An introduction to shape and topology optimization

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Part V

Topology optimization

- A glimpse at mathematical homogenization

4. Relaxation by homogenization

4.1. The G-closure problem : preliminaries

We have seen that, in 2D-periodic homogenization, the effective conductivity A^* of a mixture of 2 phases α and β is given by the resolution of PDE's

One computes the correctors χ_1, χ_2 $H^1_\#$-solutions to the cell problems

$$\begin{cases} \operatorname{div}\Big(a(y)\Big[\chi_j(y) + y_j\Big]\Big) = 0 \quad \text{in } Y \\ \chi_j \in H^1_\#(Y), \qquad i = 1,2 \end{cases}$$

and then forms

$$A^*_{ij} = \int_Y a(y)\Big(\delta_{ij} + \frac{\partial \chi_j}{\partial y_j}\Big)$$

Equivalently, one can solve the variational problem

$$A^*\xi \cdot \xi = \min\{\int_Y a(y)\Big(\xi + \nabla w(y)\Big) \cdot \Big(\xi + \nabla w(y)\Big) \quad w \in H^1_\#(Y)\}$$

The G-closure (2)

A few natural questions arise from this derivation :

- Can A^* be interpreted as the conductivity of a limiting material ?

  Does A^* posess the properties of a conductivity ?

  Does u_* solve a PDE of the same type as the u_ε's ?

- Can one characterize all the conductivities A^* that can be obtained by mixing two (or more) phases ?

  The latter question is called the problem of G-closure

The G-closure (3)

- In general, effective conductivities are matrix-valued

In particular, one can build anisotropic media as homogenized limits of mixtures of isotropic phases

- If $a(y)$ is symmetric, so is A^*
- Effective conductivities satisfy the following

Prop : Elementary Reuss-Voigt bounds

$$\forall\, \xi \in \mathbb{R}^2, \qquad \Big(\mathcal{M}(1/a)\Big)^{-1}\xi\cdot\xi \;\leq\; A^*\xi\cdot\xi \;\leq\; \Big(\mathcal{M}(a)\Big)\xi\cdot\xi \tag{1}$$

where $\quad \mathcal{M}(f) = \int_Y f(y)\,dy$

In particular, it follows that the homogenized equation is elliptic (and well-posed)

The G-closure (4)

Proof : 1. Recall the variational principle

$$A^*\xi \cdot \xi \quad = \quad \min\{ \int_Y a(y)\Big(\xi + \nabla w(y)\Big) \cdot \Big(\xi + \nabla w(y)\Big) \quad w \in H^1_\#(Y)\}$$

The choice $w = 0$ is admissible and yields

$$A^*\xi \cdot \xi \quad \leq \quad \int_Y a(y)\xi \cdot \xi \, dy \;=\; \mathcal{M}(a)\xi \cdot \xi$$

2. For the lower bound, consider $w \in H^1_\#(Y)$. Then for a.e. $y \in Y$

$$a(y)(\xi + \nabla w(y)) \cdot (\xi + \nabla w(y)) \quad = \quad \sup_{\eta \in \mathbb{R}^2} \Big\{ 2(\xi + \nabla w(y)) \cdot \eta - \frac{1}{a(y)} \eta \cdot \eta \Big\}$$

The G-closure (5)

It follows that

$$
\begin{aligned}
T &:= \int_Y a(y)\Big(\xi + \nabla w(y)\Big)\cdot\Big(\xi + \nabla w(y)\Big) \\
&\geq \int_Y \sup_{\eta(y)\in\mathbb{R}^2} \left\{ 2(\xi + \nabla w(y))\cdot\eta(y) - \frac{1}{a(y)}\eta(y)\cdot\eta(y) \right\} \\
&\geq \sup_{\eta\in\mathbb{R}^2} \int_Y 2(\xi + \nabla w(y))\cdot\eta - \frac{1}{a(y)}\eta\cdot\eta
\end{aligned}
$$

as one obtains a lower bound by choosing the same η for all y's
Using the fact that w is periodic, we further obtain that for any $w \in H^1_\#(Y)$

$$
T \geq \sup_{\eta\in\mathbb{R}^2} 2\xi\cdot\eta - \Big(\int_Y \frac{1}{a(y)}\Big)\eta\cdot\eta
$$

Taking the supremum wrt to η yields the lower bound

4.2. The G-closure problem : sequential laminates

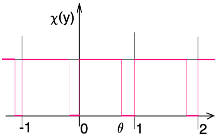
As we have seen, the effective coefficients A^* of a composite mixture of 2 phases depends on the following ingredients

