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ADDRESSING THE NON-LINEARITY AND SINGULARITY PHENOMENA OF STRESS-BASED OPTIMAL DESIGN OF MATERIAL MICROSTRUCTURES

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Abstract. Material design is an active research field since composites have met increasingly interest, for instance, in lightweight construction as it happens in aerospace industry. One assumes in the present work a given macroscopic stress or strain field (one that may occur at a certain point of a macro-structure) and computes through homogenization the micro-stress distribution across the two (weaker and stronger) composite constituents mixed in a unit-cell domain which is representative of a periodic heterogeneous material. Stress gradients depend a lot of design details but typically the stress field is highly non-linear. In the frame of finite element models for material microstructures one pursues here an investigation about mesh convergence. Since stress distribution is strongly design dependent, that motivates one to pursue optimal design of the material microstructure to comply with admissible stress criteria. The inverse homogenization method using density-based topology optimization is applied here for such purpose. This is quite a challenge not only because of the aforementioned non-linearity of the stress field but also due to the singularity phenomena which one overcomes using standard relaxation techniques. Some preliminary results are obtained in order to get some insight into the fine structure of composite materials and the influence of the stresses therein.

1 INTRODUCTION

Material design is an active research field since composites have met increasingly interest, for instance, in lightweight construction as it happens in aerospace industry [1,2]. Fully understanding the overall response of a composite demands greater insight about its microstructure behaviour. Micro-mechanical models detailing the geometry and the interfaces of base constituents of a composite allow fine measure and control of local stresses [3-6]. Homogenization models are often used to transfer data among different design scales. Multiscale analysis coupling macro, meso and micro scales can then be done [7].

For simplicity one assumes in the present work a given macroscopic stress or strain field (one that may occur at a certain point of a macro-structure) and computes through homogenization the micro-stress distribution across the two (weaker and stronger) composite constituents mixed in a unit-cell domain Y, i.e., the representative volume element (RVE) of the material heterogeneous medium Ω.

Stress gradients depend a lot of design details but typically the stress field is highly non-linear. In the frame of finite element models for material microstructures one pursues here an investigation about mesh dependence. By means of ever-increasing mesh refinements and shape functions order one evaluates convergence of micro-stress measures and concludes about mesh quality. Besides investigating the quality of numerical approximation to the stress field, one might also address the quality of the homogenization stress predictions comparing them to the actual composite by repeating an unit-cell a limited number of times and subjecting the resulting numerical model to a battery of load tests for stress assessment. The outcome of this later study is in [8,9] which indicates that it is sufficient to have a few repetitions of unit-cells to replace the non-homogeneous composite Ω by the equivalent homogeneous material with the stress field computed by homogenization.

Since stress distribution is strongly design dependent, that motivates one to pursue optimal design of the material microstructure to comply with admissible stress criteria. Stresses may be either minimized as the objective function or limited by an upper bound in the constraint function. The inverse homogenization method using density-based topology optimization is applied here for such purpose. This is quite a challenge not only because of the aforementioned non-linearity of the stress field but also due to the singularity phenomena which means that stresses tend to finite values as density design variables tend to zero due to degenerated regions of the feasible design domain. To overcome the singularity problem one may use the so-called relaxation approaches, such as the ε-relaxation or *qp*-approach [10,11], which have been applied to the optimal design of structures with success. Bearing this in mind one extends the application of these relaxation techniques to material design in order to obtain some preliminary results and get some insight into the fine structure of composite materials and the influence of the stresses therein.

2 MATERIAL MODEL

The material model considered in the present work is shown in Fig. 1. Assuming solid and void phases mixed one gets a cellular material generated through the repetition of a unit-cell which represents the smallest periodic heterogeneity of the heterogeneous medium Ω. The elastic properties of such medium are computed through homogenization assuming periodic boundary conditions and infinite periodicity of the unit-cell [5]. For optimal material design purposes one discretizes the unit-cell domain Y in a regular (square-grid) mesh of 20×20 8-node isoparametric hexahedral finite elements. Although three-dimensional elements are used here the focus is on designing optimal 2-D layouts forcing design uniformity in the normal direction. This already easies the natural extension of the problem to 3-D material microstructure designs coming as future work. One assigns a density design variable per each finite element assuming it uniform therein. Solid and void phases correspond to density equal to 1 and 0, respectively. Topology optimization can then be used to search for an unit-cell lay-out improving a measure of structural performance and complying at the same time with specific design requirements. This design method is also known as inverse homogenization and it was originally introduced by Sigmund [12].

