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CLASS SESSIONS

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1 Session 1: Topology optimization Problem

1.1 Formulation of the topology optimization problem

Let Ω be the domain of the problem and let Ω^+ and Ω^- be a partion that represents strong and weak materials respectively, such that:

$$\Omega = \Omega^+ \cup \Omega^- \quad (1)$$

The fundamental mathematical statement of a topology optimization problem is defined through the design variable, the objective function and a set of constraints. Based on linear static finite element discretization, the standard topology optimization problem may be given as:

$$P1 : \begin{cases} \min & f(\chi, U) \\ x, u \\ s.t. & K(\chi)U = F(\chi) \\ & g_i(\chi, U) \leq 0 \end{cases} \quad (2)$$

where f is the objective function, χ is the vector of integer nodal design variables (solid or void), U is the displacement vector, K is the global stiffness matrix, F is the force vector and g_i are the constraints. The characteristic function χ is defined as follows:

$$\chi(x) = \begin{cases} 1 & x \in \Omega^+ \\ 0 & x \in \Omega^- \end{cases} \quad (3)$$

Where x is the position of each point of the domain. Within this generalized statement, a number of problems can be formulated considering a variety of objectives and constraints, including compliance, stresses, volume, perimeter and inverse problems. As an example, the popular compliance problem can be setup by minimizing an objective of structural compliance as $f = U^T K U$ and constraining the amount of material usage as $g = \frac{\int \chi}{V_0} - V^* \leq 0$.

As defined in Eq. 2, the stiffness matrix is written in terms of the characteristic function χ .

$$K = \int_{\Omega} B^T C B d\Omega = \int_{\Omega^+} B^T C^+ B d\Omega + \int_{\Omega^-} B^T C^- B d\Omega \quad (4)$$

Which, if expressed over the whole volume, gives the following expression:

$$K = \int_{\Omega} \chi B^T C^+ B d\Omega + (1 - \chi) B^T C^- B d\Omega \quad (5)$$

Therefore, if comparing Eq. 5 with the definition of the stiffness matrix, the elasticity matrix C can be written in terms of the characteristic function χ , by means of C^+ and C^- :

$$C = \chi C^+ + (1 - \chi) C^- \quad (6)$$

1.2 Regularization of the problem

Fundamentally, the formulation in (2) poses an extremely challenging large-scale integer programming problem. As a result, it is desirable to replace the integer variable with continuous variables and identify a means to iteratively steer the solution towards a discrete solid/void solution. This is accomplished with a regularization function. Finally, material interpolation schemes are then used characterize the material in grey areas.

A general formulation of the regularized problem based on linear static finite element analysis may be given as:

$$P2 : \begin{cases} \min & f(\rho, U) \\ \rho, u \\ \text{s.t.} & K(\rho)U = F(\rho) \\ & g_i(\rho, U) \leq 0 \end{cases} \quad (7)$$

where f is the objective function, ρ is the vector of nodal densities, $\rho \in [0, 1]$, U is the displacement vector, K is the global stiffness matrix, F is the force vector and g_i are the constraints.

1.3 Interpolation Scheme

At this point, instead of expressing the domain by means of an integer function χ , the domain is expressed by a continuous function ρ . However, there has to be a way to interpret the physical meaning of ρ . For instance, if $\chi = 1$ represents a point in the domain where there is material, and $\chi = 0$ represents a point in the domain where there is void, then the interpretation of an intermediate value of $\rho = 0.75$ has to be determined. Interpolation schemes will allow to establish a relation between the function ρ and its corresponding constitutive tensor $C(\rho)$.