- the conductivities α, β of the constituting pure phases
- the function χ that describe the geometry of the mixture

The determination of A^* require the resolution of a PDE. In a (very) limited number of cases, one can obtain explicit formulas

Laminates (2)

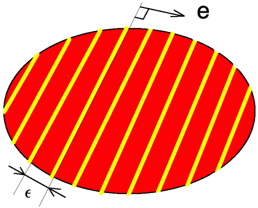
Let $e \in \mathbb{R}^d$ be a unit vector and given $0 \leq \theta \leq 1$ let χ denote the 1-periodic function (of a single variable) whose graph is



For $\varepsilon > 0$, we consider a medium defined by the conductivity

$$A_\varepsilon(x) \quad = \quad \chi(\frac{x \cdot e}{\varepsilon})\, A \,+\, (1 - \chi(\frac{x \cdot e}{\varepsilon}))\, B$$

which describes the periodic distribution of a mixture of 2 phases with conductivities A, B in layers perpendicular to the direction e



Laminates (3)

As a consequence of Tartar's compactness theorem, if u_ε is a bounded sequence of voltage potentials which satisfies

$$\mathrm{div}(A_\varepsilon(x)\nabla u_\varepsilon(x)) \quad = \quad 0 \quad \text{in } \Omega \tag{2}$$

and which converges weakly in H^1 to some u_*, then the limiting potential satisfies

$$\mathrm{div}(A^*\nabla u_*(x)) \quad = \quad 0 \quad \text{in } \Omega$$

Let us try to construct a sequence of solutions to (2) which are piecewise linear functions : we seek $\lambda, \xi \in \mathbb{R}^d$ so that in the j-th layer

$$u_\varepsilon(x) \quad = \quad \begin{cases} \lambda \cdot x + c_j & \text{in the layers of the phase } A \\ \xi \cdot x + c_j' & \text{in the layers of the phase } B \end{cases}$$

where the constants c_j, c_j' are adjusted in each layer so that the resulting function is continuous.

Laminates (4)

Actually, continuity is the sole requirement for such a function to be in H^1_{loc}
In particular, if we consider two points x and $x + te^{\perp}$ that belong to the same interface then continuity at these points yields the condition

$$\begin{aligned} \lambda \cdot x + c_j &= \xi \cdot x + c_j' \\ \lambda \cdot (x + te^{\perp}) + c_j &= \xi \cdot (x + te) + c_j' \end{aligned}$$

so that for any direction $e^{\perp}$ perpendicular to e

$$(\xi - \lambda) \cdot e^{\perp} = 0 \tag{3}$$

Notice that such u_ε has a periodic, piecewise constant gradient and that the associated current $\sigma_\varepsilon = a(y)\nabla u_\varepsilon$ has the form

$$\sigma_\varepsilon = \begin{cases} A\lambda & \text{in the layers of the phase } A \\ B\xi & \text{in the layers of the phase } B \end{cases}$$

Laminates (5)

Such a function is a solution to $\mathrm{div}(\sigma_\varepsilon) = 0$ in $\mathcal{D}'(\Omega)$ provided

$$\Big(A\lambda - B\xi\Big) \cdot e \quad = \quad 0 \tag{4}$$

Relations (3-4) show that

$$\xi = \lambda + te \quad \text{with} \quad t = \frac{(A - B)\xi \cdot e}{Be \cdot e} \tag{5}$$

In addition, since both fields ∇u_ε and σ_ε are periodic, they converge weakly in L^2 to

$$\nabla u_\varepsilon \rightharpoonup \nabla u_* := \theta\lambda + (1-\theta)\xi \qquad \text{and} \qquad \sigma_\varepsilon \rightharpoonup \sigma_* := \theta A\lambda + (1-\theta)B\xi$$

which should satisfy

$$A^* \nabla u_* = \sigma_* \qquad \text{i.e.} \qquad A^*\Big(\theta\lambda + (1-\theta)\xi\Big) \;=\; \theta\Big(A\lambda\Big) + (1-\theta)\Big(B\xi\Big)$$

Laminates (6)

