A brief overview of shape and topology optimization, with a few applications in electromagnetism

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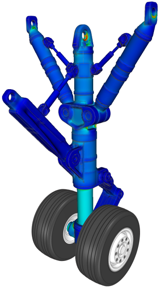
Foreword: Shape and topology optimization

- Shape optimization aims to minimize a function of the domain.
- Such problems can be traced back to the early human history...
- ... The needs to realize energy savings and get free from fossile fuels have aroused much enthusiasm for the discipline.
- It heralds promising applications in varied physical contexts.
- This presentation broaches a few of its specific issues:
  - *Modeling:* Choice of adequate design variables, of a relevant physical model.
  - *Theory:* Calculation of derivatives with respect to the design.
  - *Numerical implementation:* Efficient design updates (remeshing), large scale solution of physical equations.

Hooke's principle: "As hangs the flexible chain, so but inverted stands the rigid arch".



Optimized design of a landing gear (courtesy of Ansys*).*

Disclaimer

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- This presentation is by no means exhaustive, and it is strongly biased by the knowledge and experience of the author.
- See the References for more elaborate discussions.

A general panorama

A shape and topology optimization problem reads:

$$\min_{h \in \mathcal{U}_{\text{ad}}} J(h) \text{ s.t. } G(h) = 0. \qquad (\mathcal{P})$$

In this formulation:

- The design variable h is sought within a set $\mathcal{U}_{\text{ad}}$ of admissible designs.
- $J(h)$ is an objective function.
- $G(h) = (G_1(h), \ldots, G_p(h))$ is a collection of p (equality) constraints.
- $J(h)$ or some of the $G_i(h)$ depend on h via a state u_h, solution in a functional space V to a physical boundary value problem:

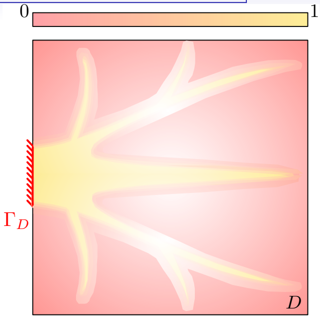
$$\text{Search for } u_h \in V \text{ s.t. } \mathcal{F}(h, u_h) = 0. \qquad (BVP)$$

This generic formulation encompasses multiple frameworks.

Let $D \subset \mathbb{R}^d$ be a thermal cavity;

- The temperature is fixed to 0 on $\Gamma_D \subset \partial D$.
- The remaining boundary $\partial D \setminus \overline{\Gamma_D}$ is insulated.
- A source $f : D \to \mathbb{R}$ is acting in the medium.
- The design variable $h : D \to [0,1]$ is related to the distribution of conducting material inside D:

$$\gamma_h(x) = \alpha + (\beta - \alpha)h(x), \text{ for some } 0 < \alpha \leq \beta.$$



The temperature $u_h : D \to \mathbb{R}$ is the solution to the conductivity equation:

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

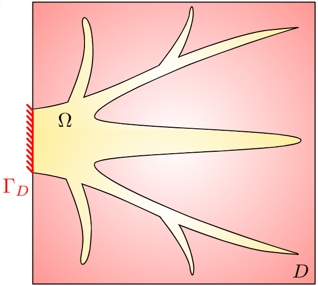
We minimize the mean temperature in D for a given amount V_T of material:

$$J(h) = \frac{1}{|D|} \int_D u_h \, \mathrm{d}x, \text{ and } G(h) = \int_D h \, \mathrm{d}x - V_T.$$

... and its shape optimization counterpart

- Concrete manufacturing processes cannot assemble arbitrary conductivities γ_h.
- Realistic patterns include distributions of two materials with conductivities α, β within D.
- The design variable h is now the shape $\Omega \subset D$ of the phase β, and the induced conductivity is:

$$\forall x \in D, \quad \gamma_\Omega(x) = \begin{cases} \beta & \text{if } x \in \Omega, \\ \alpha & \text{otherwise.} \end{cases}$$



The temperature u_Ω inside D is the solution to the two-phase conductivity equation:

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

The considered objective and constraint functions read:

$$J(\Omega) = \frac{1}{|D|} \int_D u_\Omega \, \mathrm{d}x, \text{ and } G(\Omega) = \mathrm{Vol}(\Omega) - V_T, \ \mathrm{Vol}(\Omega) := \int_\Omega \mathrm{d}x.$$

In structure mechanics, the shape is a bounded domain $\Omega \subset \mathbb{R}^d$, which is:

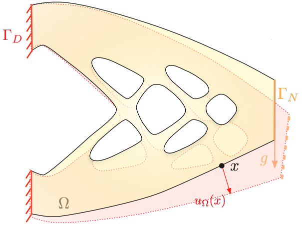
- Fixed on a part Γ_D of its boundary,
- Submitted to surface loads g, applied on another region $\Gamma_N \subset \partial\Omega$, $\Gamma_D \cap \Gamma_N = \emptyset$.

The displacement $u_\Omega : \Omega \to \mathbb{R}^d$ is the vector field governed by the linear elasticity system:

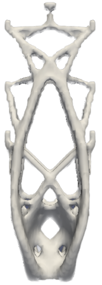
$$\left\{ \begin{array}{rcll} -\mathrm{div}(Ae(u_\Omega)) & = & 0 & \text{in } \Omega, \\ u_\Omega & = & 0 & \text{on } \Gamma_D, \\ Ae(u_\Omega)n & = & g & \text{on } \Gamma_N, \\ Ae(u_\Omega)n & = & 0 & \text{on } \Gamma, \end{array} \right. ,$$

where $e(u) = \frac{1}{2}(\nabla u^T + \nabla u)$ is the strain tensor, and A is the Hooke's law of the material:

$$\forall e \in \mathcal{S}_d(\mathbb{R}), \;\; Ae = 2\mu e + \lambda \mathrm{tr}(e)\mathrm{I}.$$



The linear elasticity model



Optimized design of a pylon

In this context, the objective function $J(\Omega)$ could be:

- The work of the external loads g or compliance $C(\Omega)$ of Ω:

$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega)\,\mathrm{d}x = \int_{\Gamma_N} g.u_\Omega\,\mathrm{d}s$$

- A least-square error between u_Ω and a target displacement $u_T \in H^1(\Omega)^d$ (useful when designing micro-mechanisms):

$$D(\Omega) = \left(\int_\Omega k(x) |u_\Omega - u_T|^\alpha \mathrm{d}x \right)^{\frac{1}{\alpha}},$$

  where α is a fixed parameter, and $k(x)$ is a weight factor.

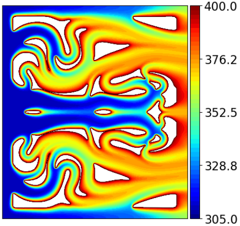
Such problems usually features a constraint on the volume ($\approx$ mass) of the shape:

$$G(\Omega) = \mathrm{Vol}(\Omega) - V_T, \text{ where } V_T \text{ is a target.}$$

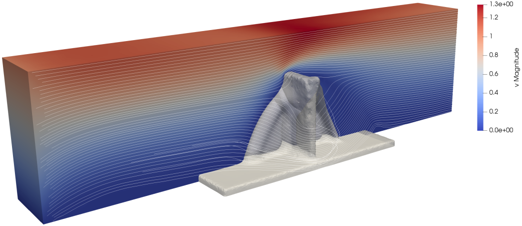
A wide variety of applications beyond

Optimal design has recently aroused burning issues in such diverse fields as:

- Fluid mechanics: external aerodynamics, fluid transport, mixing devices, etc.

