Shape optimization (Lectures 3 & 4)

François Jouve University Paris Diderot (Paris 7) & Laboratoire J.L.Lions

Grégoire Allaire, CMAP, Ecole Polytechnique (Palaiseau)

Sylvie Aubry, Sandia Lab, Livermore Eric Bonnetier, Grenoble University Gilles Francfort, Paris Nord University Hervé Maillot, Orléans University

Frédéric de Gournay, Versailles University Anca-Maria Toader, Lisbon University Nicolas Van Goethem, Lisbon University

www.cmap.polytechnique.fr/~optopo

jouve@math.jussieu.fr

Plan

- Lecture 1: Introduction to shape optimization. Homogenization method I
- Lecture 2: Homogenization method II. Algorithm and numerical issues

- Lecture 3: Domain variation. Level set method I
- Lecture 4: Level set method II and applications

Part 2: Level set method

1) Shape sensitivity optimization

• Hadamard method, revisited by many authors (Murat-Simon, Pironneau, Nice's school, etc.).

- III posed problem: many local minima, no convergence under mesh refinement.
- In practice, topology changes very difficult to handle.
- Very costly because of remeshing (3d).
- Very general: any constitutive equation or objective function.
- Widely used method.

2) Topology optimization

• Homogenization method (Murat-Tartar, Lurie-Cherkaev, Kohn-Strang, Bendsoe-Kikuchi, Allaire-Bonnetier-Francfort-FJ, etc.).

 \longrightarrow simple objective functions, linear models but well posed problem.

- Evolutionary algorithms (Schoenauer, etc.).
- Topological asymptotics, topological gradient (Sokołowski, Masmoudi, etc.).
- Very cheap because it captures shapes on a fixed mesh.

Level set method

• Combine some advantages of the shape sensitivity method and the topological method (homogenization, topological gradient, SIMP)

• Based on the shape derivative (Hadamard, Murat-Simon).

- * Easy handling of various objective functions
- * Can be adapted to any direct problem (e.g. nonlinear)

• Shape representation by the 0 level set of a scalar field on a fixed mesh (Osher-Sethian).

* Moderate cost

- * No numerical instabilities due to remeshing
- * Easy topology changes
 - Remaining drawbacks:
- 1. reduction of topology (rather than variation) in 2d,
- 2. local minima.

Hint: coupling with the topological gradient

Setting of the problem

Linearly elastic material. Isotropic Hooke's law A. u displacement field, $e(u) = \frac{1}{2} (\nabla u + \nabla u^T)$ deformation tensor.

Linearized elasticity system posed on $\omega \subset \Omega$ (a given open bounded domain):

$$\begin{cases} -\operatorname{div}(Ae(u)) &= 0 \quad \text{in } \omega \\ u &= 0 \quad \text{on } \partial \omega \cap \Gamma_D \\ (Ae(u)) \cdot n &= g \quad \text{on } \partial \omega \cup \Gamma_N \end{cases}$$

It admits a unique solution.



* Compliance: $J(\omega) = \int_{\omega} Ae(u) : e(u)dx = \int_{\omega} A^{-1}\sigma : \sigma dx = \int_{\partial \omega} g \cdot u \, ds = c(\omega)$

Global measurement of rigidity.

The most widely used in structural topology optimization.

Remark: the compliance *maximization* for 2 materials is related to damage models.

* Displacement dependent criterion: for example $J(\omega) = \left\{ \int_{\omega} k(x) |u(x) - u_0(x)|^{\alpha} dx \right\}^{1/\alpha}$

where u_0 is a given *target-displacement*, $\alpha \geq 2$ and k a given multiplier.

Geometrical advantage: J_{G}

$$_{\mathbf{A}}(\omega) = -\frac{u_{out}}{u_{in}},$$



* Stress dependent objective functions:

$$J_{\sigma}(\omega) = \left\{ \int_{\omega} |\sigma|^{\alpha} \right\}^{1/\alpha}$$

$$J_{\sigma \text{target}}(\omega) = \left\{ \int_{\omega} k(x) |\sigma - \sigma_0|^{\alpha} \right\}^{1/\alpha}$$

$$J_{\rm VM}(\omega) = \left\{ \int_{\omega} \left((\sigma_{11} - \sigma_{22})^2 + (\sigma_{22} - \sigma_{33})^2 + (\sigma_{33} - \sigma_{11})^2 + 6(\sigma_{12}^2 + \sigma_{23}^2 \sigma_{31}^2) \right)^{\alpha} \right\}^{1/\alpha}$$

* Eigenfrequency(ies) maximization:

$$J(\omega) = -\omega_1(\omega)^2$$

where $\omega_1(\omega)$ is the first eigenfrequency associated to the domain ω . It is given by the Rayleigh quotient:

$$\omega_1^2 = \min_{\substack{v \in H^1(\omega)^N, \, v \neq 0 \\ v = 0 \text{ on } \Gamma_D}} \frac{\int_{\omega} A \, e(v) \cdot e(v) \, dx}{\int_{\omega} \rho |v|^2 dx}$$

