Optimization of the shape and topology of regions supporting boundary conditions

Eric Bonnetier[1], Carlos Brito-Pacheco[2], Charles Dapogny[2], Nicolas Lebbe[2,3], Edouard Oudet[2], Michael Vogelius[4]

[1] Institut Fourier, Université Grenoble Alpes, Grenoble, France
[2] Laboratoire Jean Kuntzmann, Université Grenoble Alpes, Grenoble, France
[3] CEA, Leti, Grenoble, France
[4] Department of Mathematics, Rutgers University, USA

27th March, 2024

Foreword (I)

- Shape and topology optimization techniques are ubiquitous in industry and academics.

- Usually in practice,

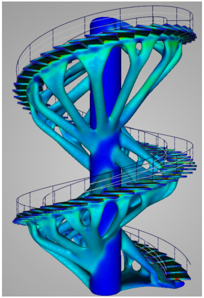
  - A domain $\Omega \subset \mathbb{R}^d$ is optimized, representing e.g. a mechanical structure, a fluid device.

  - The performance of Ω is evaluated by an objective function $J(\Omega)$.

  - $J(\Omega)$ is expressed in terms of the solution u_Ω to a boundary value problem posed on Ω.

  - The regions of $\partial\Omega$ supporting specific boundary conditions are not subject to optimization.

- We investigate a variant of this setting, where not only the shape Ω, but also the subsets of $\partial\Omega$ bearing boundary conditions are optimized.



Optimization of a staircase (courtesy of Ansys).

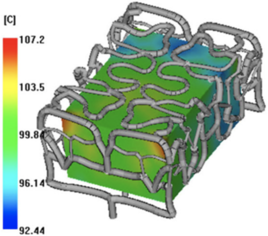
"Optimized" front-end of the Qatar National Convention Center.

Foreword (II)

Examples:

- In thermal conduction,
  - The temperature $u_\Omega : \Omega \to \mathbb{R}$ inside Ω is the solution to the conductivity equation;
  - Dirichlet b.c. account for a known profile,
  - Neumann b.c. represent an imposed heat flux.
- When Ω is a mechanical structure,
  - The displacement $u_\Omega : \Omega \to \mathbb{R}^d$ of Ω is solution to the linear elasticity system;
  - Ω is attached at the regions equipped with homogeneous Dirichlet b.c.
  - Neumann b.c. represent applied surface loads.
- Other applications arise in acoustics, in fluid mechanics, etc.

Optimization of the screws of a mandibular prosthesis [LaBa].



Optimized cooling process for a structure produced by molding [WeWuShi].

Contents

A model shape optimization problem (I)

- The considered shapes Ω are smooth, bounded domains in $\mathbb{R}^d$, with boundaries:

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

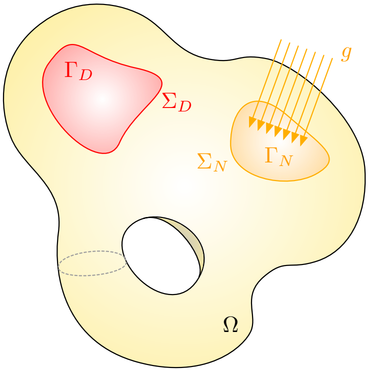
- We assume that $\overline{\Gamma_D} \cap \overline{\Gamma_N} = \emptyset$ and denote

$$\Sigma_D = \partial\Gamma_D, \text{ and } \Sigma_N = \partial\Gamma_N.$$

- The behavior of Ω is encoded in the solution $u_\Omega \in H^1(\Omega)$ to the conductivity equation:

$$\left\{ \begin{array}{rl} -\text{div}(\gamma \nabla u_\Omega) = f & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_\Omega}{\partial n} = 0 & \text{on } \Gamma, \\ \gamma \frac{\partial u_\Omega}{\partial n} = g & \text{on } \Gamma_N, \end{array} \right.$$

where
- γ is the conductivity of the medium
- $f \in L^2(\Omega)$ is a source (or a sink),
- $g \in L^2(\Gamma_N)$ is a heat flux.



A model shape optimization problem (II)

- We consider a shape optimization problem of the form

$$\boxed{\min_{\Omega} J(\Omega) \text{ s.t. } \; C(\Omega) \leq 0,}$$

where $J(\Omega)$ and $C(\Omega)$ are objective and constraint functions of the domain.

- The treatment of this task usually relies on the derivatives of $J(\Omega)$ and $G(\Omega)$ with respect to the domain, which can be accounted for in two different ways:
  - Shape derivatives account for "small" perturbations of the boundary of Ω;
  - Topological derivatives consider the nucleation of "small" holes inside Ω.

- We focus on a typical function of the domain, of the form

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

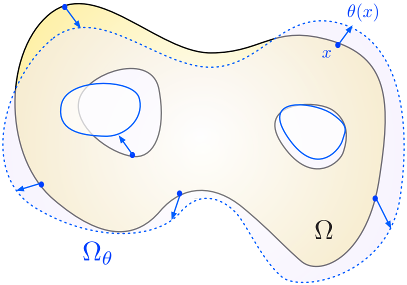
where $j : \mathbb{R} \to \mathbb{R}$ is smooth and satisfies suitable growth conditions.

Shape derivatives (I): definition

The method of Hadamard relies on variations of a shape $\Omega \subset \mathbb{R}^d$ of the form

$$\Omega_\theta := (\mathrm{Id} + \theta)(\Omega),$$

where $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ is a "small" vector field.



Definition 1.

The shape derivative of a function $J(\Omega)$ at a particular domain Ω is the Fréchet derivative at $\theta = 0$ of the underlying mapping

$$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \ni \theta \longmapsto J(\Omega_\theta) \in \mathbb{R}.$$

The following expansion holds:

$$J(\Omega_\theta) = J(\Omega) + J'(\Omega)(\theta) + \mathrm{o}(\theta), \text{ where } \frac{|\mathrm{o}(\theta)|}{||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}} \xrightarrow{\theta \to 0} 0.$$

Shape derivatives (II): a typical calculation

Most often, only the free region $\Gamma \subset \partial\Omega$ is optimized, i.e. deformations θ satisfy:

$$\theta \equiv 0 \text{ on } \Gamma_D \cup \Gamma_N.$$

Typical calculation of the derivative $J'(\Omega)(\theta)$ of $J(\Omega) = \int_\Omega j(u_\Omega)\,\mathrm{d}x$:

1. Using the implicit function theorem, one proves that the transported function

$$W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d) \ni \theta \mapsto \overline{u_\Omega}(\theta) := u_{\Omega_\theta} \circ (\mathrm{Id} + \theta) \in H^1(\Omega)$$

   is differentiable. Its derivative $\mathring{u}_\Omega(\theta) \in H^1(\Omega)$ – the Lagrangian derivative of u_Ω – is characterized as the solution to a variational problem.

2. Direct differentiation in the definition of $J(\Omega)$ then yields:

$$J'(\Omega)(\theta) = \int_\Omega \Big(\mathrm{div}(\theta) j(u_\Omega) + j'(u_\Omega)\mathring{u}_\Omega(\theta) \Big)\,\mathrm{d}x.$$

Shape derivatives (III): a typical calculation

❸ Thanks to the adjoint method, the "difficult" contribution of $\mathring{u}_\Omega(\theta)$ is eliminated from the expression of $J'(\Omega)(\theta)$, and a volume form is obtained:

$$J'(\Omega)(\theta) = \int_\Omega \Big(S(u_\Omega, p_\Omega) : \nabla\theta + R(u_\Omega, p_\Omega) \cdot \theta \Big) \, \mathrm{d}x,$$

where:

- The adjoint state p_Ω satisfies a boundary value problem similar to that for u_Ω;
- $R(u_\Omega, p_\Omega) : \Omega \to \mathbb{R}^d$, $S(u_\Omega, p_\Omega) : \Omega \to \mathbb{R}^{d \times d}$ are vector and matrix fields.

