The Adjoint Method in Calculus of Variations
and Applications

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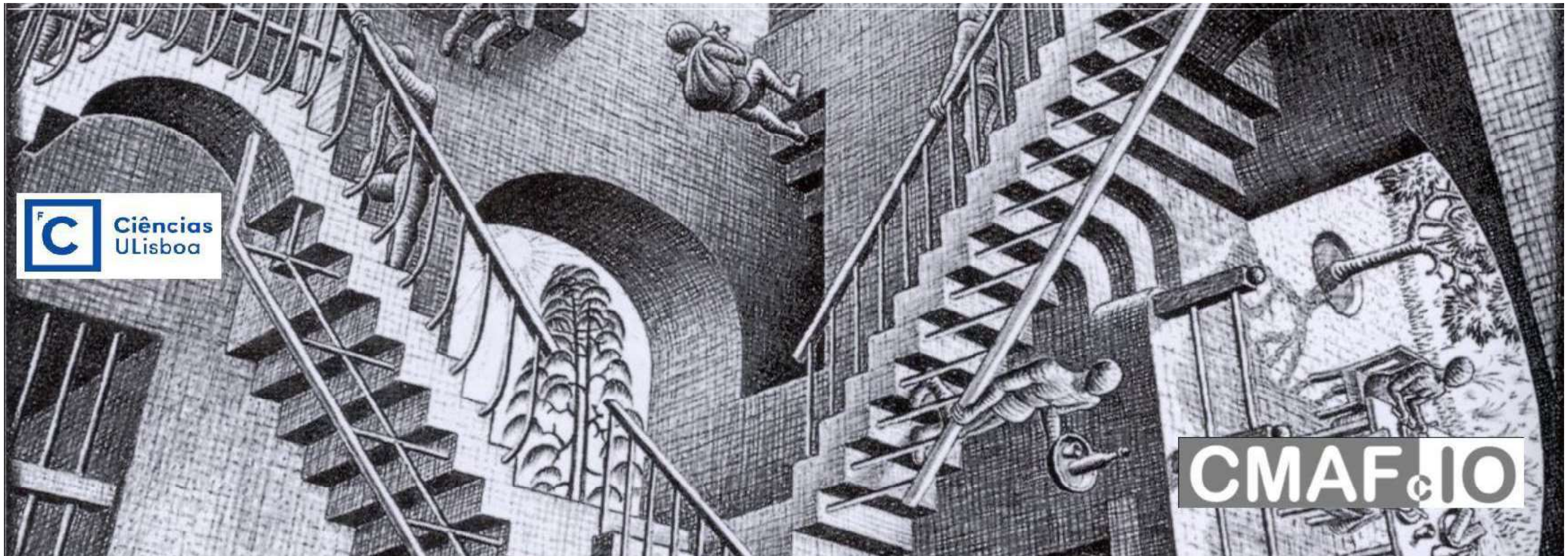


Introduction to the Adjoint Method

- Brief description of the Adjoint Method
- Pontryagin's Principle
- Lagrange Multipliers on Banach Spaces

Brief description of the Adjoint Method

The state equation, which may be a PDE with the variational formulation

$$A_\theta(u_\theta, v) = l_\theta(v), \forall v \in H, \qquad (P_\theta)$$

gives the dependency between u and θ.

- H is a Hilbert space,
- A_θ family of bilinear forms that are continuous and coercive,
- l_θ family of linear continuous forms.

Acording to [F. Murat & L. Tartar 1985] and [J. Céa 1986], the variation of the state u_θ can be described in terms of the variation of the control θ , under convenient differentiability hypothesis on the families of forms A_θ and l_θ with respect to θ .

In optimal control problems, given a functional to minimize/maximize

$$J(\theta) = \mathcal{J}(\theta, u_\theta),$$

the goal is to find a control θ producing the state u_θ that minimizes or maximizes J

Brief description of the Adjoint Method

The total derivative of J involves the derivative of u_θ with respect to θ :

$$\frac{dJ}{d\theta}(\theta)\,\tau = \frac{\partial \mathcal{J}}{\partial \theta}(\theta, u_\theta)\,\tau + \frac{\partial \mathcal{J}}{\partial u}(\theta, u_\theta)\frac{du_\theta}{d\theta}(\theta)\,\tau. \qquad (dJ)$$

The *Adjoint Method* allows one to transform the implicit dependency in the term $\frac{du_\theta}{d\theta}(\theta)\,\tau$ in an explicit one with respect to τ

Consider the adjoint problem in the form

$$A_\theta(p_\theta, w) = \frac{\partial \mathcal{J}}{\partial u}(\theta, u_\theta)w, \forall w \in H, \qquad (PA_\theta)$$

the solution $p_\theta \in H$ is called the *adjoint state*.

Brief description of the Adjoint Method

Deriving the state equation (P_θ) yields, for all $v \in H$,

$$\frac{dA_\theta}{d\theta}(u_\theta, v)\,\tau + A_\theta(\frac{du_\theta}{d\theta}(\theta)\,\tau, v) = \frac{dl_\theta}{d\theta}(v)\tau.$$

Under symmetry hypothesis on the operators A_θ it is possible to prove that the implicit term in the expression of (dJ) has the following explicit form :

$$\begin{aligned}\frac{\partial \mathcal{J}}{\partial u}(\theta, u_\theta)\frac{du_\theta}{d\theta}(\theta)\,\tau = A_\theta(p_\theta, \frac{du_\theta}{d\theta}(\theta)\,\tau) = A_\theta(\frac{du_\theta}{d\theta}(\theta)\,\tau, p_\theta)\\ = \left(-\frac{dA_\theta}{d\theta}(u_\theta, p_\theta) + \frac{dl_\theta}{d\theta}(p_\theta)\right)\tau.\end{aligned}$$

The total derivative of J has the following expression, where the dependency on τ is explicit :

$$\frac{dJ}{d\theta}(\theta)\,\tau = \left(\frac{\partial \mathcal{J}}{\partial \theta}(\theta, u_\theta) - \frac{dA_\theta}{d\theta}(u_\theta, p_\theta) + \frac{dl_\theta}{d\theta}(p_\theta)\right)\tau$$

Pontryagin's Principle

Classical control problem

The state $y \in H^1(0, T; \mathbb{R}^m)$ is solution of

$$\begin{cases} \dfrac{dy}{dt}(t) = A(t, \quad y(t), \theta(t)), \quad t \in]0, T[, \\ y(0) = y_0, \end{cases}$$

where the control $\theta \in L^\infty(0, T; [0, 1])$.
The problem is to find θ that minimizes the functional

$$F(\theta) = \int_0^T B(t, y(t), \theta(t))dt$$

Pontryagin's Principle

- $A : [0, T] \times \mathbb{R}^m \times [0, 1] \mapsto \mathbb{R}^m$ – continuously differentiable in y and θ, linear in θ and continuous in t
- $B : [0, T] \times \mathbb{R}^m \times [0, 1] \mapsto \mathbb{R}$ – continuously differentiable in y and θ, convex in θ and continuous in t

Pontryagin's Principle (1962) gives a necessary condition of optimality If $\theta^* \in L^\infty(0, T; [0, 1])$ is a solution of the above minimization problem, then for almost all $t \in [0, T]$ the application

$$\tau \in [0, 1] \mapsto p(t)A(t, y(t), \tau) + B(t, y(t), \tau)$$

atains its minimum in $\tau = \theta^*(t)$, where $p \in H^1(0, T; \mathbb{R}^m)$ denotes the adjoint state which is solution of the adjoint problem

$$\begin{cases} -\left(\dfrac{dp}{dt}(s) + \dfrac{\partial A}{\partial y}(s, y(s), \theta(s))p(s)\right) = \dfrac{\partial B}{\partial y}(s, y(s), \theta(s)), \\ p(T) = 0. \end{cases}$$

Lagrange Multipliers on Banach Spaces

The following general result may be applied in order to obtain the adjoint state p in the previous control problem

Theorem. [E. Zeidler - Springer 1995] Let X and Y be two real Banach spaces and let $U \subset X$, open. Consider two continuously differentiable applications, $f : U \mapsto \mathbb{R}$ (the functional to minimize/maximize) and $g : U \mapsto Y$ (a constraint). If u_0 is an extremal point of f when restricted to $g^{-1}(0)$ and if $Dg(u_0) \in \mathcal{L}(X, Y)$ is onto, then there exists an application $\lambda \in \mathcal{L}(Y, \mathbb{R})$, called Lagrange multiplier, with the property

$$Df(u_0) = \lambda \circ Dg(u_0).$$

Lagrange Multipliers on Banach Spaces

Consider $f : H^1(0, T; \mathbb{R}^m) \times L^\infty(0, T) \mapsto \mathbb{R}$,

$$f(y, \theta) = \int_0^T B(t, y(t), \theta(t))dt$$

and $g : H^1(0, T; \mathbb{R}^m) \times L^\infty(0, T) \mapsto L^2(0, T; \mathbb{R}^m) \times \mathbb{R}^m$,

$$g(y, \theta) = \left(\frac{dy}{dt}(t) - A(t, y(t), \theta(t)), \quad y(0) - y_0 \right)$$

