A MULTISCALE APPROACH IN TOPOLOGY OPTIMIZATION

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The most recent results were obtained in collaboration with F. de Gournay, F. Jouve, O. Pantz, A.-M. Toader.

CONTENTS

1. Introduction.
2. Classical method of shape differentiation. Link between ill-posedness and topology optimization.
3. The level set method.
4. The topological gradient.

-I- INTRODUCTION

A shape optimization problem is defined by three data:

☞ a model (a p.d.e.) in order to analyze the mechanical behavior of a structure,

☞ an objective function which measures one or several performance(s) and has to be minimized,

☞ an admissible set of shapes (the optimization variables) which takes into account additional constraints.

For simplicity, we choose to focus on single load optimization in linear elasticity.

SHAPE OPTIMIZATION

Mathematical formulation : minimize an objective function over a set of admissibles shapes Ω (including possible constraints)

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

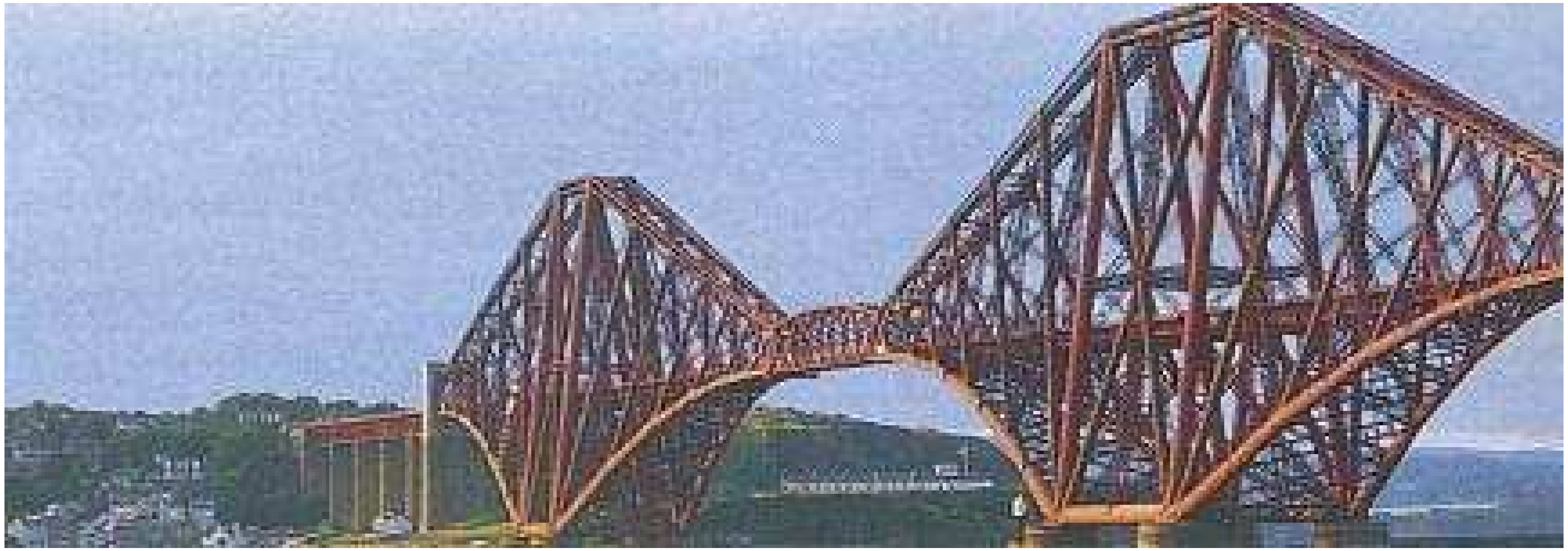
The objective function is evaluated through a partial differential equation (state equation)