1.3.1 SIMP

SIMP mathematical formulation is presented in the following equation:

$$C(\rho) = \rho^p C^+ + (1 - \rho^p) C^- \quad (8)$$

Where C is the elasticity matrix (C^+ for solid material and C^- for void), ρ is the regularized characteristic function and p is any value higher than 1. It has been showed that the a proper value for this parameter is $p = 3$. In order to satisfy the Hashin-Shtrikman (HS) bounds for two-phase materials, and following the reference book, the penalization factor is computed according to (9).

$$p(\nu^+) = \max \left\{ \frac{2}{1 - \nu^+}, \frac{4}{1 + \nu^+} \right\} \quad (9)$$

Note that the elasticity matrix can be expressed as a function of the Young modulus and the Poisson ratio, i.e.,

$$C^- = \frac{E^-}{1 - 2\nu^-} \begin{pmatrix} 1 & \nu^- & 0 \\ \nu^- & 1 & 0 \\ 0 & 0 & \frac{1 - (\nu^-)^2}{2} \end{pmatrix} \quad C^+ = \frac{E^+}{1 - 2\nu^+} \begin{pmatrix} 1 & \nu^+ & 0 \\ \nu^+ & 1 & 0 \\ 0 & 0 & \frac{1 - (\nu^+)^2}{2} \end{pmatrix} \quad (10)$$

Inserting it into to Eq. (8):

$$C(\rho) = (\rho^p E^+ + (1 - \rho^p) E^-) \frac{1}{1 - 2\nu} \begin{pmatrix} 1 & \nu^+ & 0 \\ \nu^+ & 1 & 0 \\ 0 & 0 & \frac{1 - (\nu^+)^2}{2} \end{pmatrix} = E(\rho) \frac{1}{1 - 2\nu} \begin{pmatrix} 1 & \nu^+ & 0 \\ \nu^+ & 1 & 0 \\ 0 & 0 & \frac{1 - (\nu^+)^2}{2} \end{pmatrix} \quad (11)$$

Where $\nu^- = \nu^+ = \nu$ has been assumed constant for both C^+ and C^- . Now, an expression for the Young modulus in terms of ρ and p has been obtained. In isotropic materials, the shear and bulk modulus, κ and μ , can be obtained by means of E and ν , which are used to computed the Hashin-Strikman bounds.

Hashin-Shtrikman bounds Hashin-Shtrikman bounds are the tightest bounds possible from range of composite moduli for a two-phase material, in the form of matrix and inclusion. On the one hand, the upper bound is derived by considering the solid material (μ^+ , κ^+) as the matrix, and the void material (μ^- , κ^-) is the inclusion in the form of a sphere (or circle in 2D). On the other hand, the lower bound is derived from the opposite assumption, where the void material (μ^- , κ^-) is the matrix and the solid material (μ^+ , κ^+) the inclusion. A visual representation of the concept is presented in Figure 1. And kind of interpolation must be in between the upper and lower band in order to physically understand the meaning of a grey material.

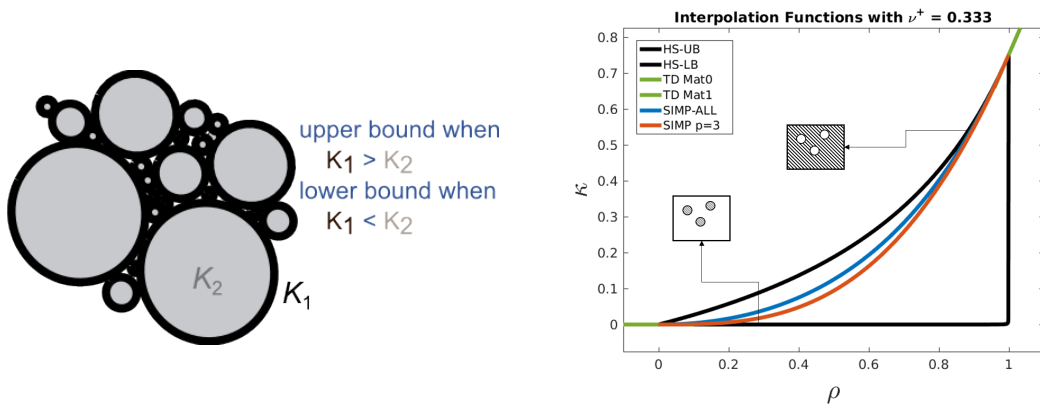


Figure 1: Visual representation of the Hashin-Shtrikman bounds

The Hashin-Shtrikman bounds are the limits of the all the possible micro-structures that, for instance, a point material with a $\rho = 0.75$ may have.