Then

$$Dg(y_0, \theta_0)(\delta y, \delta\theta) =$$

$$= \begin{pmatrix} \frac{d(\delta y)}{dt}(t) - \frac{\partial A}{\partial y}(t, y_0(t), \theta_0(t))\delta y - \frac{\partial A}{\partial \theta}(t, y_0(t), \theta_0(t))\delta\theta \\ \delta y(0) \end{pmatrix}$$

Lagrange Multipliers on Banach Spaces

Applying the Theorem there exists a Lagrange multiplier $\lambda = (\lambda_1, \lambda_2) \in \mathcal{L}(L^2(0,T;\mathbb{R}^m) \times \mathbb{R}^m; \mathbb{R})$, with the property

$$\int_0^T \lambda_1(t) \left[\frac{d}{dt}(\delta y)(t) - \frac{\partial A}{\partial y}(t, y_0(t), \theta_0(t))\delta y - \frac{\partial A}{\partial \theta}(t, y_0(t), \theta_0(t))\delta\theta \right] dt$$

$$+\lambda_2 \delta y(0) = \int_0^T \left[\frac{\partial B}{\partial y}(t, y_0(t), \theta_0(t))\delta y + \frac{\partial B}{\partial \theta}(t, y_0(t), \theta_0(t))\delta\theta \right]$$

for all $\delta y \in H^1(0,T;\mathbb{R}^m)$ and all $\delta\theta \in L^\infty(0,T)$.
Then $\lambda_1 \in H^1(0,T;\mathbb{R}^m)$ and satisfies the adjoint problem

$$\begin{cases} \lambda_1(T) = 0, \\ -\left(\frac{d\lambda_1}{dt}(s) + \frac{\partial A}{\partial y}(s, y_0(s), \theta_0(s))\lambda_1(s) \right) = \frac{\partial B}{\partial y}(s, y_0(s), \theta_0(s)) \text{ in }]0, \end{cases}$$

and the condition $\lambda_2 = \lambda_1(0)$.

The Adjoint Method in my research

- The Adjoint Method in Shape Optimization
- The Generalized Adjoint Method
- The Adjoint Method in Topology Optimization
- The Adjoint Method in Optimization of Eigenvalues and Eigenmodes
- The Adjoint Method in the framework of Bloch waves
- The Adjoint Method in Optimization - other frameworks

The Adjoint Method in Shape Optimization

One seeks to minimize an objective functional $J(\Omega)$ when the domain $\Omega \subset \mathbb{R}^N$ varies, while the volume is constant equal to a given $V > 0$

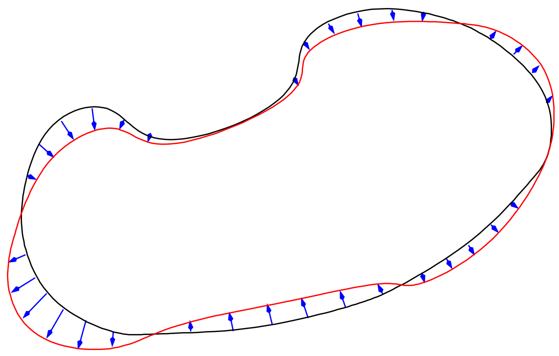
$$\inf_{\Omega \in \mathcal{U}_{ad}} J(\Omega, u(\Omega)),$$

where $\mathcal{U}_{ad}$ is the set of admissible domains and the state u is the solution of

$$\begin{cases} -div(Ae(u)) = f \text{ in } \Omega, \\ u = 0 \text{ on } \Gamma_D, \\ Ae(u)n = g \text{ on } \Gamma_N. \end{cases}$$

The Adjoint Method in Shape Optimization

Consider a reference domain Ω_0 of C^1 regularity and the set of admissible shapes obtained by deformation of Ω_0



$$\mathcal{U}_{ad} = \{\Omega \subset D, \int_\Omega dx = V, \text{ s.t. exists } T \in \mathcal{T} \text{ with } \Omega = T(\Omega_0)\},$$

where $\mathcal{T}$ is the space of diffeomorphisms given by

$$\mathcal{T} = \{T \text{ such that } T \in W^{1,\infty}_{loc}(\mathbb{R}^N;\mathbb{R}^N),\ T^{-1} \in W^{1,\infty}_{loc}(\mathbb{R}^N;\mathbb{R}^N)\}.$$

The Adjoint Method in Shape Optimization

If $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ verifies

$$\|\theta\|_{W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)} < 1,$$

the function $T = I + \theta$ is invertible and belongs to $\mathcal{T}$.
Given $J : \mathcal{U}_{ad} \to \mathbb{R}$, J is called differentiable with respect to the domain, in Ω_0 , if the function

$$\theta \mapsto J((I+\theta)\Omega_0)$$

is differentiable in $\theta = 0$.
The shape derivative of J is defined as the Fréchet derivative of the above application, that is a linear continuous form L on $W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ that satisfies :

$$J((I+\theta)(\Omega_0)) = J(\Omega_0) + L(\theta) + o(\theta), \text{ with } \lim_{\theta\to 0} \frac{|o(\theta)|}{\|\theta\|} = 0,$$

$$\text{where } L = J'(\Omega_0).$$

The Adjoint Method in Shape Optimization

Property. Given a differentiable function $J : \mathcal{U}^1_{ad} \to \mathbb{R}$ in Ω_0 , if $\theta_1, \theta_2 \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$ verify $\theta_2 - \theta_1 \in C^1(\mathbb{R}^N;\mathbb{R}^N)$ and

$$\theta_1 \cdot n = \theta_2 \cdot n \text{ on } \partial\Omega_0,$$

the shape derivative $J'(\Omega_0)$ satisfies

$$J'(\Omega_0)(\theta_1) = J'(\Omega_0)(\theta_2).$$

The Adjoint Method in Shape Optimization

Classical cases 1. If $J : \mathcal{U}^1_{ad} \to \mathbb{R}$ is defined as

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

with $f \in W^{1,1}(\mathbb{R}^N)$, then J is differentiable in Ω_0 and

$$J'(\Omega_0)(\theta) = \int_{\Omega_0} div(\theta(x)f(x))dx_0 = \int_{\partial\Omega_0} \theta(x)\cdot n(x)f(x)ds,$$

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

2. For $f \in W^{2,1}(\mathbb{R}^N)$ define $J : \mathcal{U}^1_{ad} \to \mathbb{R}$ by

$$J(\Omega) = \int_{\partial\Omega} f(x)dx.$$

Then J is differentiable in Ω_0 and for all $\theta \in W^{1,\infty}(\mathbb{R}^N;\mathbb{R}^N)$

$$J'(\Omega_0)(\theta) = \int_{\partial\Omega_0} \left(\frac{\partial f}{\partial n} + div\, nf\right)\theta\cdot nds.$$

The Adjoint Method in Shape Optimization

Assuming that $f \in H^1(\Omega)^N$, $g \in H^2(\Omega)^N$ and $u \in H^2(\Omega)^N$, where u is the solution of

$$\begin{cases} -div(Ae(u)) = f \text{ in } \Omega, \\ u = 0 \text{ on } \Gamma_D, \\ Ae(u)n = g \text{ on } \Gamma_N, \end{cases}$$

the shape derivative in Ω_0 of the compliance functional

$$J_1(\Omega) = \int_\Omega f \cdot u dx + \int_{\Gamma_N} g \cdot u ds$$

is the following (see [G. Allaire, F. Jouve & A-M T , JCP 2004])

$$J_1'(\Omega_0)(\tau) = \int_{\Gamma_{0N}} \left[2 \left(\frac{\partial (g \cdot u)}{\partial n} + H g \cdot u + f \cdot u \right) \right] \tau \cdot n \, ds -$$

$$- \int_{\Gamma_{0N}} (Ae(u) \cdot e(u)) \tau \cdot n \, ds + \int_{\Gamma_{0D}} (Ae(u) \cdot e(u)) \tau \cdot n \, ds$$

where $H = div \, n$ is the mean curvature of $\partial \Omega_0$.

