$\int_D \gamma_\varepsilon(y)\nabla_y N(x,y)\cdot\nabla r_\varepsilon(y)\,\mathrm{d}y,$$

we "insert $y \mapsto N(x,y)$ as test function" in the variational formulation for r_ε:

$$\forall v \in H^1_{\Gamma_D}(D),\;\; \int_D \gamma_\varepsilon(x)\nabla r_\varepsilon\cdot\nabla v\,\mathrm{d}x = -\frac{1}{\varepsilon^d}\int_{\omega_\varepsilon}(\gamma_1-\gamma_0)\nabla u_0\cdot\nabla v\,\mathrm{d}x.$$

This produces:

$$\int_D \gamma_\varepsilon(y)\nabla_y N(x,y)\cdot\nabla r_\varepsilon(y)\,\mathrm{d}y = -\frac{1}{\varepsilon^d}\int_{\omega_\varepsilon}(\gamma_1(y)-\gamma_0(y))\nabla u_0(y)\cdot\nabla_y N(x,y)\,\mathrm{d}y,$$

and finally

$$r_\varepsilon(x) = -\frac{1}{\varepsilon^d}\int_{\omega_\varepsilon}(\gamma_1(y)-\gamma_0(y))\nabla u_0(y)\cdot\nabla_y N(x,y)\,\mathrm{d}y - \int_{\omega_\varepsilon}(\gamma_1(y)-\gamma_0(y))\nabla_y N(x,y)\cdot\nabla r_\varepsilon(y)\,\mathrm{d}y.$$

Asymptotic expansion of u_ε: a formal calculation (III)

We finally use a change of variables to rewrite both integrals over the fixed set ω:

$$r_\varepsilon(x) = -\int_\omega (\gamma_1(\varepsilon z) - \gamma_0(\varepsilon z))\nabla u_0(\varepsilon z) \cdot \nabla_y N(x, \varepsilon z)\, \mathrm{d}z$$

$$- \int_\omega (\gamma_1(\varepsilon z) - \gamma_0(\varepsilon z))\nabla_y N(x, \varepsilon z) \cdot \nabla s_\varepsilon(z)\, \mathrm{d}z.$$

where the rescaled error $s_\varepsilon(z)$ is defined by:

$$s_\varepsilon(z) = \varepsilon^{d-1} r_\varepsilon(\varepsilon z).$$

This is the quantity that we need to study inside the rescaled inclusion set ω.

Asymptotic expansion of u_ε: a formal calculation (IV)

Step 2: *We analyze the rescaled error* $s_\varepsilon = \varepsilon^{d-1} r_\varepsilon(\varepsilon z)$.

- Recall that r_ε satisfies the following minimization problem:

$$\min_{u \in H^1_{\Gamma_D}(D)} E_\varepsilon(u), \text{ where}$$

$$E_\varepsilon(u) := \frac{1}{2}\int_D \gamma_\varepsilon |\nabla u|^2 \, \mathrm{d}x + \frac{1}{\varepsilon^d}\int_{\omega_\varepsilon} (\gamma_1 - \gamma_0)\nabla u_0 \cdot \nabla u \, \mathrm{d}x.$$

- Using a change of variables, $s_\varepsilon \in H^1_{\frac{1}{\varepsilon}\Gamma_D}(\frac{1}{\varepsilon}D)$ is the solution to:

$$\min_{u \in H^1_{\frac{1}{\varepsilon}\Gamma_D}(\frac{1}{\varepsilon}D)} F_\varepsilon(u), \text{ where}$$

$$F_\varepsilon(u) := \frac{1}{2\varepsilon^d}\int_{\frac{1}{\varepsilon}D} \gamma_\varepsilon(\varepsilon z)|\nabla u|^2 \, \mathrm{d}z + \frac{1}{\varepsilon^d}\int_{\omega_1} (\gamma_1(\varepsilon z) - \gamma_0(\varepsilon z))\nabla u_0(\varepsilon z) \cdot \nabla u \, \mathrm{d}z.$$

We approximate the latter problem by retaining only leading order terms in the energy, and in the functional space:

$$\min_{u \in W_0^{1,-1}(\mathbb{R}^d)} \widetilde{F_\varepsilon}(u), \text{ where}$$

$$\widetilde{F_\varepsilon}(u) := \frac{1}{2}\int_{\mathbb{R}^d} \widehat{\gamma}(z)|\nabla u|^2 \, \mathrm{d}z + \int_{\omega_1} (\gamma_1(0) - \gamma_0(0))\nabla u_0(0) \cdot \nabla u \, \mathrm{d}z,$$

and we have defined:

$$\forall z \in \mathbb{R}^d, \;\; \widehat{\gamma}(z) = \begin{cases} \gamma_1(0) & \text{if } z \in B(0,1), \\ \gamma_0(0) & \text{otherwise.} \end{cases}$$

Asymptotic expansion of u_ε: a formal calculation (VI)

- We use the Euler-Lagrange equation of this problem to characterize the minimizer v:

$$\forall w \in W_0^{1,-1}(\mathbb{R}^d),$$
$$\widetilde{F_\varepsilon}'(v)(w) = \int_{\mathbb{R}^d} \widehat{\gamma}(z)\nabla v \cdot \nabla w \, \mathrm{d}z + \int_{\omega_1} (\gamma_1(0) - \gamma_0(0))\nabla u_0(0) \cdot \nabla w \, \mathrm{d}z = 0.$$

- We compare the latter identity with the variational formulation for the cell function $\phi_\xi \in W_0^{1,-1}(\mathbb{R}^d)$:

$$\forall w \in W_0^{1,-1}(\mathbb{R}^d), \ \int_{\mathbb{R}^d} \widehat{\gamma}(z)\nabla \phi_\xi \cdot \nabla w \, \mathrm{d}z + \int_{\omega} (\gamma_1(0) - \gamma_0(0))\xi \cdot \nabla w \, \mathrm{d}z = 0.$$

