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ON MULTI-SCALE STRUCTURAL TOPOLOGY OPTIMIZATION AND MATERIAL DESIGN

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Abstract *Computational material design has gained considerable interest, along the last years, in the computational mechanics community. Although most of the current approaches focus on one-scale structural optimization, this work is settled in a multi-scale framework. In this sense, the goal consists of designing the micro-structure material and the macro-structure topology such that some cost function is minimized. In this case, the structural compliance is the considered cost function, so that the structural stiffness is maximized for a given weight.*

As a cost-reduction tool, an online-offline strategy, based on the off-line construction of a computational Vademecum, for the microstructural optimization problem, and the on-line resolution of the structural equilibrium, is introduced.

The topological derivative concept is used as a tool for designing the topology at both, the macro and micro, scales. A fixed-point method, based on an alternate-directions strategy, is used as numerical technique for resolution of the non-linear problem.

The presented numerical results show the availability of the proposed approach to computational material design and structural optimization in a high-performance framework.

1. INTRODUCTION

The computational mechanics community has recently showed a significant interest on macro-structure topology design, and many recent studies have been developed [1,3,6]. On the other hand, material design is still one of the cornerstones of the engineering oriented to industrial applications.
However, both fields have been often studied separately because of their complexity. Not long ago, some authors [5,7] have tried to solve them coupled through parallelism techniques but still only small meshes are able to be used.

Thanks to the computational homogenization approach, topology material design and macrostructure topology design could be thought as the same process in different levels, being the homogenized constitutive tensor of the first one used as the material property for the second one.
Both, material in the micro and the macro-structures will be defined by the characteristic functions χ and χ_μ . In this sense, the multi-scale problem will be solved by knowing the topology in both scales (χ, χ_μ) and the mechanical variables in such a way that they minimize some cost function.
For convexity issues, the equilibrium problem is preferred to be written in terms of the stresses (dual formulation) as in [1,6].
One of the most common and interesting industrial application is maximizing the structural stiffness (or compliance in dual formulation) such that its volume is below a certain value. Whereupon the formulation could be written as the following minimization problem:

$$\begin{aligned} \min_{\sigma,\chi_\mu,\chi} \quad & \int_\Omega \sigma : \mathbb{C}^h(\chi_\mu, \chi)^{-1} : \sigma \\ s.t. \quad & \nabla \cdot \sigma = 0 \\ & \int_\Omega \chi \leq V \\ & \int_{\Omega_\mu} \chi_\mu \leq V_\mu \end{aligned}$$

In this terms, the problem seems to be computational unaffordable, mainly because of the number of design variables and the non-linear relationship.
With this in mind, a computational Vademecum is introduced as a reduction model technique as done in [4].
Taking advantage of separability, the first idea is to solve offline the local micro-structure problem for each stress value.
This local problem is then written as:

$$\begin{aligned} \min_{\chi_\mu} \quad & \sigma : \mathbb{C}^h(\chi_\mu)^{-1} : \sigma \\ s.t. \quad & \int_{\Omega_\mu} \chi_\mu \leq V_{\mu,} \end{aligned}$$

where the micro-structure topology is solved through the topology derivative tool using a level-set algorithm, as done in [2,3].
Some modifications on Amstutz algorithm has been done in order to improve its robustness. Fundamentally, the selection of a new value of the step in the line search process is set using a discretization of the interval where it lives and selecting the one that has better (less) objective

function value independently if it is bigger than the last iteration. Thus, no remeshing is needed. In addition, a mixed augmented Lagrangian is scheme is used in order to fulfill the constraint with a low computational cost.
The modulus of the stress is not playing any role in the minimization problem because the solution of the design variable is not dependent on the intensity of the objective function.
In this manner, the problem can be studied only with unitary stresses (unity ball) which can be parametrized by two (spherical) coordinates (θ y φ). So for each value of V_μ, θ y φ a micro-structure topology and its homogenized constitutive tensor $\mathcal{C}^h$ is computed.
That process must be computed once forever, so it has been decided to do it accurately, solving around two thousands micro-structural optimization problems. Using symmetries and some periodicities it has been obtain at the end around eight thousands optimal micro-structures for a specific value of V_μ. In the numerical results a few of them has been shown.