The Adjoint Method in Shape Optimization

However in the case where a hydrostatic force is applied on a part of the boundary the previous result cannot be applied.

$$\begin{cases} -div(Ae(u)) = f \text{ in } \Omega, \\ u = 0 \text{ on } \Gamma_D, \\ Ae(u)n = p_h n \text{ on } \Gamma_N \end{cases}$$

the force $p_h n$ depends on the normal to the domain in the considered point, that is it depends on Ω . When the domain varies, the force follows the variations of the domain.
The shape derivative in Ω_0 of the compliance functional

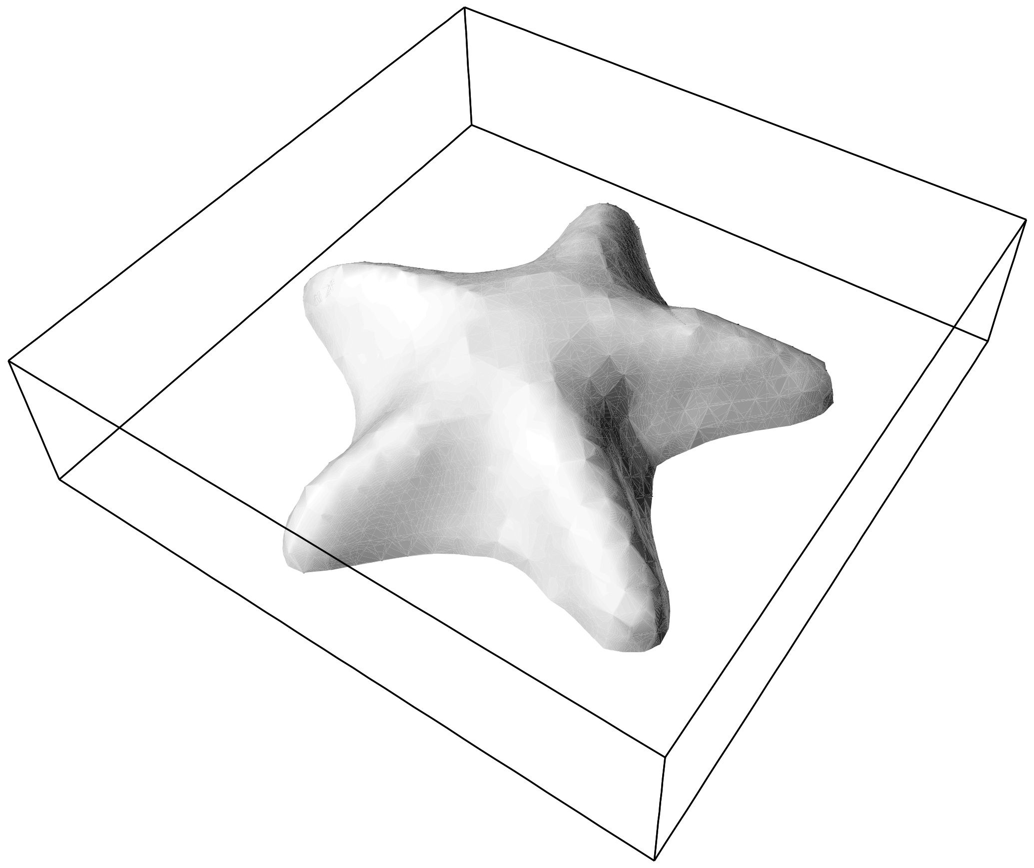
$$J_1(\Omega) = \int_\Omega f \cdot u dx + \int_{\Gamma_N} p_h n \cdot u ds$$

is (see [G. Allaire, F. Jouve & A-M T , JCP 2004])

$$J_1'(\Omega_0)(\tau) = \int_{\Gamma_{0N}} [2(f \cdot u + div(p_h u)) - Ae(u) \cdot e(u)]\tau \cdot n \, ds + \int_{\Gamma_{0D}} Ae(u) \cdot e(u) \tau \cdot n \, ds.$$

The Adjoint Method in Shape Optimization

Numerical example in Shape Optimization with following forces



Optimal shape under hydrostatic forces with five anchor points and a concentrated vertical force applied in the center of the base

The Adjoint Method in Shape Optimization

Assuming that $f \in H^1(\Omega)^N$, $g \in H^2(\Omega)^N$ and $u \in H^2(\Omega)^N$, where u is the solution of

$$\begin{cases} -div(Ae(u)) = f \text{ in } \Omega, \\ u = 0 \text{ on } \Gamma_D, \\ Ae(u)n = g \text{ on } \Gamma_N, \end{cases}$$

the shape derivative in Ω_0 of the distance type functional

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

is given by

$$J_2'(\Omega_0)(\tau) =$$

$$\int_{\Gamma_{0N}} \left(\frac{C_0}{\alpha} k|u - \bar{u}|^\alpha + Ae(p) \cdot e(u) - f \cdot p - \frac{\partial(g \cdot p)}{\partial n} - Hg \cdot p \right) \tau \cdot n$$
$$+ \int_{\Gamma_{0D}} \left(\frac{C_0}{\alpha} k|u - \bar{u}|^\alpha - Ae(p) \cdot e(u) \right) \tau \cdot n,$$

The Adjoint Method in Shape Optimization

p is the adjoint state and is the solution of the adjoint problem

$$\begin{cases} -div(Ae(p)) = -C_0 k|u-\bar{u}|^{\alpha-2}(u-\bar{u}) \text{ in } \Omega_0, \\ p = 0 \text{ on } \Gamma_{0D}, \\ Ae(p)n = 0 \text{ on } \Gamma_{0N}. \end{cases}$$

where C_0 is a constant given by

$$C_0 = \left(\int_{\Omega_0} k(x)|u(x) - \bar{u}(x)|^\alpha \right)^{1/\alpha - 1}.$$

The Generalized Adjoint Method

The Adjoint Method was generalized in order to treat variational formulations (that arose in Topology Optimization) written on an affine manifold of a Hilbert space - A-M T - SIAM, 2011.
Consider V a Hilbert space, V_0 a linear closed subspace of V and K an affine manifold of the form $K = \gamma + V_0$ for some element γ of V .

Generalization of the Lax-Milgram Lemma

Consider $a : V \times V \to \mathbb{R}$ a bilinear, symmetric continuous form on V which is coercive only on V_0 , and consider $l : V \to \mathbb{R}$ a linear continuous form on V . Then the problem

$$\begin{cases} \text{find } u \in K \text{ such that} \\ a(u, v) = l(v) \ \forall v \in V_0, \end{cases}$$

has a unique solution.

The Generalized Adjoint Method

Considering a parameter $\rho > 0$, the state equation below has a unique solution u^ρ.

$$\begin{cases} \text{find } u^\rho \in K \text{ such that} \\ a_\rho(u^\rho, v) = l_\rho(v) \ \forall v \in V_0. \end{cases}$$

Assume that

- $a_\rho : V \times V \to \mathbb{R}$ is a family of bilinear, symmetric, uniformly continuous forms that are uniformly coercive only on V_0
- $l_\rho : V \to \mathbb{R}$ is a family of linear, uniformly continuous forms
- $\delta_a : V \times V \to \mathbb{R}$ is a bilinear, symmetric and continuous form
- $\delta_l : V \to \mathbb{R}$ is a linear continuous form
- $\|a_\rho - a_0 - f(\rho)\delta_a\|_{\mathcal{L}^2(V)} = o(f(\rho))$,
- $\|l_\rho - l_0 - f(\rho)\delta_l\|_{\mathcal{L}(V)} = o(f(\rho))$

for a function $f : \mathbb{R}_+ \to \mathbb{R}_+$ with the property $\lim_{\rho\to 0} f(\rho) = 0$. Then the estimation $\|u^\rho - u^0\| = O(f(\rho))$ holds, where u^0 denotes the solution of the above problem for $\rho = 0$.

The Generalized Adjoint Method

The goal is to determine the asymptotic development of a functional $j(\rho) := J_\rho(u^\rho)$.
Assuming that there exists $\delta_J : V \to \mathbb{R}$ such that

$$J_\rho(v) - J_0(u) = DJ(u)(v-u) + f(\rho)\delta_J(u) + o(\|v-u\| + f(\rho)), \forall u, v \in V,$$

where $DJ(u)$ is the Gâteaux derivative of J_0 in u ,
the asymptotic development of $j(\rho)$ is obtained

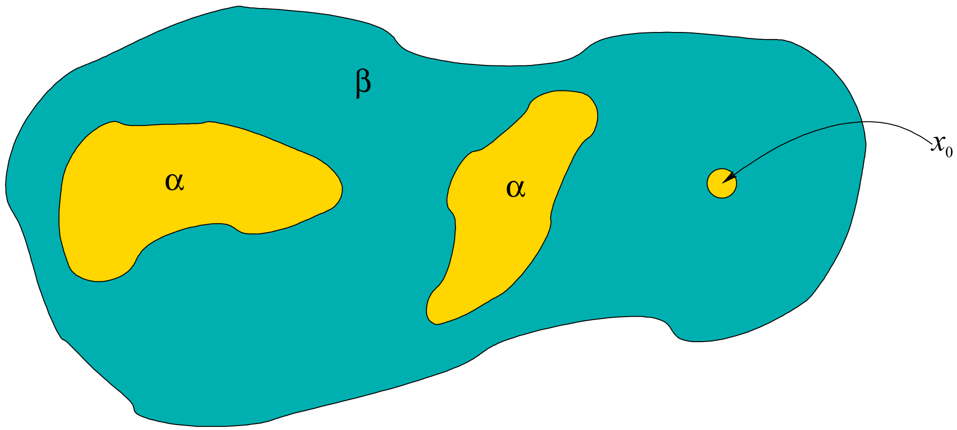
$$j(\rho) = j(0) + f(\rho)(\delta_J(u^0) + \delta_a(u^0, p) - \delta_l(p)) + o(f(\rho)),$$

where the adjoint state p is solution of the adjoint problem

$$\begin{cases} \text{find } p \in V_0 \text{ such that} \\ a_0(w, p) = -DJ(u^0)w, \ \forall w \in V_0. \end{cases}$$

The Adjoint Method in Topology Optimization

Topology optimization is another application of the Calculus of Variations which jointly with the Shape Optimization completes the general framework of structural optimization.



If in Shape Optimization the variations of the domain are made in the same class of homotopy, without changing the topology, in Topology Optimization the variations allow to change the class of homotopy. More precisely, the influence of the position of an infinitesimal perforation in the domain is studied on the functional to minimize/maximize. This problem arose first in Engineering, at a macroscopic level and was solved in mathematical rigor by M. Masmoudi and J. Sokołowski & A. Zochowski in 2001.