- The uniqueness of the solution to this problem implies that:

$$v = \phi_{\nabla u_0(0)}.$$

Asymptotic expansion of u_ε: a formal calculation (VII)

Step 3: *We pass to the limit in the representation formula for $r_\varepsilon(x)$.*

- We have proved in Step 1 that, for $x \in D \setminus \{0\}$,

$$r_\varepsilon(x) = -\int_\omega (\gamma_1(\varepsilon z) - \gamma_0(\varepsilon z))\nabla u_0(\varepsilon z) \cdot \nabla_y N(x, \varepsilon z)\,\mathrm{d}z \\ - \int_\omega (\gamma_1(\varepsilon z) - \gamma_0(\varepsilon z))\nabla s_\varepsilon(z) \cdot \nabla_y N(x, \varepsilon z)\,\mathrm{d}z,$$

- During Step 2, we have justified the convergence,

$$s_\varepsilon(z) \to v(z) = \phi_{\nabla u_0(0)}.$$

- As a result:

$$\lim_{\varepsilon \to 0} r_\varepsilon(x) = -\int_\omega (\gamma_1(0) - \gamma_0(0))\nabla u_0(0) \cdot \nabla_y N(x, 0)\,\mathrm{d}z \\ - \int_\omega (\gamma_1(0) - \gamma_0(0))\nabla \phi_{\nabla u_0(0)}(z) \cdot \nabla_y N(x, 0)\,\mathrm{d}z.$$

Asymptotic expansion of u_ε: a formal calculation (VIII)

A simple rearrangement now yields:

$$\begin{aligned}\lim_{\varepsilon\to 0} r_\varepsilon(x) &= -\int_\omega (\gamma_1(0)-\gamma_0(0))\left(\nabla u_0(0)+\nabla\phi_{\nabla u_0(0)}(z)\right)\cdot\nabla_y N(x,0)\,\mathrm{d}z,\\ &= -\left(\int_\omega (\gamma_1(0)-\gamma_0(0))\left(\nabla u_0(0)+\nabla\phi_{\nabla u_0(0)}(z)\right)\,\mathrm{d}z\right)\cdot\nabla_y N(x,0),\\ &= -\mathcal{M}\nabla u_0(0)\cdot\nabla_y N(x,0),\end{aligned}$$

where we have used the definition of the polarization tensor $\mathcal{M}\in\mathbb{R}^{d\times d}$:

$$\forall\xi\in\mathbb{R}^d,\;\; \mathcal{M}\xi = (\gamma_1(0)-\gamma_0(0))\int_\omega (\xi+\nabla\phi_\xi(y))\,\mathrm{d}y.$$

□

We consider the observable:

$$J(\varepsilon) = \int_D j(u_\varepsilon)\,\mathrm{d}x,$$

where $j : \mathbb{R} \to \mathbb{R}$ is a smooth function, satisfying growth conditions.

Proposition 4.

The function $J(\varepsilon)$ admits the following asymptotic expansion at $\varepsilon = 0$:

$$J(\varepsilon) = J(0) + \varepsilon^d J'(0) + \mathrm{o}(\varepsilon^d),$$

where the "derivative" $J'(0)$ reads:

$$J'(0) = \mathcal{M}\nabla u_0(0) \cdot \nabla p_0(0).$$

Here, $\mathcal{M}$ is the polarization tensor and the adjoint state p_0 is the unique solution in $H^1_{\Gamma_D}(D)$ to:

$$\begin{cases} -\mathrm{div}(\gamma_0 \nabla p_0) = -j'(u_0) & \text{in } D, \\ p_0 = 0 & \text{on } \Gamma_D, \\ \gamma_0 \frac{\partial p_0}{\partial n} = 0 & \text{on } \partial D \setminus \overline{\Gamma_D}. \end{cases}$$

Derivative of an observable

Sketch of proof:

- At first, Taylor's formula yields:

$$\begin{aligned}\frac{1}{\varepsilon^d}(J(\varepsilon)-J(0)) &= \frac{1}{\varepsilon^d}\int_D (j(u_\varepsilon)-j(u_0))\,\mathrm{d}x,\\ &= \int_D\int_0^1 j'(u_0+t(u_\varepsilon(x)-u_0(x)))\,\frac{u_\varepsilon(x)-u_0(x)}{\varepsilon^d}\,\mathrm{d}t\,\mathrm{d}x.\end{aligned}$$

- Using the Lebesgue dominated convergence theorem to pass to the limit (which can be justified in the present case), we obtain:

$$J'(0) := \lim_{\varepsilon\to 0}\frac{1}{\varepsilon^d}(J(\varepsilon)-J(0)) = \int_D j'(u_0(x))u_1(x)\,\mathrm{d}x,$$

where we have just calculated the sensitivity $u_1(x)$:

$$u_1(x) = -\mathcal{M}\nabla u_0(0)\cdot\nabla_y N(x,0).$$

- This expression is difficult to handle in practice, since the fundamental solution $N(x,y)$ does not have an explicit expression.

Derivative of an observable

- We now bring into play the adjoint state $p_0 \in H^1_{\Gamma_D}(D)$.
- The representation formula involving the fundamental solution $N(x, y)$ to the "background" operator yields:

$$p_0(x) = -\int_D j'(u_0)(y) N(x, y)\, \mathrm{d}y,$$

- Then, a calculation reveals:

$$\begin{aligned} J'(0) &= -\int_D j'(u_0(x)) \underbrace{\mathcal{M}\nabla u_0(0) \cdot \nabla_y N(x, 0)}_{=u_1(x)} \mathrm{d}x, \\ &= -\mathcal{M}\nabla u_0(0) \cdot \nabla_y \left(\underbrace{\int_D j'(u_0(x)) N(x, y)\, \mathrm{d}x}_{=-p_0(y)} \right)\Bigg|_{y=0}, \\ &= \mathcal{M}\nabla u_0(0) \cdot \nabla p_0(0), \end{aligned}$$

which is the desired formula.