* Robust optimization (worst case compliance):

$$J_r(\omega) = \max_{\alpha \text{ admissible perturbation}} \int_{\partial \omega} (g + \alpha) \cdot u \, ds$$

* Optimization of the buckling criterion:

$$J_b(\omega) = \frac{1}{\lambda}$$

where λ is the critical buckling load (solution of a generalized eigenvalue problem)

* Multiple loads:

$$J(\omega) = \sum_{k=1}^{n} \int_{\omega} Ae(u_k) : e(u_k) dx = \sum_{k=1}^{n} \int_{\partial \omega} g_k \cdot u_k ds$$

 $(u_k)_{k=1...n}$ are *n* displacement fields solutions of *n* different elasticity problems where $(g_k)_{k=1...n}$ are independent loadings.

* Any linear combination of the above objective functions

Existence theory

Minimal set of admissible shapes

$$\mathcal{U}_{ad} = \left\{ \omega \subset \Omega, \ \mathsf{vol}(\omega) = V_0, \ \Gamma_N \subset \partial \omega, \ meas(\Gamma_D \cap \partial \omega) > 0 \right\}$$

where Ω is open and bounded in \mathbb{R}^N .

Usually, the minimization problem has no solutions in U_{ad} .

Existence under additional conditions:

- Uniform cone condition (D.Chenais)
- *Regularity condition* (F.Murat, J.Simon)
- *Perimeter constraint* (L.Ambrosio, G.Buttazzo)
- In 2d, a uniformly bounded number of connected components of $\Omega \setminus \omega$ (A.Sverak, A.Chambolle, C.Larsen)

Existence theorem 1: Uniform cone condition

Definition: let $\theta \in (0, \pi/2)$, h > 0, $\xi \in \mathbb{R}^N$, $|\xi| = 1$, the cone of direction ξ , angle θ and height h is defined by

 $C(\theta, h, \xi) = \{ x \in \mathbb{R}^N, x.\xi > |x| \cos \theta, |x| < h \}$

Definition: $\omega \subset \mathbb{R}^N$ verifies the uniform cone condition if and only if $\exists \theta \in (0, \pi/2), h > 0, r > 0$ such that $\forall x \in \partial \omega, \exists \xi(x)$ such that

$$\forall y \in B(x,r) \cap \partial \omega, \quad y + C(\theta,h,\xi(x)) \subset \omega$$

Remark 1: the cone condition does not imply regularity (corners allowed)Remark 2: the cone condition avoids highly oscillating boundaries and cusps

Existence theorem 1: Uniform cone condition

Theorem [Chenais 75]: $D \subset \mathbb{R}^N$ a given domain. If

 $U_{ad1} = \{ \omega \in U_{ad}, \ \omega \text{ verifies the uniform cone condition} \}$

then

$$\inf_{\omega \in U_{ad1}} J(\omega)$$

admits at least one solution.

Remark:: not useful for applications



Existence theorem 2: Regularity condition

Definition: diffeomorphisms of \mathbb{R}^N :

$$\mathcal{T} = \{T: \mathbb{R}^N \to \mathbb{R}^N, \ (T - Id) \in W^{1,\infty}(\mathbb{R}^N, \mathbb{R}^N) \text{ and } (T^{-1} - Id) \in W^{1,\infty}(\mathbb{R}^N, \mathbb{R}^N)\}$$

If $\omega_0 \subset {\rm I\!R}^N$ is a given open reference domain, bounded and smooth (e.g. \mathcal{C}^1) and

$$\mathcal{D}(\omega_0) = \{ \omega \subset \mathbb{R}^N, \exists T \in \mathcal{T} \text{ such that } \omega = T(\omega_0) \}$$

then for $\omega_1,\omega_2\in\mathcal{D}(\omega_0)$ we can define the pseudo-distance

$$d(\omega_1, \omega_2) = \inf_{T \in \mathcal{T}, T(\omega_1) = \omega_2} \left(||T - Id||_{1,\infty} + ||T^{-1} - Id||_{1,\infty} \right)$$

Existence theorem 2: Regularity condition

Theorem [Murat-Simon 76]: if C > 0 and

$$U_{ad2} = \{ \omega \in U_{ad} \cap \mathcal{D}(\omega_0), \ d(\omega, \omega_0) \le C \}$$

then

$$\inf_{\omega \in U_{ad2}} J(\Omega)$$

admits at least one solution.

Remark:: not useful for applications

Existence theorem 3: Additional regularizing term

Theorem [Ambrosio-Buttazzo 93]: if $\tilde{J}(\omega) = J(\omega) + P(\partial \omega)$, where $P(\partial \omega)$ is an ad-hoc regularizing term involving the perimeter of the shape, then

$$\inf_{\omega \in U_{ad}} \tilde{J}(\omega)$$

admits at least one solution.