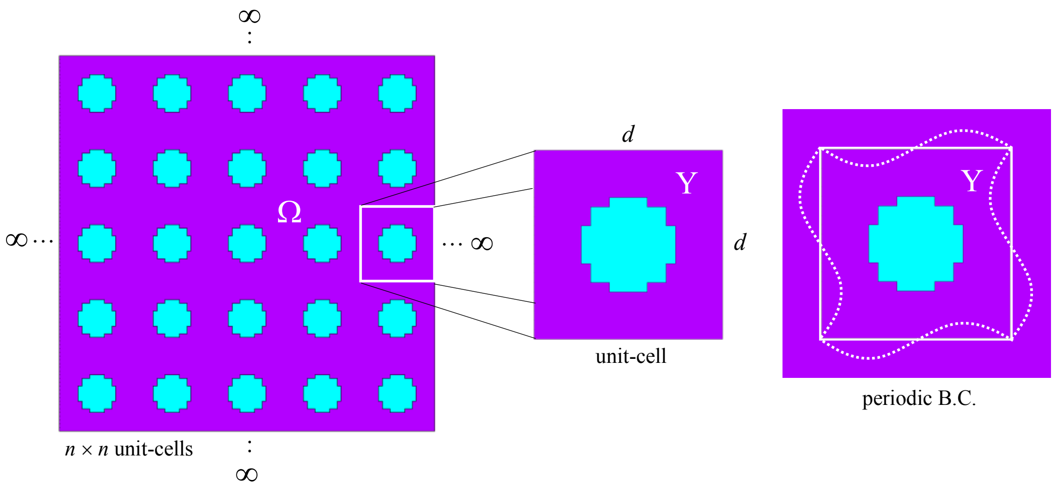


Figure 1: Material model of composite material with periodic unit-cell (array of $n \times n$ unit-cells in domain Ω of size D, in theory $n \to \infty$). Portray of periodic boundary conditions applied to the unit-cell domain Y of size d.

3 OPTIMIZATION PROBLEM FORMULATION

For the sake of demonstration purposes one selects the conventional formulation seen in topology optimization where stiffness is maximized (compliance is minimized) subjected to a volume fraction constraint [13]. While some results are revisited in the present work, using this very well-known formulation, additional results are presented too as an extension of the conventional compliance problem to include stress constraints in order to get not only stiff but also strength oriented optimal designs. In fact, engineering practice demands feasible designs on stresses too. The impact of stress criteria on the final design can be perceived later on as one plots the stress field for the stiff oriented design only where the peak stresses are higher and may exceed an admissible stress threshold.

Eq. (1) shows the optimization problem formulation where the total strain energy is maximized on density based design variables ρ ($\tilde{\rho}$ is a filtered density as explained afterwards) subjected to a volume fraction constraint $V/V^* \leq 1$ and as many stress constraints as the number of design variables in the problem, n. This way one achieves "pointwise" control over stresses in the full unit-cell domain Y although the problem can rapidly become computationally expensive or even prohibitive. There are aggregation techniques applied to stress constraints that allow reducing their number in the problem [13]. However, by doing that one lacks local control over stresses jeopardizing the admissible stress requirement. Rather than saving computational effort one meets here the worst case scenario of handling huge number of constraints leaving the matter of getting cheaper computations for future work.

$$\begin{aligned}
&\max_{\boldsymbol{\rho}} \frac{1}{2}\int_Y \mathbf{E}^{\mathrm{H}}(\tilde{\boldsymbol{\rho}})\bar{\boldsymbol{\varepsilon}}\bar{\boldsymbol{\varepsilon}}\,\mathrm{d}Y \\
&\text{s.t.}: \\
&\frac{V(\tilde{\boldsymbol{\rho}})}{V^*} \le 1 \\
&\frac{\sigma_{\mathrm{VM}}^{e}(\tilde{\boldsymbol{\rho}})}{\tilde{\rho}_e^q \sigma^*} \le 1\,, e = 1,\ldots,n \\
&0 < \rho_e \le 1\,, e = 1,\ldots,n
\end{aligned} \tag{1}$$