The Adjoint Method in Topology Optimization

At the microscopic level, however, although there were several papers dealing with numerical topology optimization, the topological derivative was computed with mathematical rigor in [A-M T - SIAM 2011]. A survey on shape and topology derivatives of the homogenized coefficients is contained in [C. Barbarosie & A-M T - SMO 2010 a].

In order to characterize periodic microstructures the following general notion of periodicity is used :

$\varphi : \mathbb{R}^N \to \mathbb{R}^m$ is called $\mathcal{G}$-periodic if

$$\varphi(x + \vec{g}) = \varphi(x), \ \forall x \in \mathbb{R}^N \ \forall \vec{g} \in \mathcal{G}.$$

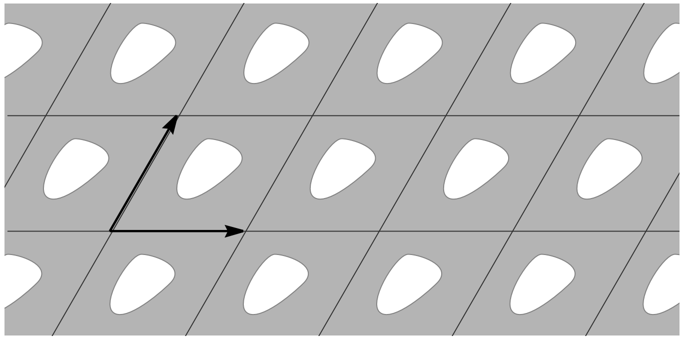
where $\mathcal{G}$ is an additive subgroup of $\mathbb{R}^N$ having d linear independent generators (a lattice).

- the notion does not depend on the set of chosen generators
- each set of generators defines a periodicity cell

The Adjoint Method in Topology Optimization

Let Y be a periodicity cell. Consider T a compact set having Lipschitz boundary and such that $T \subset \overset{\circ}{Y}$. The set $Y \setminus T$ is filled with a material having the elastic tensor C while T corresponds to a hole. $\mathbb{R}^N_{perf}(T) = \mathbb{R}^N \setminus \bigcup_{k \in \mathbb{Z}^N} (T + k_1 \vec{g}_1 + \dots k_d \vec{g}_d)$

For a small parameter $\varepsilon > 0$, one makes an ε zoom of $\mathbb{R}^N_{perf}(T)$ that is a homothety of ratio ε. This new perforated domain is filled with the material of tensor C .



When $\varepsilon \to 0$, the effective behaviour of the corresponding microstructure is characterized by the homogenized tensor C^H . According to the homogenization theory, C^H may be characterized in terms of the solution of the cellular problem.

The Adjoint Method in Topology Optimization

Homogenization Theory. *Given a matrix* $A \in \mathcal{M}^N(\mathbb{R})$ *, symmetric (effective strain), the homogenized tensor* C^H *is characterized by*

$$C^H A = \frac{1}{|Y|} \int_{Y \setminus T} Ce(u_A) dx$$

where u_A *is the solution of the cellular problem :*

$$\begin{cases} -div(Ce(u_A)) = 0 \text{ in } \mathbb{R}^N_{perf}(T) \\ Ce(u_A)n = 0 \text{ on } \partial T \\ u_A(x) = Ax + \phi_A(x), \quad \phi_A \ \mathcal{G}\text{-periodic function} \end{cases}$$

The Adjoint Method in Topology Optimization

The cellular problem in strain formulation writes

$$\begin{cases} u_A \in LP(\mathbb{R}^N_{perf}(T)) \\ -\mathrm{div}(Ce(u_A)) = 0 \text{ in } \mathbb{R}^N_{perf}(T) \\ Ce(u_A)n = 0 \text{ on } \partial T \\ \frac{1}{|Y|}\left(\int_{Y\setminus T} e(u_A)dx - \int_{\partial T} u_A \vee n\, ds(x)\right) = A \end{cases}$$

where

$$LP(\mathbb{R}^N_{perf}(T)) = \bigcup_{A\in\mathcal{M}^s_d(\mathbb{R})} LP_A(\mathbb{R}^N_{perf}(T))$$

$$LP_A(\mathbb{R}^N_{perf}(T)) = A + H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{R}^N)$$

$H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{R}^N)$ denotes the completion in the norm of $H^1(Y \setminus T, \mathbb{R}^N)$ of the space of functions in $C^\infty(\mathbb{R}^N_{perf}(T), \mathbb{R}^N)$ which are $\mathcal{G}$-periodic

The Adjoint Method in Topology Optimization

The cellular problem in stress formulation writes

$$\begin{cases} w_\sigma \in LP(\mathbb{R}^N_{perf}(T)), \\ -\mathrm{div}(Ce(w_\sigma)) = 0 \text{ in } \mathbb{R}^N_{perf}(T) \\ Ce(w_\sigma)n = 0 \text{ on } \partial T \\ \frac{1}{|Y|}\int_{Y\setminus T} Ce(w_\sigma)dx = \sigma \end{cases}$$

For $\sigma = C^H A$, which is equivalent to $A = D^H \sigma$, where $D^H = (C^H)^{-1}$ is homogenized compliance tensor, the solutions u_A and w_σ of the cellular problem in strain and respectively in stress formulation, are equal.

The Adjoint Method in Topology Optimization

The homogenized tensor C^H can also be defined through

$$\langle C^H A, B\rangle = \frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(u_A), e(u_B)\rangle \, dx,$$

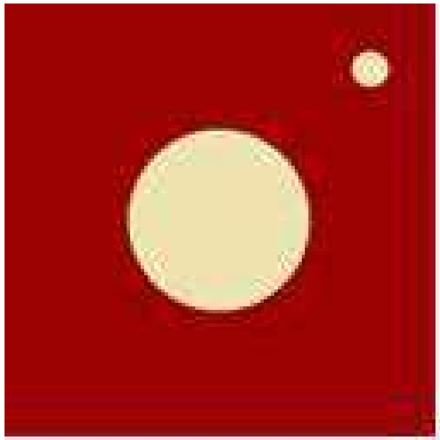
where u_A and u_B are solutions of the cellular problem for two different effective strains A and B. Considering, in particular, the matrices A and B in a basis of the space of symmetric matrices, one obtains each one of the homogenized coefficients, i.e. the entries of the homogenized tensor. In general, for A and B arbitrarily fixed one studies the functional

$$j(Y \setminus T) = \frac{1}{|Y|}\int_{Y\setminus T} \langle Ce(u_A), e(u_B)\rangle \, dx.$$

The above problem is perturbed by creating at a location x_0 lying in a zone of material, an infinitesimal hole, typically spherical, whose radius ρ tends to 0 , and on the boundary of which homogeneous Neumann conditions are applied.

The Adjoint Method in Topology Optimization

The domain varies with the parameter ρ and therefore the solution of the cellular problem will depend on ρ. These dependencies infer on the functional j and we are interested precisely in its asymptotic expansion in ρ :



$j(Y \setminus (T \cup \bar{B}(x_0, \rho)) = j(Y \setminus T) + f(\rho) D_T j(x_0) + o(f(\rho))$, where $\lim_{\rho \to 0} f(\rho) = 0$, $f(\rho) > 0$.

The second term in the asymptotic expansion involves the so called topological derivative $D_T j$ in x_0 . Using the language of control theory, the homogenized coefficients are controlled by the location x_0 of the center of a virtual newly created hole $\bar{B}(x_0, \rho)$, of infinitesimal radius $\rho \to 0$.

The Adjoint Method in Topology Optimization

The perturbed cellular problem has the form

$$\begin{cases} -\mathrm{div}(Ce(u_A^\rho)) = 0 \text{ in } \mathbb{R}^N_{perf}(T \cup \bar{B}(x_0,\rho)) \\ Ce(u_A^\rho)n = 0 \text{ on } \partial T \\ Ce(u_A^\rho)n = 0 \text{ on } \partial B(x_0,\rho) \\ u_A^\rho(x) = Ax + \phi_A^\rho(x), \quad \phi_A^\rho \ \mathcal{G}\text{-periodic function.} \end{cases}$$

The Adjoint Method in Topology Optimization

The variational formulation of the perturbed problem above is

$$\begin{cases} \text{find } u_A^\rho \in LP_A(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R))) \text{ such that} \\ a_\rho(u_A^\rho, v) = 0, \ \forall v \in H^1_\#(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N) \end{cases}$$

and the solution u_0 of the unperturbed problem is solution of the variational problem

$$\begin{cases} \text{find } u_0 \in LP_A(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R))) \text{ such that} \\ a_0(u_0, v) = 0, \ \forall v \in H^1_\#(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N) \end{cases}$$

Then the estimation

$$\|u_A^\rho - u_0\|_{LP(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)))} = O(\rho^N).$$

holds.