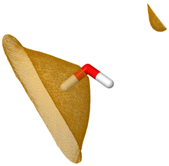


Optimized 2d section of a heat exchanger.

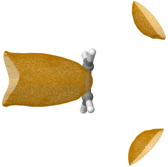


Optimized shape of a solid obstacle to a fluid flow.

- Quantum chemistry, with the theory of Maximum Probability Domains:



Maximum probability domain for the H_2O molecule.

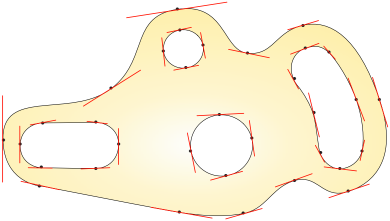


Maximum probability domain for the C_2H_4 molecule.

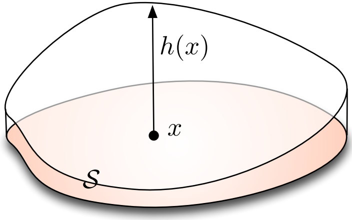
- Electromagnetism: electric machines, current sensors, photonic crystals, etc.

Parametric optimization (I)

The considered designs h are described by a collection of parameters $\{p_i\}_{i=1,\dots,N}$, typically thicknesses, curvature radii, etc...



Description of a mechanical part via the control points of a CAD model.



Parametrization of a plate with cross-section $\mathcal{S}$ via the thickness function $h : \mathcal{S} \to \mathbb{R}$.

Parametric optimization (II)

- The parameters describing shapes are the design variables, and the shape optimization problem rewrites:

$$\min_{\{p_i\}\in\mathcal{P}_{\textbf{ad}}} J(p_1, ..., p_N) \text{ s.t. } G(p_1, \ldots, p_N) = 0,$$

where $\mathcal{P}_{\text{ad}}$ is a set of admissible parameters.

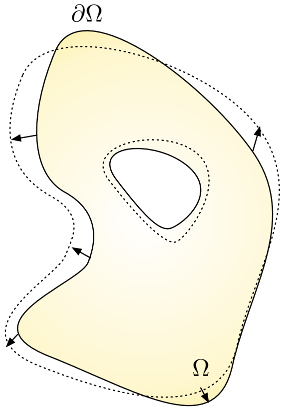
- In this framework, it is straightforward to account for variations of a shape $\{p_i\}_{i=1,\ldots,N}$:

$$\{p_i\}_{i=1,\ldots,N} \to \{p_i + \delta p_i\}_{i=1,\ldots,N}.$$

- However, the variety of possible designs is severely restricted, and the use of such methods relies on an a priori knowledge about the sought optimized design.

Geometric optimization

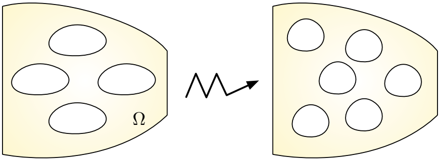
- The topology of shapes (i.e. their number of holes in 2d) is fixed.
- The whole boundary $\partial\Omega$ of shapes Ω is the optimization variable.
- This setting allows for greater freedom, since no a priori knowledge about the relevant features of the optimized shape is required.



Optimization of Ω via "free" perturbations of the boundary $\partial\Omega$.

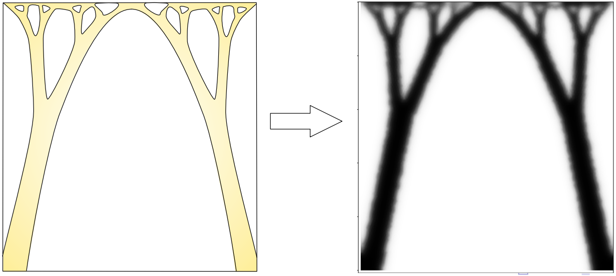
Topology optimization

- The topology of the shape is often unknown, and also subject to optimization.



- It is often preferred not to represent the boundaries of shapes, but to employ different descriptions, allowing for a more natural account of topological changes.

Example The shape Ω is replaced by a density function $h : D \to [0,1]$.



Additional comments

An optimal design framework is the combination of:

- A model (a boundary value problem) for the physical situation, which is
    - Sufficiently elaborate to be physically relevant, ...
    - ... yet simple enough to be tractable for optimization.
- A mathematical description of designs: $h =$ a set of parameters, a "true" shape, ...?
- An efficient numerical representation of h: by a mesh, a density function, ...?
- Numerical algorithms dedicated to
    - *Geometric computations:* e.g. the normal vector, the curvature of the shape;
    - *Mechanical computations:* solution of boundary value problems characterizing the physical performance of the shape;
    - *Algorithmic operations:* update (deformation) of the shape throughout the iterations of the process.

All these choices are intimately related!

Differentiation with respect to the design

- The solution of the optimal design problem ($\mathcal{P}$) often hinges on the derivatives of the functions $J(h)$ and $G(h)$.

- When the design h belongs to a vector space H (e.g. in parametric optimization), the sensitivity of a function $J(h)$ is encoded in the derivative $H \ni \widehat{h} \mapsto J'(h)(\widehat{h})$.

- The knowledge of $J'(h)$ allows to identify a descent direction $\widehat{h} \in H$ for $J(h)$:

$$J'(h)(\widehat{h}) < 0 \;\Rightarrow\; \text{For “small”} \tau > 0, \quad J(h + \tau\widehat{h}) \approx J(h) + \tau J'(h)(\widehat{h}) < J(h),$$

  and the new design $h + \tau\widehat{h}$ is better than h with respect to $J(h)$.

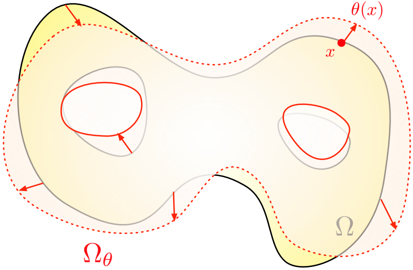
- Most constrained optimization methods use descent directions for $J(h)$ and $G(h)$.

- Differentiation w.r.t. the design is more subtle when the latter is a shape $\Omega \subset \mathbb{R}^d$.

Hadamard's boundary variation method features variations of a reference, Lipschitz domain Ω of the form:

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

for "small" $\theta \in W^{1,\infty}\left(\mathbb{R}^d, \mathbb{R}^d\right)$.



Lemma 1.

For all $\theta \in W^{1,\infty}\left(\mathbb{R}^d, \mathbb{R}^d\right)$ with norm $||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)} < 1$, $(\mathrm{Id} + \theta)$ is a Lipschitz diffeomorphism of $\mathbb{R}^d$, with Lipschitz inverse.

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

Definition 1.