Remark 1: avoids highly oscillating boundaries (like the cone condition)

Remark 2: useful in practice. The perimeter is easy to compute (e.g. using the level set representation).

Existence theorem 4: Topological condition in 2d

Theorem [Sverak 93, Chambolle-Larsen 03]: for a given $k \in \mathbb{N}$,

 $U_{ad4} = \{ \omega \in U_{ad}, \ \Omega \setminus \omega \text{ has less than } k \text{ connected components} \}$

then

$$\inf_{\omega \in U_{ad4}} J(\omega)$$

admits at least one solution.

Remark 1: strongly restricted to the 2d case

Remark 2: not (very) useful for applications

Numerical method strategy

1) Computation of the shape derivatives of the objectives functions (in a continuous framework). \rightarrow Murat-Simon method.

2) The derivatives are discretized. The shapes are modeled by a level set function on a fixed mesh. The shape is varied by advecting the level set function following the flow of the shape gradient.

 \longrightarrow transport equation of Hamilton-Jacobi type.

3) From *time to time*, additional computation of the topological gradient to guess where it may be advantageous to dig new holes (and back to point 1)).

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Shape derivative (Murat-Simon, Céa)

 ω_0 reference domain. We are interested in variations of the form

$$\omega = \{x + \theta(x) \mid x \in \omega_0\} = (\mathrm{Id} + \theta)\omega_0$$

with $\theta \in W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d).$

 $\theta(x)$ is a vector field that *deforms* the reference domain ω_0 .



Lemma: For any $\theta \in W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ such that $\|\theta\|_{W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)} < 1$, $(\operatorname{Id} + \theta)$ is a diffeomorphism in \mathbb{R}^d .

Definition:

The shape derivative of $\omega \mapsto J(\omega)$ at ω_0 is the Fréchet derivative of $\theta \mapsto J((\operatorname{Id} + \theta)\omega_0)$ at 0.

Shape derivative (Murat-Simon)



Lemma: Let ω_0 be a smooth bounded open set and $J(\omega)$ at differentiable function at ω_0 . Its derivative satisfies

$$J'(\omega_0)(\theta_1) = J'(\omega_0)(\theta_2)$$

if $\theta_1, \theta_2 \in W^{1,\infty}({\rm I\!R}^N; {\rm I\!R}^N)$ are such that

$$\left\{ \begin{array}{l} \theta_2 - \theta_1 \in \mathcal{C}^1(\mathbb{R}^N; \mathbb{R}^N) \\ \theta_1 \cdot n = \theta_2 \cdot n \quad \text{on } \partial \omega_0. \end{array} \right.$$

Examples of shape derivatives (I)

Objective-function defined in the domain: Let ω_0 be a smooth bounded open set of class \mathcal{C}^1 of \mathbb{R}^N . Let $f(x) \in W^{1,1}(\mathbb{R}^N)$ and J defined by

$$J(\omega) = \int_{\omega} f(x) \, dx$$

Then J is differentiable at ω_0 and

$$J'(\omega_0)(\theta) = \int_{\omega_0} \operatorname{div} \left(\theta(x) f(x)\right) dx = \int_{\partial \omega_0} \theta(x) \cdot n(x) f(x) ds$$

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

Examples of shape derivatives (II)

Objective-function defined on the boundary: Let ω_0 be a smooth bounded open set of class \mathcal{C}^1 of \mathbb{R}^N . Let $f(x) \in W^{2,1}(\mathbb{R}^N)$ and J defined by

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

Then J is differentiable at ω_0 and

$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} \left(\nabla f \cdot \theta + f \left(\operatorname{div} \theta - \nabla \theta n \cdot n \right) \right) ds$$

for all $\theta \in W^{1,\infty}(\mathbb{R}^N; \mathbb{R}^N)$. Moreover if ω_0 is smooth of class \mathcal{C}^2 , then

$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} \theta \cdot n\left(\frac{\partial f}{\partial n} + Hf\right) ds,$$

where H is the mean curvature of $\partial \omega_0$ defined by $H = \operatorname{div} n$.

Shape derivative of the compliance

$$J(\omega) = \int_{\partial \omega \cup \Gamma_N} g \cdot u \, ds = \int_{\omega} A \, e(u) \cdot e(u) \, dx,$$

$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} \left(2 \left[\frac{\partial (g \cdot u)}{\partial n} + Hg \cdot u \right] - Ae(u) \cdot e(u) \right) \theta \cdot n \, ds,$$

where u is the state (displacement field) in ω_0 , and H the mean curvature of $\partial \omega_0$.

No adjoint state involved. The compliance problem is self-adjoint.