For a given macro-structure a fix point iteration scheme is used in order to find the best micro-structure for its Gauss point. In fact, the algorithm is first solving for a fixed micro-structure distribution an equilibrium iteration and then for each Gauss point is selecting the optimal micro-structure from the Vademecum, depending on its stress value until convergence.

On the other hand, the macrostructure topology is changing on the same terms as the micro-structure optimization problem, i.e, a topology derivative using a level set approach with a mixed augmented Lagrangian formulation.

Thus, the global algorithm could be thought as an alternate direction as in [1]. Fixed macro, alternating equilibrium and stresses until convergence, then an iteration of the macro, and a new internal loop of stresses and micro-structure topologies, and this until global convergence.

Finally, the goal of this theory is to see, for a fixed micro and macro fixed fraction volume, the improvement of the stiffness of the structure selecting optimal micro-structure instead of taking a fixed one. These differences are also illustrated in the numerical results.

2. NUMERICAL RESULTS

- Computational Vademecum

All the micro-structures computed in the Vademecum, and then used in the macro-structure, have the same elastic material properties, i.e. a Young modulus $E_\mu = 1$ and a Poisson's ratio $\nu_\mu = 0.3$. In addition, all of them have the specified volume value $V_\mu = 0.6$.

Some of them are shown in the Fig. 5. More information on initial values of the level-set and other parameters are detailed in [3].

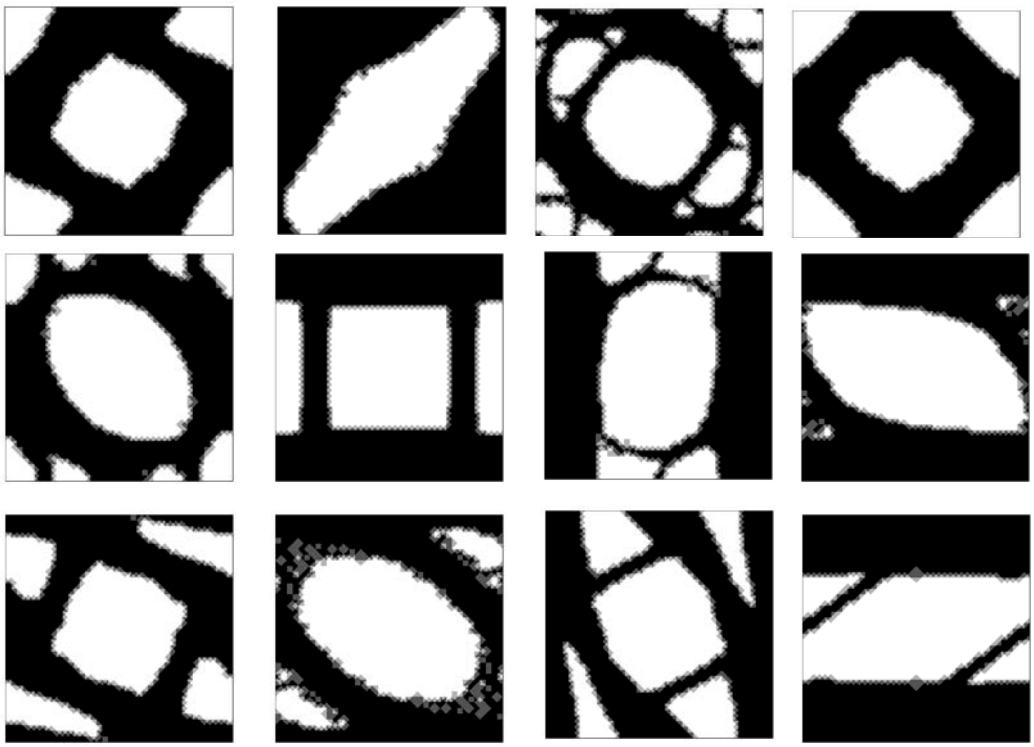

Fig.5 Different optimized micro-structures topologies of the Vademecum with fraction volume $V_\mu = 0.6$

- Macro-structure and material design

The theoretical development and its algorithm has been tested with the widely used cantilever problem [1,3,5,6]. The domain is of the size 2 x 1 box, with homogenous Dirichlet conditions in the left hand side and a vertical, pointwise, unitary force on the center of the right hand side as shown in the Fig .1. More details of the level-set initialization parameters could be found in [3].