Let $\Omega \subset \mathbb{R}^d$ be a smooth domain. A function $\Omega \mapsto J(\Omega)$ is shape differentiable at Ω if the mapping

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

is Fréchet-differentiable at 0, i.e. the following expansion holds:

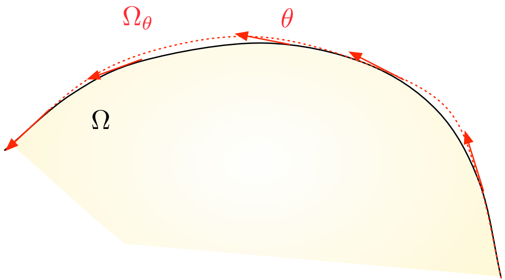
$$J(\Omega_\theta) = J(\Omega) + J'(\Omega)(\theta) + \mathrm{o}\left(||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}\right), \text{ where } \frac{\mathrm{o}(\theta)}{||\theta||_{W^{1,\infty}(\mathbb{R}^d,\mathbb{R}^d)}} \xrightarrow{\theta \to 0} 0.$$

The mapping $\theta \mapsto J'(\Omega)(\theta)$ is the shape derivative of $J(\Omega)$ at Ω.

Differentiation with respect to the domain: Hadamard's method (III)

- The shape derivative of "most" functions of the domain has the surface form:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega \, \theta \cdot n \, \mathrm{d}s, \text{ for some scalar field } v_\Omega : \partial\Omega \to \mathbb{R}.$$



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

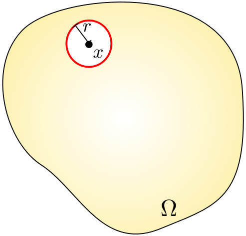
- A descent direction for $J(\Omega)$ is readily revealed from this expression:

$$\theta = -v_\Omega n \;\Rightarrow J'(\Omega)(\theta) < 0.$$

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 the point $x \in \Omega$ if there exists $\mathrm{d}J_T(\Omega)(x) \in \mathbb{R}$ such that:

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

Intuition: If $\mathrm{d}J_T(\Omega)(x) < 0$, it is beneficial to drill a tiny hole around x.

A. A. Novotny and J. Sokołowski, *Topological derivatives in shape optimization*, Springer Science & Business Media, 2012.

The adjoint method in an abstract framework (I)

- "Many" useful functionals in shape and topology optimization are of the form:

$$J(h) = j(u_h),$$

  where

  - The design h belongs to a Hilbert space $(H, \langle \cdot, \cdot \rangle_H)$.
  - The state u_h belongs to another Hilbert space $(V, \langle \cdot, \cdot \rangle_V)$.
  - It is the solution to a boundary value problem

$$\text{Search for } u_h \in V \text{ s.t. } \mathcal{F}(h, u_h) = 0, \qquad (BVP)$$

    where $\mathcal{F} : H \times V \to V$ is a suitable operator.
  - The observable $j : V \to \mathbb{R}$ is smooth enough.

- We aim to calculate the derivative $J'(h)(\widehat{h})$ and to find a descent direction for $J(h)$.

- We present the adjoint method in an abstract setting, agnostic of the nature of h.

R.-E. Plessix, *A review of the adjoint-state method for computing the gradient of a functional with geophysical applications*, Geophysical Journal International, 167 (2006), pp. 495–503.

The adjoint method in an abstract framework (II)

- The implicit function theorem ensures that the mapping $h \mapsto u_h$ is differentiable.

- Differentiation in (BVP) yields a characterization of the derivative $u_h'(\widehat{h}) \in V$:

$$\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right](\widehat{h}) + \left[\frac{\partial \mathcal{F}}{\partial u}(h, u_h)\right] u_h'(\widehat{h}) = 0.$$

- Likewise, by applying the chain rule, we calculate the derivative of $J(h)$:

$$J'(h)(\widehat{h}) = \left\langle j'(u_h), u_h'(\widehat{h}) \right\rangle_V .$$

- This expression does not lend itself to identification of a descent direction.

$\Rightarrow$ One would have to try multiple $\widehat{h} \in H$, calculate $u_h'(\widehat{h})$, ... until finding one such that $J'(h)(\widehat{h}) < 0$.

The adjoint method in an abstract framework (III)

- To overcome this issue, we introduce the adjoint state $p_h \in V$ as the solution to:

$$\left[\frac{\partial \mathcal{F}}{\partial u}(h, u_h)\right]^* p_h = -j'(u_h).$$

- An elementary calculation yields:

$$\begin{aligned} J'(h)(\widehat{h}) &= \left\langle j'(u_h), u_h'(\widehat{h})\right\rangle_V \\ &= -\left\langle \left[\tfrac{\partial \mathcal{F}}{\partial u}(h, u_h)\right]^* p_h, u_h'(\widehat{h})\right\rangle_V \\ &= -\left\langle \left[\tfrac{\partial \mathcal{F}}{\partial u}(h, u_h)\right] u_h'(\widehat{h}), p_h\right\rangle_V \end{aligned}$$

where we have used the definitions of p_h and of the adjoint operator $\left[\frac{\partial \mathcal{F}}{\partial u}(h, u_h)\right]^*$.

- Using now the problem satisfied by $u_h'(\widehat{h})$, we obtain:

$$J'(h)(\widehat{h}) = \left\langle \left[\frac{\partial \mathcal{F}}{\partial h}(h, u(h))\right] \widehat{h}, p_h\right\rangle_V.$$

The adjoint method in an abstract framework (IV)

- Introducing the adjoint $\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right]^* : V \to H$ of $\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right] H \to V$, we end up with:

$$J'(h)(\widehat{h}) = \left\langle \left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right]^* p_h, \widehat{h} \right\rangle_H .$$

- Now, a descent direction $\widehat{h}$ for $J(h)$ is immediately revealed:

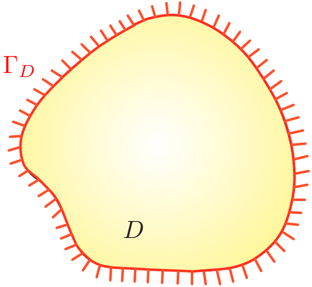
$$\widehat{h} = -\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right]^* p_h \;\Rightarrow J'(h)(\widehat{h}) = -\left|\left|\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right]^* p_h\right|\right|_H^2 .$$

- The evaluation of $\widehat{h}$ demands:
  - The calculation of u_h (finite element solution);
  - The calculation of p_h (finite element solution);
  - The calculation of the operator $\left[\frac{\partial \mathcal{F}}{\partial h}(h, u_h)\right]^*$ (derivative of the explicit dependence of the boundary value problem w.r.t the design).

The adjoint method: worked example (I)

- Let $D \subset \mathbb{R}^d$ be a fixed domain.
- The temperature is set to 0 on ∂D.
- A source $f : D \to \mathbb{R}$ is acting in the medium.
- The considered designs are conductivity coefficients:

$$h \in \mathcal{U}_{\mathrm{ad}} := L^\infty(D, [0,1]).$$



- We consider the functional:

$$J(h) = \int_D j(u_h)\,\mathrm{d}x,$$

where u_h is the temperature.

- It is the solution in $H^1_0(D)$ to:

$$\left\{ \begin{array}{rcll} -\mathrm{div}(\gamma_h \nabla u_h) & = & f & \text{in } D, \\ u_h & = & 0 & \text{on } \partial D, \end{array} \right. \quad \text{where } \gamma_h(x) := \alpha + h(x)(\beta - \alpha).$$

The adjoint method: worked example (II)

For a fixed design $h \in \mathcal{U}_{\mathrm{ad}}$,

- The variational formulation characterizing u_h reads:

$$\text{Search for } u_h \in H^1_0(D) \text{ s.t. } \forall v \in H^1_0(D), \quad \int_D \gamma_h \nabla u_h \cdot \nabla v \, \mathrm{d}x = \int_D f v \, \mathrm{d}x.$$

- This problem has a unique solution $u_h \in H^1_0(D)$, which satisfies:

$$||u_h||_{H^1_0(D)} \leq C||f||_{L^2(D)},$$

for some constant $C > 0$, owing to the Lax-Milgram theorem.