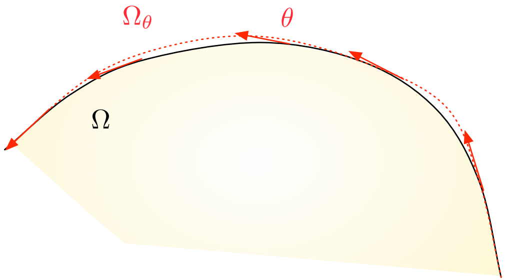
❹ *Assuming sufficient regularity from u_Ω and p_Ω (typically $H^2(\Omega)$)*, integration by parts in the volume form lead to a surface form for $J'(\Omega)(\theta)$:

$$J'(\Omega)(\theta) = \int_\Gamma v(u_\Omega, p_\Omega) \, \theta \cdot n \, \mathrm{d}s,$$

for a certain scalar field $v(u_\Omega, p_\Omega) : \Gamma \to \mathbb{R}$.

Shape derivatives (IV): structure

- (When available) The surface form highlights the fact that $J'(\Omega)(\theta)$ depends on the normal component of θ on Γ.



A tangential vector field θ, (i.e. $\theta \cdot n = 0$) only accounts for a convection of the shape Ω and $J'(\Omega)(\theta) = 0$.

- A descent direction for $J(\Omega)$ is readily supplied by the surface form of $J'(\Omega)(\theta)$:

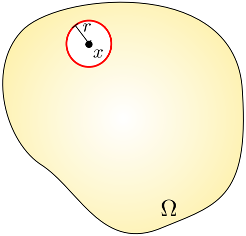
$$\theta = -v(u_\Omega, p_\Omega)n \ \Rightarrow J'(\Omega)(\theta) < 0.$$

Topological derivatives

The notion of topological derivative features variations of a shape $\Omega \subset \mathbb{R}^d$ of the form

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

where $x \in \Omega$, and $\varepsilon \ll 1$.



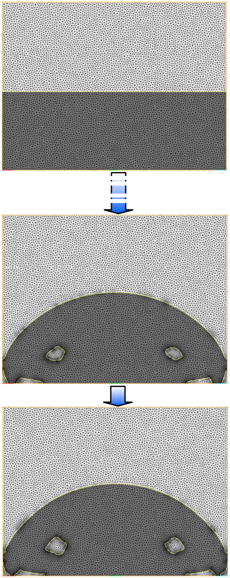
Definition 2.

The function $J(\Omega)$ has a topological derivative at Ω and at point $x \in \Omega$ if there exists $\mathrm{d}J_T(\Omega)(x) \in \mathbb{R}$ such that:

$$J(\Omega_{x,\varepsilon}) = J(\Omega) + \varepsilon^d \mathrm{d}J_T(\Omega)(x) + \mathrm{o}(\varepsilon^d).$$

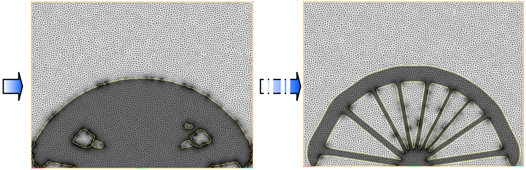
Remark Depending on the context, different rates may occur for $J(\Omega_{x,\varepsilon})$ as $\varepsilon \to 0$.

A representative shape and topology optimization workflow



A standard gradient strategy is used.

- At each iteration $n = 0, \dots,$ the shape Ω^n is equipped with a mesh $\mathcal{T}^n$.
- The finite element computations for u_{Ω^n} and p_{Ω^n} are performed on $\mathcal{T}^n$.
- A descent direction θ^n is obtained from $J'(\Omega^n)$.
- The mesh updates $\mathcal{T}^n \to \mathcal{T}^{n+1}$ rely on a mesh evolution algorithm [AlDaFre].
- At times, the topological derivative $\mathrm{d}J_T(\Omega)$ is calculated to nucleate a small hole inside Ω.



Goals of this work

Besides the shape Ω, We aim to optimize the repartition of the regions Γ_D and Γ_N of $\partial\Omega$ where homogeneous Dirichlet and inhomogeneous Neumann b.c. are applied, in two different ways:

1. We analyze the shape derivative of $J(\Omega)$ when deformations θ that do not vanish near Σ_D and Σ_N are allowed.

2. We consider "topological derivatives", accounting for singular changes in the type of applied b.c.:

   "How to account for the insertion of a "small" region ω_ε bearing homogeneous Dirichlet b.c. inside Γ?"

We consider again the model functional

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

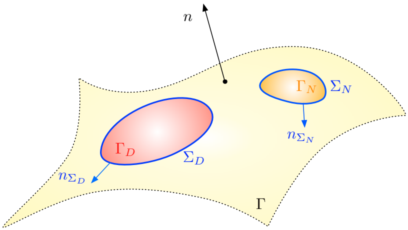
where $u_\Omega \in H^1(\Omega)$ is the solution to the conductivity equation.

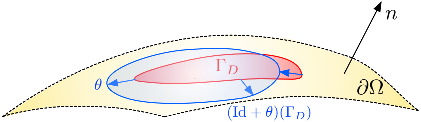
We aim to calculate the shape derivative $J'(\Omega)(\theta)$ when θ is either in

$$\Theta_{DN} := \left\{\theta \in \mathcal{C}^{2,\infty}(\mathbb{R}^d,\mathbb{R}^d),\ \ \theta = 0 \text{ on } \overline{\Gamma_N}\right\},$$

or in

$$\Theta_{NN} := \left\{\theta \in \mathcal{C}^{2,\infty}(\mathbb{R}^d,\mathbb{R}^d),\ \ \theta = 0 \text{ on } \overline{\Gamma_D}\right\},$$





Tangential deformations leave the room for modifications of Γ_D.

Notation

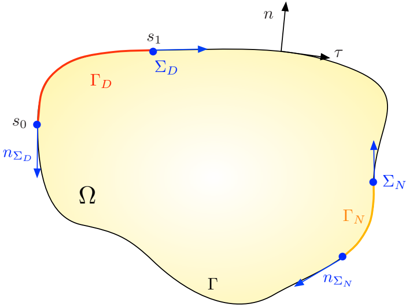
The notations u_Ω, $J(\Omega)$, ... only reflect dependences with respect to Ω, but the associated objects also depend on the repartition of Γ_D, Γ_N and Γ on $\partial\Omega$.

Setting (II)

- We focus on the most difficult situation where the Dirichlet – Neumann transition Σ_D is subject to optimization, i.e. deformations θ belong to Θ_{DN}.

- The analysis will often be simplified by the following assumptions:

(H)
- $d = 2$;
- The conductivity γ is constant in Ω;
- $\Sigma_D = \partial\Gamma_D = \{s_0, s_1\}$;
- $\partial\Omega$ is flat around s_0 and s_1.



Fractional Sobolev spaces on the boundary of Ω (I)

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain.

- For $0 < s < 1$, $H^s(\partial\Omega)$ is the space of $L^2(\partial\Omega)$ functions such that

$$||u||^2_{H^s(\partial\Omega)} := \int_{\partial\Omega} u^2 \,\mathrm{d}s + \int_{\partial\Omega}\int_{\partial\Omega} \frac{|u(x)-u(y)|^2}{|x-y|^{d-1+2s}} \,\mathrm{d}s(x)\mathrm{d}s(y) < \infty.$$

- For $0 < s < 1$, $H^{-s}(\partial\Omega)$ is the topological dual of $H^s(\partial\Omega)$.