One assumes a solid, isotropic and ductile behavior for the base material used to fabricate the composite. Thus, in terms of the material failure criteria, the stress constraints in Eq. (1) relate the Von-Mises stress with the admissible stress value. This equivalent stress measure depends on the micro-stresses σ_{ij} (at the level of the material microstructure) which are obtained from asymptotic homogenization theory, by considering the displacement test fields χ_k^{rs} as already done in a previous work [6], see Eq. (2).

$$\sigma_{ij} = E_{ijkm}\left(\delta_{kr}\delta_{ms} - \frac{\partial \chi_k^{rs}}{\partial y_m}\right)\varepsilon_{rs}^0 \tag{2}$$

In Eq. (2), ε_{rs}^0 is a given macroscopic (average) strain field. The tensor σ_{ij} represent the stress state varying throughout the unit-cell domain Y. Here, the methodology used for obtaining such stresses is based on the software POSTMAT [5,6].

The density term $\tilde{\rho}^q$ introduces the *qp*-approach [11] as a relaxation technique to deal with the well-known singularity phenomena in stress-based optimization problems [13]. Exponent q is lower that p in order to relax the constraint and in turn exponent p figures in the SIMP (Solid Isotropic Model with Penalization) model used to interpolate between density and the base material stiffness E^0, i.e., $E=\rho^p E^0$ [14]. The following values are used in the present study, $q = 2.5$ and $p = 3$. In turn, the homogenized stiffness tensor $\mathbf{E}^{\mathrm{H}}$ is computed through the homogenization formulas that can be seen in [5,6].

In problem (1) is used a density filter according to [15,16] to avoid checkerboard problems as well as to smooth enough the density and stress fields such that stress singularities are not prone to occur inside the unit-cell domain while its lay-out changes along the iterations of the optimization process. This filter is given by Eq. (3) where ω is a weighting factor based on a given filter radius $R_{\min}$ and the distance between centers of elements i and e.

Gradient-based algorithms, such as MMA [17], are used to solve problem (1) and thus sensitivities of constraints and objective functions are required. Deriving analytical sensitivities is quite straightforward as regards compliance and volume functions [13]. Getting this data for stresses is a non-trivial calculus which is beyond the preliminary study presented here. Therefore, as regards stress sensitivity one relays here on the finite difference method that proves to be accurate enough as shown later on. Since one uses here a density filter bear in mind that one has to apply accordingly the chain rule while computing sensitivities, see for details [16].

$$\tilde{\rho}_e = \frac{\sum_{i \in N_e} \omega(x_i)\rho_i}{\sum_{i \in N_e} \omega(x_i)}, \quad \omega(x_i) = \max\{0, R_{\min} - \|x_i - x_e\|\} \tag{3}$$

4 MESH CONVERGENCE ANALYSIS

Engineers and scientists use finite element analysis to build predictive computational models of real-world scenarios. The accuracy that can be obtained from a finite element model is directly related to the finite element mesh that is used. As the finite elements are made smaller and smaller, as the mesh is refined, the computed solution will approach the true solution. While the same problem is resolved with successively finer and finer meshes one may compare the results between the different meshes. This comparison can be done by analyzing the fields at one or more points in the model or by evaluating the integral of a field over the domain. This leads one to choose an appropriate mesh refinement metric, which can be either local or global.

In the present study one focus on the stress field which can be quite non-linear over the physical domain of the unit-cell and thus the distribution of stress or its peak may easily become mesh dependent. Therefore, here one evaluates how good a stress approximation is by reducing the element size of the mesh successively (h-refinement method), dividing in the present study each existing element into four elements (two per edge) without changing the type and shape of the elements (only the size changes). To compare the quality of the different meshes obtained one uses the total Strain Energy S, as a global metric, and the Von-Mises stress, as a local metric, evaluated at some predefined nodal points or simply one selects the maximum value in the domain. This convergence analysis is specially relevant as one eventually optimizes the topology of a material microstructure for a given strength criteria and that must relay on a regular grid of FE (see e.g. Fig. 2a) accurate enough to provide reliable stress values which must be kept under an admissible value.