Theorem 2.

The objective function

$$J(h) = \int_D j(u_h)\,\mathrm{d}x$$

is differentiable at any $h \in \mathcal{U}_{\mathrm{ad}}$*, and its derivative reads*

$$\forall \widehat{h} \in L^\infty(D),\;\; J'(h)(\widehat{h}) = (\beta - \alpha) \int_D (\nabla u_h \cdot \nabla p_h)\widehat{h}\,\mathrm{d}x,$$

where the adjoint state $p_h \in H^1_0(D)$ *is the solution to the boundary value problem:*

$$\begin{cases} -\mathrm{div}(\gamma_h \nabla p_h) = -j'(u_h) & \text{in } D, \\ p_h = 0 & \text{on } \partial D. \end{cases}$$

Proof: The proof is divided into three steps:

1. We use the implicit function theorem to prove that the state mapping

$$\mathcal{U}_{\text{ad}} \ni h \longmapsto u_h \in H_0^1(D)$$

is Fréchet differentiable, with derivative $\widehat{h} \mapsto u_h'(\widehat{h})$.

2. We calculate the derivative of $J(h)$ by using the chain rule.

3. We give a more convenient structure to this derivative, by introducing an adjoint state p_h to eliminate the occurrence of $u_h'(\widehat{h})$.

Step 1: *Differentiability of $h \mapsto u_h$:*

For any $h \in \mathcal{U}_{\text{ad}}$, u_h is the unique solution in $H_0^1(D)$ to the variational problem:

$$\forall v \in H_0^1(D), \;\; \int_D \gamma_h \nabla u_h \cdot \nabla v \, \mathrm{d}x = \int_D f v \, \mathrm{d}x.$$

The adjoint method: worked example (V)

Let

$$\mathcal{F} : \mathcal{U}_{\mathrm{ad}} \times H^1_0(D) \to H^{-1}(D)$$

be the mapping defined by:

$$\mathcal{F}(h,u) : v \mapsto \int_D \gamma_h \nabla u \cdot \nabla v \,\mathrm{d}x - \int_D fv \,\mathrm{d}x.$$

One verifies that

- $\mathcal{F}$ is a mapping of class $\mathcal{C}^1$.
- For given $h \in \mathcal{U}_{\mathrm{ad}}$, u_h is the unique solution u to the equation
$$\mathcal{F}(h,u) = 0.$$
- The derivative of the partial mapping $u \mapsto \mathcal{F}(h,u)$ reads:
$$H^1_0(D) \ni \widehat{u} \longmapsto \left[v \mapsto \int_D \gamma_h \nabla \widehat{u} \cdot \nabla v \,\mathrm{d}x \right] \in H^{-1}(D).$$
It is an isomorphism, owing to the Lax-Milgram theorem:

For all $g \in H^{-1}(D)$, there exists a unique $u \in H^1_0(D)$ s.t.

$$\forall v \in H^1_0(D), \ \int_D \gamma_h \nabla u \cdot \nabla v \,\mathrm{d}x = \langle g, v \rangle_{H^{-1}(D), H^1_0(D)}.$$

The adjoint method: worked example (VI)

The implicit function theorem guarantees that the mapping $h \mapsto u_h$ is of class $\mathcal{C}^1$.

To calculate the derivative $\widehat{h} \mapsto u_h'(\widehat{h})$, we return to the variational formulation for u_h:

$$\forall v \in H_0^1(D), \;\; \int_D \gamma_h \nabla u_h \cdot \nabla v \,\mathrm{d}x = \int_D f v \,\mathrm{d}x.$$

Taking derivatives with respect to h in a direction $\widehat{h} \in L^\infty(D)$ yields:

$$(\beta - \alpha) \int_D \widehat{h} \nabla u_h \cdot \nabla v \,\mathrm{d}x + \int_D h \nabla u_h'(\widehat{h}) \cdot \nabla v \,\mathrm{d}x = 0,$$

and so, for all $\widehat{h} \in L^\infty(D)$, $u_h'(\widehat{h})$ is the unique solution in $H_0^1(D)$ to:

$$\boxed{\forall v \in H_0^1(D), \;\; \int_D h \nabla u_h'(\widehat{h}) \cdot \nabla v \,\mathrm{d}x = -(\beta - \alpha) \int_D \widehat{h} \nabla u_h \cdot \nabla v \,\mathrm{d}x.}$$

The adjoint method: worked example (VII)

Step 2: *Calculation of the derivative of $J(h)$:*

Since $h \mapsto u_h$ is of class $\mathcal{C}^1$, the chain rule yields immediately:

$$\forall \widehat{h} \in L^\infty(D), \;\; J'(h)(\widehat{h}) = \int_D j'(u_h) u_h'(\widehat{h}) \, \mathrm{d}x.$$

- This expression is awkward: the dependence $\widehat{h} \mapsto J'(h)(\widehat{h})$ is not explicit and it is difficult to find a descent direction, i.e. a $\widehat{h} \in L^\infty(D)$ such that:

$$J'(h)(\widehat{h}) < 0.$$

- Fortunately, the expression of $J'(h)$ can be simplified thanks to the introduction of the adjoint state p_h.

The adjoint method: worked example (VIII)

Step 3: *Reformulation of $J'(h)$ using an adjoint state:*

The adjoint state p_h is the unique solution in $H^1_0(D)$ to the variational problem:

$$\forall v \in H^1_0(D), \quad \int_D \gamma_h \nabla p_h \cdot \nabla v \, \mathrm{d}x = -\int_D j'(u_h) v \, \mathrm{d}x,$$

to be compared with the variational formulation for $u_h'(\widehat{h}) \in H^1_0(D)$:

$$\forall v \in H^1_0(D), \quad \int_D \gamma_h \nabla u_h'(\widehat{h}) \cdot \nabla v \, \mathrm{d}x = -(\beta - \alpha) \int_D \widehat{h} \nabla u_h \cdot \nabla v \, \mathrm{d}x.$$

Then, we calculate:

$$\begin{aligned} J'(h)(\widehat{h}) &= \int_D j'(u_h) u_h'(\widehat{h}) \, \mathrm{d}x, \\ &= -\int_D \gamma_h \nabla p_h \cdot \nabla u_h'(\widehat{h}) \, \mathrm{d}x, \\ &= -\int_D \gamma_h \nabla u_h'(\widehat{h}) \cdot \nabla p_h \, \mathrm{d}x, \\ &= (\beta - \alpha) \int_D \widehat{h} \nabla u_h \cdot \nabla p_h \, \mathrm{d}x. \end{aligned}$$

where the last line uses the variational formulation of $u_h'(\widehat{h})$ with p_h as test function.

The adjoint method: final comments

- The adjoint state p_h can be interpreted as the Lagrange multiplier associated to the PDE constraint if we formulate the minimization problem of $J(h)$ as:

$$\min_{(h,u)} \int_D j(u)\,\mathrm{d}x \text{ s.t. } \begin{cases} -\mathrm{div}(h\nabla u) = f & \text{in } D, \\ u = 0 & \text{on } \partial D. \end{cases}$$

- This general methodology allows to deal with
  - Different physical situations,
  - Other optimal design frameworks, including "true" geometric optimization.

