Shape optimization by the level set method

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1 Introduction

Classical domain variation methods have a great advantage over the topological methods based on homogenization theory: they can handle a large number of direct models and almost any objective function. Their major weaknesses are the numerical cost and the numerical instabilities due to the necessary remeshing each time the shape is changing (especially in 3d), and the tendency to find local minima and solution strongly dependent of the initial guess. On the other hand optimization methods based on homogenization avoid these two flaws but are more restrictive in the choice of constitutive equations (limited to linear models) and objective functions.

The representation of shapes by a level set of a scalar field over a fixed mesh is an efficient way to avoid one of the flaws of the classical methods, preserving all their other qualities.

In this summary we concentrate on the problem of structural shape design in linear elasticity, i.e. find a shape included in a given bounded domain that minimizes an objective function. Many extensions including nonlinear constitutive models, layout optimization of two materials with application to damage modeling and fracture propagation, electronic devices optimization, etc, will be presented at the conference.

The basic idea is to compute the shape derivative introduced in the context of the classical domain variation methods and use this shape derivative as a descent direction to evolve the shape represented by a level set of a scalar field (the level set function). The shape derivative is classically computed using the Murat-Simon [15][21] and Céa [8] results. It involves the solutions of the direct and adjoint problems posed on the current shape. The shape evolution amounts the resolution of an Hamilton-Jacobi equation for the level set function.

The second flaw of the classical methods (local minima and dependency to the initial guess) is addressed by the introduction of the topological gradient that allows the creation of new holes inside the domain, which is almost impossible by evolving a given shape through boundary variations (cf. [12], [9], [13], [22], [23]).

Let f and g be respectively the volume and surface forces, and A the Hooke law of the (given) constitutive material. Denote by u the displacement field solution of the linearized elasticity problem posed on the domain Ω:

$$\left\{\begin{array}{rcll} -\mathrm{div}\,(A\,e(u)) & = & f & \text{in } \Omega \\ u & = & 0 & \text{on } \Gamma_D \\ \big(A\,e(u)\big)n & = & g & \text{on } \Gamma_N. \end{array}\right. \tag{1.1}$$

As Ω varies during the optimization process, f and g have to be well defined for all the admissible configurations. Let D be an open bounded domain in $\mathbb{R}^d$ containing all the admissible Ω. If $f \in L^2(D)^d$, $g \in H^1(D)^d$ and $\Gamma_D \neq \emptyset$ then (1.1) has a unique solution in $H^1(\Omega)^d$.

2 Shape derivative

We aim to apply a gradient method to a shape optimization problem of the type

$$\inf_{\Omega \in \left\{\Omega \subset D \text{ such that } |\Omega| = V\right\}} J(\Omega)\,. \tag{2.1}$$

We recall the notion of shape derivative. The basic idea was given by Hadamard and many authors have contributed to its formalization (cf. e.g. textbooks [18], [24]). We follow here the Murat-Simon approach [15], [21]. Starting from an initial open domain, smooth enough, let us consider variations of the type

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

where $\theta \in W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$. For θ small enough, $(\,\mathrm{Id} + \theta)$ is a diffeomorphism in $\mathbb{R}^d$.

Definition 1. *The shape derivative of $J(\Omega)$ at Ω is defined as the Fréchet derivative in $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$ at 0 of $\theta \to J\big((\,\mathrm{Id} + \theta)(\Omega)\big)$*, i.e.

$$J\big((\,\mathrm{Id} + \theta)(\Omega)\big) = J(\Omega) + J'(\Omega)(\theta) + o(\theta) \quad \textit{with} \quad \lim_{\theta \to 0} \frac{\|o(\theta)\|}{\|\theta\|} = 0\,,$$

where $J'(\Omega)$ is a continuous linear form over $W^{1,\infty}(\mathbb{R}^d, \mathbb{R}^d)$.

A classical result says that the directional derivative $J'(\Omega)(\theta)$ only depends on the trace of $\theta \cdot n$ on the boundary $\partial\Omega$.

Lemma 1. *Let Ω be a smooth bounded open domain and $J(\Omega)$ a derivable function at Ω. Its derivative satisfies*

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

as soon as $\theta_1, \theta_2 \in W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$ are such that $\theta_2 - \theta_1 \in \mathcal{C}^1(\mathbb{R}^d; \mathbb{R}^d)$ and

$$\theta_1 \cdot n = \theta_2 \cdot n \qquad \textit{on } \partial\Omega.$$

We give below two examples of shape derivatives for two classes of objective functions that will be useful in the following:

Lemma 2. *Let Ω be a smooth bounded open domain and $\phi(x) \in W^{1,1}(\mathbb{R}^d)$. If*

$$J(\Omega) = \int_\Omega \phi(x)\, dx,$$

then J is differentiable at Ω and

$$J'(\Omega)(\theta) = \int_\Omega \mathrm{div}\big(\theta(x)\,\phi(x)\big)\, dx = \int_{\partial\Omega} \theta(x) \cdot n(x)\,\phi(x)\, ds\,,$$