To proceed with the mesh convergence analysis one selects a lay-out simple enough to practice the mesh refinement without compromising any geometric descriptions avoiding that way the "modeling error" and bringing forth as desired the "discretization error" only. Fig. 2b shows such a lay-out where a centered square hole is placed in the unit-cell domain Y matching a volume fraction of 75%. On the top of this lay-out one fits easily regular (square) grid meshes as 8×8, 16×16, 32×32, 64×64 and 128×128. All these meshes preserve the design boundary or contour which is quite reassuring for the success of the proposed mesh convergence study. However, this coincidence is very difficult to achieve in practice when optimizing topology on the top of square grid meshes which often gives mesh dependent lay-outs. This motivates further mesh convergence analyses beyond the scope of the present study once some feedback is provided by the topology optimization design solution.

The properties of the base material selected are E = 290MPa and ν = 0.3. The void region (hole) has a very small stiffness value to prevent any singular matrixes in the FE model. For each mesh one uses either 8-node or 20-node isoparametric hexahedral finite elements. The material microstructure is subjected to a macroscopic in-plane hydrostatic stress field, i.e., $\sigma_1 = \sigma_2$ = 1MPa. Fig. 2c shows specific node locations, not mesh dependent, where Von-Mises stress values are collected for comparison purposes.

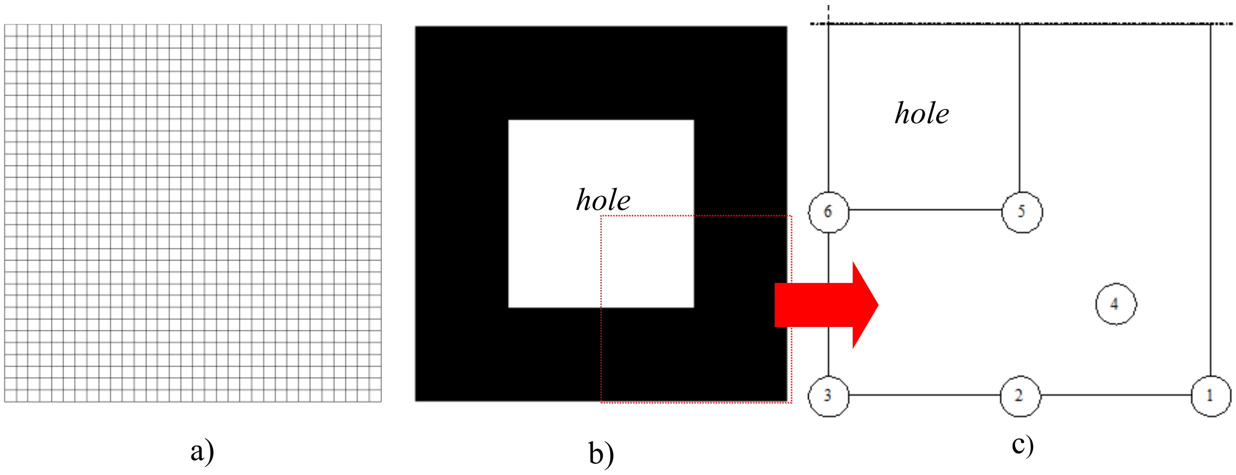


Figure 2: Numerical model for mesh convergence analysis; a) Example of square grid meshes considered (case 32×32 is displayed); b) Lay-out considered: unit-cell with square hole and 75% of volume fraction; c) Location of nodes where Von-Mises stresses are measured (a quarter of the unit-cell is shown).

Fig. 3 plots the element solution of the Von-Mises stress. The element solution is the volume average of the Von-Mises stresses measured at the element gauss points, 2×2×2 and 3×3×3 gauss points for 8-node and 20-node hexahedral elements, respectively.