- Another (formal and sometimes dangerous) method allows to calculate shape derivatives: Céa's method.

J. Céa, *Conception optimale ou identification de formes, calcul rapide de la dérivée directionnelle de la fonction coût*, ESAIM: M2AN, 20(3), (1986), pp. 371–402.

A generic numerical algorithm

The numerical solution of $(\mathcal{P})$ hinges on a constrained optimization algorithm:

Initialization: Start from an initial design h^0,

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

1. Calculate the derivatives $J'(h^n)$ and $G'(h^n)$ of $J(h)$ and $G(h)$ at $h = h^n$;
2. Identify descent directions $\widehat{h}_J^n$ and $\widehat{h}_G^n$ for $J(h)$ and $G(h)$ from h^n;
3. Infer a descent direction $\widehat{h}^n$ for the optimization problem $(\mathcal{P})$;
4. Select an appropriate time step $\tau^n > 0$;
5. Update the design as:

$$h^{n+1} = h^n - \tau^n \widehat{h}^n.$$

The main difficulty is to find a numerical discretization of shapes which lends itself to:

- Step ❷: Finite element solutions;
- Step ❺: Deformation of the shape.

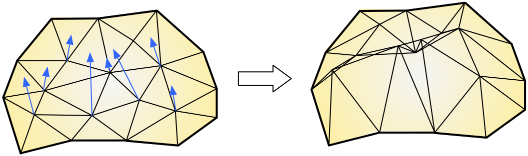
"Lagrangian" approaches

- Each shape Ω^n is represented by a (triangular) mesh $\mathcal{T}^n$.
- The Finite Element method is applied on $\mathcal{T}^n$ for computing u_{Ω^n} (and p_{Ω^n}).
- The descent direction θ^n is obtained from the surface form of the shape derivative:

$$J'(\Omega)(\theta) = \int_{\partial\Omega} v_\Omega \, \theta \cdot n \, \mathrm{d}s \quad \Rightarrow \quad \theta^n = -v_{\Omega^n} n \text{ on } \partial\Omega^n.$$

- The shape advection step $\Omega^n \overset{(\mathrm{Id}+\tau^n\theta^n)}{\longmapsto} \Omega^{n+1}$ is performed by pushing the nodes of $\mathcal{T}^n$ along $\tau^n\theta^n$, to obtain the new mesh $\mathcal{T}^{n+1}$:

$$\forall \text{ vertex } x \in \mathcal{T}^n, \; x \longmapsto x + \tau^n\theta^n(x).$$

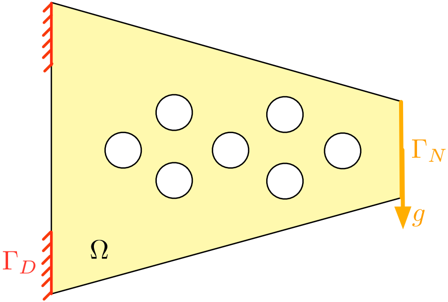


Pushing nodes according to the velocity field may result in an invalid configuration.

- In the context of linear elasticity, one aims at minimizing the compliance $C(\Omega)$ of a cantilever beam:

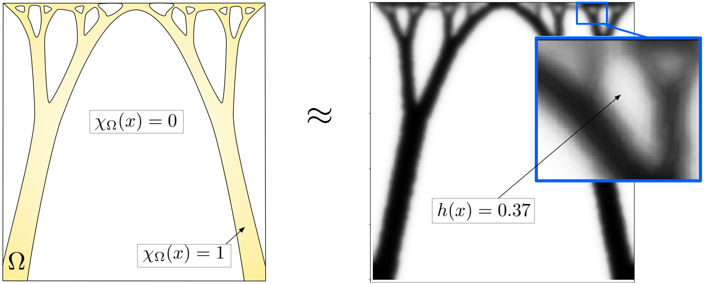
$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega)\,\mathrm{d}x.$$

- A volume constraint is imposed: $G(\Omega) = \mathrm{Vol}(\Omega) - V_T$.



Density-based topology optimization (I)

- The design variable h is a density function $h : D \to [0,1]$ defined on a fixed hold-all domain D.
- $h \approx$ relaxed version of the characteristic function $\chi_\Omega : D \to \{0,1\}$ of a shape Ω.



- The cornerstone of these methods is to endow intermediate regions $h(x) \in (0,1)$ with a physical meaning.
- We present this methodology in the context of the conductivity equation.
- It can be adapted to multiple physical contexts beyond.

- We consider an unconstrained shape optimization problem in the two-phase conductivity setting:

$$\min_{\Omega \subset D} J(\Omega), \text{ where } J(\Omega) = \int_D j(u_\Omega)\, dx. \qquad \text{(SO)}$$

- In here, the temperature u_Ω is the solution to:

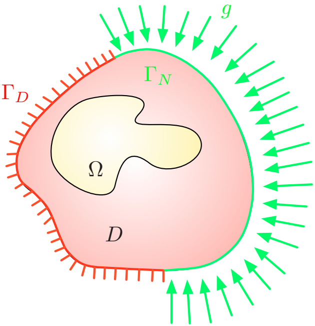
$$\begin{cases} -\text{div}(\gamma_\Omega \nabla u_\Omega) = f & \text{in } D, \\ u_\Omega = 0 & \text{on } \Gamma_D, \\ \gamma_\Omega \frac{\partial u_\Omega}{\partial n} = g & \text{on } \Gamma_N, \end{cases}$$

where the conductivity γ_Ω reads:

$$\gamma_\Omega = \alpha + \chi_\Omega(\beta - \alpha),$$

and χ_Ω is the characteristic function of Ω:

$$\forall x \in D, \quad \chi_\Omega(x) = \begin{cases} 1 & \text{if } x \in \Omega, \\ 0 & \text{otherwise.} \end{cases}$$



Density-based topology optimization (III)

- The "black-and-white" characteristic function $\chi_\Omega : D \to \{0,1\}$ of the shape Ω, is replaced by a "grayscale" density function $h : D \to [0,1]$.
- The properties of a region with intermediate density $h(x) \in (0,1)$ are described via an empirical interpolation law $\zeta(h)$ between α and β:

$$\zeta \text{ is smooth and } \zeta(0) = \alpha, \text{ and } \zeta(1) = \beta.$$

- The problem rewrites:

$$\min_{h \in \mathcal{U}_{\mathrm{ad}}} J(h), \text{ where } \mathcal{U}_{\mathrm{ad}} = L^\infty(D,[0,1]), \;\; J(h) = \int_D j(u_h)\,\mathrm{d}x, \qquad (\text{TO})$$

and $u_h \in H^1(D)$ is the solution to:

$$\begin{cases} -\mathrm{div}(\zeta(h)\nabla u_h) = f & \text{in } D, \\ u_h = 0 & \text{on } \Gamma_D, \\ \zeta(h)\frac{\partial u_h}{\partial n} = g & \text{on } \Gamma_N. \end{cases}$$

- The problem (TO) falls in the realm of parametric optimization!