Let Γ be a proper open and Lipschitz subset of $\partial\Omega$;

- For all $-1 < s < 1$, $H^s(\Gamma)$ is the space of restrictions $U|_\Gamma$ to Γ of functions of $H^s(\partial\Omega)$, equipped with the quotient norm:

$$||u||_{H^s(\Gamma)} := \inf\left\{ ||U||_{H^s(\partial\Omega)},\ \ U \in H^s(\partial\Omega),\ \ U|_\Gamma = u \right\}.$$

- For $-1 < s < 1$, $\widetilde{H}^s(\Gamma)$ is the subspace of $H^s(\Gamma)$ defined as, equivalently:
  - The space of elements $u \in H^s(\partial\Omega)$ with compact support inside $\overline{\Gamma}$;
  - The space of elements $u \in L^2(\Gamma)$ whose extension $\tilde{u}$ by 0 belongs to $H^s(\partial\Omega)$.

Fractional Sobolev spaces on the boundary of Ω (II)

For all $s > 0$, $\widetilde{H}^{-s}(\Gamma)$ $(H^{-s}(\Gamma))$ is the dual of $H^s(\Gamma)$ $(\widetilde{H}^s(\Gamma))$ for the duality:

$$\langle u, v\rangle_{\widetilde{H}^{-s}(\Gamma),H^s(\Gamma)} = \Big\langle \underbrace{\tilde{u}}_{\substack{\text{extension}\\ \text{of } u \text{ by } 0}} , \underbrace{V}_{\substack{\text{any extension}\\ \text{of } v \text{ to } \partial\Omega}} \Big\rangle_{H^{-s}(\partial\Omega),H^s(\partial\Omega)}.$$

Example: Let $u_\Omega \in H^1(\Omega)$ be the variational solution to the conductivity equation:

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

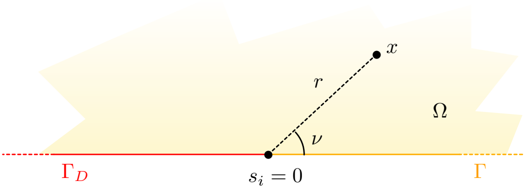
Then:

- $u_\Omega \in \widetilde{H}^{1/2}(\Gamma \cup \Gamma_N)$;
- $\gamma\frac{\partial u_\Omega}{\partial n} \in \widetilde{H}^{-1/2}(\Gamma_D \cup \Gamma_N)$.

About the regularity of u_Ω

- For any point $x \in \overline{\Omega} \setminus \Sigma_D \cup \Sigma_N$, there exists a neighborhood W of x in $\mathbb{R}^d$ such that u_Ω is in $H^2(\Omega \cap W)$ (smooth).
- u_Ω is weakly singular near Σ_D: let (H) hold and, without loss of generality, let V be a small enough neighborhood of s_i such that:

$$s_i = 0, \;\; \Omega \cap V = \{x \in V, \text{ s.t. } x_2 > 0\}, \text{ and } \Gamma_D \cap V = \{x \in V, \text{ s.t. } x_2 = 0, \; x_1 < 0\}.$$



Then, for any $\eta > 0$, $u_\Omega \in H^{3/2-\eta}(V)$ and

$$u_\Omega = u_r^i + c^i S^i \text{ on } \Omega \cap V, \text{ where } u_r^i \in H^2(\Omega \cap V), c_i \in \mathbb{R} \text{ and } S^i(r,\nu) = r^{\frac{1}{2}} \cos\left(\frac{\nu}{2}\right).$$

P. Grisvard, *Elliptic problems in nonsmooth domains*, SIAM, (2011).

Exact shape derivative

Proposition 1.

The function $J(\Omega)$ is shape differentiable and its shape derivative reads (volume form): for all $\theta \in \Theta_{DN}$,

$$J'(\Omega)(\theta) = \int_{\partial\Omega} (j(u_\Omega) - fp_\Omega)\theta \cdot n \, \mathrm{d}s - \int_\Omega j'(u_\Omega)\nabla u_\Omega \cdot \theta \, \mathrm{d}x + \int_\Omega (\nabla\gamma \cdot \theta)\nabla u_\Omega \cdot \nabla p_\Omega \mathrm{d}x$$
$$+ \int_\Omega \gamma((\mathrm{div}\theta)\mathrm{I} - \nabla\theta - \nabla\theta^T)\nabla u_\Omega \cdot \nabla p_\Omega \, \mathrm{d}x + \int_\Omega f\nabla p_\Omega \cdot \theta \, \mathrm{d}x,$$

where the adjoint state p_Ω is the $H^1(\Omega)$ solution to the problem:

$$\begin{cases} -\mathrm{div}(\gamma\nabla p_\Omega) = -j'(u_\Omega) & \text{in } \Omega, \\ p_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial p_\Omega}{\partial n} = 0 & \text{on } \Gamma_N \cup \Gamma. \end{cases}$$

Moreover, under the assumption (H), this rewrites (surface form):

$$J'(\Omega)(\theta) = \int_{\Gamma_D \cup \Gamma} \Big(j(u_\Omega) - fp_\Omega\Big)\theta \cdot n \, \mathrm{d}s - \int_{\Gamma_D} \frac{\partial p_\Omega}{\partial n}\frac{\partial u_\Omega}{\partial n}\theta \cdot n \, \mathrm{d}s$$
$$+ \int_\Gamma \frac{\partial u_\Omega}{\partial \tau}\frac{\partial p_\Omega}{\partial \tau}\theta \cdot n \, \mathrm{d}s + \frac{\pi}{4}\sum_{i=0,1} c_u^i c_p^i (\theta \cdot n_{\Sigma_D})(s_i).$$

Remarks

- A formal calculation of $J'(\Omega)(\theta)$ (with Céa's method) ignoring the weak singularity of u_Ω and p_Ω yields:
$$J'(\Omega)(\theta) = 0 \text{ if } \theta \cdot n = 0,$$
i.e. $J(\Omega)$ does not depend on the repartition of boundary conditions!

  $\Rightarrow$ The sensitivities of u_Ω and $J(\Omega)$ with respect to Γ_D are entirely encoded in the weak singularity of u_Ω (and p_Ω).

- The dependence of $J'(\Omega)(\theta)$ on the singularities of u_Ω and p_Ω makes its numerical evaluation awkward.

  $\Rightarrow$ Need to construct smooth approximations $u_{\Omega,\varepsilon}$ and $J_\varepsilon(\Omega)$ of u_Ω and $J(\Omega)$.

- Different (simpler) situations could be considered:
  - Transition homogeneous Neumann – inhomogeneous Neumann b.c.
  - Transition homogeneous Neumann – homogeneous Robin b.c. (for models of corrosion / Helmholtz)

The geodesic signed distance function

Let $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain.

- The geodesic distance $d^{\partial\Omega}(x,y)$ on $\partial\Omega$ between two points $x, y \in \partial\Omega$ is:

$$d^{\partial\Omega}(x,y) = \inf_{\substack{\gamma:[0,1]\to\partial\Omega, \\ \gamma(0)=x, \ \gamma(1)=y}} \ell(\gamma), \text{ where } \ell(\gamma) = \int_0^1 |\gamma'(t)| \, \mathrm{d}t.$$

- The geodesic distance $d^{\partial\Omega}(x,K)$ of $x \in \partial\Omega$ to a compact subset $K \subset \partial\Omega$ is:

$$d^{\partial\Omega}(x,K) = \inf_{y \in K} d^{\partial\Omega}(x,y).$$

- When the minimizer is unique in the above definition, it is denoted by $p_K(x)$ and called the projection of x onto K.