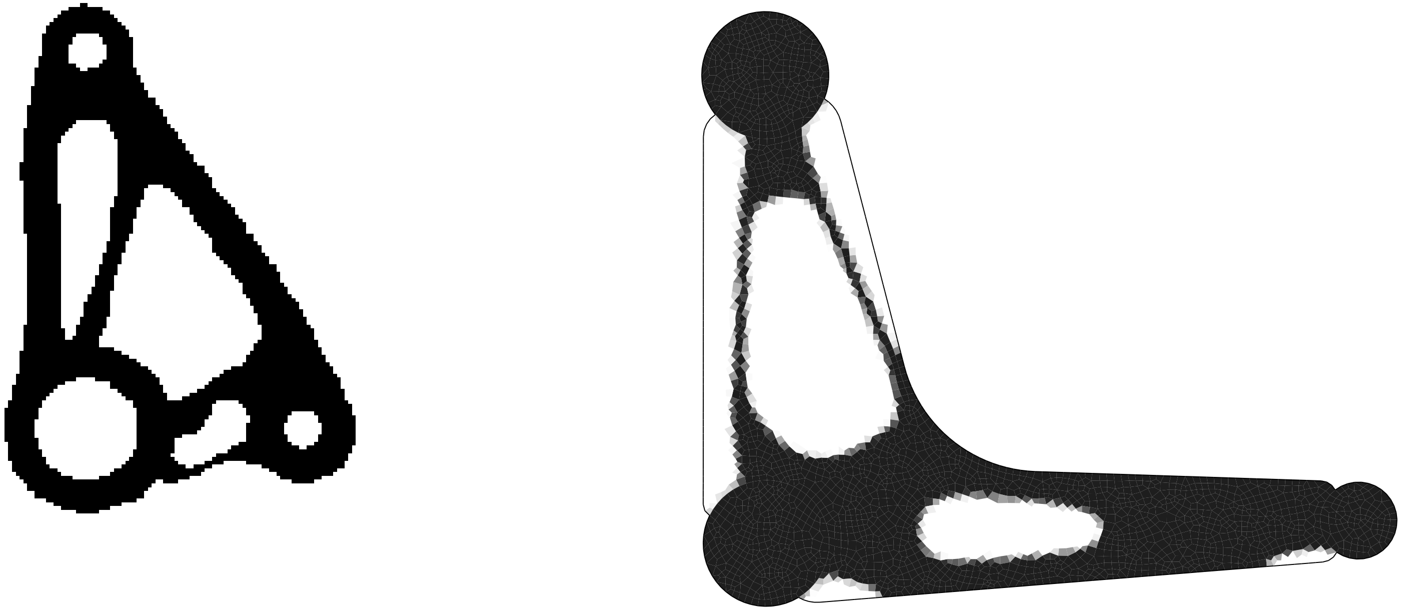
$$J(\Omega) = \int_\Omega j(u_\Omega)\, dx$$

where u_Ω is the solution of

$$PDE(u_\Omega) = 0 \quad \text{in} \quad \Omega$$

Topology optimization : the optimal topology is unknown.





The model of linear elasticity

Shape $\Omega \subset \mathbb{R}^d$ with boundary

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

where Γ_D and Γ_N are fixed.