The interpolation profile

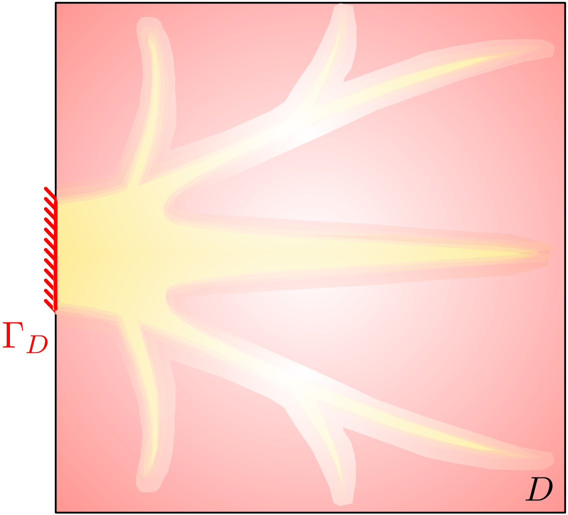
- The interpolation profile $\zeta(h)$ prescribes material properties (diffusion, etc.) to regions with (fictitious) intermediate densities.

- In the practice of the Solid Isotropic Method with Penalization (SIMP), a power law of the form
$$\zeta(h) = \alpha + h^p(\beta - \alpha)$$
is used (often, $p = 3$).

- This has the effect to penalize the presence of "grayscale" intermediate regions, and to steer the optimized density towards a "black-and white" function.

- This interpolation law is empirical: there is no guarantee that a material with such properties does exist!

Density-based topology optimization of a heat diffuser



Density-based topology optimization (IV)

Assets of density-based methods

- Simplicity of the mathematical analysis (calculation of derivatives, etc).
- They allow for the use of efficient mathematical programming routines.
- Simplicity and robustness of the implementation: everything takes place on a fixed mesh, no mesh deformation is required.

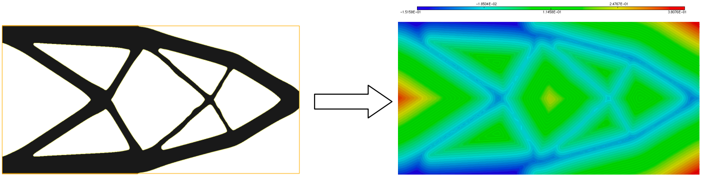
Drawbacks

- A reformulation and approximation of the physical equations are necessary.
- The geometry of shapes is lost, which may make it difficult to formulate, e.g. geometric constraints.

The level set method for geometric optimization (I)

- At the continuous level, the design variable h is a domain $\Omega \subset \mathbb{R}^d$, inside a fixed 'hold-all" domain D.
- The sensitivity of a function $J(\Omega)$ is captured by the notion of shape derivative.
- At the discrete level, Ω is represented by a "level set " function

$$\phi : D \to \mathbb{R}, \text{ on a fixed mesh } \mathcal{T} \text{ of } D.$$



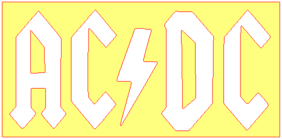
- The motion of Ω along the descent direction θ is translated by a partial differential equation for ϕ.

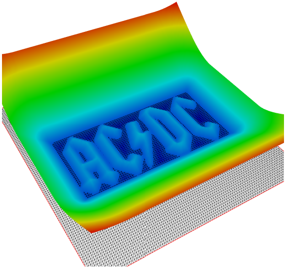
A short detour by the Level Set Method

A paradigm: [OSe] *the motion of an evolving domain is best described in an* *implicit* *way.*

One domain $\Omega \subset \mathbb{R}^d$ is equivalently defined by a function $\phi : \mathbb{R}^d \to \mathbb{R}$ such that:

$$\phi(x) < 0 \quad \text{if } x \in \Omega \quad ; \quad \phi(x) = 0 \quad \text{if } x \in \partial\Omega \quad ; \quad \phi(x) > 0 \quad \text{if } x \in {}^c\overline{\Omega}$$





(Left) A bounded domain $\Omega \subset \mathbb{R}^2$; (right) Graph of an associated level set function.

Surface evolution equations in the level set framework

- Let $\Omega(t) \subset \mathbb{R}^d$ be a domain moving according to a velocity field $v(t,x) \in \mathbb{R}^d$.
- Let $\phi(t,x)$ be a level set function for $\Omega(t)$.
- The motion of $\Omega(t)$ translates in terms of ϕ as the level set advection equation:

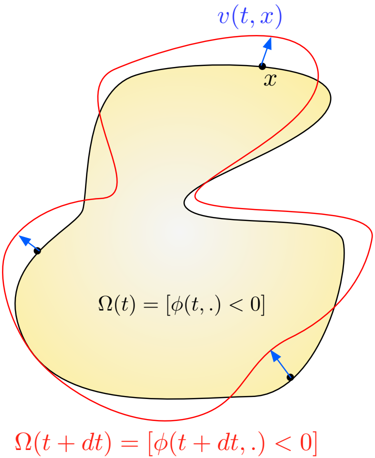
$$\boxed{\frac{\partial \phi}{\partial t}(t,x) + v(t,x).\nabla\phi(t,x) = 0}$$

- If $v(t,x)$ is normal to the boundary $\partial\Omega(t)$, i.e.:

$$\boxed{v(t,x) := V(t,x)\frac{\nabla\phi(t,x)}{|\nabla\phi(t,x)|},}$$

this rewrites as a Hamilton-Jacobi equation:

$$\boxed{\frac{\partial \phi}{\partial t}(t,x) + V(t,x)|\nabla\phi(t,x)| = 0}$$



The level set method of Allaire-Jouve-Toader [AlJouToa]

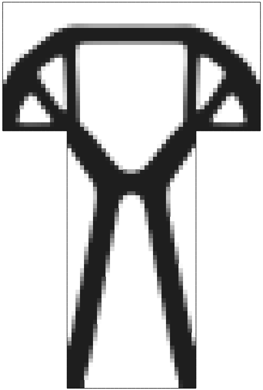
- The shapes Ω^n are embedded in a working domain D equipped with a fixed mesh.

- The successive shapes Ω^n are accounted for in the level set framework, i.e. via a function $\phi^n : D \to \mathbb{R}$ which implicitly defines them.

- At each step n, the exact linear elasticity system for u_{Ω^n}, posed on Ω^n, is approximated by the Ersatz material approach: the void $D \setminus \Omega^n$ is filled by a very "soft" material.

  $\Rightarrow$ Approximate system posed on D.

- This approach is very versatile and does not require a mesh of the shapes at each iteration.

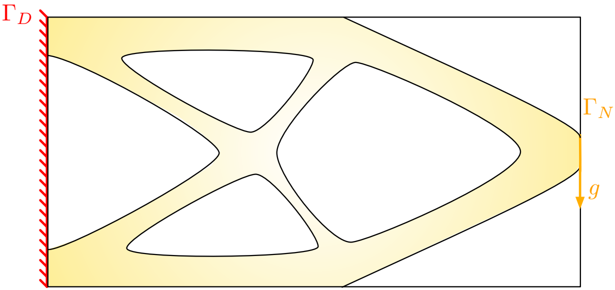


Shape accounted for by a level set description

- In the context of linear elasticity, one aims to minimize the compliance $C(\Omega)$ of a cantilever beam:

$$C(\Omega) = \int_\Omega Ae(u_\Omega) : e(u_\Omega)\,\mathrm{d}x.$$

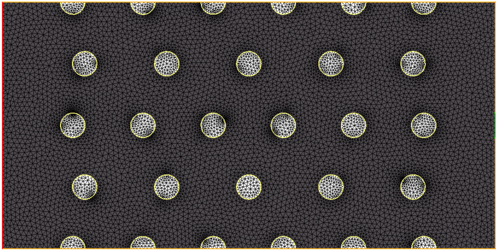
- A volume constraint is imposed.