The adjoint problem is

$$\begin{cases} \text{find } p \in H^1_{\#}(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N) \text{ such that} \\ a_0(w, p) = -DJ_0(u_0)w, \ \forall w \in H^1_{\#}(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N). \end{cases}$$

where the Gâteaux derivative of J_0 is

$$DJ_0(u)w = \frac{2}{|Y|} \int_{Y \setminus T} \langle Ce(u), e(w) \rangle dx$$

Note that $DJ_0(u_0)w = 0$ for all $w \in H^1_{\#}(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$. Therefore $a_0(w, p) = 0$ for all $w \in H^1_{\#}(\mathbb{R}^N_{perf}(T \cup \bar{B}(x_0, R)), \mathbb{R}^N)$, consequently $p = 0$. The problem is null-adjoint.

The Adjoint Method in Topology Optimization

Theorem. *The functional*

$$j(\rho) = \frac{1}{|Y|} \int_{Y \setminus (T \cup \bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_A^\rho) \rangle dx$$

has the following asymptotic expansion

$$j(\rho) = j(0) + \rho^N D_T j(x_0) + o(\rho^N),$$

where the topological derivative $D_T j$ *in* x_0 *writes in terms of the operator* $\mathcal{T}$ *as*

$$D_T j(x_0) = \frac{1}{|Y|} \int_{\partial B(x_0,R)} \delta_{\mathcal{T}} u_0 u_0 ds(x)$$

with u_0 *solution of the unperturbed problem.*

The Adjoint Method in Topology Optimization

Corollary. Consider that the elastic tensor C corresponds to an isotropic material with Lamé constants λ and μ. Consider the functional $j(\rho) := \frac{1}{|Y|}\int_{Y\setminus(T\cup\bar{B}(x_0,\rho))} \langle Ce(u_A^\rho), e(u_B^\rho)\rangle dx$ where u_A^ρ and u_B^ρ are the corresponding solutions of the cellular problem for the effective strains A and B. Then j admits the asymptotic development $j(\rho) = j(0) + \rho^N D_T j(x_0) + o(\rho^N)$, where the topological derivative $D_T j$ in x_0 for $d = 2$, has the form :

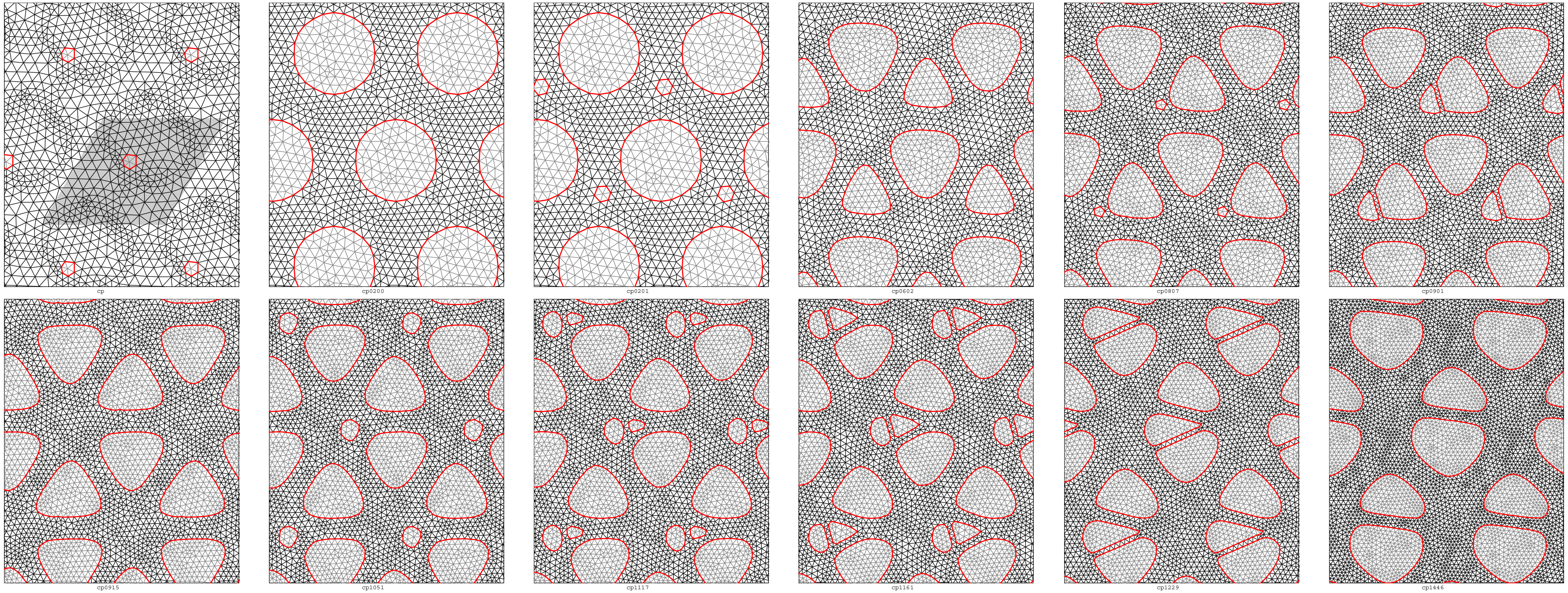
$$D_T j(x_0) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{\lambda+\mu}\Big[4\mu e(u_A(x_0))e(u_B(x_0)) + [(\lambda^2+2\lambda\mu-\mu^2)/\mu]\,\mathrm{tr}\,e(u_A(x_0))\,\mathrm{tr}\,e(u_B(x_0))\Big].$$

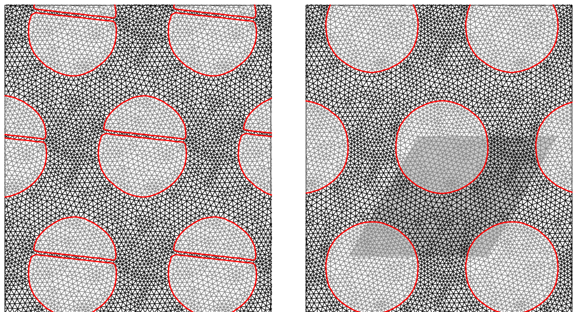
For $d = 3$ the topological derivative has the form

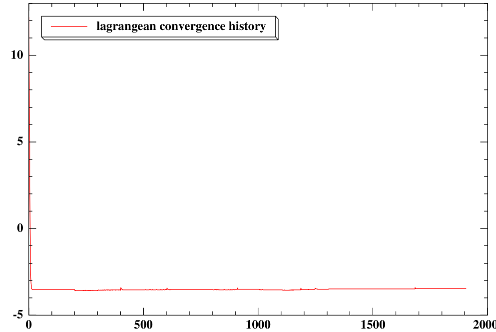
$$D_T j(x_0) = -\frac{\pi}{|Y|}\frac{\lambda+2\mu}{9\lambda+14\mu}\Big[40\mu e(u_A(x_0))e(u_B(x_0)) + [(9\lambda^2+20\lambda\mu-4\mu^2)/\mu]\,\mathrm{tr}\,e(u_A(x_0))\,\mathrm{tr}\,e(u_B(x_0))\Big].$$

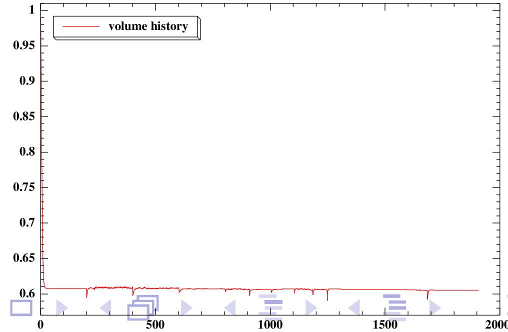
The Adjoint Method in Topology Optimization

The topological derivative was implemented in an algorithm of shape and topology optimization of microstructures [C. Barbarosie & A-M T - SMO 2009 II] and [C. Barbarosie & A-M T - MAMS 2011]. Maximization of the bulk modulus – parallelogram cell









The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

Consider the eigenvalue problem in $\Omega \subset \mathbb{R}^3$.

$$\begin{cases} -div(\mathbf{C}\epsilon(u)) = \lambda u \ \text{ in } \Omega, \\ u = 0 \quad \text{on } \Gamma_D, \\ \mathbf{C}\epsilon(u) \cdot n = 0 \quad \text{on } \Gamma_N. \end{cases}$$

This problem models the behaviour of a dam fixed on Γ_D and with an empty reservoir (there are no forces applied on Γ_N). The elastic tensor $\mathbf{C} = \mathbf{C}(s)$ depends on a vectorial parameter s that models the material coefficients. The eigenvalues $\lambda_i(s)$ and the eigenvectors (eigenmodes of vibration) $u_i(s)$ depend on s .

Goal : find the parameters s that produce prescribed eigenvalues and eigenmodes (physically measured in the dam), see [S. Oliveira, A-M T & P. Vieira, NAn:RWAp 2012].

The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

From the practical point of view, the resolution of the above problem would allow for a non-destructive method of identification of coefficients, that is, it could predict the degree of damage in the dam by using the eigenvalues and eigenmodes of the dam measured by installed sensors.
The variational formulation of the eigenvalue problem is

$$\left\{ \begin{array}{c} \text{find } \ \lambda(s) \in \mathbb{R} \ \text{ and } \ u(s) \in V \text{ such that} \\ \displaystyle\int_\Omega \mathbf{C}(s)\,\epsilon(u(s)) \cdot \epsilon(v)\,dx = \lambda(s) \int_\Omega u(s) \cdot v\,dx, \ \ \forall v \in V, \end{array} \right.$$

where

$$V = \{v \in H^1(\Omega)^3 : v_{|\Gamma_D} = 0\}.$$

By a classical result it turns out that there exists an infinite, countable set of solutions of the above problem with the property that $(\lambda_i)_{i\geq 1}$ is an increasing sequence and $(u_i)_{i\geq 1}$ forms a Hilbert basis of $(L^2(\Omega))^3$.