Setting $\zeta = \theta\lambda + (1-\theta)\xi$, so that

$$\lambda \quad = \quad \zeta - (1-\theta)\frac{(A - B\zeta \cdot e}{(1-\theta)Ae \cdot e + \theta Be \cdot e} e$$

and working out the algebra yields

$$A^*\zeta \quad = \quad \theta\Big(A\zeta\Big) + (1-\theta)\Big(B\zeta\Big) - \frac{\theta(1-\theta)\Big(A - B\Big)\zeta \cdot e}{(1-\theta)Ae \cdot e + \theta Be \cdot e}(A-B)e$$

This formula can be rewritten in a more interesting form when $A - B$ is invertible

$$\theta(A^* - B)^{-1} \quad = \quad (A-B)^{-1} + (1-\theta)\frac{e \otimes e}{Be \cdot e}$$

where the notation $e \otimes e$ stands for the matrix with entries $(e_i e_j)_{1 \leq i,j \leq d}$

Laminates (7)

This construction can be iterated : Suppose we laminate phases A and B with a proportion θ_1 of A in a direction e_1 : we obtain a composite with effective conductivity A_1^* given by the previous expression

$$\theta_1(A_1^* - B)^{-1} \quad = \quad (A - B)^{-1} + (1 - \theta_1)\frac{e_1 \otimes e_1}{Be_1 \cdot e_1}$$

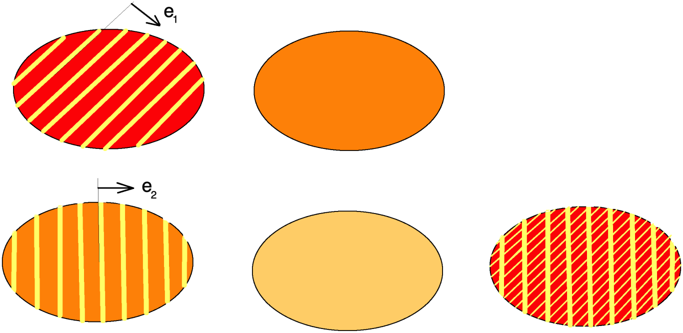
We can then construct a new material by layering A_1^* and the same background phase B, with a proportion θ_2 of A_1^* in a direction e_2 to obtain an effective conductivity A_2^* given by

$$\theta_2(A_2^* - B)^{-1} \quad = \quad (A_1^* - B)^{-1} + (1 - \theta_2)\frac{e_2 \otimes e_2}{Be_2 \cdot e_2}$$

The overal proportion of the original phase A in the resulting composite is now $\theta = \theta_1\theta_2$ and one sees that

$$\theta_1\theta_2(A_2^* - B)^{-1} \quad = \quad (A - B)^{-1} + (1 - \theta_1)\frac{e_1 \otimes e_1}{Be_1 \cdot e_1} + (1 - \theta_2)\theta_1\frac{e_2 \otimes e_2}{Be_2 \cdot e_2}$$

Laminates (8)



Laminates (9)

Iterating this procedure (keeping the same phase B as background material) one can construct a laminate of rank p :

Let $e_1, \ldots, e_p$ be a set of unit vectors, $\theta \in [0,1]$ and $m_i, 1 \leq i \leq p \in [0,1]$ with $\sum_{i=1}^{p} m_i = 1$, the laminate of rank p with lamination parameters m_i is defined by

$$\theta(A_p^* - B)^{-1} \quad = \quad (A - B)^{-1} + (1-\theta) \sum_{i=1}^{p} m_i \frac{e_i \otimes e_i}{Be_i \cdot e_i}$$

Laminates (10)

The same procedure can be carried out for the operator of linearized elasticity

Given 2 materials with isotropic Hooke's laws A and B, p unit vectors $e_1, \dots, e_p \in \mathbf{R}^d$, $\theta \in [0,1]$ and $m_i, 1 \le i \le p \in [0,1]$ with $\sum_{i=1}^p m_i = 1$, the laminate of rank p with lamination parameters m_i is defined by

$$(1-\theta)(A_p^* - B)^{-1} \quad = \quad (B-A)^{-1} + \theta \sum_{i=1}^{p} m_i f_A(e_i)$$

where for any $d \times d$ symmetric matrix ξ

$$f_A(e)\xi : \xi \quad = \quad \frac{1}{\mu_A}\left(|\xi e|^2 - (\xi e \cdot e)^2\right) + \frac{1}{2\mu_A\lambda_A}(\xi e \cdot e)^2$$

4.3. The G-closure problem : optimal bounds

Laminates composites provide a class of homogenized materials for which explicit formulas are available and the properties of which depend on a finite number of parameters

We recall the question of $G-$closure : what is the set G_θ of effective conductivities or effective Hookes'laws that can be reached as homogenized limits of (periodic) mixtures of two phases A and B in proportion θ and $(1-\theta)$?