- The geodesic signed distance function $d_G^{\partial\Omega}$ to an open region $G \subset \partial\Omega$ is:

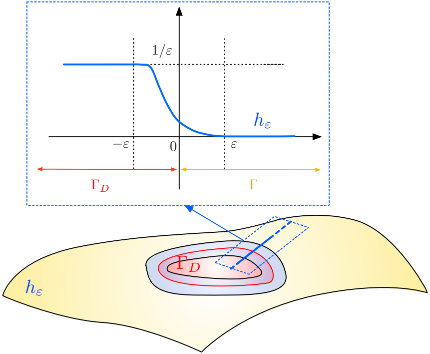
$$\forall x \in \partial\Omega, \quad d^{\partial\Omega}(x) = \begin{cases} -d^{\partial\Omega}(x,\partial G) & \text{if } x \in G, \\ 0 & \text{if } x \in \partial G, \\ d^{\partial\Omega}(x,\partial G) & \text{if } x \in \partial\Omega \setminus \overline{G}. \end{cases}$$

Remark "Many" basic properties of $d_G^{\partial\Omega}$ are mere adaptations of those of the "usual" signed distance function to a domain of $\mathbb{R}^d$.

An approximate optimization problem (I)

- Let the approximate conductivity equation:

$$\begin{cases} -\mathrm{div}(\gamma \nabla u_{\Omega,\varepsilon}) = f & \text{in } \Omega, \\ \gamma \frac{\partial u_{\Omega,\varepsilon}}{\partial n} + h_\varepsilon u_{\Omega,\varepsilon} = 0 & \text{on } \Gamma \cup \Gamma_D, \\ \gamma \frac{\partial u_{\Omega,\varepsilon}}{\partial n} = g & \text{on } \Gamma_N. \end{cases}$$



- $h_\varepsilon(x) := \frac{1}{\varepsilon} h\left(\frac{d^{\partial\Omega}_{\Gamma_D}(x)}{\varepsilon}\right)$ is made from a smooth profile $h : \mathbb{R} \to \mathbb{R}$ such that:

$$0 \leq h \leq 1, \quad \begin{cases} h \equiv 1 & \text{on } (-\infty, -1], \\ h(0) > 0, & \\ h \equiv 0 & \text{on } [1, \infty). \end{cases}$$

- Intuitively,
  - $h_\varepsilon = 0$ well inside Γ ($\approx$ homogeneous Neumann b.c.),
  - $h_\varepsilon = \frac{1}{\varepsilon} \approx \infty$ well inside Γ_D ($\approx$ homogeneous Dirichlet b.c.).

- For a fixed $\varepsilon > 0$, standard elliptic regularity implies that $u_{\Omega,\varepsilon}$ is smooth on $\overline{\Omega}$.

An approximate optimization problem (II)

Proposition 2.

The functional $J_\varepsilon(\Omega)$ is shape differentiable, with shape derivative (surface form):

$$\forall \theta \in \Theta_{DN}, \quad J_\varepsilon'(\Omega)(\theta) =$$

$$\int_{\Gamma \cup \Gamma_D} \left(j(u_{\Omega,\varepsilon}) - f p_{\Omega,\varepsilon} + \gamma \nabla_{\partial\Omega} u_{\Omega,\varepsilon} \cdot \nabla_{\partial\Omega} p_{\Omega,\varepsilon} - \gamma \frac{\partial u_{\Omega,\varepsilon}}{\partial n} \frac{\partial p_{\Omega,\varepsilon}}{\partial n} - \kappa p_{\Omega,\varepsilon} \frac{\partial u_{\Omega,\varepsilon}}{\partial n} \right) \theta \cdot n \, \mathrm{d}s$$

$$+ \frac{1}{\varepsilon^2} \int_{\Gamma \cup \Gamma_D} h'\left(\frac{d_{\Gamma_D}}{\varepsilon}\right) \Bigg(-\theta(p_{\Sigma_D}(x)) \cdot n_{\Sigma_D}(p_{\Sigma_D}(x)) +$$

$$\int_0^{d_{\Gamma_D}(x)} \Pi^{\partial\Omega}_{\sigma_x(t)}(\sigma_x'(t), \sigma_x'(t)) \, (\theta \cdot n)(\sigma_x(t)) \, \mathrm{d}t \Bigg) u_{\Omega,\varepsilon} p_{\Omega,\varepsilon} \, \mathrm{d}s(x),$$

where

- $\sigma_x(t) = \exp_{p_{\Sigma_D(x)}}(t n_{\Sigma_D}(p_{\Sigma_D}(x)))$ *is the geodesic curve between x and $p_{\Sigma_D}(x)$,*
- *The adjoint state $p_{\Omega,\varepsilon}$ is the unique solution in $H^1(\Omega)$ to the equation:*

$$\begin{cases} -\mathrm{div}(\gamma \nabla p_{\Omega,\varepsilon}) = -j(u_{\Omega,\varepsilon}) & \text{in } \Omega, \\ \gamma \frac{\partial p_{\Omega,\varepsilon}}{\partial n} + h_\varepsilon p_{\Omega,\varepsilon} = 0 & \text{on } \Gamma_D \cup \Gamma, \\ \gamma \frac{\partial p_{\Omega,\varepsilon}}{\partial n} = 0 & \text{on } \Gamma_N. \end{cases}$$

An approximate optimization problem (III)

Under Assumption (H),

- The function $u_{\Omega,\varepsilon}$ converges to u_Ω strongly in $H^1(\Omega)$: for any $0 < s < \frac{1}{4}$,

$$||u_{\Omega,\varepsilon} - u_\Omega||_{H^1(\Omega)} \leq C_s \varepsilon^s ||f||_{L^2(\Omega)}.$$

- As a result, for any given shape Ω, the approximate shape functional $J_\varepsilon(\Omega)$ converges to its exact counterpart $J(\Omega)$.

- Going further, the approximate shape derivative $J'_\varepsilon(\Omega)$ converges to its exact counterpart $J'(\Omega)$, i.e.:

$$\sup_{||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} \leq 1} |J'_\varepsilon(\Omega)(\theta) - J'(\Omega)(\theta)| = 0.$$

An example in thermal conduction (I)

- During cooling, the temperature u_Ω within a device $\Omega \subset \mathbb{R}^3$ satisfies:

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

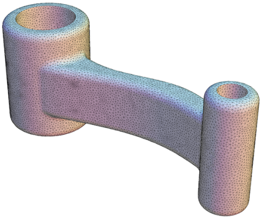
  where Γ_D is the region of $\partial\Omega$ in contact with cooling channels.

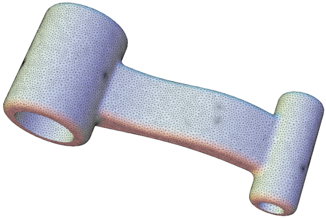
- We minimize the mean temperature:

$$\min T(\Omega) + \ell \mathrm{Per}(\Gamma_D), \text{ where}$$

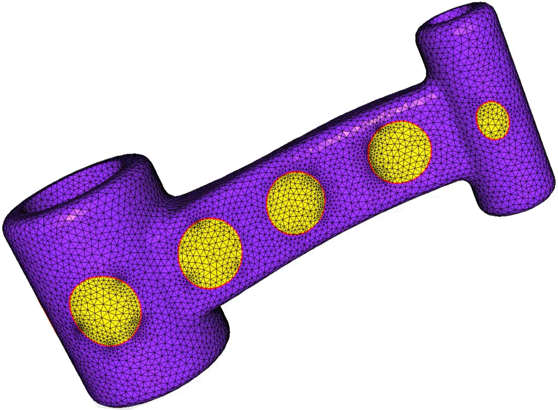
$$T(\Omega) = \frac{1}{|\Omega|} \int_\Omega u_\Omega \,\mathrm{d}x.$$

- Tangential deformations θ are used: only $\Gamma_D \subset \partial\Omega$ is optimized (not Ω).