Shape derivative of the least-square criterion

$$J(\omega) = \left(\int_{\omega} k(x)|u - u_0|^{\alpha} dx\right)^{1/\alpha},$$
$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} \left(\frac{\partial (g \cdot p)}{\partial n} + Hg \cdot p - Ae(p) \cdot e(u) + \frac{C_0}{\alpha} k|u - u_0|^{\alpha}\right) \theta \cdot n \, ds,$$

where the state \boldsymbol{u} is solution of the elasticity system and the adjoint state \boldsymbol{p} is solution of

$$\begin{cases} -\operatorname{div} (A e(p)) &= C_0 k(x) |u - u_0|^{\alpha - 2} (u - u_0) & \text{in } \omega_0 \\ p &= 0 & \text{on } \Gamma_D \\ (A e(p)) \cdot n &= 0 & \text{on } \Gamma_N \cup \partial \omega_0, \end{cases}$$

•

with
$$C_0 = \left(\int_{\omega_0} k(x) |u(x) - u_0(x)|^{\alpha} dx \right)^{1/\alpha - 1}$$

Consider a general objective function

$$J(\omega) = \int_{\omega} j(x, u(x)) \, dx + \int_{\partial \omega} l(x, u(x)) \, ds,$$

Introduce the Lagrangian defined for $(v,q) \in \left(H^1(\mathbb{R}^d;\mathbb{R}^d)\right)^2$ by

$$\mathcal{L}(\omega, v, q) = \int_{\omega} j(v) \, dx + \int_{\partial \omega} l(v) \, ds + \int_{\omega} Ae(v) \cdot e(q) \, dx - \int_{\omega} q \cdot f \, dx \\ - \int_{\Gamma_N} q \cdot g \, ds - \int_{\Gamma_D} \Big(q \cdot Ae(v)n + v \cdot Ae(q)n \Big) ds.$$

v and q belong to a functional space that does not depend on ω , so we can apply the usual differentiation rule to \mathcal{L} .

The stationarity of the Lagrangian gives the optimality conditions of the minimization problem.

$$\begin{split} \langle \frac{\partial \mathcal{L}}{\partial q}(\omega, u, p), \phi \rangle &= 0 = -\int_{\omega} \phi \cdot \left(\operatorname{div} \left(Ae(u) \right) + f \right) dx \\ &+ \int_{\Gamma_N} \phi \cdot \left(\left(Ae(u) \right) n - g \right) ds \\ &- \int_{\Gamma_D} u \cdot Ae(\phi) n \, ds. \end{split}$$

- $\bullet~\phi$ with compact support in ω \rightarrow state equation
- vary the trace of ϕ on $\Gamma_N \to \mathsf{Neumann}$ boundary condition on u
- vary $(Ae(\phi))n$ on $\Gamma_D \to \text{Dirichlet boundary condition on } u$

$$\begin{split} \langle \frac{\partial \mathcal{L}}{\partial v}(\omega, u, p), \phi \rangle &= 0 \quad = \int_{\omega} j'(u) \cdot \phi \, dx + \int_{\partial \omega} l'(u) \cdot \phi \, ds \\ &+ \int_{\omega} Ae(\phi) \cdot e(p) \, dx \\ &- \int_{\Gamma_D} \left(p \cdot Ae(\phi)n + \phi \cdot Ae(p)n \right) ds. \end{split}$$

Integration by parts leads to

$$\begin{split} \langle \frac{\partial \mathcal{L}}{\partial v}(\omega, u, p), \phi \rangle &= \int_{\omega} \left(j'(u) - \operatorname{div} \left(Ae(p) \right) \right) \cdot \phi \, dx + \int_{\Gamma_N} \phi \cdot \left(Ae(p)n + l'(u) \right) ds \\ &+ \int_{\Gamma_D} \left(\phi \cdot l'(u) - p \cdot Ae(\phi)n \right) ds. \end{split}$$

• ϕ with compact support in $\omega \rightarrow$ adjoint state equation:

$$-\operatorname{div}(Ae(p)) = -j'(u)$$
 in ω .

• vary the trace of ϕ on $\Gamma_N \rightarrow$ Neumann boundary condition on p:

$$(Ae(p))n = -l'(u)$$
 on Γ_N .

• vary $(Ae(\phi))n$ on $\Gamma_D \to \text{Dirichlet boundary condition on } p$:

$$p=0$$
 on Γ_D .

We have found a well-posed boundary value problem for the adjoint state p.

The shape derivative of the objective function is obtained by differentiating ${\cal L}$ with respect to ω in the direction θ

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \omega}(\omega, u, p)(\theta) &= \int_{\partial \omega} \theta \cdot n \left(j(u) + Ae(u) \cdot e(p) - p \cdot f \right) ds \\ &+ \int_{\partial \omega} \theta \cdot n \left(\frac{\partial l(u)}{\partial n} + H \, l(u) \right) ds \\ &- \int_{\Gamma_N} \theta \cdot n \left(\frac{\partial (g \cdot p)}{\partial n} + H \, g \cdot p \right) ds \\ &- \int_{\Gamma_D} \theta \cdot n \left(\frac{\partial h}{\partial n} + H h \right) ds, \end{split}$$

where $h = u \cdot Ae(p)n + p \cdot Ae(u)n$ and $H = \operatorname{div} n$ is the mean curvature of the boundary.