If we cannot fully characterize G_θ, can we get optimal estimates on some functions of A^* ?

Such estimates are called Hashin-Shtrikman bounds

Thm : Hashin-Strickman bounds in conductivity [Murat Tartar 85, Lurie and Cherkaev 84]

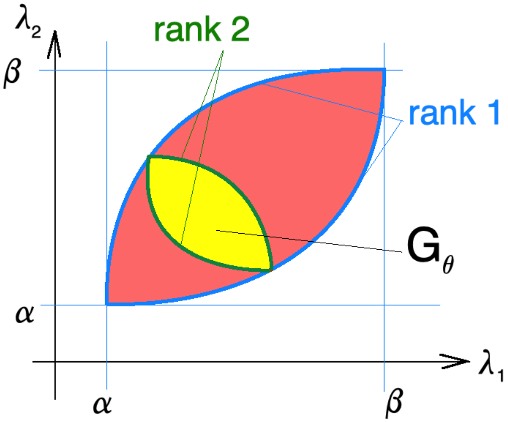
Let A^* be a $d \times d$ matrix that can be realized as the mixture of 2 isotropic conductivities $\alpha < \beta$ in volume fraction θ and $(1-\theta)$ (we say $A^* \in G_\theta$)

Then the eigenvalues $\lambda_1, \ldots \lambda_d$ of A^* satisfy

$$\begin{cases} \lambda_\theta^- \leq \lambda_j \leq \lambda_\theta^+ \\ 1 \leq j \leq d \end{cases} \quad \text{and} \quad \begin{cases} \sum_{j=1}^d \frac{1}{\lambda_j - \alpha} & \leq & \frac{1}{\lambda_\theta^- - \alpha} + \frac{d-1}{\lambda_\theta^+ - \alpha} \\ \sum_{j=1}^d \frac{1}{\beta - \lambda_j} & \leq & \frac{1}{\beta - \lambda_\theta^-} + \frac{d-1}{\beta - \lambda_\theta^+} \end{cases}$$

where $\lambda_\theta^- = \left(\theta\alpha^{-1} + (1-\theta)\beta^{-1}\right)^{-1}$ and $\lambda_\theta^+ = \theta\alpha + (1-\theta)\beta$

Representation of the bounds in 2D : note that laminates describe the enveloppe of the sets G_θ



Optimal Bounds (4)

For linearized elasticity, the situation is more complex : there is no complete characterization of G_θ

However, one can characterize those effective Hooke's laws that whose energy is optimal

Thm : [Allaire-Kohn 93]

Let A^* denote the effective Hooke's law of a mixture of 2 well-ordered materials with Hooke's laws $A \leq B$ (in the sense of quadratic forms) then

$$A^*\xi : \xi \quad \geq \quad A\xi : \xi + (1-\theta) \max_{\eta \in \mathbf{M}_s^d} \left[2\xi : \eta + (B-A)^{-1}\eta : \eta - \theta \max_{|e|=1} f_A(e)\eta : \eta \right]$$

$$A^*\xi : \xi \quad \leq \quad B\xi : \xi + \theta \min_{\eta \in \mathbf{M}_s^d} \left[2\xi : \eta + (B-A)^{-1}\eta : \eta - (1-\theta) \min_{|e|=1} f_B(e)\eta : \eta \right]$$

Furthermore, these bounds are attained by sequential laminates of rank d in dimension d, whose directions of lamination are aligned with the eigendirections of the symmetric matrix ξ

4.4. A strategy for structural optimization

To summarize the insight we have gained in the previous paragraphs, let us consider again the problem of finding the optimal distribution of a material with Hooke's law A and a very soft material with Hooke's law $B = \eta A$, $\eta << 1$, in a given set Ω

$$\text{Find } \chi_{opt} \in L^\infty(\Omega, \{0,1\}) \text{ such that}$$

$$\begin{aligned} J(\chi_{opt}) &= \min \left\{ J(\chi)\ \chi \in L^\infty(\Omega, \{0,1\}) \right\} \\ &= \min_{\chi} \left\{ \int_\Omega A_\chi e(u_\chi) : e(u_\chi) + \lambda \int_\Omega \chi \right\} \end{aligned}$$