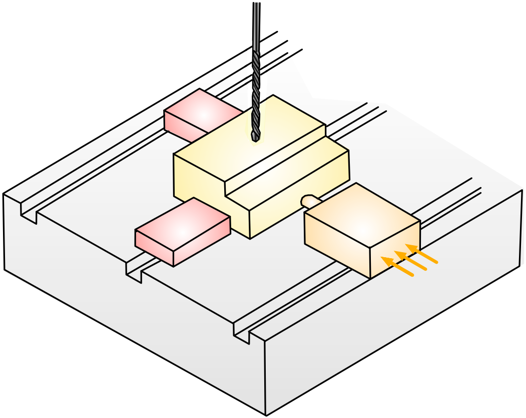
An example in thermal conduction (II)



Optimization of a fixture system (I)

During its construction, a mechanical structure $\Omega \subset \mathbb{R}^3$ is stilled by a clamp-locator system:

- Locators are regions of $\partial\Omega$ where the displacement is prevented;
- Clamps are regions where a surface load is applied to maintain the part.

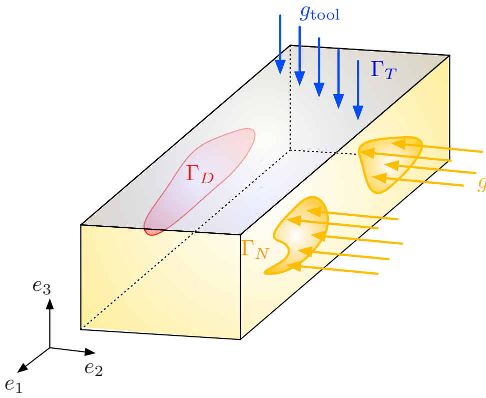


Optimization of a fixture system (II)

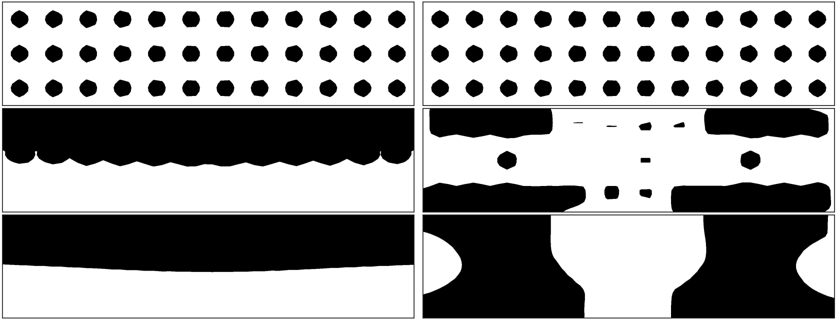
- Let $\Omega \subset \mathbb{R}^3$ be a fixed structure.
- A load g_{tool} is applied on $\Gamma_T \subset \partial\Omega$ by the machine tool.
- Ω is located on Γ_D, and clamped on Γ_N: a load g is applied.
- The displacement u_Ω of Ω is solution to the linear elasticity system.
- We aim to minimize the displacement of the structure,

$$J(\Omega) = \int_\Omega |u_\Omega|^2 \, \mathrm{d}x,$$

under constraints on the perimeters of Γ_D and Γ_N.

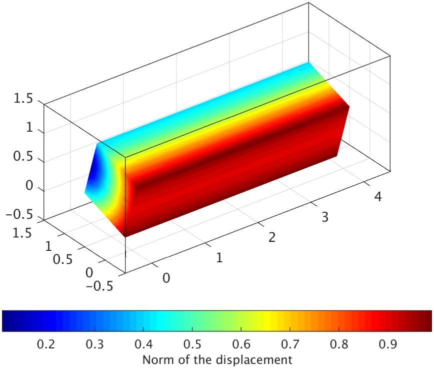


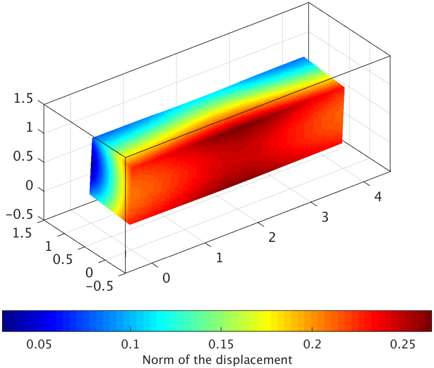
Optimization of a fixture system (III)



Designs of (left column) clamps and (right column) locators at iterations 1, 20 and 100.

Optimization of a fixture system (IV)





Deformed configurations of (left) the initial and (right) optimized designs.

Concurrent optimization of shape and boundary conditions (I)

- The design of an elastic force inverter is optimized.

- We minimize the least-square functional

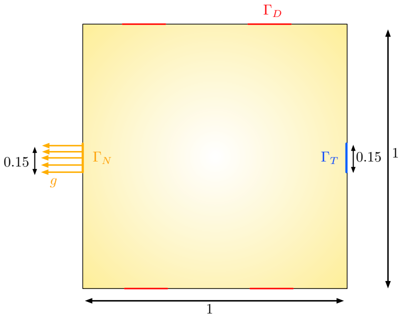
$$J(\Omega) = \alpha \int_{\Gamma_T} |u_\Omega - u_T|^2 \, \mathrm{d}s - \beta \int_{\Gamma_N} u_1 \, \mathrm{d}s,$$

  where

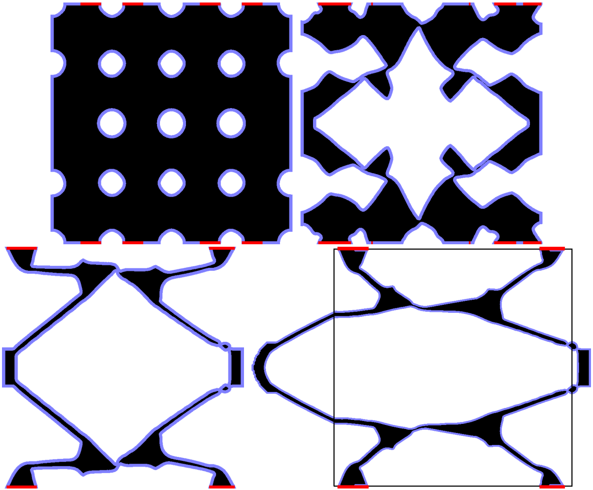
  - The displacement u_Ω is expected to match a target $u_T = (1, 0)$ on Γ_T,
  - The displacement u_1 of Ω to the right is penalized on Γ_N:

- We concurrently optimize the shape Ω and the fixation region $\Gamma_D \subset \partial\Omega$.

- A constraint on the perimeter of Γ_D is added.