The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

Consider the objective functionals :

$$F_1(s) = \sum_{i=1}^{n} |\lambda_i(s) - \tilde{\lambda}_i|^2,$$

and

$$F_2(s) = \sum_{i=1}^{n} |\lambda_i(s) - \tilde{\lambda}_i|^2 + \|u_i(s) - \tilde{u}_i\|_{L^2}^2 .$$

depending on the first n eigenvalues and eigenmodes (λ_i, u_i) of the elastic model. The physically measured eigenvalues and eigenmodes are $\tilde{\lambda}_i$ and $\tilde{u}_i$.
Both functionals F_1 and F_2 are non-negative and attain the minimum value (zero) when the values of the eigenvalues and eigenmodes calculated in the model and the measured ones coincide. Therefore it is necessary to derive the functionals with respect to the parameter s .

The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

Theorem. Assuming the differentiability of $\mathbf{C}(s)$ and that the problem has only simple eigenvalues then the eigenvalues and eigenmodes are differentiable with respect to s . One has $\dfrac{d\lambda_i}{ds} = \displaystyle\int_\Omega \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i)\cdot\epsilon(u_i)\,dx$, where the eigenmode is normalized in L^2 . The derivative of the eigenmode $\dfrac{du_i}{ds}$ is solution of

$$
\left\{
\begin{array}{c}
\text{find } \dfrac{du_i}{ds} \in < u_i >^\perp \text{ such that } \forall v \in V, \\[2ex]
\displaystyle\int_\Omega \mathbf{C}(s)\epsilon(\frac{du_i}{ds})\cdot\epsilon(v)\,dx - \lambda_i \int_\Omega \frac{du_i}{ds}\cdot v\,dx = \\[2ex]
\displaystyle\frac{d\lambda_i}{ds}\int_\Omega u_i\cdot v\,dx - \int_\Omega \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i)\cdot\epsilon(v)\,dx.
\end{array}
\right.
$$

where $< u_i >^\perp$ is the orthogonal complement of the eigenspace

The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

The derivative of F_1 is

$$\frac{dF_1}{ds}(s) = 2\sum_{i=1}^{n}(\lambda_i(s) - \tilde{\lambda}_i)\int_\Omega \frac{d\mathbf{C}}{ds}\epsilon(u_i)\cdot\epsilon(u_i)\,dx,$$

and the derivative of F_2

$$\frac{dF_2}{ds}(s) = \frac{dF_1}{ds}(s) + 2\sum_{i=1}^{n}\int_\Omega \frac{du_i}{ds}(s)\cdot(u_i(s) - \tilde{u}_i)\,dx,$$

The formula of $\frac{dF_2}{ds}$ has little utility since for its implementation is necessary to solve $n \times k$ elliptic problems, where n – number of eigenvalues tooken into account and k – number of parameters (components of s).

The Adjoint Method in Optimization of Eigenvalues and Eigenmodes

The Adjoint Method permits to obtain the derivative of F_2 by solving only n problems, independently of the number k of parameters s .

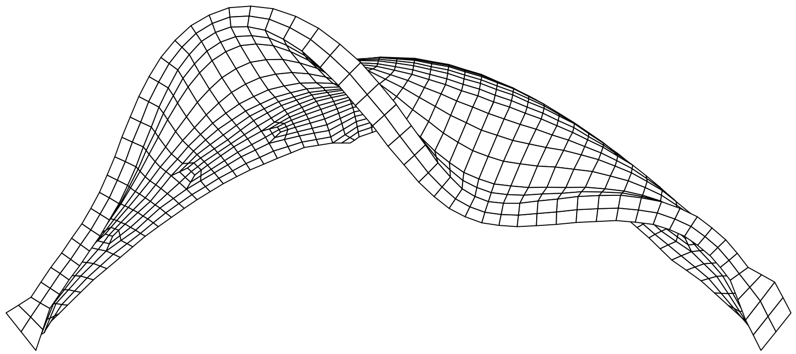
Theorem. *Consider* n *adjoint problems, for* $1 \leq i \leq n$ *, of the form :*

$$\left\{ \begin{array}{l} \textit{find } p_i \in V, \ \textit{with} \int_\Omega p_i \cdot u_i(s) dx = 0 \ s. \ t. \ \forall w \in V, \\ \int_\Omega \mathbf{C}(s)\epsilon(p_i) \cdot \epsilon(w) dx - \lambda_i(s) \int_\Omega p_i \cdot w dx = \\ \quad -2 \int_\Omega w \cdot \tilde{u}_i dx + 2 \int_\Omega u_i(s) \cdot \tilde{u}_i dx \int_\Omega w \cdot u_i(s) dx. \end{array} \right.$$

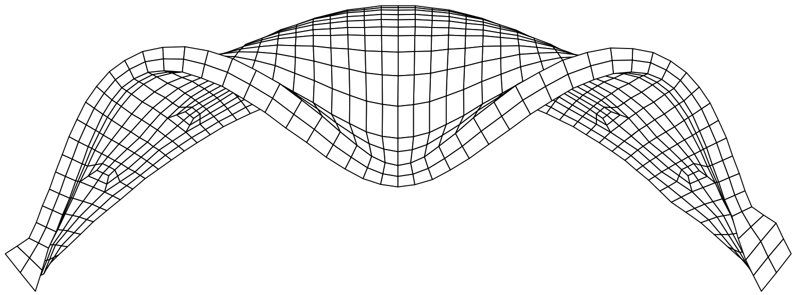
The adjoint problems have unique solution in $< u_i >^\perp$ *, and*

$$\frac{dF_2}{ds}(s) = \frac{dF_1}{ds}(s) - \sum_{i=1}^{n} \int_\Omega \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i(s)) \cdot \epsilon(p_i)\, dx.$$

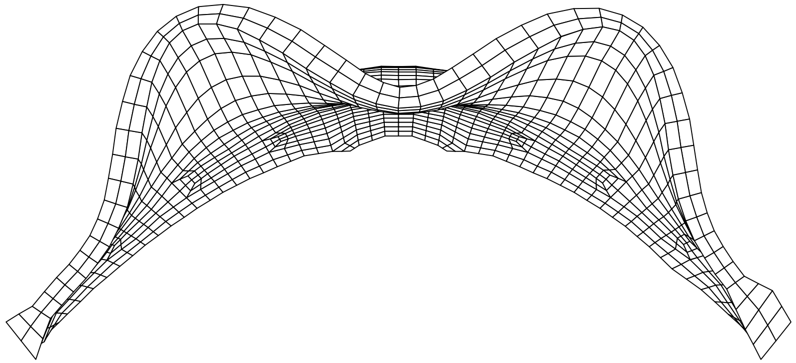
The Adjoint Method in Optimization of Eigenvalues and Eigenmodes



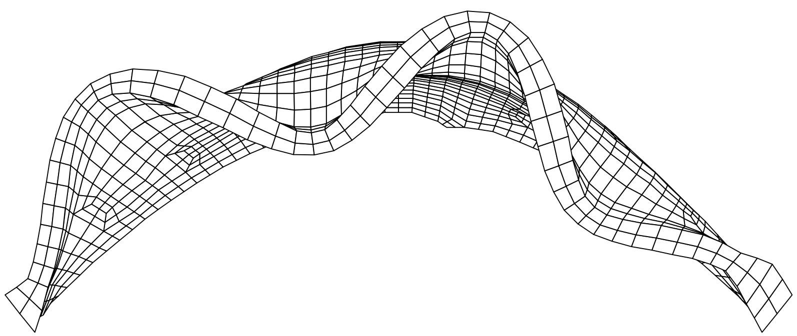
1-st mode 2.52 Hz.



2-nd mode 2.64 Hz.

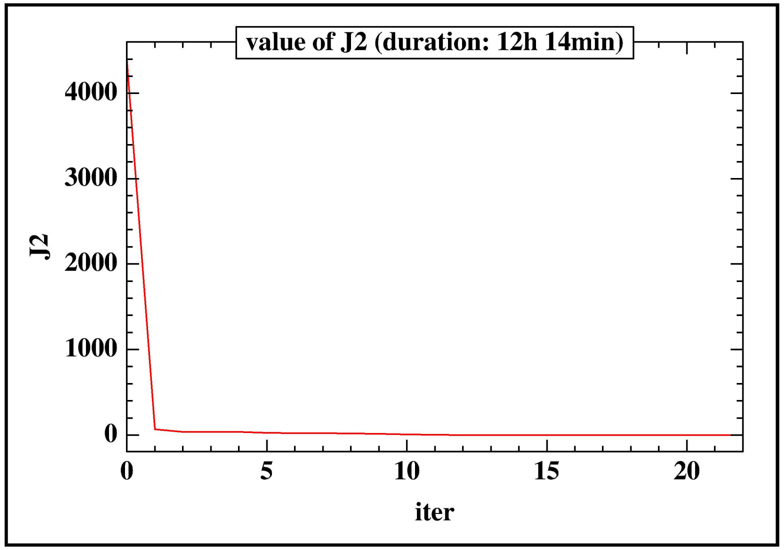


3-rd mode 3.75 Hz.