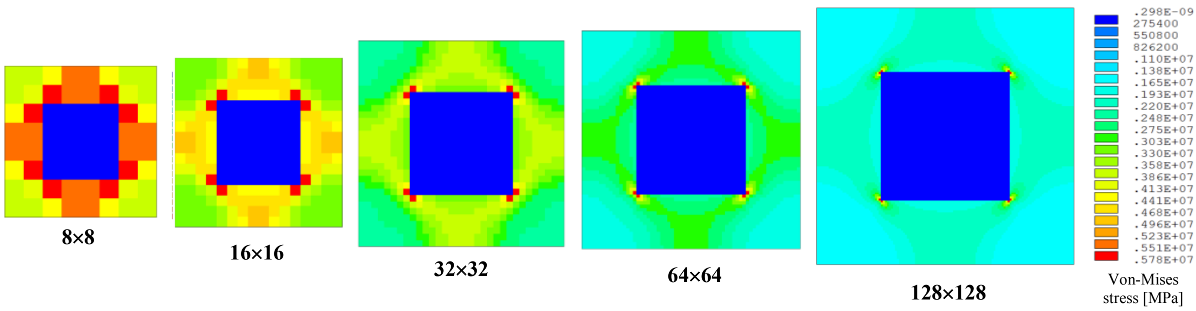
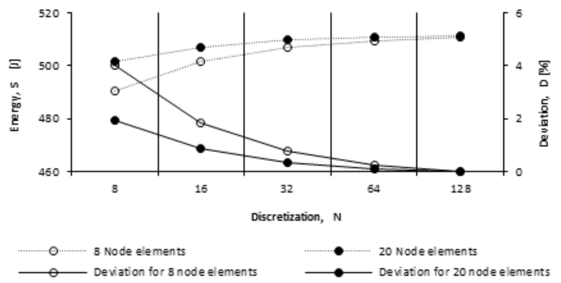
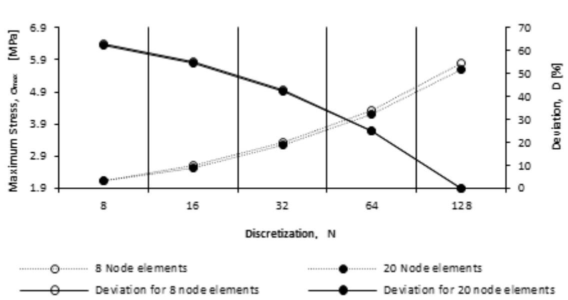


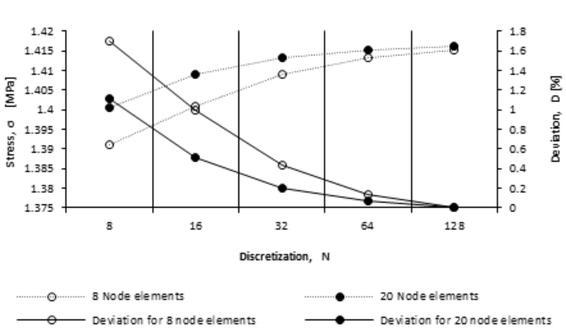
Figure 3: Von-Mises stress plots for meshes of N×N FE with N increasing from 8 to 128. The images get bigger just for the sake of enlarging finer meshes, bear in mind that the unit-cell size is always unitary |Y|=1. Stress scale on the right refers to 128×128 results.



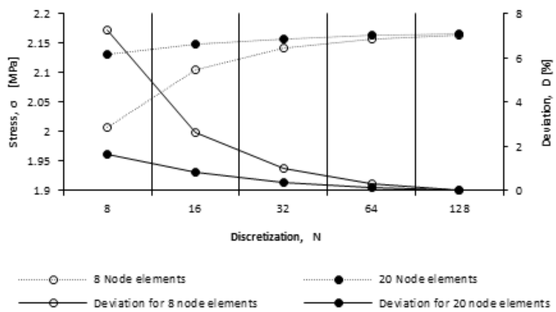
a) Strain Energy



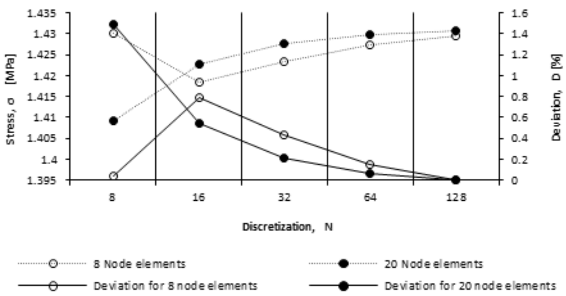
b) Maximum Von-Mises Stress (element solution)