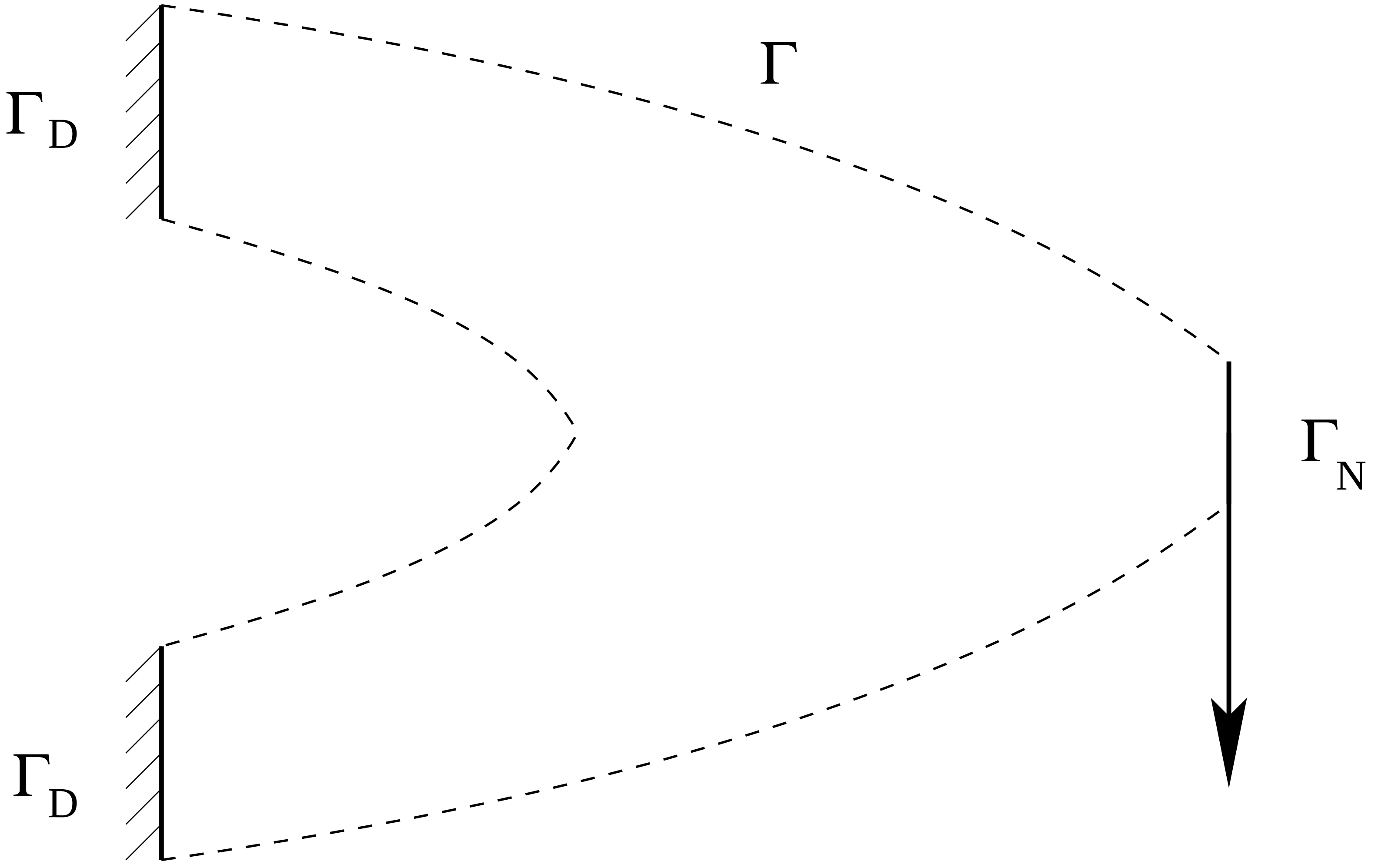
Only Γ is optimized (free boundary).

For a given applied load $g : \Gamma_N \to \mathbb{R}^d$, the displacement $u : \Omega \to \mathbb{R}^d$ is the solution of

$$\begin{cases} -\operatorname{div}\left(A\,e(u)\right) = 0 & \text{in } \Omega \\ u = 0 & \text{on } \Gamma_D \\ \big(A\,e(u)\big)n = g & \text{on } \Gamma_N \\ \big(A\,e(u)\big)n = 0 & \text{on } \Gamma \end{cases}$$

with the strain tensor $e(u) = \frac{1}{2}\left(\nabla u + \nabla^t u\right)$, the stress tensor $\sigma = Ae(u)$, and A an homogeneous isotropic elasticity tensor.

Example: the cantilever



Admissible set and objective function

The set of admissible shapes is typically

$$\mathcal{U}_{ad} = \left\{ \Omega \subset D \text{ open set such that } \Gamma_D \bigcup \Gamma_N \subset \partial\Omega \text{ and } \int_\Omega dx = V_0 \right\},$$

where $D \subset \mathbb{R}^d$ is a given "working domain" and V_0 is a prescribed volume.