2 Session 3: The SLERP Method

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11/10/2017

The SLERP algorithm is used in Topology Optimization when a level-set function describes the topology of the domain. It consist in using the Topological Derivative to minimize a function ($J(\chi)$) in the whole domain providing a topology which has optimal stiffness for a certain value of volume. In the next paragraphs this method is explained.

Firstly, the Topological Derivative has to be defined as the difference between the actual state of the topology and any infinitesimal change in it. Equation (12) represents the definition of this derivative.

$$J(\chi + \tilde{\chi}_\epsilon) - J(\chi) = D_T J(\chi) |Be| \quad (12)$$

Where,

- $\tilde{\chi}_\epsilon$ is any infinitesimal topology change.
- $J(\chi)$ is the actual topology.
- D_T is the Topological Derivative.
- Be is the ball inserted in the domain

The aim of the whole process is to minimize the topology function, therefore, the optimal condition is expressed as Equation 13 states.

$$J(\chi + \tilde{\chi}_\epsilon) - J(\chi) = D_T J(\chi) |Be| \geq 0 \quad \forall \tilde{\chi} \quad (13)$$

Following reference work a g function is defined from the Topological Derivative as:

$$g = \begin{cases} D_T J & \Psi > 0 \quad (X \in \Omega^-) \\ -D_T J & \Psi < 0 \quad (X \in \Omega^+) \end{cases} \quad (14)$$

Notice that Ψ is the level-set function that defines the topology. As a result, the new definition of the optimal condition becomes:

$$g(\chi) \begin{cases} > 0 & \Psi > 0 \quad (\chi \in \Omega^-) \\ < 0 & \Psi < 0 \quad (\chi \in \Omega^+) \end{cases} \quad (15)$$

Alternative as:

$$\text{sign}(g(\chi(\Psi))) = \text{sign}(\Psi) \quad (16)$$

Thus, in order to find the optimal solution only the signs must coincide between g and Ψ . Moreover, in order to solve the problem, a strong optimality condition is imposed through the following requirements.

1. To satisfy the same sign of the gradient and the level-set, it is imposed to be the same.

2. Transform the optimal condition represented in Equation (16) as the following expression:

$$R(\Psi) = g(\chi(\Psi^*)) - \Psi^* = 0 \quad (17)$$

By this new definition, the problem can be solved by a Fix Point method, performing the iteration: $\Psi_{n+1} = g(\chi(\Psi_n))$.

3. Reduce level-set possible infinite values by making unitary its $L^2(\Omega)$ norm:

$$\|\psi\|_L^2(\Omega) = 1 \quad \rightarrow \quad (\Psi, \Psi) = \int_{\Omega} \Psi^2 = 1 \quad (18)$$

Where (\cdot, \cdot) is the scalar product.

Having introduced these changes, we can rewrite Equation (17) in its general case as:

$$R(\Psi) = \frac{g(\chi(\Psi))}{\|g(\chi(\Psi))\|} - \Psi = 0 \quad (19)$$

It must be commented that when the optimal solution is reached using Equation (19), $\|g(\chi(\Psi))\|$ becomes equal to 1. Therefore, Equation (17), which is the original optimal condition remains invariant. Trying to solve the problem with this configuration with a Fix-point method would lead to:

$$\Psi_{n+1} = \frac{g(\chi(\Psi_n))}{\|g(\chi(\Psi_n))\|} \quad (20)$$

The above equation would be too aggressive to solve directly in some cases. Thus, a relaxation the algorithm (20) is proposed through a line-search method. The values α and β are computed by explicitly impose $\|\psi\| = 1$, leading to the final expression of the SLERP algorithm (21).

$$\Psi_{n+1} = \beta\Psi_n + \alpha \frac{g(\chi(\Psi_n))}{\|g(\chi(\Psi_n))\|} \quad (21)$$

Where $\theta_n = \arccos\left(\frac{(\Psi_n, g_n)}{\|\Psi_n\| \|g_n\|}\right)$ and plays the role of the line search parameter.