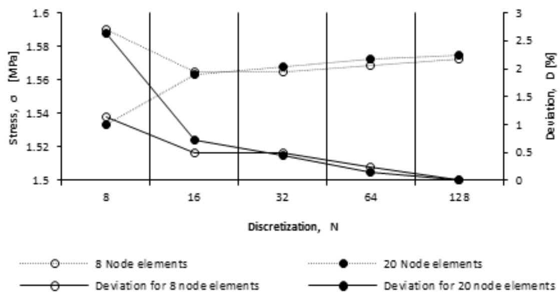
c) Nodal stress at **point 1**



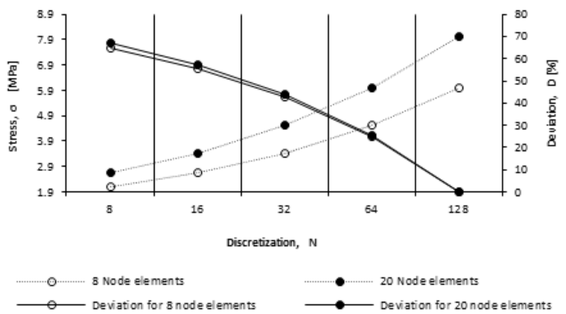
d) Nodal stress at **point 2**



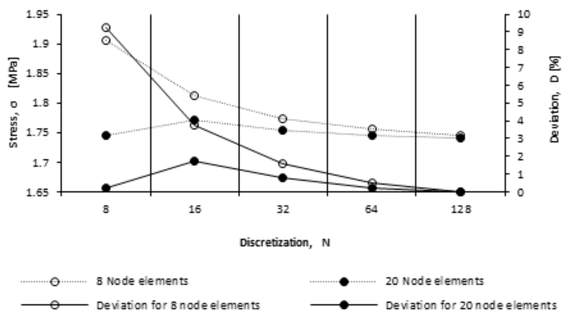
e) Nodal stress at **point 3**



f) Nodal stress at **point 4**



g) Nodal stress at **point 5**



h) Nodal stress at **point 6**

Figure 4: Plots of mesh refinement metrics. Global metric is Strain Energy (*S*). Local metrics are maximum Von-Mises Stress (σ_{max}) measured in the element and nodal Von-Mises stresses measured at specific locations according to Fig. 2c). Respective deviations in [%] having the finest mesh refinement as the reference.

Fig. 4 shows a set of charts providing the results for the different metrics used as the mesh is refined. The nodal values plotted should be interpreted with the help of Fig. 2c. Monotonic convergence of the strain energy is obtained as expected from a FE solution (see Fig. 4a).

Analyzing the plotted contours in Fig. 3 one easily perceives a red spot associated to a singularity which could be actually anticipated due to the sharp corner of the hole (see Fig. 4b and 4g). The maximum stress that is actually measured at this corner is non-convergent as the mesh gets finer and finer (theoretically tends to infinite). An experienced analyst may determine that such a red spot (singularity) can be safely ignored once in the real world there are seldom perfectly sharp corners (fillets instead). Thus such high peak stress tend actually to obscure more interesting features in the FE solution (see plots for the remaining nodal points selected: 1,2,3,4 and 6). Anyway, one anticipates here that the singularity existence may become a critical issue when running a stress-based optimization problem where the overall stress level should be kept to a maximum, i.e. under an allowable stress value. A singularity in such optimization problem formulation will lead to solutions that are only optimal in terms of reducing the amplitude of the unphysical peak stress. The procedure of identifying and excluding regions of singularities from the search for a maximum stress will lead to an optimization problem not well posed either. It is preferable that by no means a singularity comes to the fore during the form finding process executed by the optimization algorithm. This motivates further research concerning "red spots" influence while designing material microstructure via topology optimization. As mentioned in the previous section, the use of density filters may play an important role in that regard.

Apart from the singularity noticed, mesh convergence is clearly recognized taking the results obtained with the finest mesh, 128×128, as reference to plot the deviation in %. This also helps to see how rapidly the metrics used converge. Typically, convergent curves show deviations less than 1% above 32×32 meshes which is quite low and results are even better for 20-node brick elements in the mesh.