The **shape optimization** problem is

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

with, as an objective function, the compliance

$$J(\Omega) = \int_{\Gamma_N} g \cdot u \, dx,$$

or a least square criteria for a target displacement $u_0(x)$

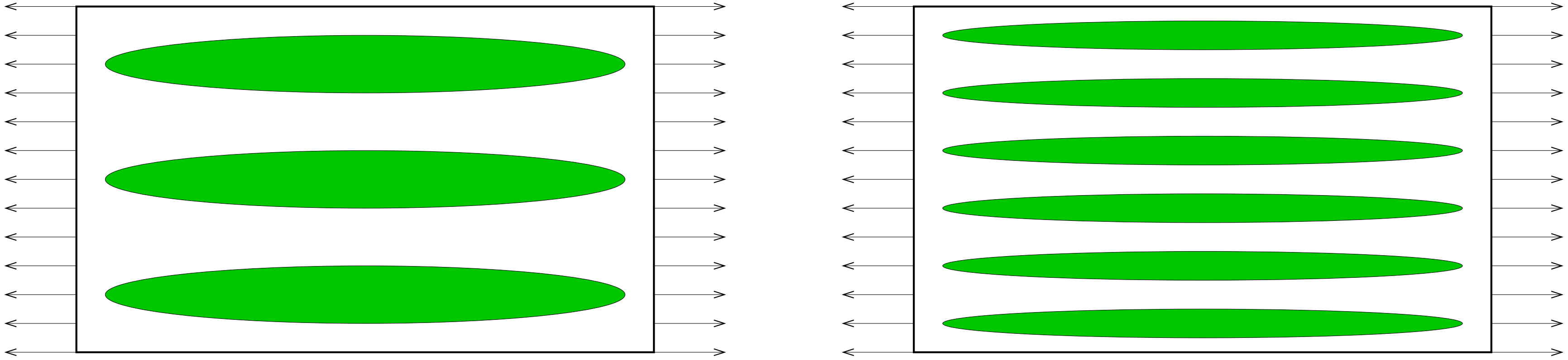
$$J(\Omega) = \int_\Omega k(x)|u - u_0|^2 dx.$$

The true optimization variable is the free boundary Γ.

Generic non-existence of optimal shapes

Without further constraint, there does not exist an optimal shape !
(Counter-examples of F. Murat, 1972, 1977)

$$J(\Omega_3) > J(\Omega_6)$$



Mechanical intuition: for minimal compliance, a minimizing sequence is made of more and more, thinner and thinner, horizontal holes, but the minimum can not be attained.

Consequences of ill-posedness

- ☞ Deep interplay between mathematical and computational issues !
- ☞ Ill-posedness can be seen numerically in the occurence of many local minima.
- ☞ Very often local minima correspond to different topologies.
- ☞ A microstructure appears in the minimizing sequences.
- ☞ Need a multiscale approach to numerically solve this difficulty.

Two possible numerical remedies:

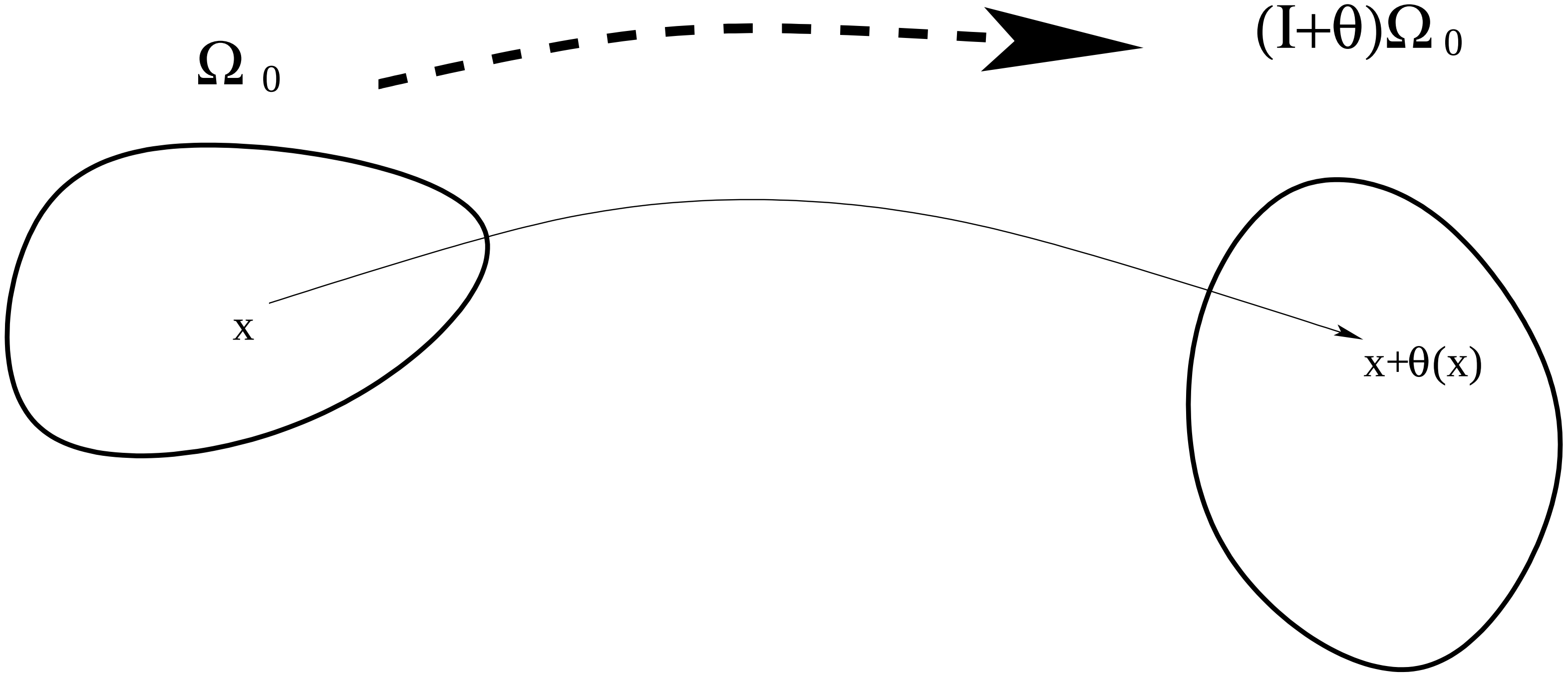
1. The homogenization method: composite materials with a microstructure are introduced (relaxation of the problem).
2. Level set method with a topological gradient: possible topology changes with a nucleation mechanism for new holes.