Taking into account the boundary conditions u = p = 0 on Γ_D gives (after computation)

$$\begin{split} \frac{\partial \mathcal{L}}{\partial \omega}(\omega, u, p)(\theta) &= \int_{\Gamma_N} \theta \cdot n \left(j(u) + Ae(u) \cdot e(p) - p \cdot f - \frac{\partial (g \cdot p)}{\partial n} - H \, g \cdot p \right) ds \\ &+ \int_{\Gamma_D} \theta \cdot n \left(j(u) - Ae(u) \cdot e(p) \right) ds \\ &+ \int_{\partial \omega} \theta \cdot n \left(\frac{\partial l(u)}{\partial n} + H \, l(u) \right) ds. \end{split}$$

Remark: this computation is only valid for a domain (1 phase + void). In the 2 phases case, the spirit is the same but the result is much more complicated (see damage evolution problem).

Front propagation by level set

Shapes are not meshed, but captured on a fixed mesh of a large box Ω .

Parameterization of the shape ω by a level set function:

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

- Exterior normal to ω : $n = \nabla \psi / |\nabla \psi|$.
- Mean curvature: $H = \operatorname{div} n$.
- These formula make sense everywhere in Ω , not only on the boundary $\partial \omega$.
- \longrightarrow natural extension

Level set



Hamilton-Jacobi equation

If the shape $\omega(t)$ evolves in pseudo-time t with a normal speed V(t, x), then ψ satisfies a Hamilton-Jacobi equation:

$$\psi(t, x(t)) = 0$$
 for all $x(t) \in \partial \omega(t)$.

deriving in t yields

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

As $n=\nabla\psi/|\nabla\psi|$ we obtain

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

This equation is valid on the whole domain Ω , not only on the boundary $\partial \omega$, assuming that the velocity is known everywhere.

 \rightarrow the description of the boundary of ω can remain implicit during the algorithm.

Application to shape optimization

If the shape derivative can be expressed as an integral of the form:

$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} v \,\theta \cdot n \, ds,$$

then a valid descent direction, allowing J to decrease at the first order, is

$$\theta = -v \cdot n$$

Thus, solving

$$\frac{\partial \psi}{\partial t} - v |\nabla \psi| = 0 \quad \text{ in } \Omega$$

is equivalent to perform a descent algorithm where t is a descent parameter
Numerical algorithm

- 1. Initialization of the level set function ψ_0 (e.g. a product of sinus).
- 2. Iterations until convergence for $k \ge 1$:
 - (a) Computation of u_k and eventually p_k by solving a linearized elasticity problem on the shape ψ_k . Computation of the shape gradient \rightarrow normal velocity V_k
 - (b) Transport of the shape by the speed V_k (Hamilton-Jacobi equation) to obtain a new shape ψ_{k+1} . (Several successive time steps can be applied for a same velocity field). The descent step is controlled by the CFL condition on the transport equation and by the decreasing of the objective function.
 - (c) Possible reinitialization of the level set function such that ψ_{k+1} is the signed distance to the interface.
- 3. Optionally: computation of the topological gradient to guess where holes may be dig, and return to loop 2.

Topological Gradient (Sokołowski et al., Masmoudi et al.)

A scalar criterion used to guess where it may be useful to dig additional holes in a converged solution that could be a local minimum.

Examples of topological gradients (2d elasticity, plane strains, Neuman boundary conditions for the holes):

• Example 1 (Compliance optimization):

$$TG = \frac{\pi(\lambda + 2\mu)}{2\mu(\lambda + \mu)} \left\{ 4\mu\sigma(u) : e(u) + (\lambda - \mu)\mathrm{tr}\sigma(u)\mathrm{tr}e(u) \right\}$$

• Example 2 (Minimization of $\int k(x)|u-u_0|^{\alpha}$):

$$TG = \frac{\pi}{\alpha} C_0 k(x) |u(x) - u_0(x)|^{\alpha} + \frac{\pi(\lambda + 2\mu)}{2\mu(\lambda + \mu)} \left\{ 4\mu\sigma(u) : e(p) + (\lambda - \mu) \operatorname{tr}\sigma(u) \operatorname{tr}e(p) \right\}$$









Some technical points

• Q1 quadangular structured meshes $(2d-3d) \longrightarrow$ classical upwind transport schemes.

 \bullet Possibilities of unstructured meshes \longrightarrow more complicated schemes for Hamilton-Jacobi equation (Abgrall).