5 STRESS-BASED OPTIMAL DESIGN

Strength oriented design of material microstructures is the ultimate goal here. To better compare how stress constraints change an optimal design, one solves first the problem (1) simplified, i.e. minimizing compliance subjected to the volume constraint alone. The outcome is a design initially oriented to meet stiffness criteria only.

In the strain formulation used in problem (1) one chooses the macroscopic strain field $\bar{\boldsymbol{\varepsilon}}$ where the longitudinal strains in plane x_1x_2 are equal (hydrostatic case), i.e. $(\bar{\varepsilon}_{11},\bar{\varepsilon}_{22},\bar{\varepsilon}_{33},\bar{\varepsilon}_{12},\bar{\varepsilon}_{13},\bar{\varepsilon}_{23})=(0.2414,0.2414,-0.2069,0,0,0)\times 10^{-2}$. In the volume fraction constraint one selects an upper bound of V*=0.8 (80% of solid phase). The base material properties are E = 290MPa and ν = 0.3. The Method of Moving Asymptotes [17] is chosen as the optimizer to update the density design variables. Although the previous mesh convergence study may provide an indication about what a good mesh is to perform optimization with stress criteria, one decides here to simply come up with some preliminary optimized designs regardless the quality of the mesh. Problem formulation in (1) deals with a rapidly increasing number of constraints as the mesh gets finer and finer. Therefore, for the sake of demonstration purposes only, here one chooses a reasonable number of constraints, 400 = 20×20 mesh, see Fig. 5a. This allow one to get some initial insight about stress criteria influence on the design without getting a too expensive problem to solve. As a future work, finer meshes are recommended for use as well as techniques to reduce the computational cost.

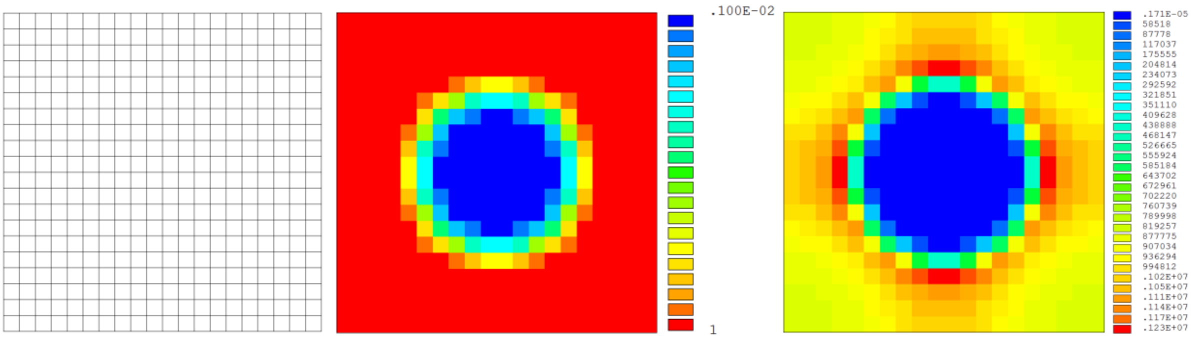


Figure 5: Topology optimization without stress constraints; a) Finite element mesh used 20×20, b) Optimal density distribution, $\rho_{\min}$, c) Equivalent (Von-Mises) stress field, $\sigma_{VM}^{max} = 1.23MPa$.

Fig. 5b shows the stiffness-oriented optimal design solution, basically a square with a round hole, and Fig. 5c displays the respective equivalent stress distribution where higher stresses are concentrated in the boundary of the hole. Supposing now that the maximum stress value found of 1.23MPa is actually exceeding the admissible stress in 23% i.e., σ_{adm} = 1MPa, one adds a "battery" of constraints as in Eq. (1) to ensure that no point in the design domain violates such stress limit. Imposing the stress constraints, the outcome is a strength-oriented optimal design solution as can be seen in Fig. 6. The history of optimization is shown in terms of the density and stress changes along the algorithm iterations. The regions in "blue" identify density or stress close to zero while "red" regions correspond to full density (=1) or maximum stress (=σ_{adm}). Intermediate colors represent intermediate density and stress values interpreted the same way as in Fig. 5b and 5c. The initial design has two square regions of uniform density such that a material volume fraction of 80% is attained. Furthermore, this design is feasible too regarding stresses as one can easily inspect visually for no red spot is found in the initial stress distribution shown in Fig.6 (left side).