The level set method for geometric optimization (IV)

Assets of the level set method

- A clear representation of the shape Ω is possible.
- Yet, the method is robust, and arbitrary deformations of Ω are possible.
- Recent progress in remeshing techniques make it possible to additionally enjoy an exact mesh of the shape throughout the process.



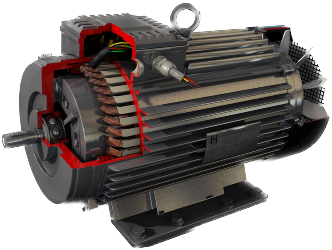
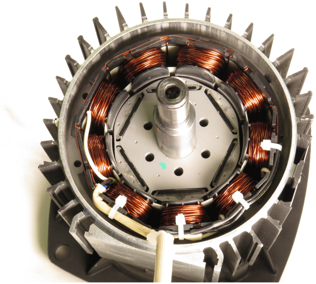
Drawbacks

- The mathematical framework is more difficult.
- The implementation is slightly more subtle too.

Optimization of the shape of an electric motor (I)

Joint work with A. Cesarano & P. Gangl

- Electric machines convert electrical energy into mechanical work.
- The physics at play is magneto-quasi-static electromagnetism:
  - An electric current is powered in the coils of the outermost stator part.
  - It induces a magnetic field in the inner, rotor part, provoking its rotation.
  - The resulting mechanical energy is collected by a central shaft.
- Electric motors are seen as promising answers to the environmental crisis and the needs for energy savings.

(Left) Overview of a motor [Hau]; (right) Cross-section of a motor, by Hanning Elektro-Werke GmbH & Co KG.

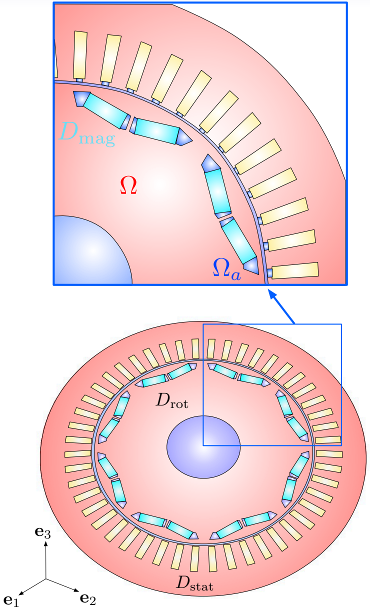
Optimization of the shape of an electric motor (II)

- The cross-section D of a motor is made of the stator, the rotor, separated by an air gap:

$$\overline{D} = \overline{D_{\text{rot}}} \cup \overline{D_{\text{gap}}} \cup \overline{D_{\text{stat}}}.$$

- The stator D_{stat} consists of:
  - A region filled with ferromagnetic material;
  - A region made of air;
  - The coils, featuring copper wires.
- At rest, the rotor D_{rot} is composed of:
  - A ferromagnetic core, occupying the optimized region Ω;
  - Air, occupying the region Ω_{a};
  - Permanent magnets in D_{mag}.
- The internal geometry of the rotor undergoes a rotating motion φ_t:

$$\Omega(t) = \varphi_t(\Omega),\ \Omega_a(t) = \varphi_t(\Omega_a),\ \text{etc.}$$



Optimization of the shape of an electric motor (III)

- Due to the cylindrical structure of the motor, the problem amounts to a 2d evolution problem for the transverse component u_Ω of the vector potential:

$$\begin{cases} \sigma_{\Omega(t)} \frac{\mathrm{d}u_\Omega}{\mathrm{d}t} - \mathrm{div}\left(\nu_{\Omega(t)}(x, |\nabla u_\Omega|)\nabla u_\Omega\right) = f & \text{in } (0,T) \times D, \\ u_\Omega(t,x) = 0 & \text{for } t \in (0,T),\ x \in \partial D, \\ u_\Omega(0,x) = u_\Omega(T,x) & \text{for } x \in D_{\mathsf{mag}}, \end{cases} \qquad \text{(MQS)}$$

  where σ and ν are the conductivity and reluctivity coefficients.

- This problem is non linear, because of the behavior of the ferromagnetic material.

- It is of mixed parabolic – elliptic type:

$$\sigma_{\Omega(t)}(x) = \begin{cases} \sigma_m & \text{for } x \in D_{\mathrm{mag}}(t), \\ 0 & \text{otherwise.} \end{cases}$$

- It is posed on a moving geometry:

$$\sigma_{\Omega(t)} \text{ and } \nu_{\Omega(t)}(x, |\nabla u_\Omega|) \text{ depend on the motion of the rotor.}$$

- The mechanical torque is maximized:

$$\max_{\Omega \subset D_{\mathrm{rot}}} J(\Omega), \text{ where } J(\Omega) = \int_0^T \int_D j(\nabla u_\Omega)\,\mathrm{d}x\,\mathrm{d}t, \text{ for a function } j : \mathbb{R}^2 \to \mathbb{R}.$$

Optimization of the shape of an electric motor (IV)

- Since "small" deformations of Ω are expected, a Lagrangian mesh deformation method is used.

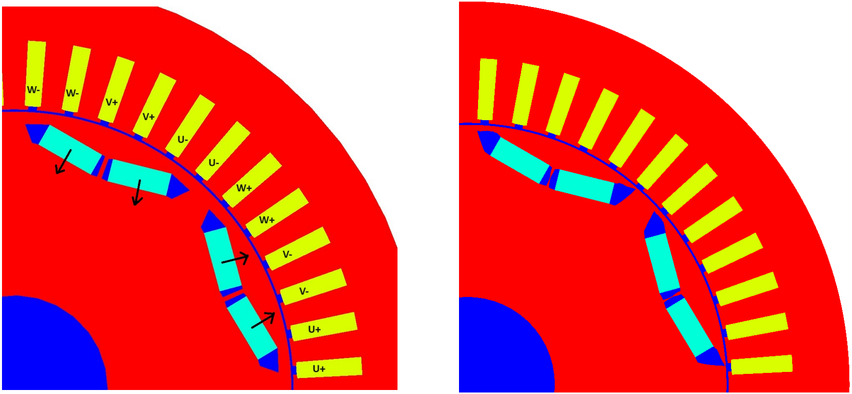
- The solution of (MQS) is tackled by a space-time finite element method:

  "The whole space-time cylinder $D \times (0, T)$ *is meshed by a tetrahedral* $(2+1)$ *dimensional mesh".*

  - This practice naturally incorporates time periodic boundary conditions.
  - It allows to handle moving in time geometries.
  - It leaves the room for mesh adaptation and domain decomposition in space-time.

- A Newton-Raphson method is used to treat the non linear term.