Where for a given χ, u_χ is defined as the solution to

$$\left\{ \begin{aligned} -\mathrm{div}(A_\chi e(u_\chi)) &= f \quad \text{in } \Omega \\ u_\chi &= 0 \quad \text{on } \partial\Omega \end{aligned} \right.$$

Structural optimization (2)

If (χ_n) is a minimizing sequence, then weak compactness and the compactness theorem of Tartar imply that a subsequece of (χ_n, A_{χ_n}) converges to some limiting composite structure (θ, A^*)

The latter convergence holds in the sense of H-convergence : the sequence of equilibrium states u_n converge weakly in H^1 to the equilibrium state u_* associated to A^*

Moreover, the energies converge, so that

$$J(\chi_n) \quad \to \quad \int_\Omega A^* e(u_*) : e(u_*) \; + \; \lambda \int_\Omega \theta \; =: J^*(\theta, A^*)$$

Structural optimization (3)

We are thus led to consider the relaxed optimization problem

$$\text{Find } \theta_{opt} \in L^\infty(\Omega,[0,1]) \text{ and } A^*_{opt} \in G_\theta, \text{ such that}$$

$$\begin{aligned} J^*(\theta_{opt}, A^*_{opt}) &= \min\left\{ J^*(\theta, A^*), \quad \theta \in L^\infty(\Omega,[0,1]), A^* \in G_\theta \right\} \\ &:= \min_{\theta, A^*} \left\{ \int_\Omega A^* e(u_*) : e(u_*) \; + \; \lambda \int_\Omega \theta \right\} \end{aligned}$$

Structural Optimization (4)

Remarks :

- The condition $A^* \in G_\theta$ means $A^*(x) \in G_{\theta(x)} \quad$ for a.e. x
- There is a catch : for linear elasticiy, we do not know explicitely the set G_θ
- However, when the cost functional is the compliance (or a sum of compliances) we do know that optimal values of the compliance may be achieved with laminated composites of rank d
- So we may replace the condition $A^* \in G_\theta$ by $A^* \in L_\theta$ the set of rank d laminates : recall that such materials are characterized by d directions and d proportions of lamination at each point

Structural Optimization (5)

Given θ, A^*, recall that u_* is defined as the solution to

$$\begin{cases} -\mathrm{div}(A^* e(u_*)) & = & f & \text{in } \Omega \\ u_* & = & 0 & \text{on } \partial\Omega \end{cases} \tag{6}$$

so that by the principle of minimal complementary energy

$$\int_\Omega A^* e(u_*) : e(u_*) \quad = \quad \int_\Omega f \cdot u_* = \min_{\sigma \in \Sigma_{adm}} \int_\Omega (A^*)^{-1} \sigma : \sigma$$

where

$$\Sigma_{adm} \quad = \quad \{\sigma \in L^2(\Omega), -\mathrm{div}(\sigma) = f \text{ in } \Omega\}$$

It follows that the relaxed problem can be cast in the form :

$$\min_{\theta, A^* \in G_\theta} \left\{ \int_\Omega A^* e(u_*) : e(u_*) \; + \; \lambda \int_\Omega \theta \right\}$$

$$= \quad \min_{\theta, A^* \in L_\theta} \min_{\sigma \in \Sigma_{adm}} \left\{ \int_\Omega (A^*)^{-1} \sigma : \sigma \; + \; \lambda \int_\Omega \theta \right\}$$

$$= \quad \min_{\sigma \in \Sigma_{adm}} \int_\Omega \min_\theta \left[\min_{A^* \in L_\theta} \left((A^*)^{-1} \sigma : \sigma \right) \; + \; \lambda \theta \right]$$

Structural Optimization (7)

When $\eta \to 0$, one can show that given $\tau \in \mathbf{M}_s^d$ and $0 \leq \theta \leq 1$

$$\min_{A^* \in L_\theta} (A^*)^{1} \tau : \tau \quad \to \quad A^{-1}\tau : \tau + \frac{1-\theta}{\theta} g^*(\tau)$$

where

$$g^*(\tau) \quad = \quad \min_{\left\{ \begin{array}{c} 0 \leq m_i \leq 1 \\ \sum_{i=1}^d m_i = 1 \end{array} \right.} \quad \sum_{i=1}^{d} m_i f_A^c(e_i) \tau : \tau$$

Structural Optimization (8)

In 2D and 3D this $g^*(\tau)$ can be computed explicitely

For example in 2D, denoting τ_1 and τ_2 the eigenvalues of the (symmetric) matrix τ