- $\bullet~\psi$ discretized at mesh nodes.
- Resolution of elasticity systems by finite elements:

$$\begin{aligned} -\operatorname{div} (\theta(x) A e(u)) &= 0 \quad \text{in } \Omega \\ + B.C. \end{aligned}$$

with $\theta(x)$ a piecewise constant field defined by

 $\left\{ \begin{array}{ll} \theta &=& \varepsilon \ (\approx 10^{-3}) & \mbox{if } \psi > 0 \ \mbox{for all the nodes of the element} \\ \theta &=& \mbox{ad-hoc proportion} & \mbox{if the 0 level set goes through the element} \\ \theta &=& 1 & \mbox{si } \psi < 0 \ \mbox{for all the nodes of the element} \end{array} \right.$

Transport (structured mesh)

Resolution of

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

by an explicit upwind scheme of 1st or 2nd order

$$\frac{\psi_i^{n+1} - \psi_i^n}{\Delta t} - \max(j_i^n, 0) g^+ (D_x^+ \psi_i^n, D_x^- \psi_i^n) - \min(j_i^n, 0) g^- (D_x^+ \psi_i^n, D_x^- \psi_i^n) = 0$$

with
$$D_x^+ \psi_i^n = \frac{\psi_{i+1}^n - \psi_i^n}{\Delta x}$$
, $D_x^- \psi_i^n = \frac{\psi_i^n - \psi_{i-1}^n}{\Delta x}$, and
 $g^-(d^+, d^-) = \sqrt{\min(d^+, 0)^2 + \max(d^-, 0)^2}$,
 $g^+(d^+, d^-) = \sqrt{\max(d^+, 0)^2 + \min(d^-, 0)^2}$.

Complex geometries

To deal with complex geometries of the design domain (i.e. non rectangular geometries), 2 possibilities :

 \bullet Use an unstructured mesh (triangular or tetrahedral) \rightarrow special schemes for Hamilton-Jacobi resolution

• Use a large rectangular bounding box and a structured rectangular mesh. Introduce an additional level set to define the fixed domain

Example of use of an additional level set (optimization of the inner part of a wing) :



• The level set function is periodically reinitialized to avoid it to be *too flat* (\rightarrow poor precision on ψ) or *too steep* (\rightarrow poor precision on $\nabla \psi$ i.e. the normal) after some transport steps. It is done by solving

$$\frac{\partial \psi}{\partial t} + \operatorname{sign}(\psi) \Big(|\nabla \psi| - 1 \Big) = 0 \quad \text{ in } \Omega,$$



whose stationary solution is the signed distance to the interface $\{\psi(t=0,x)=0\}$.

Well well well... That's what you read in all the papers dealing with level sets That is certainly true at the continuous level *Let's see what happens for the discrete problem*



Example of function ψ on a rough mesh



Manual and exact computation of the signed distance and plot of the new level sets !



Level set after 100 iterations of exact computation of the signed distance !!

No reinitialization !



Natural extension vs regularized velocity

• The natural extension of the velocity in the whole domain is less efficient than an Hilbertian extension obtained by solving an elliptic problem taking the velocity at the interface as Dirichlet boundary conditions.

 \longrightarrow better convergence properties.

• Natural extension: the formula of the shape gradient is established on $\partial\Omega$, but it can be computed on the whole computational domain Ω .

• Hilbertian extension: obtained by solving an elliptic problem taking the velocity at the interface $\partial \omega$ as a Dirichlet boundary condition.

 \longrightarrow better convergence properties.



First eigenfrequency maximization



Boundary conditions, initialization and optimal shape of the double cantilever

Multi loads



Single load

Multi loads

Additional perimeter term









No perimeter term

3 different perimeter terms

Nonlinear elasticity



No trick. You can see the large displacements



Robust optimization

Optimize the structure for the "worst" perturbation of a given load.



Pressure applied on the (variable) boundary





Other objective-function: micromechanism design (MEMS)



What about the "weak material" ?



Multi loads MEMS



Why a stress based criterion ?



Why a stress based criterion ?



Shape derivative of a criterion depending on the stresses

$$J(\omega) = \left(\int_{\omega} k(x)|\sigma - \sigma_0|^{\alpha} dx\right)^{1/\alpha},$$
$$J'(\omega_0)(\theta) = \int_{\partial \omega_0} \left(\frac{\partial (g \cdot p)}{\partial n} + Hg \cdot p - Ae(p) \cdot e(u) + \frac{C_0}{\alpha} k|\sigma - \sigma_0|^2\right) \theta \cdot n \, ds,$$

where p is the adjoint state, solution of the adjoint problem:

$$\begin{cases} -\operatorname{div} (A e(p)) &= C_0 k(x) |\sigma - \sigma_0|^{\alpha - 2} (\sigma - \sigma_0) & \operatorname{dans} \omega_0 \\ p &= 0 & \operatorname{sur} \Gamma_D \\ (A e(p)) \cdot n &= 0 & \operatorname{sur} \Gamma_N \cup \partial \omega_0, \end{cases}$$

avec
$$C_0 = \left(\int_{\omega_0} k(x) |\sigma(x) - \sigma_0(x)|^{\alpha} dx\right)^{1/\alpha - 1}$$
.