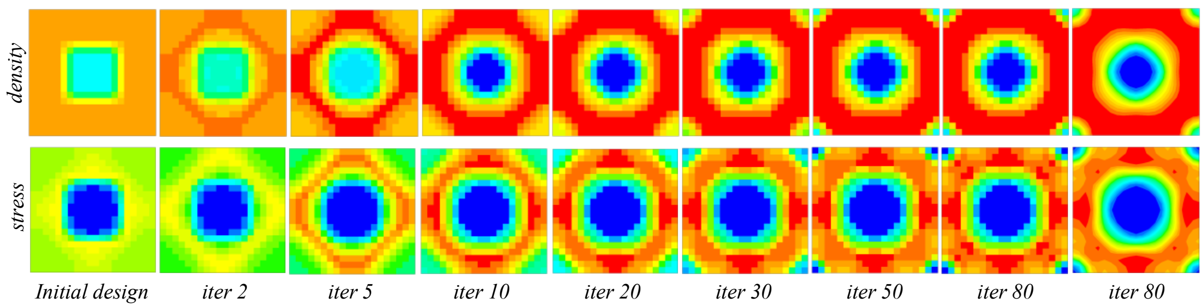
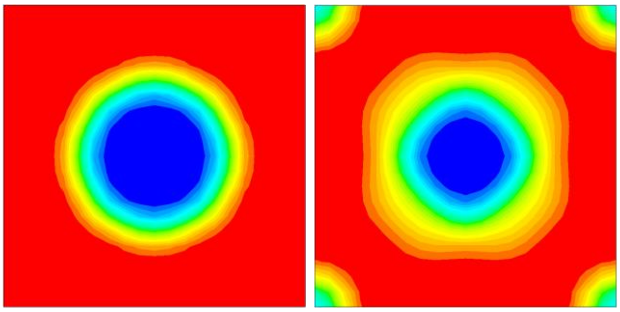


Figure 6: Topology optimization with stress constraints. Changes on the density and stress fields along the algorithm iterations are displayed. Last iteration is repeated here twice to show at last how both fields are smoothed when an image processing technique based on averaging is applied.

Finally, the stiffness and strength oriented optimal designs are compared side by side in Fig. 7. Here one clearly sees the effect of stress constraints on rounding the sharp corners of the initial design of the unit-cell. At these corners, where the stress level is lower, the density is reduced and the region where the hole is located gets more undefined as the gray zone enlarges. This demands for further investigation as regards the size of the mesh used as well as the filter used. Although the optimal microstructure in Fig. 7b is not that much defined as regards its boundary, one has here a preliminary result of stresses constrained (feasible design) which is actually obtained at the expense of getting lower level of stiffness in the objective function value in comparison to Fig. 7a (12% less).



a) b)

Figure 7: Comparison between the non-based and based stress optimization problem; a) without stress constraints; b) with stress constraints.

6 CONCLUSIONS

In this paper periodic composite materials mixing solid and void phases are considered. Homogenization is used to compute equivalent elastic properties as well as to estimate stresses at a local level, i.e. in the unit-cell domain. A mesh convergence analysis is conducted to conclude that metrics such as strain energy and pointwise stresses converge rapidly enough. However, results are shown for a very simple geometry that is a square unit-cell with a square hole which proves to be very convenient because one preserves geometry as the mesh is refined spotting that way discretization errors only. More complex designs should also be taken into account as future work to see also if density filters can smooth the stress field enough to prevent singularities from occurring during the optimization process. Mesh convergence studies in the future should also allow one to conclude what is the best mesh to be used in subsequent microstructure optimization. The optimization process can be quite demanding of computational resources due to the huge number of stress constraints one may face. In order to have a lighter computational load here one used a coarser mesh which motivates further studies with finer meshes. Anyway, results are shown for an optimal design complying with stress requirements considering an in-plane hydrostatic loading case. The unit-cell design differences obtained between stiffness and strength oriented design problems are highlighted. Further developments should include other loading conditions too.

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