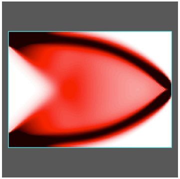
$$g^*(\tau) \quad = \quad \frac{\lambda}{4\mu(\lambda+\mu)}\left(|\tau_1| + |\tau_2|\right)^2$$

and the minimum is achieved by a rank-2 laminate aligned with the eigenvectors of τ and with parameters

$$m_1 = \frac{|\tau_2|}{|\tau_1| + |\tau_2|}, \quad m_2 = \frac{|\tau_1|}{|\tau_1| + |\tau_2|}$$

Note that

- The minimization with respect to the structural parameters (local volume fraction of phase A, lamination parameters) is local
- Given the pointwise values $\theta(x)$ and $\sigma(x)$, the minimization wrt the lamination parameters is explicit. These are the composites that achieve the optimal bounds for the complementary energy
- Existence of a minimum can be established for this relaxed optimization problem
- This formulation leads to efficient algorithms that will be the described next



4.5. An algorithm for topological optimization

We consider optimization of the compliance under given load + BC's

$$\min_{\theta, A^* \in G_\theta} \left\{ \int_\Omega A^* e(u_*) : e(u_*) \, + \, \lambda \int_\Omega \theta \right\}$$

$$= \min_{\theta, A^* \in L_\theta} \min_{\sigma \in \Sigma_{adm}} \left\{ \int_\Omega (A^*)^{-1} \sigma : \sigma \, + \, \lambda \int_\Omega \theta \right\}$$

where u_* is the solution to

$$\begin{cases} -\mathrm{div}(A^* e(u_*)) & = & f & \text{in } \Omega \\ u_* & = & 0 & \text{on } \partial\Omega \end{cases}$$

An alternate direction algorithm (2)

The bounded domain Ω is discretized with quadrangular elements

Alternate directions algorithm

- Initialisation of the design parameters θ_0, A_0^*

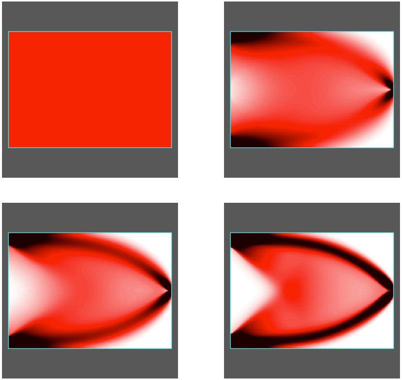
  (for example $\theta_0 = 1, A_n^* = A$ everywhere in Ω)

- Iteration until convergence:

  a) Computation of $u_{*,n}$ solution to the problem of linear elasticity with design parameters θ_n, A_n^*

  b) update of the design variables θ_n, A_n^* using the explicit formulas for the lamination parameters, which are locally optimal for the field $\tau_n = A^* n e(u_{*,n})$

An alternate direction algorithm (3)



An alternate direction algorithm (4)

Note that the resulting shape is a composite structure

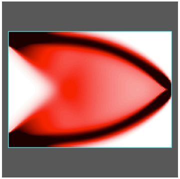
Upon convergence, once can obtain quasi-optimal black-and-white shapes by performing a few more iterations of the algorithms where composites are penalized :

In the (local) optimization with respect to θ, one forces the values of the optimal density to move closer to 0 or 1

$$\theta_n = \frac{1 - \cos(\pi \theta_o pt)}{2}$$

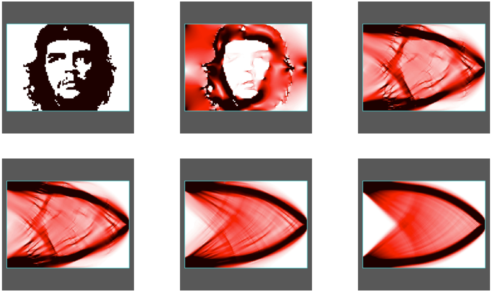
Of course, the resulting shapes do not perform as well, but one can have a practical estimate of the loss of performance

An alternate direction algorithm (5)



An alternate direction algorithm (6)

Experimentally, one observes less local minima and robustness with respect to the initial design parameters



An alternate direction algorithm (7))

Remarks :

- Explicit formulas are only available for the compliance (or a sum of compliance)
- There are many open questions concerning the numerical implementation of such methods and its coupling with level set/parametric methods
- The idea of looking into generalized composite designs, may give ideas of original designs that may prove interesting