-II- SHAPE DIFFERENTIATION

We recall the well-known Hadamard's method.

Let Ω_0 be a reference domain. Shapes are parametrized by a vector field θ

$$\Omega = (\,\mathrm{Id} + \theta)\Omega_0 \quad \text{with} \quad \theta \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d).$$



Shape derivative

Definition: the shape derivative of $J(\Omega)$ at Ω_0 is the Fréchet differential of $\theta \to J\big((\,\mathrm{Id} + \theta)\Omega_0\big)$ at 0.

Lemma. For any $\theta \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$ such that $\|\theta\|_{W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)} < 1$, $(\,\mathrm{Id} + \theta)$ is a diffeomorphism in $\mathbb{R}^d$. In particular, it implies that there are no topology variations.

Many authors have contributed to this setting: Hadamard (1907), Murat-Simon (1976), Pironneau (1984), Sokolowski-Zolesio (1992), etc.

Examples of shape derivatives

Let Ω_0 be a smooth bounded open set and $f(x) \in W^{2,1}(\mathbb{R}^d)$. Define

$$J_1(\Omega) = \int_\Omega f(x)\,dx \quad \text{and} \quad J_2(\Omega) = \int_{\partial\Omega} f(x)\,ds.$$

Then J_1 and J_2 are differentiable at Ω_0 and, for any $\theta \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$,

$$J_1'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta(x)\cdot n(x)\,f(x)\,ds$$

$$J_2'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \theta(x)\cdot n(x)\left(\frac{\partial f}{\partial n} + Hf\right)(x)\,ds,$$

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

SHAPE DERIVATIVE OF THE COMPLIANCE

$$J(\Omega) = \int_{\Gamma_N} g \cdot u_\Omega \, ds = \int_\Omega A\, e(u_\Omega) \cdot e(u_\Omega) \, dx,$$

$$J'(\Omega_0)(\theta) = - \int_\Gamma Ae(u) \cdot e(u) \, \theta \cdot n \, ds,$$

where u is the state variable in Ω_0.

Remark: self-adjoint problem (no adjoint state is required).

Without volume constraint: the bigger the domain, the smaller the compliance.