A closer look to the polarization tensor $\mathcal{M}$

- The polarization tensor

$$\mathcal{M}\xi = (\gamma_1(0) - \gamma_0(0)) \int_\omega (\xi + \nabla\phi_\xi(y))\,\mathrm{d}y,$$

$$\text{where } \begin{cases} -\Delta\phi_\xi = 0 & \text{in } \omega \cup (\mathbb{R}^d \setminus \overline{\omega}), \\ \gamma_0(0)\frac{\partial\phi_\xi^+}{\partial n} - \gamma_1(0)\frac{\partial\phi_\xi^-}{\partial n} = -(\gamma_0(0) - \gamma_1(0))\xi\cdot n & \text{on } \partial\omega, \\ |\phi_\xi(y)| \to 0 & \text{when } y \to \infty, \end{cases}$$

can be calculated explicitly in some particular situations.

- When ω is the unit disk in $\mathbb{R}^2$, an explicit calculation using polar coordinates yields:

$$\phi_\xi(y) = \begin{cases} \frac{\gamma_0(0)-\gamma_1(0)}{\gamma_0(0)+\gamma_1(0)}\xi\cdot y & \text{if } y \in \omega, \\ \frac{\gamma_0(0)-\gamma_1(0)}{\gamma_0(0)+\gamma_1(0)}\frac{\xi\cdot y}{|y|^2} & \text{otherwise,} \end{cases} \quad \text{and } \mathcal{M} = 2\pi\gamma_0(0)\frac{\gamma_1(0)-\gamma_0(0)}{\gamma_1(0)+\gamma_0(0)}\mathrm{I}.$$

The asymptotic expansion of $J(\varepsilon)$ reads in this case:

$$J(\varepsilon) = J(0) + \varepsilon^d 2\pi\gamma_0(0)\frac{\gamma_1(0)-\gamma_0(0)}{\gamma_1(0)+\gamma_0(0)}\nabla u_0(0)\cdot\nabla p_0(0) + \mathrm{o}(\varepsilon^d).$$

Part IV

Topological derivatives

Extension to the linearized elasticity system (I)

The above study can be generalized to the two-phase linear elasticity system.

- The boundary of the "hold-all' domain $D \subset \mathbb{R}^d$ reads:

$$\partial D = \overline{\Gamma_D} \cup \overline{\Gamma_N} \cup \overline{\Gamma}.$$

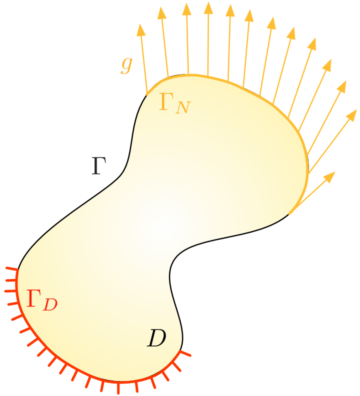
- The "background" displacement u_0 is the unique solution in $H^1_{\Gamma_D}(D)^d$ to the system:

$$\begin{cases} -\text{div}(A_0 e(u_0)) = f & \text{in } D, \\ u_0 = 0 & \text{on } \Gamma_D, \\ Ae(u_0)n = g & \text{on } \Gamma_N, \\ Ae(u_0)n = 0 & \text{on } \Gamma, \end{cases}$$

with

  - Smooth data $f : D \to \mathbb{R}^d$, $g : \Gamma_N \to \mathbb{R}^d$;
  - A smooth, elliptic Hooke's tensor A_0:

$$A_0(x)e = 2\mu_0(x)e + \lambda_0(x)\text{tr}(e)\text{I}.$$



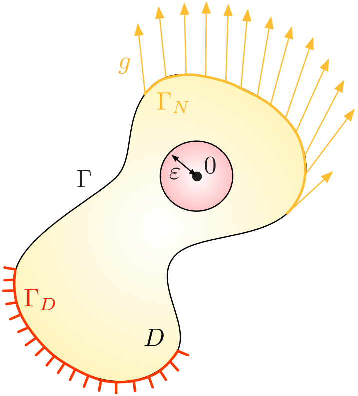
Extension to the linearized elasticity system (I)

- In the perturbed situation, the displacement u_ε is the unique solution in $H^1_{\Gamma_D}(D)^d$ to:

$$\left\{\begin{array}{ll} -\text{div}(A_\varepsilon e(u_\varepsilon)) = f & \text{in } D, \\ u_\varepsilon = 0 & \text{on } \Gamma_D, \\ A_\varepsilon e(u_\varepsilon) n = g & \text{on } \Gamma_N, \\ A_\varepsilon e(u_\varepsilon) n = 0 & \text{on } \Gamma. \end{array}\right.$$

- The perturbed Hooke's tensor reads:

$$\forall x \in D, \;\; A_\varepsilon(x) = \left\{\begin{array}{ll} A_1(x) & \text{if } x \in B(0,\varepsilon), \\ A_0(x) & \text{otherwise.} \end{array}\right.$$



Let us consider the quantity of interest

$$J(\varepsilon) = \int_D j(u_\varepsilon)\,\mathrm{d}x,$$

where $j : \mathbb{R}^d \to \mathbb{R}$ is a smooth function, satisfying adequate growth conditions.

Proposition 5.