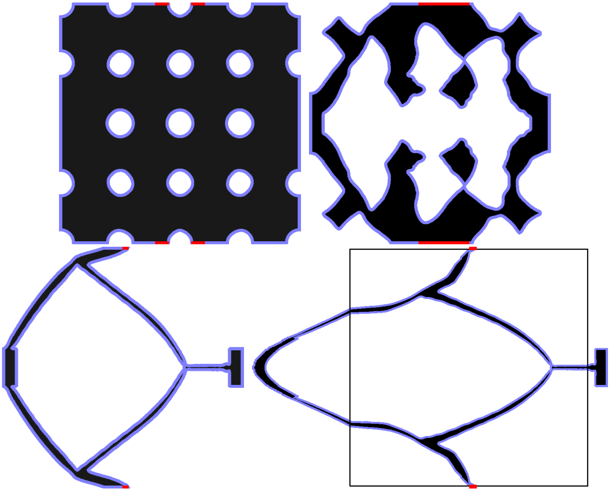


Concurrent optimization of shape and boundary conditions (II)



Concurrent optimization of the shape and the fixation regions of the force inverter, with an initial configuration for Γ_D *composed of* 8 *line segments.*

Concurrent optimization of shape and boundary conditions (III)



Concurrent optimization of the shape and the fixation regions of the force inverter, with an initial configuration for Γ_D composed of 4 line segments.

Foreword

- We inquire about the sensitivity of u_Ω – and that of a related quantity of interest $J(\Omega)$ – with respect to a "small" singular perturbation of the b.c. for u_Ω.
- This study leverages techniques from the field of asymptotic analysis.

These issues raises questions of two sorts:

- At the theoretical level, what is the general structure of the perturbed field?
- For a particular geometry of the inclusion set ω_ε, what is the precise asymptotic expansion of u_ε and a related quantity of interest?

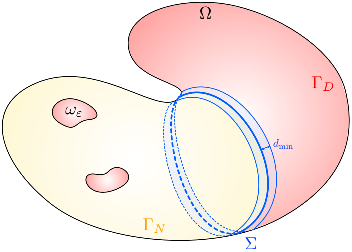
We focus on the situation of the replacement of homogeneous Neumann b. c. by homogeneous Dirichlet b. c.

- Ω is a smooth bounded domain in $\mathbb{R}^d$, $d = 2, 3$;
- Its boundary is decomposed as

$$\partial\Omega = \Gamma_D \cup \Gamma_N, \ \ \Gamma_D \cap \Gamma_N = \emptyset.$$

- The ω_ε are open, Lipschitz subsets of $\partial\Omega$;
- They are contained in Γ_N, and stay well-separated from $\Sigma := \overline{\Gamma_D} \cap \overline{\Gamma_N}$:

$$\exists d_{\min} > 0 \text{ s.t. } \forall\ \varepsilon > 0, \quad \text{dist}(\omega_\varepsilon, \Sigma) \geq d_{\min}.$$



The background and perturbed potentials $u_0 = u_\Omega$ and $u_\varepsilon \in H^1(\Omega)$ are solution to:

$$\left\{ \begin{array}{ll} -\text{div}(\gamma \nabla u_\Omega) = f & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_\Omega}{\partial n} = 0 & \text{on } \Gamma_N, \end{array} \right. \quad \text{and} \quad \left\{ \begin{array}{ll} -\text{div}(\gamma \nabla u_\varepsilon) = f & \text{in } \Omega, \\ u_\varepsilon = 0 & \text{on } \Gamma_D \cup \omega_\varepsilon, \\ \gamma \frac{\partial u_\varepsilon}{\partial n} = 0 & \text{on } \Gamma_N \setminus \overline{\omega_\varepsilon}. \end{array} \right.$$

The Green's function of the background problem

- For a fixed $x \in \Omega$, the Green's function $y \mapsto N(x,y)$ of the background problem is the solution to:

$$\begin{cases} -\mathrm{div}_y(\gamma(y)\nabla_y N(x,y)) = \delta_{y=x} & \text{in } \Omega, \\ N(x,y) = 0 & \text{for } y \in \Gamma_D, \\ \gamma(y)\frac{\partial N}{\partial n_y}(x,y) = 0 & \text{for } y \in \Gamma_N. \end{cases}$$

- The solution to the boundary value problem

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

  reads:

$$u(x) = \int_\Omega N(x,y) f(y) \, \mathrm{d}y.$$

- *Physically*, $N(x,\cdot)$ is the response of the medium to a point source at x.
- $N(x,y)$ is symmetric in its arguments: $N(x,y) = N(y,x)$.
- $N(x,y)$ can be constructed from the fundamental solution of the Laplace operator.

The capacity of a subset of $\mathbb{R}^d$ (I)

The relevant quantity to measure the "smallness" of ω_ε in this context is the capacity [HenPi] [Lan].

Definition 3.

The capacity $\text{cap}(E)$ *of an arbitrary subset* $E \subset \mathbb{R}^d$ *is defined by:*

$$\text{cap}(E) = \inf \left\{ ||v||^2_{H^1(\mathbb{R}^d)}, \;\; v(x) \geq 1 \textit{ a.e. on an open neighborhood of } E \right\}.$$

Intuition: $\text{cap}(E)$ is the energy of the function $v : \mathbb{R}^d \to \mathbb{R}$ such that:

- v equals 1 on E;
- v "tends to 0 at ∞";
- v is harmonic on $\mathbb{R}^d \setminus E$.

A. Henrot and M. Pierre, *Shape Variation and Optimization*, EMS Tracts in Mathematics, Vol. 28, (2018).

N. S. Landkof, *Foundations of modern potential theory*, Vol. 180, Springer, (1972).

The capacity of a subset of $\mathbb{R}^d$ (II): example

Let $\mathbb{D}_\varepsilon \subset \mathbb{R}^d$ be defined by:

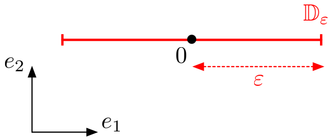
$$\mathbb{D}_\varepsilon = \left\{ x = (x_1, \ldots, x_{d-1}, 0) \in \mathbb{R}^d, \;\; |x| < \varepsilon \right\},$$

i.e.

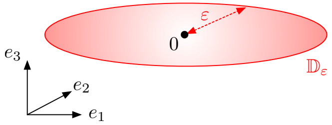
- $\mathbb{D}_\varepsilon$ is a segment with length 2ε if $d = 2$;
- $\mathbb{D}_\varepsilon$ is a planar disk with radius ε if $d = 3$.

The capacity of $\mathbb{D}_\varepsilon$ satisfies:

- If $d = 2$, $\mathrm{cap}(\mathbb{D}_\varepsilon) \le \frac{C_2}{|\log \varepsilon|}$;
- If $d = 3$, $\mathrm{cap}(\mathbb{D}_\varepsilon) \le C_3 \varepsilon$.



$\mathbb{D}_\varepsilon$ when $d = 2$



$\mathbb{D}_\varepsilon$ when $d = 3$

A general structure formula

Theorem 3.

Let ω_ε be such that $\mathrm{cap}(\omega_\varepsilon) \to 0$ as $\varepsilon \to 0$. Then there exists a subsequence, still denoted by ε, and a Radon measure μ on $\partial\Omega$, such that for any point $x \in \Omega$:

$$u_\varepsilon(x) = u_\Omega(x) - \mathrm{cap}(\omega_\varepsilon) \int_{\partial\Omega} u_\Omega(y)\gamma(y)N(x,y)\,\mathrm{d}\mu(y) + \mathrm{o}(\mathrm{cap}(\omega_\varepsilon)).$$

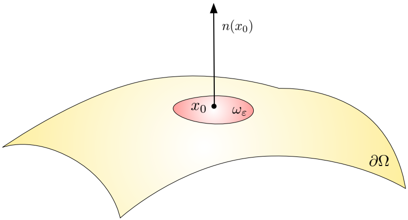
In this formula,

- *The measure μ is non negative and non trivial; it depends only on the subsequence ω_ε, Ω, and Γ_N;*
- *The support of μ lies inside any compact subset $K \subset \partial\Omega$ containing the ω_ε for $\varepsilon > 0$ small enough;*
- *The remainder $\mathrm{o}(\mathrm{cap}(\omega_\varepsilon))$ is uniform when x lies in compact subsets of Ω.*

Asymptotic formulas for quantities of interest

A more specific situation about the nature of ω_ε is considered:

- ω_ε is a surfacic disk with center $x_0 \in \partial\Omega$ and radius ε;
- It is contained in Γ_N.