SHAPE DERIVATIVE OF THE LEAST-SQUARE CRITERIA

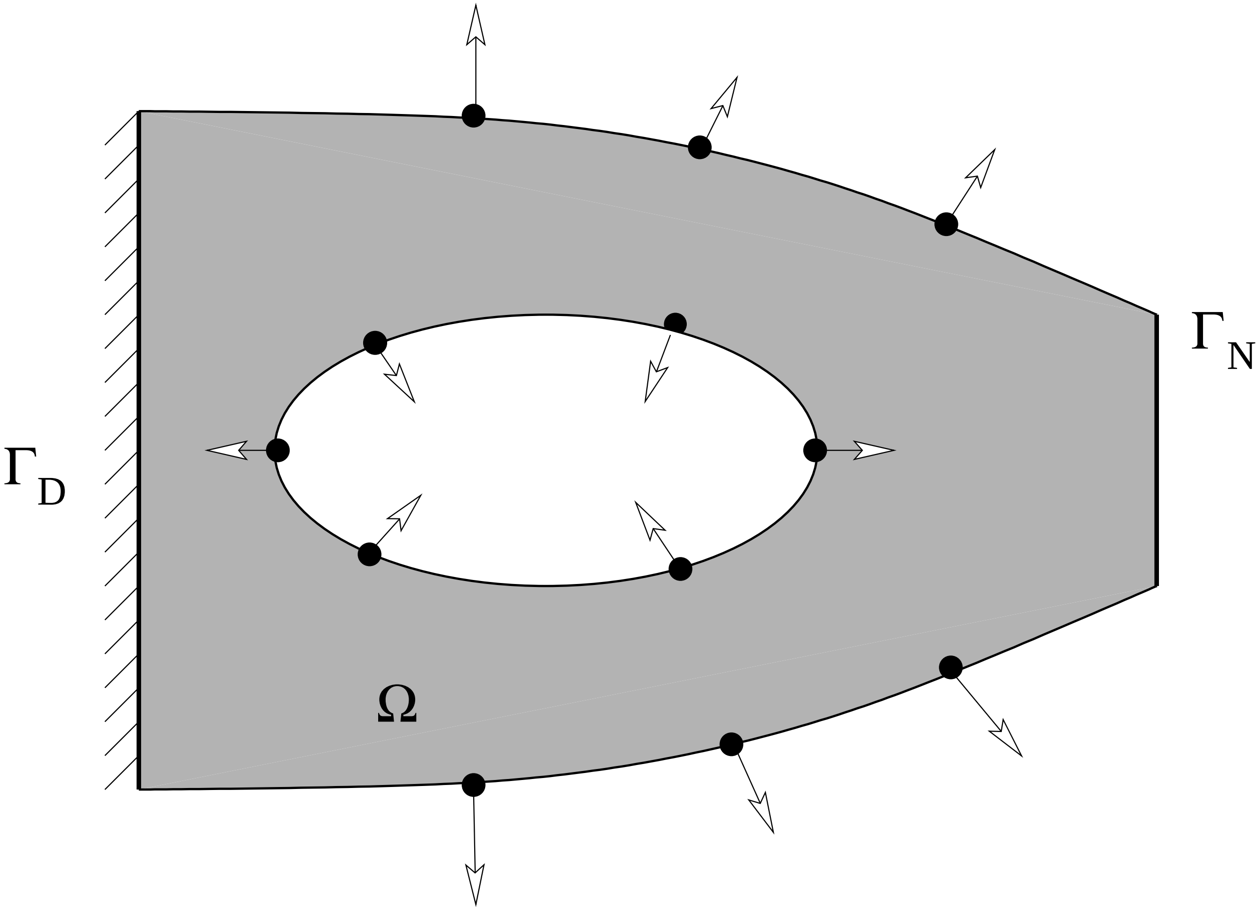
$$J(\Omega) = \int_{\Omega} k(x)|u_{\Omega} - u_0|^2 dx,$$

$$J'(\Omega_0)(\theta) = \int_{\Gamma} \left(-Ae(p)\cdot e(u) + k(x)|u-u_0|^2\right) \theta \cdot n \, ds,$$

with the state u and the adjoint state p defined by

$$\begin{cases} -\operatorname{div}\left(A\, e(p)\right) = 2k(x)(u-u_0) & \text{in } \Omega_0 \\ p = 0 & \text{on } \Gamma_D \\ \big(Ae(p)\big)n = 0 & \text{on } \Gamma_N \cup \Gamma. \end{cases}$$

Classical numerical algorithm



The boundary is parametrized by control nodes which are moved in the direction of the shape gradient (steepest descent algorithm).

Principles

- ☞ Iterative algorithm: the shape derivative is computed (by solving a p.d.e.), and accordingly the shape is deformed.
- ☞ Convergence to a local minimum.
- ☞ Strong influence of the initial design and of the mesh size.
- ☞ The topology (number of holes in 2-d) can not change.
- ☞ The shape must be re-meshed in case of large deformations: this is too costly in 3-d.