Optimal cantilevers for $||\sigma||_{\alpha}$



Optimal "L" for $||\sigma||_{\alpha}$



Reentering corner for $||\sigma||_{\alpha}$



A compliant gripper





 $\int (|\sigma|^4)^{1/4}$

GA

A compliant gripper (deformed configuration)



 $\int (|\sigma|^4)^{1/4}$

GA

Compliant gripper (stress distribution for free jaws)





 $\int (|\sigma|^4)^{1/4}$

GA

Compliant gripper (stress distribution for blocked jaws)





GA

 $\int (|\sigma|^4)^{1/4}$

Compliance optimization of an electric mast



Stress optimization of an electric mast



Damage



Damage

• Damage of an healthy elastic material under a static or variable exterior force field

• Micro-structural phenomenons (e.g. micro-cracks) preserving a residual elasticity in the damaged zones

• Irreversibility of the process: once damaged, a zone remains damaged for the rest of the evolution

• Many mechanical models
The Francfort-Marigo model (1993)

• Quasi-static: dynamic and thermal effects are neglected.

• Two phases: "healthy" and "damaged" material, both linear elastic. Hooke's laws A_0 and A_1 well ordonned (in the sense of the quadratic forms): $A_1 \ge A_0$.

- Typical rigidity ratio = 3 to 10, but $A_0 \rightarrow 0$ is also interesting.
- At each point $x \in \Omega$, the material is damaged if the strain tensor e(u(x)) verifies

$$\frac{1}{2} (A_1 - A_0) e(u(x)) : e(u(x)) \ge \kappa,$$

where κ is the release of elastic energy per unit mass at critical strain values.

 \rightarrow Griffith criterion = energetic criterion of damage.

Damage model ⇔ design problem Layout of two materials in a given domain

The Francfort-Marigo model (1993)

• Linear elasticity but nonlinear model: the damaged zone depends on the strain tensor, that depends on the damaged zone...

• Minimization problem: χ characteristic function of the damaged zone:

$$A_{\chi}(x) = \chi(x)A_0 + (1 - \chi(x))A_1,$$

$$\inf_{\chi} \left(J_D(\chi) + \kappa \int_{\Omega} \chi(x) dx \right)$$
$$J_D(\chi) = \min_{u \in V} \left(\frac{1}{2} \int_{\Omega} \left(A_{\chi}(x) e(u) : e(u) - fu \right) dx - \int_{\Gamma_N} g.u \, ds \right)$$

where

$$V = \{ u \in H^1(\Omega)^d, u = u_D \text{ on } \Gamma_d \}$$
$$e(u) = \frac{1}{2} (\nabla u + \nabla u^T)$$

The Francfort-Marigo model (1993)

Double minimum (over u and χ). If there is an interface between the two materials, for a given $u, \forall x \in \Omega$:

$$\min_{\chi \in \{0,1\}} \{ \frac{1}{2} A_{\chi} e(u) : e(u) + \kappa \chi \}(x)$$

and the functionnal to minimize over all $u \in V$:

$$\frac{1}{2}\int_{\Omega}\min\left(A_{1}e(u):e(u),\,A_{0}e(u):e(u)+2\kappa\right)dx-\int_{\Omega}fu\,dx-\int_{\Gamma_{N}}gu\,ds$$

• III posed problem

• Francfort-Marigo: relaxation by homogenization (use of fine mixtures of the two phases and optimal microstructures)

• Global minima

Numerical example with homogenization (Allaire, Aubry, FJ 1998)



Propagation of interfaces

- We are looking for local minima: quasi-static evolution of a damaged zone.
- Interface between two materials.
- Admissible interface variations: domain derivation (Hadamard, Murat-Simon)
- No new damage zones not connected to initialy damaged zones.
- Interface representation and propagation using level set techniques.









Compliance minimization vs damage evolution

The variational formulation of the Francfort-Marigo is similar to the classical problem of compliance minimization in topology structural optimization:

• Compliance minimization: find the best compromise between rigidity and weight. The parameter κ governs the total volume of the optimized structure.

• Damage model: find the least rigid structure minimizing the volume of the damaged zone under the constraint of the Griffith criterion.

• Main differences:

* Sign

* Time discretization + Irreversibility of the damaged zone

* Two non degenerated phases (\rightarrow more complicated formula for the shape derivative).

Outline of the numerical algorithm (classical level set method)

- 1. Initialization of the level set function ψ_0 .
- 2. Iterations for $k \ge 1$:
 - (a) Computation of u_k : for a given layout associated to ψ_k , solve the elasticity problem.
 - (b) Computation of the shape derivative.
 - (c) Propagation of the interface using the shape derivative (Hamilton-Jacobi equation)
 - \rightarrow New interface characterized by ψ_{k+1} .