The background and perturbed potentials $u_0 = u_\Omega$ and u_ε are the $H^1(\Omega)$ solutions to:

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

We look for an explicit asymptotic expansion of u_ε as $\varepsilon \to 0$.

Theorem 4.

The following asymptotic expansion holds, at any point $x \in \overline{\Omega}$, $x \notin \Sigma \cup \{0\}$:

$$u_\varepsilon(x) = u_\Omega(x) - \frac{\pi}{|\log \varepsilon|}\gamma(x_0)u_\Omega(x_0)N(x,x_0) + \mathrm{o}\left(\frac{1}{|\log \varepsilon|}\right) \quad \textit{if} \quad d = 2,$$

and

$$u_\varepsilon(x) = u_\Omega(x) - 4\varepsilon\gamma(x_0)u_\Omega(x_0)N(x,x_0) \quad \textit{if } d = 3,$$

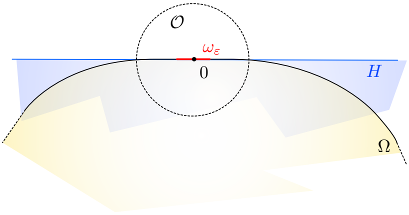
where $N(x,y)$ *is the Green's function of the background problem.*

Asymptotic formulas for the potential

Sketch of proof:

For simplicity, we assume that

- The space dimension is $d = 3$;
- $x_0 = 0$;
- $\partial\Omega$ is completely flat near 0.
- γ is constant near 0.



The error $r_\varepsilon := u_\varepsilon - u_\Omega \in H^1(\Omega)$ is the solution to:

$$\begin{cases} -\mathrm{div}(\gamma \nabla r_\varepsilon) = 0 & \text{in } \Omega, \\ r_\varepsilon = 0 & \text{on } \Gamma_D, \\ r_\varepsilon = -u_\Omega & \text{on } \omega_\varepsilon, \\ \gamma \frac{\partial r_\varepsilon}{\partial n} = 0 & \text{on } \Gamma_N \setminus \overline{\omega_\varepsilon}. \end{cases}$$

Asymptotic formulas for the potential

Step 1: We represent $r_\varepsilon(x)$ at $x \neq 0$ in terms of the values of r_ε inside ω_ε.

Using the Green's function $N(x,y)$ of the background problem,

$$\begin{aligned}
r_\varepsilon(x) &= -\int_\Omega \mathrm{div}_y(\gamma \nabla_y N(x,y)) r_\varepsilon(y)\,\mathrm{d}y \\
&= -\int_{\partial\Omega} \underbrace{\gamma \frac{\partial N}{\partial n_y}(x,y)}_{=0 \text{ on } \Gamma_N} \underbrace{r_\varepsilon(y)}_{=0 \text{ on } \Gamma_D} \,\mathrm{d}s(y) + \int_\Omega \gamma \nabla_y N(x,y)\cdot \nabla r_\varepsilon(y)\,\mathrm{d}y \\
&= \int_{\partial\Omega} \underbrace{\gamma \frac{\partial r_\varepsilon}{\partial n}(y)}_{=0 \text{ on } \Gamma_N \setminus \overline{\omega_\varepsilon}} \underbrace{N(x,y)}_{=0 \text{ on } \Gamma_D} \,\mathrm{d}s(y) - \int_\Omega \underbrace{\mathrm{div}(\gamma \nabla r_\varepsilon)(y)}_{=0} N(x,y)\,\mathrm{d}y \\
&= \int_{\omega_\varepsilon} \gamma \frac{\partial r_\varepsilon}{\partial n}(y) N(x,y)\,\mathrm{d}s(y)
\end{aligned}$$

and introducing $\varphi_\varepsilon(z) := \varepsilon^{d-1}\left(\gamma \frac{\partial r_\varepsilon}{\partial n}\right)(\varepsilon z) \in \widetilde{H}^{-1/2}(\mathbb{D}_1)$, we obtain:

$$\boxed{r_\varepsilon(x) = \int_{\mathbb{D}_1} \varphi_\varepsilon(z) N(x, \varepsilon z)\,\mathrm{d}s(z).}$$

Step 2: We characterize φ_ε by an integral equation.

Letting x approach ω_ε and replacing x with εx, $x \in \mathbb{D}_1$, this becomes:

$$\forall x \in \mathbb{D}_1, \qquad \underbrace{r_\varepsilon(\varepsilon x)}_{=-u_\Omega(\varepsilon x)} = \int_{\mathbb{D}_1} \varphi_\varepsilon(z) N(\varepsilon x, \varepsilon z)\,\mathrm{d}s(z).$$

Hence,

$$\forall x \in \mathbb{D}_1, \qquad \int_{\mathbb{D}_1} \varphi_\varepsilon(z) N(\varepsilon x, \varepsilon z)\,\mathrm{d}s(z) = -u_\Omega(0) + \mathrm{o}(1).$$

Since $\partial\Omega$ is flat near 0, we can replace $N(\varepsilon x, \varepsilon z)$ with $L(\varepsilon x, \varepsilon z)$, where

$$L(x,y) = \frac{1}{\gamma}\Big(G(x,y) + G(x,\widetilde{y})\Big), \quad G(x,y) = \frac{1}{4\pi}\frac{1}{|x-y|} \text{ and } \widetilde{y} := (y_1, \ldots y_{d-1}, -y_d)$$

is the Green's function of the lower half-space H. Eventually:

$$\boxed{\frac{1}{2\pi}\int_{\mathbb{D}_1} \frac{1}{|x-z|}\varphi_\varepsilon(z)\,\mathrm{d}s(z) = -\varepsilon\gamma u_\Omega(0) + \mathrm{o}(\varepsilon).}$$

Step 3: We solve this integral equation.

The solution to this equation is known as an equilibrium distribution:

$$\varphi_\varepsilon(z) = -\frac{2\varepsilon\gamma u_\Omega(0)}{\pi\sqrt{1-|x|^2}} + \mathrm{o}(\varepsilon).$$

In particular,

$$\int_{\mathbb{D}_1} \varphi_\varepsilon(z)\,\mathrm{d}s(z) = -4\gamma\varepsilon u_\Omega(0) + \mathrm{o}(\varepsilon).$$

Step 4: We pass to the limit in the representation formula for $r_\varepsilon(x)$.

The Lebesgue dominated convergence theorem yields:

$$\begin{aligned} r_\varepsilon(x) = \int_{\mathbb{D}_1} \varphi_\varepsilon(z) N(x, \varepsilon z)\,\mathrm{d}s(z) = \left(\int_{\mathbb{D}_1} \varphi_\varepsilon(z)\,\mathrm{d}s(z)\right) N(x,0) + \mathrm{o}(\varepsilon) \\ = -4\varepsilon\gamma u_\Omega(0) N(x,0) + \mathrm{o}(\varepsilon). \end{aligned}$$

□

Asymptotic formulas for a quantity of interest

Let us introduce the quantity of interest depending on u_ε:

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

i.e. $J(\varepsilon)$ is a version of $J(\Omega)$ where the boundary conditions of u_Ω are perturbed.