NUMERICAL RESULTS

Illustration of ill-posedness: local minima and impossibility of topology changes. (Results obtained with FreeFem++ in collaboration with O. Pantz.)

Cantilever problem: compliance minimization.

Consequence: we must optimize both the shape and the topology.

Two possible directions (among others):

- ☞ Relaxation by the homogenization method.
- ☞ The level set method with a topological gradient.

They both rely on a multiscale approach. We focus on the latter one. (Similar idea in the context of inverse problems by Burger, Hackl and Ring, JCP 2004).

-III- LEVEL SET METHOD

A new numerical implementation of an old idea...

- ☞ Still in the framework of Hadamard's method.
- ☞ Shape capturing algorithm.
- ☞ Fixed mesh: low computational cost.

Main tool: the level set method of Osher and Sethian (JCP 1988).

- ☞ Some references: Sethian and Wiegmann (JCP 2000), Osher and Santosa (JCP 2001), Allaire, Jouve and Toader (CRAS 2002, JCP 2003), Wang, Wang and Guo (CMAME 2003).
- ☞ Similar (but different) from the phase field approach of Bourdin and Chambolle (COCV 2003).
- ☞ Some drawbacks remain: reduction of topology rather than variation (mainly in 2-d), many local minima.

FRONT PROPAGATION BY LEVEL SET

Shape capturing method on a fixed mesh of the “working domain” D.

A shape Ω is parametrized by a **level set** function

$$\begin{cases} \psi(x) = 0 & \Leftrightarrow x \in \partial\Omega \cap D \\ \psi(x) < 0 & \Leftrightarrow x \in \Omega \\ \psi(x) > 0 & \Leftrightarrow x \in (D \setminus \Omega) \end{cases}$$

The normal n to Ω is given by $\nabla\psi/|\nabla\psi|$ and the curvature H is the divergence of n.

These formulas make sense everywhere in D on not only on the boundary $\partial\Omega$.

Hamilton Jacobi equation

Assume that the shape $\Omega(t)$ evolves in time t with a normal velocity $V(t,x)$. Then

$$\psi\Big(t,x(t)\Big) = 0 \quad \text{for any } x(t) \in \partial\Omega(t).$$

Deriving in t yields

$$\frac{\partial\psi}{\partial t} + \dot{x}(t)\cdot\nabla_x\psi = \frac{\partial\psi}{\partial t} + Vn\cdot\nabla_x\psi = 0.$$

Since $n = \nabla_x\psi/|\nabla_x\psi|$ we obtain

$$\frac{\partial\psi}{\partial t} + V|\nabla_x\psi| = 0.$$

This Hamilton Jacobi equation is posed in the whole box D, and not only on the boundary $\partial\Omega$, if the velocity V is known everywhere.

Idea of the method

Shape derivative

$$J'(\Omega_0)(\theta) = \int_\Gamma j(u,p)\,\theta\cdot n\,ds.$$

Gradient algorithm for the shape:

$$\Omega_{k+1} = \Big(\mathrm{Id} - j(u_k,p_k)n_k\Big)\Omega_k$$

The normal advection velocity of the shape is $-j$.

Introducing a “pseudo-time” (a descent parameter), we solve the Hamilton-Jacobi equation

$$\frac{\partial\psi}{\partial t} - j|\nabla_x\psi| = 0 \quad \text{in } D$$

NUMERICAL ALGORITHM

1. Initialization of the level set function ψ_0 (including holes).
2. Iteration until convergence for $k \geq 1$:
   - (a) Computation of u_k and p_k by solving linearized elasticity problem with the shape ψ_k. Evaluation of the shape gradient = normal velocity $= -j(u_k, p_k)$
   - (b) Transport of the shape by $-j(u_k, p_k)$ (Hamilton Jacobi equation) to obtain a new shape ψ_{k+1}.

Algorithmic issues

- ✗ Finite difference scheme, upwind of order 2, for the Hamilton Jacobi equation (ψ is discretized at the nodes of a quadrangular mesh).