The function $J(\varepsilon)$ has the following expansion at $\varepsilon = 0$:

$$J(\varepsilon) = J(0) + \varepsilon^d J'(0) + \mathrm{o}(\varepsilon^d),$$

where the "derivative" $J'(0)$ reads:

$$J'(0) = \mathcal{M}e(u_0)(0) : e(p_0)(0),$$

$\mathcal{M}$ is the polarization tensor and the adjoint p_0 is the unique solution in $H^1_{\Gamma_D}(D)^d$ to:

$$\left\{ \begin{array}{cl} -\mathrm{div}(A_0 e(p_0)) = -j'(u_0) & \text{in } D, \\ p_0 = 0 & \text{on } \Gamma_D, \\ A_0 e(p_0) n = 0 & \text{on } \Gamma \cup \Gamma_N. \end{array} \right.$$

Asymptotic expansion in the linear elasticity context (II)

- In the linearized elasticity context, the polarization tensor $\mathcal{M}$ is a fourth-order tensor, i.e. a mapping $\mathcal{M} : \mathcal{S}_d(\mathbb{R}) \to \mathcal{S}_d(\mathbb{R})$.

- In the particular case where $d = 2$, and $\omega = B(0, 1)$ is the unit disk, this tensor can be calculated explicitly:

$$\forall e \in \mathcal{S}(\mathbb{R}^d), \;\; \mathcal{M}e = \alpha \text{tr}(e)\text{I} + \beta e,$$

where the coefficients α and β read:

$$\alpha = \pi \left(\frac{(\lambda_0 + 2\mu_0)(\lambda_1 + \mu_1 - (\lambda_0 + \mu_0))}{\mu_0 + \lambda_1 + \mu_1} - \frac{2\mu_0(\mu_1 - \mu_0)(\lambda_0 + 2\mu_0)}{\mu_1(\lambda_0 + 3\mu_0) + \mu_0(\lambda_0 + \mu_0)} \right) \text{ and}$$

$$\beta = 4\pi \frac{\mu_0(\lambda_0 + 2\mu_0)(\mu_1 - \mu_0)}{\mu_0(\lambda_0 + \mu_0) + \mu_1(\lambda_0 + 3\mu_0)},$$

and we have taken the shortcuts $\lambda_0 \equiv \lambda_0(0)$, $\lambda_1 \equiv \lambda_1(0)$, etc.

For further reference, we denote this polarization tensor by:

$$\mathcal{M}(\underbrace{\lambda_0, \mu_0}_{\text{Background properties}}, \underbrace{\lambda_1, \mu_1}_{\text{Inclusion properties}}),$$

so that the sensitivity of $J(\varepsilon)$ reads

$$J'(0) = \mathcal{M}(\lambda_0, \mu_0, \lambda_1, \mu_1) e(u_0)(0) : e(p_0)(0).$$

Remark As in the context of shape sensitivity analysis, when

$$J(\varepsilon) = \int_D A_\varepsilon e(u_\varepsilon) : e(u_\varepsilon)\, \mathrm{d}x = \int_D f \cdot u_\varepsilon \, \mathrm{d}x + \int_{\Gamma_N} g \cdot u_\varepsilon \, \mathrm{d}s,$$

is the compliance, one has $u_0 = -p_0$.

The limiting one-phase and void situation

The case of an inclusion of void is a formal limit of the previous analysis.

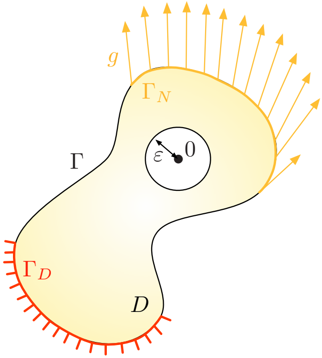
- The state $u_\varepsilon \in H^1_{\Gamma_D}(D \setminus \overline{B(0,\varepsilon)})^d$ then fulfills:

$$\begin{cases} -\mathrm{div}(Ae(u_\varepsilon)) = f & \text{in } D, \\ u_\varepsilon = 0 & \text{on } \Gamma_D, \\ Ae(u_\varepsilon)n = g & \text{on } \Gamma_N, \\ Ae(u_\varepsilon)n = 0 & \text{on } \Gamma \cup \partial B(0,\varepsilon). \end{cases}$$

where the Hooke's tensor A reads:

$$Ae = 2\mu e + \mathrm{tr}(e)\mathrm{I},$$

and the source f has support "far" 0.



- Using the previous results with $\lambda_0 = \lambda$, $\mu_0 = \mu$ and $\lambda_1, \mu_1 \to 0$, we obtain:

$$J(\varepsilon) = J(0) + \varepsilon^d J'(0) + \mathrm{o}(\varepsilon^d), \text{ where}$$

$$J'(0) = \lim_{\eta \to 0} \mathcal{M}(\lambda, \mu, \eta\lambda, \eta\mu) e(u_0)(0) : e(p_0)(0).$$

Part IV

Topological derivatives

- We consider the optimization of an elastic structure Ω.

- The displacement u_Ω of Ω satisfies the linearized elasticity system:

$$\begin{cases} -\mathrm{div}(Ae(u_\Omega)) = f & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ Ae(u_\Omega)n = g & \text{on } \Gamma_N, \\ Ae(u_\Omega)n = 0 & \text{on } \Gamma, \end{cases}$$

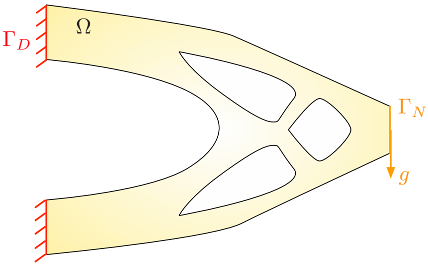
where the Hooke's law A reads:

$$Ae = 2\mu e + \lambda \mathrm{tr}(e)\mathrm{I}.$$

- We optimize the function $J(\Omega)$ defined by:

$$J(\Omega) = \int_\Omega j(u_\Omega)\,\mathrm{d}x,$$

under a constraint on $\mathrm{Vol}(\Omega)$.