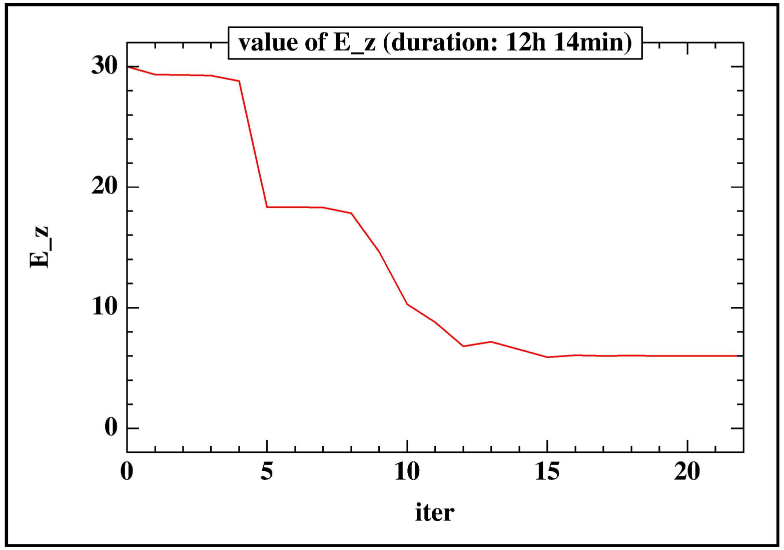


4-th mode 3.81 Hz.

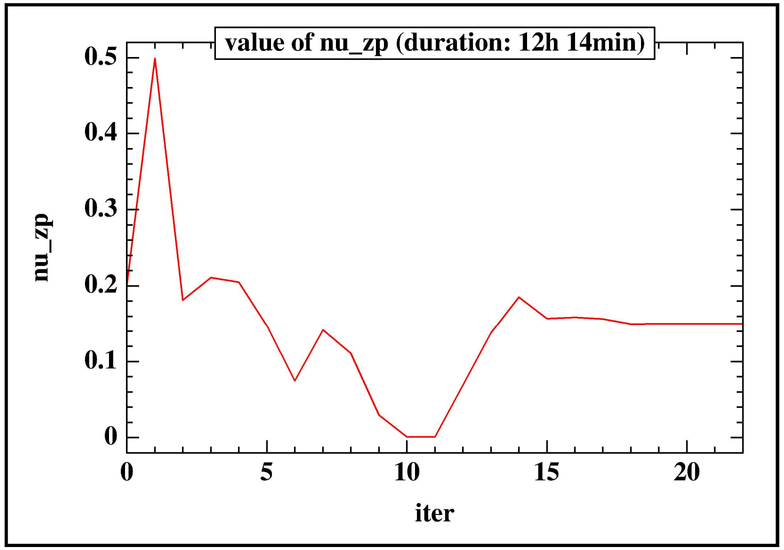
The Adjoint Method in Optimization of Eigenvalues and Eigenmodes



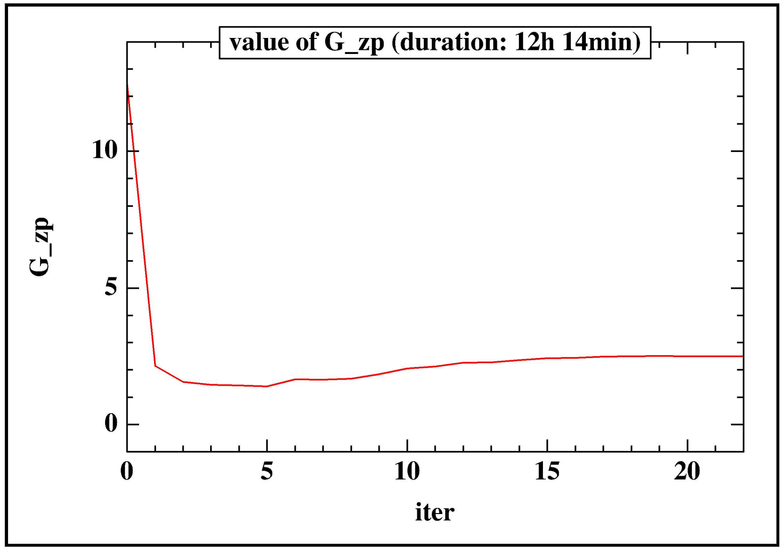
$J_{2\ \mathrm{final}} = 6.27 \times 10^{-10}$



$E_{z\ \mathrm{final}} = 6.0$



$\nu_{zp\ \mathrm{final}} = 0.15$



$G_{zp\ \mathrm{final}} = 2.5$

Adjoint method in the framework of Bloch waves

Consider a body in $\mathbb{R}^N$ ($N = 2$ or 3) made of a periodic material, that is, a material whose inhomogeneities are periodically distributed. Suppose that the period is small when compared to the overall size of the body.
An elastic Bloch wave is the superposition of a plane wave of the form $e^{i\langle \vec{k}, x\rangle}$ and a perturbation φ which is a $\mathcal{G}$ -periodic function. Thus, a Bloch wave writes :

$$u(x) = e^{i\langle \vec{k}, x\rangle}\varphi(x).$$

Note that this is equivalent to the following conditions on u :

$$u(x + \vec{g}_j) = e^{i\langle \vec{k}, \vec{g}_j\rangle}u(x), \forall x \in \mathbb{R}^N, \forall j = 1, \dots N.$$

Adjoint method in the framework of Bloch waves

When an elastic Bloch wave propagates through a body made of a $\mathcal{G}$ -periodic material, and supposing that the wavelength is comparable to the size of the periodicity cell, then the following problem, called Bloch cellular problem, characterizes the propagation phenomenon :

$$\begin{cases} -div(\mathbf{C}\epsilon(u)) & = & \lambda\rho u \ \text{ in } \mathbb{R}^N_{perf}(T), \\ \mathbf{C}\epsilon(u)\cdot n & = & 0 \ \text{ on } \partial T, \\ u(x+\vec{g}_j) & = & e^{i\langle\vec{k},\vec{g}_j\rangle}u(x),\ \forall x\in\mathbb{R}^N_{perf}(T),\ \forall j=1,\dots N. \end{cases} \quad (1)$$

In the above, T is a compact set representing a model hole in the periodicity cell Y and $\mathbb{R}^N_{perf}(T)$ is the perforated space defined by

$$\mathbb{R}^N_{perf}(T) = \mathbb{R}^N \setminus \bigcup_{k\in\mathbb{Z}^N} (T + k_1\vec{g}_1 + \dots k_N\vec{g}_N).$$

Adjoint method in the framework of Bloch waves

Recall that $H^1_{\#}(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)$ is the completion in the norm of $H^1(Y \setminus T, \mathbb{C}^N)$ of the space of functions in $C^\infty(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)$ which are $\mathcal{G}$ -periodic.
For $\vec{k} \in \mathbb{R}^N$ arbitrarily fixed, denote by $W_{\vec{k}}(\mathbb{R}^N_{perf}(T))$ the set of Bloch waves having the plane wave in the direction $\vec{k}$:

$$W_{\vec{k}}(\mathbb{R}^N_{perf}(T)) =$$
$$= \{u : \mathbb{R}^N_{perf}(T) \to \mathbb{C}^N \mid u(x) = e^{i\langle \vec{k}, x\rangle}\varphi(x), \varphi \in H^1_{\#}(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)\}.$$

Thus the last equation in (1) is equivalent to $u \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T))$.
Note that $W_0(\mathbb{R}^N_{perf}(T)) = H^1_{\#}(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)$ and $W_{\vec{k}}(\mathbb{R}^N_{perf}(T))$ is a Hilbert space, obtained from $H^1_{\#}(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)$ by multiplication with the fixed function $e^{i\langle \vec{k}, x\rangle}$
.

Adjoint method in the framework of Bloch waves

The natural norm $\|\cdot\|_{L^2_\rho}$ on the space $L^2(\mathbb{R}^N_{perf}(T), \mathbb{C}^N)$ is induced by the following inner product associated to the function $\rho \in L^\infty(\mathbb{R}^N_{perf})$ representing the specific mass ($\rho(x) \geq \rho_0 > 0$ almost everywhere in $\mathbb{R}^N_{perf}$):

$$(u, v) \mapsto \int_{Y \setminus T} \rho u \cdot \bar{v} \, dx \, .$$

In this section, the bar denotes the complex conjugate.