Outline of the numerical algorithm (damage evolution)

Time loop: at time t^i , initialization of the level set function ψ_0^i associated to the domain χ^{i-1} found at the previous time step

- 1. Initialization of the level set function ψ_0^i .
- 2. Iterations for $k \ge 1$:
 - (a) Computation of u_k^i : for a given layout associated to ψ_k^i , solve the elasticity problem.
 - (b) Computation of the shape derivative.
 - (c) Propagation of the interface using the shape derivative (Hamilton-Jacobi equation) \rightarrow New interface characterized by ψ_{k+1}^{i} .

Irreversibility: $\chi_k^i(x) \ge \chi^{i-1}(x), \quad \forall k, \forall x \in \Omega.$

Shape derivative of the compliance

$$J_C(\omega) = \int_{\Gamma \cup \Gamma_N} f \cdot u \, ds = \int_{\omega} A \, e(u) \cdot e(u) \, dx,$$

$$J'_{C}(\omega_{0})(\theta) = \int_{\partial \omega_{0}} \left(-Ae(u) \cdot e(u) \right) \theta \cdot n \, ds,$$

Shape derivative for the damage model

Additional difficulty: two materials instead of one material + void. \rightarrow more terms...

$$J'_D(\omega_0)(\theta) = \int_{\Sigma} d(x)\theta.n\,ds$$

with

$$d(x) = \left[\frac{1}{2(\lambda+2\mu)}\right] |\sigma_{nn}(u)|^2 + \left[\frac{1}{2\mu}\right] |\sigma_{tn}(u)|^2 - [\mu] |e_{tt}(u)|^2 - \left[\frac{\lambda\mu}{\lambda+2\mu}\right] |\operatorname{tr}(e_{tt}(u))|^2 - \left[\frac{\lambda}{\lambda+2\mu}\right] \sigma_{nn}(u) \operatorname{tr}(e_{tt}(u)),$$

$$e_{nn} = e(u)n.n \in \mathbb{R}, \quad e_{tt} = e(u)t.t \in \mathbb{R}^{(d-1) \times (d-1)}, \quad e_{nt} = e(u)n.t \in \mathbb{R}^{d-1}$$

 $[\mu] = \mu_1 - \mu_0$

Shape derivative for the damage model

Alternative expression to avoid degeneracy when Young modulus of A_0 tends to 0:

$$d(x) = \frac{1}{2} \Big(\sigma_{nn}(u) \cdot [e_{nn}(u)] - e_{tt}(u) \cdot [\sigma_{tt}(u)] + 2\sigma_{tn}(u) \cdot [e_{tn}(u)] \Big).$$

 $J'_D \rightarrow -\frac{1}{2}J'_C$ when $A_0 \rightarrow 0$.

Shape derivative for the damage model

Alternative expression to avoid degeneracy when Young modulus of A_0 tends to 0:

$$d(x) = \frac{1}{2} \Big(\sigma_{nn}(u) \cdot [e_{nn}(u)] - e_{tt}(u) \cdot [\sigma_{tt}(u)] + 2\sigma_{tn}(u) \cdot [e_{tn}(u)] \Big).$$

$$J'_D \to -\frac{1}{2}J'_C$$
 when $A_0 \to 0$.

Remaining implementation problem: how to compute the jump terms (e.g. $[\sigma_{tt}(u)]$) across the implicit interface ?

 \rightarrow Extension and regularization of the velocity. The regularized velocity have to preserve the positivity of some terms in the above expression.

Remarks

• The limit of the Francfort-Marigo model implemented using the level set representation seem to numerically converge to a quite efficient model of crack propagation

 \bullet Mesh refinement \rightarrow scaling of κ with the mesh size

• The shape derivative for the interface between two materials could be useful to make two-phases shape optimization

2d cracks



2d cracks (mode 2 - mesh refinements



Damage with a non-degenerated material



2d cracks



2d cracks



Bittencourt problem 1



Bittencourt problem 2



3d cracks - Mode 1



3d cracks - Mode 2



3d cracks - Mode 3



One technical issue

• The level set method can only evolve an existing interface. It includes damage initiation starting from the boundary of the domain or evolution of existing damaged areas.

But it cannot create a new damaged zone inside the domain starting from a fully healthy structure.

• Solution: topological gradient: a scalar criterion that allows to guess where it *may* be advantageous to dig new infinitesimally small holes (Sokołowski et al., Masmoudi et al., Ammari).

Topological gradient



Without topological gradient

With topological gradient

Topological gradient



Another technical issue

Real materials show different behaviours in traction and compression: they are more prone to damage under traction than compression.

 \rightarrow Simple numerical trick: introduce 2 Griffith constants $\kappa_1 < \kappa_2$ for traction and compression to get more realistic simulations.