- Shapes and their evolutions are accounted for by the level set method.

  (The ersatz material trick is used only to approximate u_Ω and p_Ω.)

- The sensitivity of a shape Ω with respect to nucleation of a hole at $x \in \Omega$ reads:

$$J(\Omega \setminus \overline{B(x,\varepsilon)}) = J(\Omega) + \varepsilon^d g_\Omega^T(x) + \mathrm{o}(\varepsilon^d),$$

  where we have seen that, in the example case of the compliance:

$$g_\Omega^T(x) = \frac{\pi(\lambda+2\mu)}{2\mu(\lambda+\mu)}\Big(4\mu Ae(u_\Omega):e(u_\Omega) + (\lambda-\mu)\mathrm{tr}(Ae(u_\Omega))\mathrm{tr}(e(u_\Omega))\Big)(x).$$

- Every now and then (say, every 4, 5 iteration), we test whether it is beneficial to nucleate a small hole inside Ω.

Initialization: Start from an initial shape Ω^0,

For $n = 0, \ldots$ **convergence,**

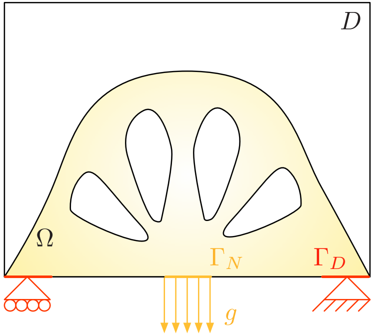
- Calculate the state u_{Ω^n} (and possibly the adjoint p_{Ω^n}) on Ω^n;
- **If** $n \bmod n_{\text{top}} = 0$**:**
  1. Calculate the topological derivative $g^T_{\Omega^n}(x)$ at every point $x \in \Omega$;
  2. The new shape Ω^{n+1} is obtained as:
  $$\Omega^{n+1} = \Omega^n \setminus \overline{B(x_0, r)},$$
  where $g^T_\Omega(x_0)$ is minimum at x_0, and $r > 0$ is a "small" parameter.
- **Else:**
  1. Calculate $J'(\Omega^n)$, and infer a descent direction θ^n for $J(\Omega)$.
  2. Advect the shape Ω^n along θ^n for a small pseudo-time step τ^n:
  $$\Omega^{n+1} = (\mathrm{Id} + \tau^n \theta^n)(\Omega^n).$$

- The wheel bridge example is considered.
- Shapes are attached on the lower-right corner, and they are free to slide on the lower left corner.
- Body forces f are omitted.
- A surface load g is applied on the middle Γ_N of the bottom side.
- We minimize a weighted sum of the compliance of the structure and its volume:

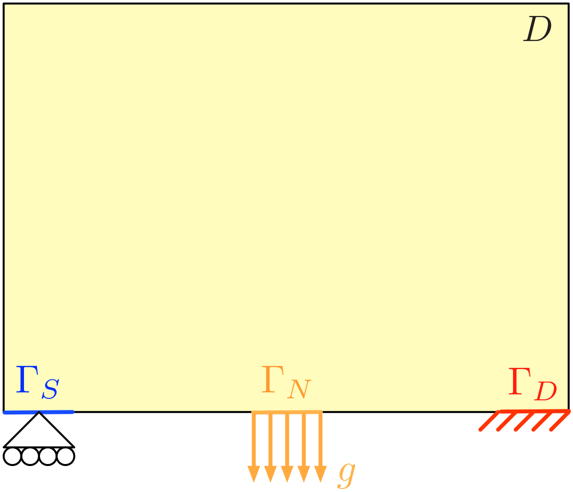
$$\min_{\Omega} C(\Omega) + \ell \mathrm{Vol}(\Omega),$$

where

$$C(\Omega) = \int_{\Gamma_N} g \cdot u_\Omega \, \mathrm{d}s.$$



Coupling topological derivatives with boundary variation methods (IV)



Part IV

Topological derivatives

A fixed-point algorithm based on topological derivatives (I)

- All the considered shapes Ω are enclosed in the fixed computational domain D.
- The displacement u_Ω of a structure $\Omega \subset D$ is approximated by the two-phase problem:

$$\begin{cases} -\text{div}(A_0 e(u_0)) = f & \text{in } D, \\ u_0 = 0 & \text{on } \Gamma_D, \\ A_0 e(u_0) n = g & \text{on } \Gamma_N, \\ A_0 e(u_0) n = 0 & \text{on } \partial D \setminus (\overline{\Gamma_D} \cup \overline{\Gamma_N}), \end{cases}$$

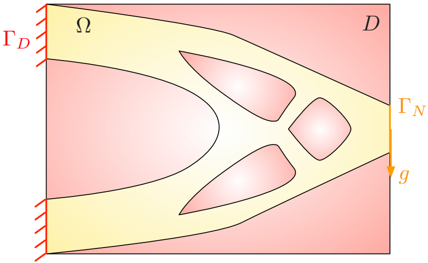
where

$$A_0(x) = \begin{cases} A & \text{if } x \in \Omega, \\ \eta A & \text{if } x \in D \setminus \overline{\Omega}, \end{cases}$$

for a small ersatz parameter $\eta \ll 1$.