Fig.1 Cantilever beam boundary conditions

An 8000 triangular elements mesh, at the upper half of the domain due to its symmetry, has been used for the whole optimization process (no remeshing needed).

Fig. 2 shows some macroscopic topologies in different stages revealing how the algorithm tries to decrease the compliance and satisfy the volume constraint at the same time.

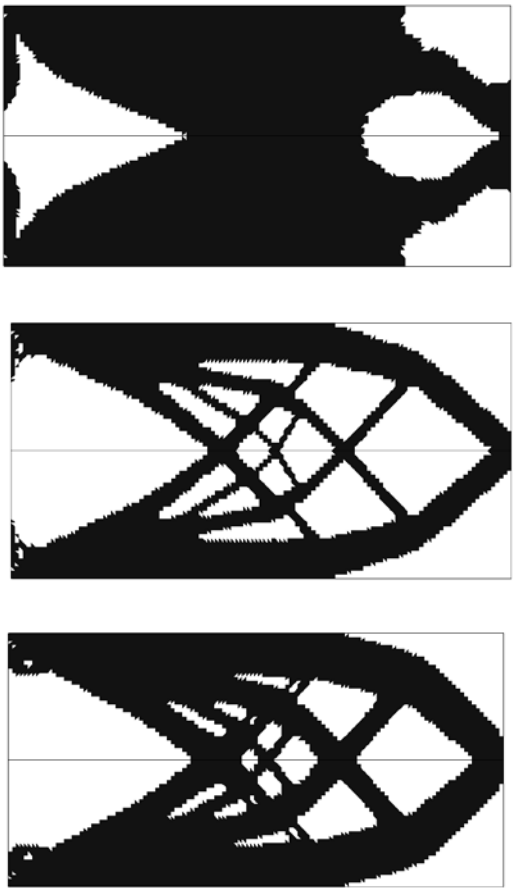

Fig.2 Iteration 3, 38 and 181 of the macroscopic topology

Moreover, the evolution of the objective function $J(\chi_\mu, \chi, \sigma)$ (compliance) and the macroscopic volume $|\Omega|$ is shown in Fig 3. Their behavior is similar highlighting its strong dependency.

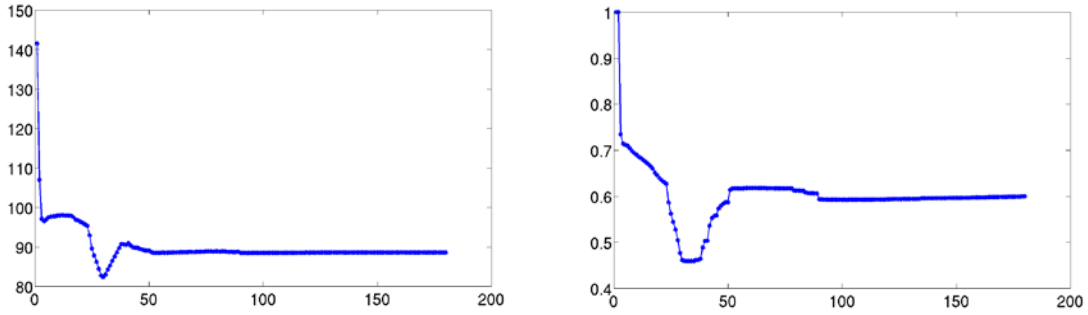

Fig.3 Compliance and volume iterations of the macro-structure

The variation of the microstructures has been decided to show in Fig 4 through its C_{11}^h field. For a better understanding, some representative micro-structures are also represented.