3 Session 4: Numerical methods

3.1 SLERP - Part II

Applying a trigonometric equivalence to the SLERP method, a new function Ψ_{n+1} , can be computed from Eq. (21) as:

$$\begin{aligned}\Psi_{n+1} &= f(\Psi_n, g_n) \\ \Psi_{n+1} &= \frac{1}{\sin \theta_n} \left[\sin((1 - k_n)\theta_n) \Psi_n + \sin(k_n \theta_n) \frac{g_n}{\|g_n\|} \right] \\ \theta_n &= \cos^{-1} \left(\frac{(\Psi_n, g_n)}{\|\Psi_n\| \|g_n\|} \right)\end{aligned}\quad (22)$$

3.2 Constraint optimization

In the topology optimization problem, constraints have been defined in terms of the design variable, χ or ρ , and fixed to a certain value. Let $c(\rho)$ be a function such that:

$$c(\rho) = \int x d\Omega - V = 0 \quad (23)$$

Where x is the design variable and V is the volume of the domain. Therefore, the topology optimization problem can be written in terms of $c(x)$

$$\begin{aligned}\min \quad & J(x) \\ \text{over } & x \\ \text{s.t.} \quad & c(x) = 0\end{aligned}\quad (24)$$

3.3 Satelle-point Lagrangian

Let \mathcal{L} be a function such that:

$$\mathcal{L}(x, \lambda) = J(x) + \lambda c(x) \quad (25)$$

Where $c(x)$ is the constraint function and $J(x)$ is the energy deformation. \mathcal{L} is defined as the Lagrangian function. Therefore, the topology optimization problem can be defined as:

$$\max_{\lambda} \min_x \mathcal{L}(x, \lambda) \quad (26)$$

The dependence of the function in terms of the constraint is evaluated as a partial derivative of \mathcal{L} :

$$\frac{\partial \mathcal{L}}{\partial c} = \lambda \rightarrow \begin{cases} \lambda > 0 & \text{high dependence on } c \\ \lambda < 0 & \text{low dependence on } c \\ \lambda = 0 & \text{no dependence on } c \end{cases} \quad (27)$$

No dependence on the constraint c can be interpreted as an indicator of which constraint may be removed.

3.4 KKT

KKT problem is defined as follows:

$$\left. \begin{aligned} \frac{\partial \mathcal{L}}{\partial x} &= \frac{\partial J}{\partial x} + \lambda \frac{\partial c}{\partial x} = 0 \\ \frac{\partial \mathcal{L}}{\partial \lambda} &= c(x) = 0 \end{aligned} \right\} \rightarrow F(x, \lambda) = 0 \quad (28)$$

This function gives the stationary points of function \mathcal{L} in terms of x and λ .

3.5 Augmented Lagrangian

The Augmented Lagrangian is an extension of the Lagrangian function \mathcal{L} , which is defined as follows:

$$\mathcal{L}_u(x, \lambda) = J(x) + \lambda c(x) + \frac{1}{2}\mu c(x)^2 \quad (29)$$

And its gradient:

$$F_x = \frac{\partial \mathcal{L}}{\partial x} = \frac{\partial J}{\partial x} + \lambda \frac{\partial c}{\partial x} + \mu c(x) \frac{\partial c}{\partial x} = 0 \quad (30)$$

$$F_\lambda = \frac{\partial \mathcal{L}}{\partial \lambda} = c(x) = 0 \quad (31)$$

4 Session 5: Compliance gradient computation

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31/10/2017

4.1 Problem Definition

In order to solve a topological optimization problem the gradient of the cost function must be computed, performing this calculation in order to minimize the compliance (as an example), the following steps must be executed to find out which is the gradient of the function. Firstly, defining:

$$l(v) = \int_{\Gamma_N} t \cdot v$$

$$a(\rho, u, v) = \int_{\Omega} J' u : C(\rho) : \nabla^s u$$

In fact, the initial problem we have is the following:

$$\min l(u)$$

subject to

$$\left. \begin{array}{l} \int_{\Omega} \rho \leq V \\ a(\rho, u, v) = l(v) \end{array} \right\} \quad \forall v \in \gamma \quad \text{and} \quad \forall \rho \in \chi$$