- We aim to optimize the function

$$J(\Omega) = \int_\Omega j(u_\Omega)\,\mathrm{d}x \approx \int_D j(u_0)\,\mathrm{d}x.$$



- We define the variation $\Omega_{x,\varepsilon}$ of a shape $\Omega \subset D$ by:

$$\Omega_{x,\varepsilon} = \begin{cases} \Omega \setminus \overline{B(x,\varepsilon)} & \text{if } x \in \Omega, \\ \Omega \cup B(x,\varepsilon) & \text{if } x \in D \setminus \overline{\Omega}. \end{cases}$$

- The previous investigations allow to write the topological expansion:

$$J(\Omega_{x,\varepsilon}) = J(\Omega) + \varepsilon^d s_\Omega(x) g_\Omega^T(x) + \mathrm{o}(\varepsilon^d), \text{ where } s_\Omega(x) = \begin{cases} -1 & \text{if } x \in \Omega, \\ 1 & \text{if } x \in D \setminus \overline{\Omega}, \end{cases}$$

and

$$g_\Omega^T = \begin{cases} -\mathcal{M}(\lambda,\mu,\eta\lambda,\eta\mu)e(u_0) : e(p_0) & \text{on } \Omega, \\ \mathcal{M}(\eta\lambda,\eta\mu,\lambda,\mu)e(u_0) : e(p_0) & \text{on } D \setminus \overline{\Omega}. \end{cases}$$

A fixed-point algorithm based on topological derivatives (II)

- The necessary first-order optimality conditions for one shape $\Omega \subset D$ read:
  - If $x \in \Omega$, then $g_\Omega^T(x) < 0$;
  - If $x \in D \setminus \overline{\Omega}$, then $g_\Omega^T(x) > 0$.

- Hence, if Ω is optimal, the shape gradient g_Ω^T is one level set function for Ω:

$$\begin{cases} g_\Omega^T(x) < 0 & \text{if } x \in \Omega, \\ g_\Omega^T(x) > 0 & \text{if } x \in D \setminus \overline{\Omega}. \end{cases}$$

- We devise a fixed point algorithm which enforces this necessary condition.

A fixed-point algorithm based on topological derivatives (III)

- The shape Ω is represented by means of a level set function ϕ:

$$\forall x \in D, \begin{cases} \phi(x) < 0 & \text{if } \ x \in \Omega, \\ \phi(x) = 0 & \text{if } x \in \partial\Omega, \\ \phi(x) > 0 & \text{if } \ x \in D \setminus \overline{\Omega}. \end{cases}$$

- The necessary condition for optimality of Ω is in turn implied by:

$$\phi = \frac{1}{||g_\Omega^T||_{L^2(D)}} g_\Omega^T(x), \text{ where } \Omega := \{x \in D, \ \phi(x) < 0\}.$$

- We enforce this condition by a fixed-point algorithm with relaxation:

$$\phi^{n+1} = \frac{\widetilde{\phi^{n+1}}}{||\widetilde{\phi^{n+1}}||_{L^2(D)}}, \text{ where } \widetilde{\phi^{n+1}} = \alpha^n \phi^n + (1 - \alpha^n) g^n,$$

and $\alpha^n \in (0, 1)$ is a relaxation step.

A fixed-point algorithm based on topological derivatives (IV)

The so-called spherical linear interpolation trick allows for an elegant reformulation of the previous formulas; see [Shoe].

- Introducing $a^n := \arccos(\phi^n, g^n)_{L^2(D)}$, we observe that:

$$\|\widetilde{\phi^{n+1}}\|^2_{L^2(D)} = (1-\alpha^n)^2 + (\alpha^n)^2 + 2\alpha^n(1-\alpha^n)(\phi^n, g^n)_{L^2(D)}.$$

- We then define the "new" pseudo time-step $\tau^n > 0$ via the relation

$$\frac{\sin(\tau^n a^n)}{\sin a^n} := \frac{\alpha_k}{\left((1-\alpha^n)^2 + (\alpha^n)^2 + 2\alpha^n(1-\alpha^n)\cos a^n\right)^{1/2}},$$

  and an elementary calculation yields:

$$\frac{\sin((1-\tau^n)a^n)}{\sin a^n} = \frac{(1-\alpha^n)}{\left((1-\alpha^n)^2 + (\alpha^n)^2 + 2\alpha^n(1-\alpha^n)\cos a^n\right)^{1/2}}.$$

- Finally, the updated level set function φ^{n+1} is obtained directly as:

$$\phi^{n+1} = \frac{1}{\sin a^n}\Big(\sin((1-\tau^n)a^n)\phi^n + \sin(\tau^n a^n)g^n\Big).$$

Topological derivatives (V)

Initialization: Initial level set function ϕ^0,

For $n = 0, \ldots$ **convergence,**

- Calculate the state u_{Ω^n} (and possibly the adjoint p_{Ω^n}) on Ω^n;
- Calculate the topological derivative $g^T_{\Omega^n}(x)$ at every point $x \in \Omega$, as well as $g^n := \frac{1}{||g^T_{\Omega^n}||_{L^2(D)}} g^T_{\Omega^n}$.
- Calculate $a^n := \arccos(\phi^n, g^n)_{L^2(D)}$;
- Choose a relaxation step $0 < \tau^n < 1$;
- The updated level set function ϕ^{n+1} is

$$\phi^{n+1} = \frac{1}{\sin a^n}\Big(\sin((1-\tau^n)a^n)\phi^n + \sin(\tau^n a^n) g^n\Big),$$

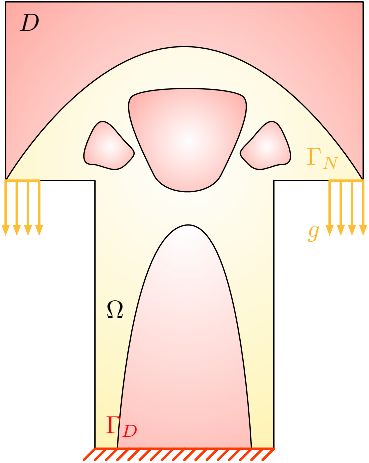
corresponding to the updated shape $\Omega^{n+1} = \left\{\phi^{n+1} < 0\right\}$.