Adjoint method in the framework of Bloch waves

The variational formulation of the Bloch cellular problem (1) is

$$\left\{ \begin{array}{c} \text{find} \quad \lambda \in \mathbb{R} \quad \text{and} \quad u \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T)) \text{ such that} \\ \displaystyle\int_{Y \setminus T} \mathbf{C}(s)\, \epsilon(u) \cdot \epsilon(\bar{v})\, dx = \lambda \int_{Y \setminus T} \rho u \cdot \bar{v}\, dx, \quad \forall v \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T)). \end{array} \right.$$

Adjoint method in the framework of Bloch waves

Theorem.[C. Barbarosie & A-M T - RICAM, De Gruyter 2017]
Provided differentiability properties of the elasticity tensor $\mathbf{C} = \mathbf{C}(s)$ *with respect to a general material parameter* s *and assuming that the eigenvalues of the Bloch cellular problem (1) are simple, then the eigenvalues and the eigenvectors are differentiable with respect to* s *.*
The derivative of the eigenvalue $\lambda_i = \lambda_i(s)$ *is*

$$\frac{d\lambda_i}{ds}(s) = \int_{Y\setminus T} \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i) \cdot \epsilon(\bar{u}_i)\, dx,$$

where the corresponding eigenvector u_i *is normalized in the* L^2_ρ *norm of* $L^2(\mathbb{R}^N_{perf}(T))$ *:* $\|u_i\|_{L^2_\rho} = 1$ *.*

Adjoint method in the framework of Bloch waves

The derivative $\dfrac{du_i}{ds}$ *of the eigenvector* $u_i = u_i(s)$ *is the solution of the problem below:*

$$
\begin{cases}
\textit{find } \dfrac{du_i}{ds} \textit{ in } W_{\vec{k}}(\mathbb{R}^N_{perf}(T)), \textit{ such that } \displaystyle\int_{Y\setminus T} \rho \frac{du_i}{ds} \bar{u}_i \, dx = 0 \textit{ and} \\[2ex]
\displaystyle\int_{Y\setminus T} \mathbf{C}(s)\epsilon\Big(\frac{du_i}{ds}\Big) \cdot \epsilon(\bar{v}) \, dx - \lambda_i \int_{Y\setminus T} \rho \frac{du_i}{ds} \cdot \bar{v} \, dx = \\
\displaystyle\frac{d\lambda_i}{ds}(s) \int_{Y\setminus T} \rho \, u_i \cdot \bar{v} \, dx - \int_{Y\setminus T} \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i) \cdot \epsilon(\bar{v}) \, dx, \\
\qquad\qquad\qquad\qquad\qquad\qquad \forall v \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T)).
\end{cases}
\tag{2}
$$

Adjoint method in the framework of Bloch waves

The derivative of a functional $F(\lambda_i(s), u_i(s))$ depending on the first n eigenvalues and on the corresponding n eigenvectors may be written in terms of n adjoint states p_i , as :

$$\frac{dF}{ds}(s) = \sum_{i=1}^{n} \frac{\partial F}{\partial \lambda_i} \int_{Y \setminus T} \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i(s)) \cdot \epsilon(\bar{u}_i(s))\, dx$$
$$- \sum_{i=1}^{n} \int_{Y \setminus T} \frac{d\mathbf{C}}{ds}(s)\epsilon(u_i(s)) \cdot \epsilon(\bar{p}_i)\, dx.$$

Adjoint method in the framework of Bloch waves

Each adjoint state p_i is the solution of the following adjoint problem, for $1 \leq i \leq n$:

$$\begin{cases} \text{find } p_i \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T)), \text{ with } \displaystyle\int_{Y \setminus T} \rho p_i \cdot \bar{u}_i(s) dx = 0 \text{ such that} \\ \displaystyle\int_{Y \setminus T} \mathbf{C}(s) \epsilon(p_i) \cdot \epsilon(\bar{w}) dx - \lambda_i(s) \int_{Y \setminus T} \rho p_i \cdot \bar{w} dx = \frac{\partial F}{\partial u_i} w, \\ \forall w \in W_{\vec{k}}(\mathbb{R}^N_{perf}(T)). \end{cases} \tag{3}$$

Adjoint method in the framework of Bloch waves

A special interesting case is when the parameter is the vector $\vec{k}$ itself. Making variations in $\vec{k}$ would allow to treat problems of the form :

$$\max_{s} \min_{\vec{k}} F(\lambda_l(s), u_l(s)) \tag{4}$$

In order to compute the derivatives of λ_l and u_l with respect to $\vec{k}$, it is preferable to write $u(x)$ in the form of Bloch wave $u(x) = e^{i\langle \vec{k},x\rangle}\varphi(x)$. Thus, the cellular problem may be written as :

$$\left\{ \begin{array}{r} \text{find} \quad \lambda \in \mathbb{R} \quad \text{and} \quad \varphi \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N) \text{ such that} \\ \displaystyle\int_{Y\setminus T} \mathbf{C}_{\alpha\beta\gamma\delta}\,(e^{i\langle \vec{k},x\rangle}\varphi_\alpha)_{,\beta}(e^{-i\langle \vec{k},x\rangle}\psi_\gamma)_{,\delta}\,dx = \lambda \int_{Y\setminus T} \rho\varphi_\alpha\psi_\alpha\,dx, \\ \forall \psi \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N). \end{array} \right.$$

Adjoint method in the framework of Bloch waves

The derivative of λ_l is obtained as

$$\frac{\partial \lambda_l}{\partial k_j} = 2Re \int_{Y\setminus T} i\mathbf{C}_{\alpha j\gamma\delta} u_{l\alpha} \bar{u}_{l\gamma,\delta};$$

while the problem that defines the derivative of φ_l, $\dfrac{\partial \varphi_l}{\partial k_j}$, writes

$$\begin{cases} \text{find } \dfrac{\partial \varphi_l}{\partial k_j} \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N) \text{ s. t. } \displaystyle\int_{Y\setminus T} \rho \frac{\partial \varphi_{l\alpha}}{\partial k_j} \bar{\varphi}_{l\alpha}\, dx = 0 \text{ and} \\ \displaystyle\int_{Y\setminus T} \mathbf{C}_{\alpha\beta\gamma\delta} \left(e^{i\langle \vec{k},x\rangle} \frac{\partial \varphi_{l\alpha}}{\partial k_j}\right)_{,\beta} (e^{-i\langle \vec{k},x\rangle} \psi_\gamma)_{,\delta}\, dx - \lambda_l \int_{Y\setminus T} \rho \frac{\partial \varphi_{l\alpha}}{\partial k_j} \psi_\alpha\, dx = \\ \qquad \dfrac{\partial \lambda_l}{\partial k_j} \displaystyle\int_{Y\setminus T} \rho\, \varphi_{l\alpha} \psi_\alpha\, dx - \\ - \displaystyle\int_{Y\setminus T} i\, \mathbf{C}_{\alpha\beta\gamma\delta} \left(\delta_{\beta j} \varphi_{l\alpha} e^{i\langle \vec{k},x\rangle} (e^{-i\langle \vec{k},x\rangle} \psi_\gamma)_{,\delta} - \delta_{\delta j} (e^{i\langle \vec{k},x\rangle} \varphi_{l\alpha})_{,\beta}\, e^{-i\langle \vec{k},x\rangle} \psi_\gamma\right) dx \\ \qquad \forall \psi \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N). \end{cases}$$

Adjoint method in the framework of Bloch waves

Consider the adjoint problem in the form

$$\begin{cases} \text{find } \; p_l \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N) \text{ with } \displaystyle\int_{Y\setminus T} \rho p_l \bar{\varphi}_l \, dx = 0 \text{ such that} \\ \displaystyle\int_{Y\setminus T} \mathbf{C}_{\alpha\beta\gamma\delta} \left(e^{i\langle \vec{k}, x\rangle} p_{l\alpha}\right)_{,\beta} (e^{-i\langle \vec{k}, x\rangle} \bar{\psi}_\gamma)_{,\delta} \, dx - \\ \qquad\qquad -\lambda \displaystyle\int_{Y\setminus T} \rho p_{l\alpha} \bar{\psi}_\alpha \, dx = \frac{\partial F}{\partial \varphi_\alpha} \psi_\alpha, \\ \qquad \forall \psi \in H^1_\#(\mathbb{R}^N_{perf}(T), \mathbb{C}^N). \end{cases}$$

Adjoint method in the framework of Bloch waves

Therefore the derivative of the functional F may be expressed as

$$\frac{dF}{dk_j}(\vec{k}) = \sum_{l=1}^{n} \frac{\partial F}{\partial \lambda_l} 2Re \int_{Y \setminus T} i\, \mathbf{C}_{\alpha j \gamma \delta}\, u_{l\alpha} \bar{u}_{l\gamma,\delta}\, dx$$

$$-\sum_{l=1}^{n} \int_{Y \setminus T} i\, \mathbf{C}_{\alpha\beta\gamma\delta} \Big(\delta_{\beta j} \varphi_{l\alpha} e^{i\langle \vec{k},x \rangle} (e^{-i\langle \vec{k},x \rangle} \bar{p}_{l\gamma})_{,\delta} -$$

$$-\delta_{\delta j} (e^{i\langle \vec{k},x \rangle} \varphi_{l\alpha})_{,\beta}\, e^{-i\langle \vec{k},x \rangle} \bar{p}_{l\gamma} \Big)\, dx.$$

The Adjoint Method in Optimization - other frameworks

- Optimization of the homogenized coefficients by varying the periodicity pattern – C. Barbarosie & A-M T – NHM 2014
- Inverse problems : domain identification using eigenvalues and eigenmodes - P. Antunes, C. Barbarosie & A-M T – JCP 2017
- Microstructures having minimum Poisson coefficient in several directions of the plane – C. Barbarosie, A-M T & S. Lopes – DCDS-B 2020

Thank you !!!!!