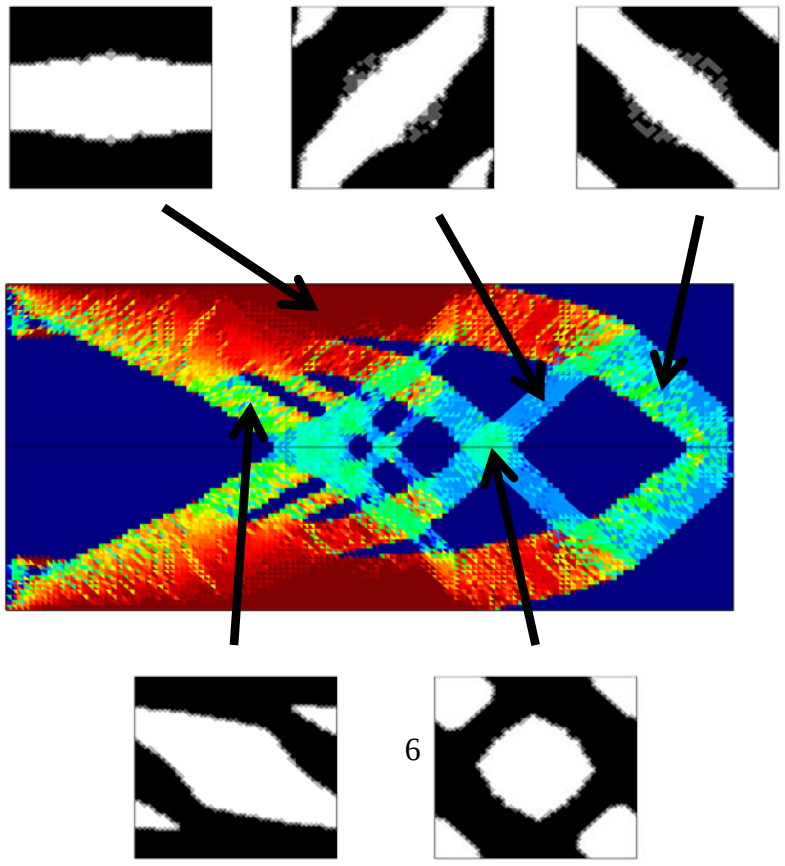

Fig.4 C_{11}^h distribution and some optimized micro-structure topologies

The algorithm has been initiated with full material ($\chi(\mathrm{x})=1 \ \forall \mathrm{x}$) on the macroscopic domain and a prefixed micro-structure topology shown in Fig 5. The radius of the circle is such that the prescribed $V_\mu = 0.6$ is fulfilled.

Fig.5 Initial microstructure with a fraction volume $V_\mu = 0.6$

A fixed micro-structure topology (circle) on the macro-structure has been also computed, in order to measure the improvement of using different optimal micro-structures. Compliance and volume are illustrated in Fig. 6.

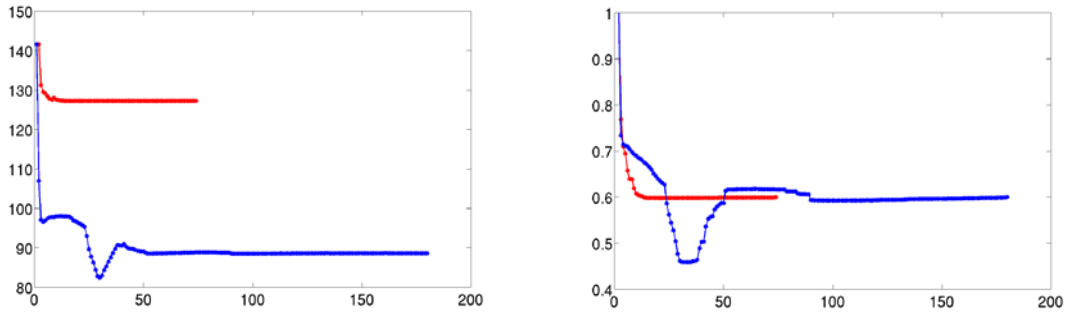

Fig.6 Compliance and volume iterations of the macro-structure

A considerable gain (around 30%) in the objective function has reached strengthening the importance of the idea of designing the optimal micro-structure material and selecting it properly.

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