- We consider the T-shaped mast example;
- Shapes are attached on their bottom side Γ_D;
- Body forces are omitted: $f = 0$;
- A vertical load g is applied at the end Γ_N of each arm;
- We minimize a weighted sum of the compliance of the structure and its volume:

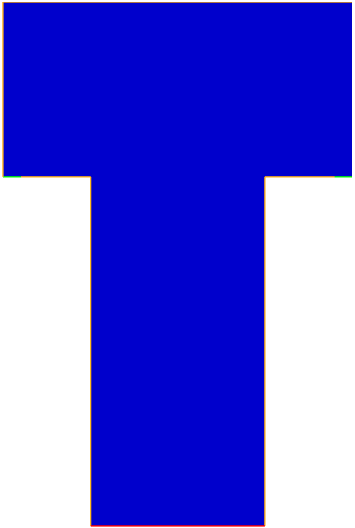
$$\min_{\Omega} C(\Omega) + \ell \mathrm{Vol}(\Omega),$$

where

$$C(\Omega) = \int_{\Gamma_N} g \cdot u_\Omega \, \mathrm{d}s.$$



The mast example using the fixed point algorithm



Appendix

Exterior problems ([Ne], §2.5.4)

- Problems posed in infinite domains often feature conditions at infinity, such as:

$$|u(x)| \to 0 \text{ as } |x| \to \infty.$$

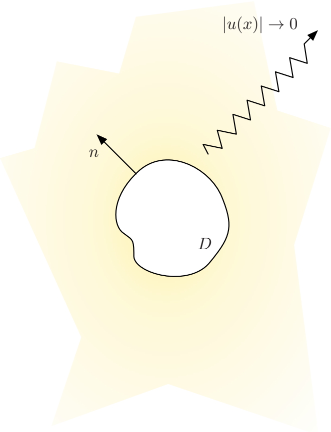
- Such exterior problems typically arise in the study of acoustic, elastic or electromagnetic waves.

- One example is the exterior Dirichlet problem

$$\begin{cases} -\Delta u = f & \text{in } \mathbb{R}^d \setminus \overline{D}, \\ u = 0 & \text{on } \partial D, \\ |u(x)| \to 0 & \text{as } |x| \to \infty, \end{cases}$$

where $D \subset \mathbb{R}^d$ is a bounded domain.

- This condition at infinity is endoded in exterior Sobolev spaces.



A glimpse to exterior spaces (I)

- We introduce the weighted Sobolev spaces $W^{1,-1}(\mathbb{R}^d)$ for $d = 2$ or 3:
$$W^{1,-1}(\mathbb{R}^2) = \left\{ u \in L^2_{\text{loc}}(\mathbb{R}^2),\ \frac{1}{(1+|x|^2)^{\frac{1}{2}} \log(2+|x|^2)} u \in L^2(\mathbb{R}^2),\ \nabla u \in L^2(\mathbb{R}^2)^2 \right\},$$
$$W^{1,-1}(\mathbb{R}^3) = \left\{ u \in L^2_{\text{loc}}(\mathbb{R}^3),\ \frac{1}{(1+|x|^2)^{\frac{1}{2}}} u \in L^2(\mathbb{R}^3),\ \nabla u \in L^2(\mathbb{R}^3)^3 \right\}.$$

- Functions $u \in W^{1,-1}(\mathbb{R}^3)$ vanish at infinity, while functions $u \in W^{1,-1}(\mathbb{R}^2)$ may not, since the latter space contains constant functions.

- The space of $W^{1,-1}(\mathbb{R}^d)$ functions "vanishing at infinity" is then:
$$W_0^{1,-1}(\mathbb{R}^d) := \begin{cases} W^{1,-1}(\mathbb{R}^2)/\mathbb{R} & \text{if } d = 2, \\ W^{1,-1}(\mathbb{R}^3) & \text{if } d = 3. \end{cases}$$

- Similar exterior spaces $W^{1,-1}(\mathbb{R}^d \setminus \overline{D})$ and $W_0^{1,-1}(\mathbb{R}^d \setminus \overline{D})$ are defined on the complement $\mathbb{R}^d \setminus \overline{D}$ of a bounded domain D.

A glimpse to exterior spaces (II)

- The restriction of $u \in W^{1,-1}(\mathbb{R}^d)$ to a bounded domain $D \subset \mathbb{R}^d$ lies in $H^1(D)$.
- The weights in the definition of $W^{1,-1}(\mathbb{R}^d)$ account for the decay of u at infinity.
- This is illustrated by the following calculation (from [NgVo]) in the case $d = 3$:

$$||\nabla u||_{L^2(\mathbb{R}^d)^2} < \infty \;\Rightarrow\; \int_{B(0,2R)\setminus\overline{B(0,R)}} \frac{1}{1+|x|^2}|u(x)|^2 \,\mathrm{d}x \xrightarrow{R\to\infty} 0.$$

Hence, using the polar coordinates $(r,\theta) \in (0,\infty)\times\mathbb{S}^2$ of points $x \in \mathbb{R}^d \setminus \{0\}$:

$$\int_R^{2R}\int_{\mathbb{S}^2} \frac{r^2}{1+r^2}|u(x+r\theta)|^2 \,\mathrm{d}r\mathrm{d}\theta \xrightarrow{\mathbb{R}\to 0} 0.$$

The mean value theorem implies that there exists a sequence $R_n \to \infty$ such that:

$$R_n \int_{\mathbb{S}^2} |u(x+R_n\theta)|^2 \,\mathrm{d}\theta \xrightarrow{n\to\infty} 0.$$

The same argument reveals that:

$$R_n^3 \int_{\mathbb{S}^2} |\nabla u(x+R_n\theta)|^2 \,\mathrm{d}\theta \xrightarrow{n\to\infty} 0.$$

A glimpse to exterior spaces (III)

Functions in exterior spaces satisfy quite familiar Poincaré-like inequalities.