Corollary 5.

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

$$\text{If } d = 2, \quad J(\varepsilon) = J(0) + \frac{\pi}{|\log\varepsilon|}\gamma(x_0)u_\Omega(x_0)p_\Omega(x_0) + \mathrm{o}\left(\frac{1}{|\log\varepsilon|}\right),$$

and

$$\text{If } d = 3, \quad J(\varepsilon) = J(0) + 4\varepsilon\gamma(x_0)u_\Omega(x_0)p_\Omega(x_0) + \mathrm{o}(\varepsilon),$$

where p_Ω is the unique solution in $H^1(\Omega)$ to the boundary value problem:

$$\begin{cases} -\mathrm{div}(\gamma\nabla p_\Omega) = -j'(u_\Omega) & \text{in } \Omega, \\ p_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma\frac{\partial p_\Omega}{\partial n} = 0 & \text{on } \Gamma_N. \end{cases}$$

Sketch of proof (in the case $d = 3$):

The Lebesgue dominated convergence theorem yields

$$\frac{J(\varepsilon) - J(0)}{\varepsilon} = \int_\Omega \frac{j(u_\varepsilon) - j(u_\Omega)}{\varepsilon} \, \mathrm{d}x \xrightarrow{\varepsilon \to 0} -4\gamma(x_0) u_0(x_0) \int_\Omega j'(u_\Omega(x)) N(x, x_0) \, \mathrm{d}x.$$

Besides, by the definition of the Green's function and its symmetry,

$$p_\Omega(x_0) = -\int_\Omega j'(u_\Omega(y)) N(y, x_0) \, \mathrm{d}y.$$

□

Numerical example (I)

- We revisit the example in cooling.
- The temperature u_Ω within Ω satisfies:

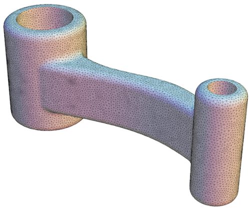
$$\begin{cases} -\mathrm{div}(\gamma \nabla u_\Omega) = f & \text{in } \Omega, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma \frac{\partial u_\Omega}{\partial n} = 0 & \text{on } \partial\Omega \setminus \overline{\Gamma_D}. \end{cases}$$

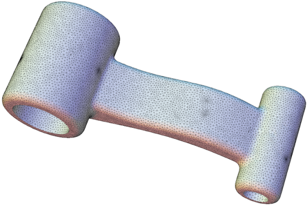
- The mean temperature is minimized:

$$\min T(\Omega) + \ell \mathrm{Per}(\Gamma_D), \text{ where}$$

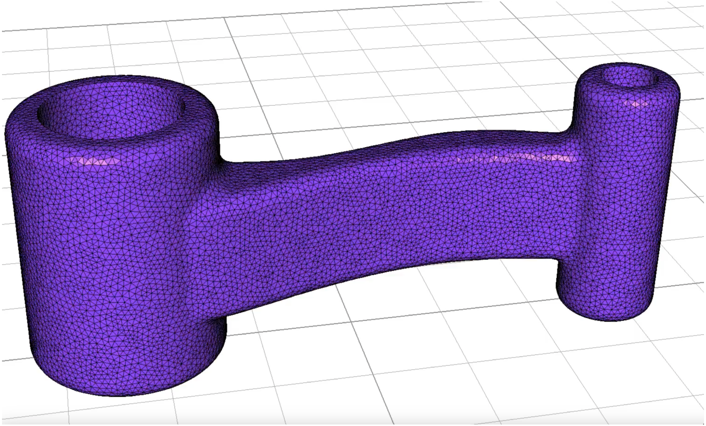
$$T(\Omega) = \frac{1}{|\Omega|} \int_\Omega u_\Omega \, \mathrm{d}x.$$

- Only tangential deformations θ are considered in the use of shape derivatives.
- Occasionally, a small Dirichlet region is nucleated inside $\partial\Omega \setminus \overline{\Gamma_D}$ thanks to the previous topological derivative.





Numerical example (II)



A word of advertisement

- All the numerical realizations are based on open-source libraries.
- A webpage gathering lecture notes, slides, demonstration codes, etc.

https://membres-ljk.imag.fr/Charles.Dapogny/tutosto.html

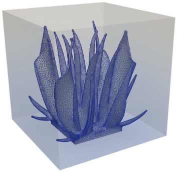
https://membres-ljk.imag.fr/Charles.Dapogny/tutosto.html

Shape and topology optimization: online resources

The discipline of shape and topology optimization has aroused a growing enthusiasm among mathematicians, physicists and engineers since the seventies, fostered by its impressive technological and industrial achievements. Nowadays, problems pertaining to fields so diverse as mechanical engineering, fluid mechanics or quantum chemistry are currently tackled with such techniques, and raise new, challenging issues.

This webpage gather useful resources of various nature, with the aim to popularize this subject and disseminate possible numerical implementations. In particular, you will find:

- Lecture notes and review articles.
- Slides and records of graduate courses.
- Open source implementations, ranging from simple, educational toy codes, to more involved frameworks allowing to deal with challenging personal test cases.
- Useful links to similar resources, emanating from other researchers.



Pedagogical articles and presentations

Article in the "Gazette des mathématiciens"	Large-audience presentation in prep. school	Review chapter about level set based shape optimization

Thank you for your attention!

References I

[AlDaFre] G. Allaire, C. Dapogny, and P. Frey, *Shape optimization with a level set based mesh evolution method*, Computer Methods in Applied Mechanics and Engineering, 282 (2014), pp. 22–53.

[BonDaVo] E. Bonnetier, C. Dapogny, and M. S. Vogelius, *Small perturbations in the type of boundary conditions for an elliptic operator*, Journal de Mathématiques Pures et Appliquées, 167 (2022), pp. 101–174.

[BriDa] C. Brito-Pacheco and C. Dapogny, *Body-fitted tracking within a surface via a level set based mesh evolution method*, submitted, (2023).

[DaLeOu] C. Dapogny, N. Lebbe and E. Oudet, *Optimization of the shape of regions supporting boundary conditions*, Numer. Math., 146, (2020), pp. 51–104.

[FreSo] G. Fremiot and J. Sokolowski, *Shape sensitivity analysis of problems with singularities*, Lecture notes in pure and applied mathematics, (2001), pp. 255–276.

[Gri] P. Grisvard, *Elliptic problems in nonsmooth domains*, SIAM, (2011).

References II

[HenPi] A. Henrot and M. Pierre, *Shape Variation and Optimization*, EMS Tracts in Mathematics, Vol. 28, (2018).

[Lan] N. S. Landkof, *Foundations of modern potential theory*, Vol. 180, Springer, (1972).

[LaBa] J. J. Lang, M. Bastian, P. Foehr, M. Seebach, et al, *Improving mandibular reconstruction by using topology optimization, patient specific design and additive manufacturing?—A biomechanical comparison against miniplates on human specimen*. Plos one, 16(6),(2021), e0253002.

[RaAlOr] L. Rakotondrainibe, G. Allaire and P. Orval, *Topology optimization of connections in mechanical systems*, Struct. and Multidisc. Optim., 61(6), (2020), pp. 2253–2269.

[WeWuShi] Z. Wei, J. Wu, N. Shi et al, *Review of conformal cooling system design and additive manufacturing for injection molds*, Math. Biosci. Eng, 17(5), (2020), pp. 5414–5431.