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

Lemma 3. *Let Ω be a smooth bounded open domain and $\phi(x) \in W^{1,1}(\mathbb{R}^d)$. If*

$$J(\Omega) = \int_{\partial\Omega} \phi(x)\, ds,$$

then J is differentiable at Ω and

$$J'(\Omega)(\theta) = \int_{\partial\Omega} \theta \cdot n \left(\frac{\partial \phi}{\partial n} + H\phi\right) ds,$$

$\forall \theta \in W^{1,\infty}(\mathbb{R}^d; \mathbb{R}^d)$, *where H is the mean curvature of $\partial\Omega$ defined by $H = \mathrm{div} n$.*

Theorem 4. *Let Ω be a smooth bounded open domain and $\theta \in W^{1,\infty}(\mathbb{R}^d;\mathbb{R}^d)$. Suppose that the data f and g as well as the solution u of (1.1) are smooth enough, (i.e. $f \in H^1(\Omega)^d$, $g \in H^2(\Omega)^d$, $u \in H^2(\Omega)^d$). Then the shape derivative of*

$$J_1(\Omega) = \int_\Omega f \cdot u \, dx + \int_{\Gamma_N} g \cdot u \, ds = \int_\Omega A\, e(u) \cdot e(u) \, dx, \tag{2.2}$$

is

$$\begin{aligned} J_1'(\Omega)(\theta) = & \int_{\Gamma_N} \left(2 \left[\frac{\partial (g \cdot u)}{\partial n} + H g \cdot u + f \cdot u \right] - Ae(u) \cdot e(u) \right) \theta \cdot n \, ds \\ & + \int_{\Gamma_D} Ae(u) \cdot e(u) \, \theta \cdot n \, ds. \end{aligned} \tag{2.3}$$

For given $u_0 \in L^\alpha(\Omega)$, $k \in L^\infty(\Omega)$ and $\alpha \geq 2$, the shape derivative of

$$J_2(\Omega) = \left(\int_\Omega k(x) |u - u_0|^\alpha dx \right)^{1/\alpha}, \tag{2.4}$$

is

$$\begin{aligned} J_2'(\Omega)(\theta) = & \int_{\Gamma_N} \left(\frac{C_0}{\alpha} k |u - u_0|^\alpha + Ae(p) \cdot e(u) - f \cdot p - \frac{\partial (g \cdot p)}{\partial n} - H g \cdot p \right) \theta \cdot n \, ds \\ & + \int_{\Gamma_D} \left(\frac{C_0}{\alpha} k |u - u_0|^\alpha - Ae(u) \cdot e(p) \right) \theta \cdot n \, ds \,, \end{aligned} \tag{2.5}$$

where p is the adjoint, supposed to be smooth i.e. $p \in H^2(\Omega)^d$, defined as the solution of the adjoint problem

$$\left\{ \begin{array}{rcll} -\mathrm{div}\,(A\, e(p)) & = & -C_0 k(x) |u - u_0|^{\alpha - 2} (u - u_0) & \text{in } \Omega \\ p & = & 0 & \text{on } \Gamma_D \\ \big(Ae(p)\big) n & = & 0 & \text{on } \Gamma_N, \end{array} \right. \tag{2.6}$$

with

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

Remark: If two given materials are involved, i.e. if we try to optimize the interface between two non degenerate materials, equivalent formulas for the shape derivative can be established, although they are much more complicated [2].

We can now describe a gradient method for the minimization of an objective function $J(\Omega)$. The expression for the shape derivative is

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

where v is given by a formula of the type shown in theorem 4. If regularity problems are neglected, a valid descent direction is for example

$$\theta = -v\,n. \tag{2.7}$$

We use this vector field to evolve the shape Ω as

$$\Omega_t = (\,\mathrm{Id} + t\theta)\Omega,$$

where $t > 0$ is the descent parameter. Formally we obtain

$$J(\Omega_t) = J(\Omega) - t\int_{\partial\Omega} v^2\,ds + \mathcal{O}(t^2)$$

that ensures that the objective function is decreasing as soon as the descent parameter is small.

3 Shape parametrization by level set

As described above, the gradient method can be implemented in a Lagrangian framework using the shape derivative as a descent direction. From a numerical point of view it is possible to mesh the initial shape and deform the mesh using the successive derivatives. This method has two flaws: when the deformation is large it is necessary to remesh the shape, which could be costly in 3d and add some extraneous oscillations to the algorithm due to the changes in the discretization. Topology changes are almost impossible to handle, especially in 3d. The level set method can be viewed as an Eulerian method, allowing the capture of the shape on a fixed discretization, that avoids the two above flaws.

Let $D \subset \mathbb{R}^d$ be a bounded domain. All the admissible shapes Ω will be included into D. The boundary of Ω is implicitly described by a level set function defined over D:

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

The elasticity system and the adjoint system are extended over the whole domain D using a fictitious material –a very weak material– that fills the voids $D \setminus \Omega$.