Where,

$$\gamma = \{\phi \in H^1(\rho) : \phi|_{\Gamma_0} = 0\}$$

$$\chi = L^\infty(\Omega, \{0, 1\})$$

4.2 Differential definition

Performing the calculation of the differential of the cost function:

$$l(u(\rho + \tilde{\rho})) - l(u(\rho)) = l[u(\rho + \tilde{\rho}) - u(\rho)] =$$

$$l[D_\rho u(\rho) \tilde{\rho} + O(\rho^2)] = l[D_\rho u(\rho) \tilde{\rho}] + O(\rho^2)$$

Therefore,

$$Dl(\rho) \tilde{\rho} = l[D_\rho u(\rho) \tilde{\rho}] \tag{32}$$

Where D_ρ is the derivative respect to ρ .

4.3 Gradient Computation

Defining,

$$F(\rho) = a(\rho, u(\rho), v) - l(v) = 0 \quad \forall v, \forall \rho$$

Therefore, computing the differential:

$$\begin{aligned}
 \underbrace{F(\rho + \tilde{\rho})}_{=0} - \underbrace{F(\rho)}_{=0} &= a(\rho + \tilde{\rho}, u(\rho + \tilde{\rho}), v) - a(\rho, u(\rho), v) = \\
 a(\rho + \tilde{\rho}, u(\rho + \tilde{\rho}), v) - a(\rho + \tilde{\rho}, u(\rho), v) &+ a(\rho + \tilde{\rho}, u(\rho), v) - a(\rho, u(\rho), v) = \\
 a(\rho + \tilde{\rho}, Du(\rho)\tilde{\rho}, v) + D_\rho a(\rho, u(\rho), v)\tilde{\rho} + O(\tilde{\rho}^2) &= \\
 a(\rho, Du(\rho)\tilde{\rho}, v) + D_\rho a(\rho, u(\rho), v)\tilde{\rho} + O(\tilde{\rho}^2) &= 0
 \end{aligned}$$

Which lasts in

$$a(\rho, Du(\rho)\tilde{\rho}, v) = \boxed{-D_\rho a(\rho, u(\rho), v)\tilde{\rho}} + O(\tilde{\rho}^2) \quad \forall v \in \gamma, \forall \rho \in \mathbb{R} \quad (33)$$

Continuing with Equation 32:

$$\begin{aligned}
 l(u(\rho + \tilde{\rho})) - l(u(\rho)) &= l[D_\rho u(\rho)\tilde{\rho}] + O(\tilde{\rho}^2) = a(\rho, u(\rho), D_\rho u(\rho)\tilde{\rho}) + O(\tilde{\rho}^2) = \\
 a(\rho, D_\rho u(\rho)\tilde{\rho}, u(\rho)) + O(\tilde{\rho}^2) &= -D_\rho a(\rho, u(\rho)\tilde{\rho}, u(\rho)) + O(\tilde{\rho}^2) = \\
 -[a(\rho + \tilde{\rho}, u(\rho), v) - a(\rho, u(\rho), v)] + O(\tilde{\rho}^2) &= \\
 -\int_{\Omega} \nabla^s u : [C(\rho + \tilde{\rho}) - C(\rho)] : \nabla^s u + O(\tilde{\rho}^2) &= \\
 -\int_{\Omega} \nabla^s u : C'(\rho)\tilde{\rho} : \nabla^s u + O(\tilde{\rho}^2) &= \\
 = Dl(\rho)\tilde{\rho} + O(\rho^2) &
 \end{aligned}$$

Therefore,

$$Dl(\rho)\tilde{\rho} = \int_{\Omega} \underbrace{(\nabla^s u : C'(\rho) : \nabla^s u)}_g \tilde{\rho} = (g, \tilde{\rho})_{L^2}$$

Finally, the computed gradient is:

$$\boxed{g = \nabla^s u : C'(\rho) : \nabla^s u} \quad (34)$$

Where,

$$C(\rho) = 2\mu(\rho)I + [\kappa(\rho) - \mu(\rho)]I \otimes I$$