Proposition 6 (Poincaré's inequality for functions in $W^{1,-1}(\mathbb{R}^d)$).

Let $D \in \mathbb{R}^d$ be a bounded Lipschitz domain; there exists a constant $C > 0$ such that for all functions $u \in W^{1,-1}(\mathbb{R}^d \setminus \overline{D})$ with $u = 0$ on ∂D,

$$||u||_{W^{1,-1}(\mathbb{R}^d \setminus \overline{D})} \leq C \left(\int_{\mathbb{R}^d \setminus \overline{D}} |\nabla u|^2 \, \mathrm{d}x \right)^{1/2}.$$

Proposition 7 (Poincaré-Wirtinger's inequality in $W_0^{1,-1}(\mathbb{R}^d)$).

Let $D \in \mathbb{R}^d$ be a bounded Lipschitz domain; there exists a constant $C > 0$ such that for all functions $u \in W_0^{1,-1}(\mathbb{R}^d \setminus \overline{D})$:

$$||u||_{W^{1,-1}(\mathbb{R}^d \setminus \overline{D})} \leq C \left(\int_{\mathbb{R}^d \setminus \overline{D}} |\nabla u|^2 \, \mathrm{d}x \right)^{1/2}.$$

Resolution of the exterior Dirichlet problem

- Consider the exterior Dirichlet problem

$$\begin{cases} -\Delta u = f & \text{in } \mathbb{R}^d \setminus \overline{D}, \\ u = 0 & \text{on } \partial D, \\ |u(x)| \to 0 & \text{as } |x| \to \infty, \end{cases}$$

  with

  - A source $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$;
  - Homogeneous Dirichlet boundary conditions on ∂D (for simplicity).

- This problem has the following variational formulation: search for $u \in W^{1,-1}(\mathbb{R}^d)$ s.t. $u = 0$ on ∂D and:

$$\forall v \in W^{1,-1}(\mathbb{R}^d) \text{ with } v = 0 \text{ on } \partial D, \int_{\mathbb{R}^d \setminus \overline{D}} \nabla u \cdot \nabla v \, \mathrm{d}x = \int_{\mathbb{R}^d \setminus \overline{D}} fv \, \mathrm{d}x.$$

- This problem is well-posed, owing to the Lax-Milgram theorem and the Poincaré's inequality in $W^{1,-1}(\mathbb{R}^d)$.

Resolution of the exterior Neumann problem

- Let us turn to the exterior Neumann problem:

$$\begin{cases} -\Delta u = f & \text{in } \mathbb{R}^d \setminus \overline{D}, \\ \frac{\partial u}{\partial n} = g & \text{on } \partial D, \\ |u(x)| \to 0 & \text{as } |x| \to \infty, \end{cases}$$

where $f \in \mathcal{C}_c^\infty(\mathbb{R}^d)$ is a source, and $g \in H^{-1/2}(\partial D)$ stands for boundary data.

- The variational formulation for this problem is: search for $u \in W_0^{1,-1}(\mathbb{R}^d)$ s.t.

$$\forall v \in W_0^{1,-1}(\mathbb{R}^d), \ \int_{\mathbb{R}^d \setminus \overline{D}} \nabla u \cdot \nabla v \, \mathrm{d}x = \int_{\mathbb{R}^d \setminus \overline{D}} fv \, \mathrm{d}x - \int_{\partial D} gv \, \mathrm{d}s.$$

- The data f and g have to satisfy the equilibrium condition in 2d:

$$\int_{\mathbb{R}^d \setminus \overline{D}} f \, dx - \int_{\partial D} g \, \mathrm{d}s = 0.$$

- This problem is well-posed by the Lax-Milgram theorem and the Poincaré Wirtinger's inequality.

Fixed point algorithms

- Let $(X, ||\cdot||_X)$ be a Banach space, and consider a function $F : X \to X$.
- We aim to find a fixed point $x^* \in X$ of F, i.e. one point such that:

$$x^* = F(x^*).$$

- The fixed point iteration method simply reads:

Initialization: Initial point x^0.

For $n = 0, \dots$ **convergence,** set $x^{n+1} = F(x^n)$.

Return x^n.

- This method converges under the quite restrictive assumption that F be a strict contraction:

$$\forall x, y \in X, ||F(x) - F(y)||_X \leq L||x - y||_X \text{ for some fixed } 0 < L < 1.$$

- Other, slightly less restrictive frameworks exist, such as that of the Krasnoselskii-Mann theorem.

Fixed point algorithms

- These conditions are rarely met in practice.
- The fixed point iteration method generally converges to one fixed point x^* of F (if any), provided the initial state x^0 is "close enough" to x^*.
- The fixed point method is usually more stable when relaxation is used.

Initialization: Initial point x^0.

For $n = 0, \dots$ **convergence,**

1. Choose a relaxation parameter $\alpha^n \in [0, 1)$;
2. set $x^{n+1} = \alpha x^n + (1 - \alpha^n) F(x^n)$.

Return x^n.

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Online resources I

- [Course] *Web page of the course, for demonstration programs* , `https://ljk.imag.fr/membres/Charles.Dapogny/coursoptim.html`.
- [FreeFem++] *Web page of the* `FreeFem` *project*, `https://freefem.org/`.