If the descent parameter $t > 0$ is used to index the successive shapes, we can consider that the sequence of shapes are $\Omega(t)$ that evolve with a pseudo-time t and a normal velocity $V(t,x)$. Then, as the shape is characterized by the level set 0 of ψ, we have

$$\psi\Big(t, x(t)\Big) = 0 \quad \forall x(t) \in \partial\Omega(t).$$

Differentiating with respect to t, and using the expression of the normal $n = \nabla\psi/|\nabla\psi|$ we find

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

This Hamilton-Jacobi equation is valid on the whole domain D if the velocity is defined on D. In the same spirit, the mean curvature $H = \operatorname{div} n$ can be extended in the whole domain D. The mean curvature appears naturally in the expression of the shape derivative if a perimeter term is involved added the objective function in order to regularize the solutions.

4 Optimization algorithm

The shape derivative of the optimization problem (2.1) has been computed:

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

where the expression for $v(u, p, n, H)$ is given by a similar result as Theorem 4. As n, H, u and p have been extended in the whole domain D, v can also be defined over D and not only on $\partial\Omega$. The descent direction

$$\theta = -v\, n,$$

can also be extended to D and its normal component $\theta \cdot n = -v$ is thus the advection velocity involved in the Hamilton-Jacobi equation

$$\frac{\partial\psi}{\partial t} - v|\nabla\psi| = 0. \tag{4.1}$$

Advect ψ through (4.1) is equivalent to evolve $\partial\Omega$ with the descent direction $-J'(\Omega)$. The numerical algorithm is the following:

1. Initialization of the level set function ψ_0 characterizing the initial shape Ω_0.

2. Iteration up to convergence, for $k \geq 0$:

(a) compute the state u_k and the adjoint state p_k over Ω_k. All the computations are done on D using a weak material in voids.

(b) modify Ω_k through ψ_k by solving Hamilton-Jacobi equation (4.1). The new shape Ω_{k+1} is characterized by the level set function ψ_{k+1}. The velocity $-v_k$ depends on u_k and p_k. The time step Δt_k is chosen such that $J(\Omega_{k+1}) \leq J(\Omega_k)$.

3. From time to time, reinitialization of ψ to the signed distance to the level set 0.

Many extensions and refinements of the basic algorithm above, and also many applications, will be presented during the talk. One of the recent applications is illustrated by the figure below.

Acknowledgement: *all this work has been done in collaboration with Grégoire Allaire. Many other persons have also been involved at different stages of the work. Among them I must cite: F. de Gournay, N. Van Goethem and A.M. Toader. Thanks to all of them.*

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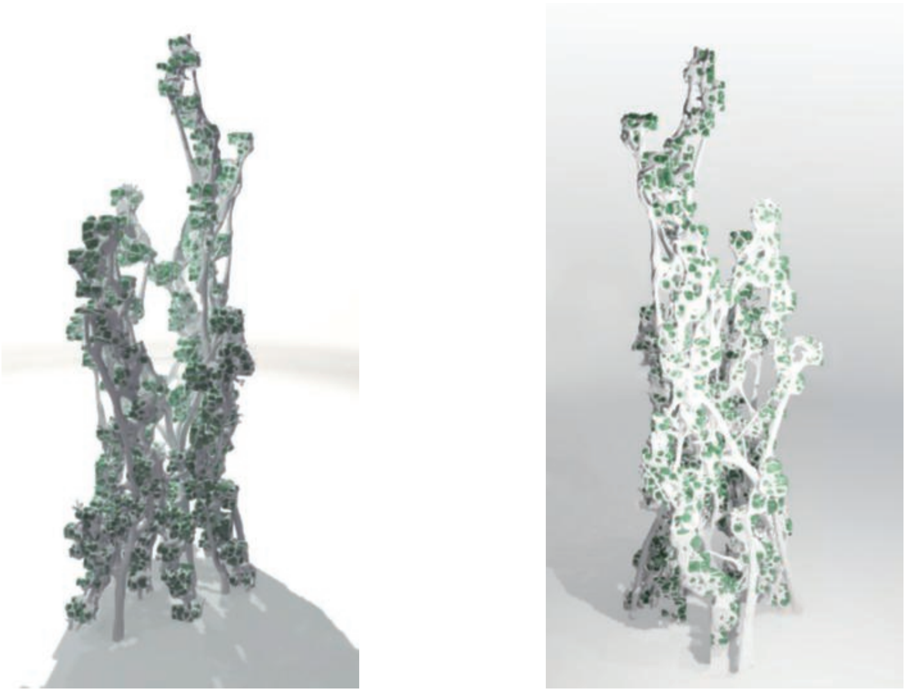

Figure 1: Shape optimization of tall buildings using level sets. (Thanks to François Roche and the architecture studio R&Sie, Paris)

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