- ✗ Q1 finite elements for the elasticity problems in D

$$\begin{cases} -\operatorname{div}\left(A^* \, e(u)\right) = 0 & \text{in } D \\ u = 0 & \text{on } \Gamma_D \\ \big(A^* e(u)\big)n = g & \text{on } \Gamma_N \\ \big(A^* e(u)\big)n = 0 & \text{on } \partial D \setminus (\Gamma_N \cup \Gamma_D). \end{cases}$$

- ✗ Tensor A^* = mixture of A and a weak material mimicking holes

$$A^*(x) = \begin{cases} A & \text{if } x \in \Omega \\ \epsilon A & \text{if } x \in D \setminus \Omega \end{cases} \qquad \text{with, e.g., } \epsilon = 10^{-3}.$$

- ✗ Descent step = several (≈ 20) explicit time steps of the transport equation (each of them controlled by the CFL condition).

NUMERICAL EXAMPLES

See the web page:

http://www.cmap.polytechnique.fr/~optopo/level_en.html

Reference: Allaire G., Jouve F., Toader A.-M., *Structural optimization using sensitivity analysis and a level-set method,* J. Comp. Phys., Vol 194/1, pp.363-393 (2004).

-IV- TOPOLOGICAL GRADIENT

Idea introduced by Eschenauer-Schumacher (1994), Guillaume-Masmoudi (2001), Sokolowski-Zochowski (1999).

This is a microscopic ingredient that we couple with the macroscopic level set method: **multiscale approach**.

Consider an open set $\Omega \subset \mathbb{R}^d$ and a point $x_0 \in \Omega$. Let $\omega \subset \mathbb{R}^d$ be a fixed smooth hole (containing the origin) and $\rho > 0$. Define the perforated domain

$$\Omega_\rho = \Omega \setminus \bar{\omega}_\rho \quad \text{with} \quad \omega_\rho = x_0 + \rho\omega.$$

Definition. If the objective function admits the following so-called topological asymptotic expansion for small $\rho > 0$

$$J(\Omega_\rho) = J(\Omega) + \rho^d D_T J(x_0) + o(\rho^d),$$

then $D_T J(x_0)$ is called the topological derivative at point x_0.

If $D_T J(x_0) < 0$, then a small hole should be inserted at x_0 to decrease the objective function.

Examples

Lemma. The topological derivative of $V(\Omega) = \int_\Omega dx$ is

$$D_T V(x) = -|\omega|.$$

Theorem (Garreau-Guillaume-Masmoudi, Sokolowski-Zochowski). Take ω to be the unit ball of $\mathbb{R}^d$. For any $x \in \Omega$ the topological derivative of the compliance is, for $d = 2$,

$$D_T J(x) = \tfrac{\pi(\lambda+2\mu)}{2\mu(\lambda+\mu)} \Big\{ 4\mu A e(u) \cdot e(u) + (\lambda - \mu) tr(Ae(u)) tr(e(u)) \Big\}(x),$$

and for $d = 3$,

$$D_T J(x) = \tfrac{\pi(\lambda+2\mu)}{\mu(9\lambda+14\mu)} \Big\{ 20\mu A e(u) \cdot e(u) + (3\lambda - 2\mu) tr(Ae(u)) tr(e(u)) \Big\}(x).$$

NUMERICAL ALGORITHM

The topological gradient is coupled to the level set method.

1. Initialization of the level set function ψ_0 (usually with no holes).
2. Iteration until convergence, for $k \geq 0$:
    - (a) **Elasticity analysis.** Computation of u_k and p_k in Ω_k. Evaluation of the shape gradient $J'(\Omega_k)$ and of the topological gradient $D_T J_k$.
    - (b) **Shape gradient.** If $\mod(k, n_{top}) < n_{top}$, the current shape Ω_k, characterized by the level set function ψ_k, is transported into a new shape Ω_{k+1}, characterized by ψ_{k+1}, by solving the transport Hamilton-Jacobi equation with velocity $-J'(\Omega_k)$.
    - (c) **Topological gradient.** If $\mod(k, n_{top}) = 0$, we insert new holes in the current shape Ω_k where the topological derivative $D_T J_k$ has minimum negative values.

NUMERICAL EXAMPLES

See the web page:

http://www.cmap.polytechnique.fr/~optopo/level_en.html

Reference: Allaire G., de Gournay F., Jouve F., Toader A.-M., *Structural optimization using topological and shape sensitivity via a level set method*, to appear in Control and Cybernetics.