Optimization of the shape of an electric motor (V)

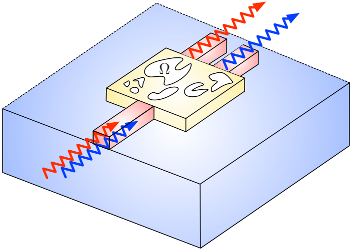


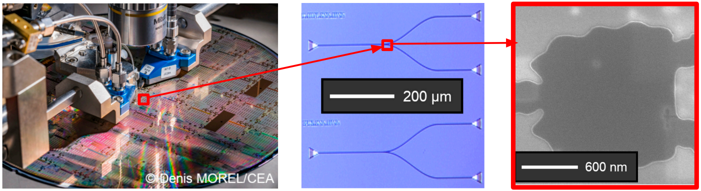
(Left) Initial, (right) Optimized design of the rotor part; the torque is increased by 12% during the process.

Optimization of nanophotonic devices (I)

Joint work with A. Gliere, K. Hassan, N. Lebbe & E. Oudet

- Nanophotonic devices are the basic components of photonic integrated circuits.
- In these, light is transported by wave guides.
- The electric and magnetic fields are governed by the time-harmonic Maxwell's equations.
- The shape Ω of air inclusions in the Si core is optimized to achieve particular effects.

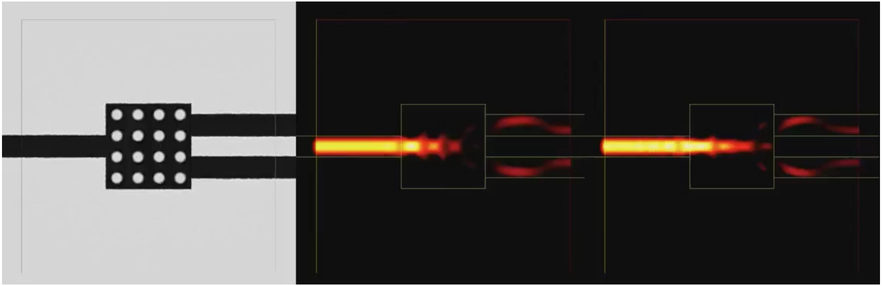




One nanophotonic component inside a complete photonic circuit.

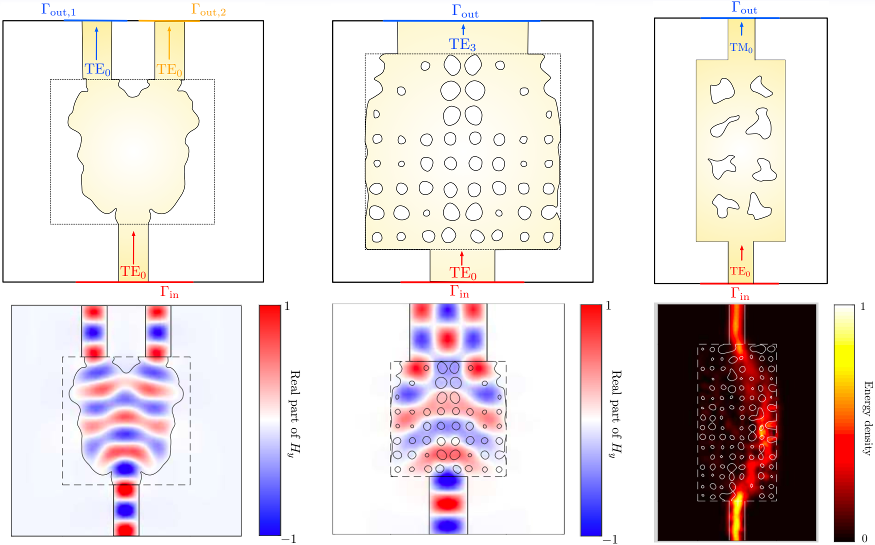
Optimization of nanophotonic devices (II)

Duplexers steer incoming waves to different out- put channels, depending on their wavelength.



Optimization of the shape of a nanophotonic duplexer.

Optimization of other nanophotonic devices

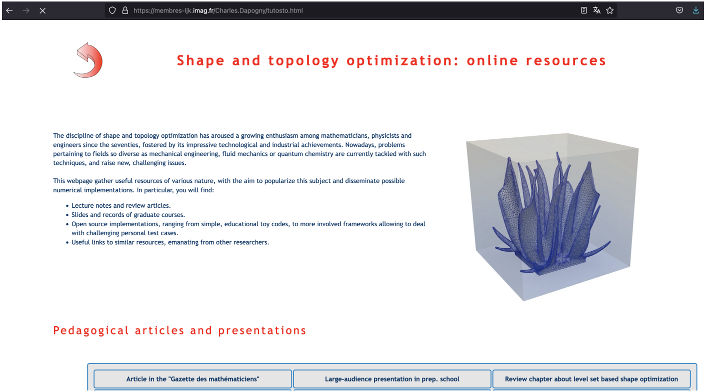


Optimization of (left) A power divider; (center) A mode converter; (right) A polarization converter.

A word of advertisement

A webpage gathering lecture notes, slides, demonstration codes, etc.

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



Thank you for your attention!

Technical appendix

The Lax Milgram theorem

In a Hilbert space H, let $a : H \times H \to \mathbb{R}$ be a bilinear form and $\ell : H \to \mathbb{R}$ be a linear form such that:

- a is continuous, i.e. there exists $M > 0$ such that:
$$\forall u, v \in H, \ \ |a(u,v)| \leq M||u||_H||v||_H.$$
- a is coercive, i.e. there exists $\alpha > 0$ such that:
$$\forall u \in H, \ \ \alpha||u||_H^2 \leq a(u,u).$$
- ℓ is continuous (i.e. ℓ belongs to the dual space H^*):
$$||\ell||_{H^*} := \sup_{\substack{v \in H \\ v \neq \mathbf{0}}} \frac{|\ell(v)|}{||v||_H} < \infty.$$

Theorem 3.

Under the above hypotheses, the variational problem

$$\textit{Search for } u \in H \textit{ s.t. for all } v \in H, \ \ a(u,v) = \ell(v)$$

has a unique solution $u \in H$, which depends continuously on ℓ:

$$||u||_H \leq \frac{M}{\alpha}||\ell||_{H^*}.$$

The implicit function theorem

The implicit function theorem ensures the existence and smoothness of a solution $u = u_\theta$ to a parametrized, non linear equation of the form:

$$\mathcal{F}(\theta, u) = 0,$$

where u is the unknown and θ is a "parameter".

Theorem 4 (Implicit function theorem).

Let Θ, E, F be Banach spaces, $\mathcal{V} \subset \Theta$, $U \subset E$ be open sets. and $\mathcal{F} : \mathcal{V} \times U \to F$ be a function of class $\mathcal{C}^p$ for $p \geq 1$. Let $(\theta_0, u_0) \in \mathcal{V} \times U$ be such that $\mathcal{F}(\theta_0, u_0) = 0$ and:

$$\text{The derivative } \frac{\partial \mathcal{F}}{\partial u}(\theta_0, u_0) : E \to F \text{ is a linear isomorphism.}$$

Then there exist open subsets $\mathcal{V}' \subset \mathcal{V}$ of θ_0 in Θ and $U' \subset U$ of u_0 in E, and a mapping $g : \mathcal{V}' \to U'$ of class $\mathcal{C}^p$ satisfying the properties:

1. $g(\theta_0) = u_0$,
2. *For all $\theta \in \mathcal{V}'$, the equation $\mathcal{F}(\theta, u) = 0$ has unique solution $u = g(\theta) \in U'$.*

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