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► **To cite this version:**

A. Ferrer, P. Geoffroy-Donders, Grégoire Allaire. Stress minimization for lattice structures. Part I: Micro-structure design. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, 2021, 379 (2201), pp.20200109. 10.1098/rsta.2020.0109 . hal-02889138v2

**HAL Id: hal-02889138**

**<https://hal.science/hal-02889138v2>**

Submitted on 12 Nov 2020

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# Stress minimization for lattice structures. Part I: Micro-structure design

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November 12, 2020

## Abstract

Lattice structures are periodic porous bodies which are becoming popular since they are a good compromise between rigidity and weight and can be built by additive manufacturing techniques. Their optimization has recently attracted some attention, based on the homogenization method, mostly for compliance minimization. The goal of our two-parts work is to extend lattice optimization to stress minimization problems in 2-d. The present first part is devoted to the choice of a parametrized periodicity cell that will be used for structural optimization in the second part of our work. In order to avoid stress concentration, we propose a square cell micro-structure with a super-ellipsoidal hole instead of the standard rectangular hole often used for compliance minimization. This type of cell is parametrized in 2-d by one orientation angle, two semi-axis and a corner smoothing parameter. We first analyse their influence on the stress amplification factor by performing some numerical experiments. Second, we compute the optimal corner smoothing parameter for each possible micro-structure and macroscopic stress. Then, we average (with specific weights) the optimal smoothing exponent with respect to the macroscopic stress. Finally, to validate the results, we compare our optimal super-ellipsoidal hole with the Vigdergauz micro-structure which is known to be optimal for stress minimization in some special cases.

## 1 Introduction

Limiting the maximum stress value that could appear in a structural domain is a crucial issue in mechanical engineering. Indeed many undesired effects, like damage, plasticity and fracture, may appear if the maximum stress exceeds a certain threshold value. For this reason it is very important that the design of structures takes into account the control of some measure or norm of the stress field. Typically, an optimal design process takes into account some stress constraint or directly minimizes the point-wise maximum stress or some approximating averaged norm. It turns out that this problem is extremely hard to solve.

Many different approaches have been developed to solve it. Based on the SIMP method (Solid Isotropic Material with Penalization), the early work [1] proposed a relaxation of the stress constraint for avoiding the singularity problem. However the stress constraints were considered point-wise which makes the problem intractable as the mesh size increases. To deal with this aspect, in [2], the point-wise constraint was substituted by a finite  $L^p$ -norm ( $p = 4$  in the examples). A comprehensive review of the topic and a SIMP-based interpolation for dealing with the singularity problem is presented in [3]. More recently, compliant mechanisms were optimized in [4] for stress constraints with a finite  $L^p$ -norm ( $p = 12$ ). Typically, in the SIMP approach for stress minimization, two different material interpolations are used: one for the constitutive tensor (usually the elasticity tensor is proportional to  $\rho^p$  where  $\rho$  is the material density) and another one for the stress evaluation. The first interpolation is known, in some cases, to correspond to real microstructures. However, the second interpolation

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(for the stress) cannot be interpreted in terms of homogenized stresses for the previous, or any other, micro-structures.

An alternative to the use of SIMP and intermediate densities is the level-set method. This was demonstrated in [5] where a  $L^p$ -norm ( $p = 10$ ) of the stress was minimized for 2-d and 3-d examples. Instead of using the classical shape derivative, the authors of [6] proposed a variant of the level-set algorithm based on the notion of topological derivative. In [7], the authors also used a level-set algorithm for multiple load cases and proposed different stress criteria in different regions of the structure. Of course, other approaches are also possible like combining the Non-Uniform Rational Basis Spline (NURBS) hyper-surfaces framework with the SIMP method, as in [8], [9], [10], which are devoted to the design of periodic microstructures.

In any case, these previous works, either with the SIMP or the level-set approach, were focusing on macroscopic structures. They did not consider domains with fine details or, more precisely, in such cases they would require significantly fine meshes. Consequently, for computational cost reasons these methods cannot be applied to the so-called lattice materials which are finely graded structures with a porous microstructure. Lattice materials recently appear as a serious alternative to more classical materials since they can be built thanks to the most advanced additive manufacturing technologies. The goal of the present work is to propose an homogenization method for stress minimization applied to these lattice structures. Homogenization is known to be a convenient theory to describe averaged of effective behaviour of graded structures or composite materials and has been successfully used in topology optimization since many years (see the textbook [11] for a brief history of this method). The homogenization method has already been applied for some stress optimization problems. For example, [12] maximized the torsional rigidity of functional graded composite materials made by a matrix with fibres inclusions, [13] extended the previous theory by additionally solving its corresponding inverse homogenization problem and [14] used composites (rank- $n$  laminates) for minimizing the stress norm. A key point in these contributions is that homogenization theory does not only define averaged or effective properties for the elastic properties but also introduce the concept of corrector terms for approaching the true stress and strain tensors in an heterogeneous medium, beyond the simple homogenized or averaged stress or strain tensor. In particular, it yields the notion of amplification stress factors, or amplifiers, which corrects the averaged macroscopic stress in order to have a reliable evaluation of the local microscopic stress concentration. Indeed, it is well known that microscopic heterogeneities may cause stress concentrations. Thus, in contrast with interpolation approaches like the SIMP method, [14] proposed a mechanically sound evaluation of microscopic stress effects. However, the stress norm used was not very large ( $L^p$  with  $p = 2$ ) and the final shapes are intrinsically multi-scale (use of rank- $n$  laminates) and thus hard to manufacture. Actually these previous works were concerned with the stress optimization of macroscopic structures, through a penalization approach which eliminates intermediate densities.

On the contrary, the present work is interested in lattice structures which are porous materials with varying macroscopic material densities. Following the pioneer work [15], it fits in the framework of the so-called de-homogenization method, which has recently been applied in [16], [17] for compliance minimization of lattice structures. The main feature of the de-homogenization method is that, after optimizing an homogenized model based on a parametrized and orientable periodicity cell, it reconstructs a globally smooth, graded and curved lattice, which is near optimal. The main novelty of our work is to extend this de-homogenization approach to stress minimization problems, introducing the additional ingredient of stress amplification factors. Let us acknowledge that there are other works on stress constraints in the optimization of lattice structures (see e.g. [18] and [19]). However, they do not consider the orientation of the cells as a design variable and they do not rely on the de-homogenization approach.

Let us describe in some more details the de-homogenization method of [16], [17], [15] which is a very efficient technique for designing lattice structures. This method consists in pre-computing first the homogenized properties of a family of micro-structures parametrized by a few geometrical variables. Then, a standard macroscopic optimization problem is solved in terms of these geometrical variables in combination with the orientation of the micro-structure. Finally, a de-homogenization technique is used for describing the global structure in terms of a porous microscopic geometry with a clear

interface and full details. As already mentioned, we extend these previous works to the context of stress minimization. Note that some promising results can already be found in [20]. Our contribution is split in two parts. Part I focuses on the design of an appropriate periodic microstructure in 2-d which, apart from being nearly optimal for stress minimization, perfectly fits in the framework of [16], [17], [15]. On the other hand, Part II [21] is devoted to the optimization of a plane macroscopic structure for stress minimization, where at each point the design variables are the geometric parameters and the orientation of an underlying periodic cell (the optimal super-ellipsoidal hole, obtained in the present Part I).

The 2-d periodic microstructure proposed in the present work are merely *nearly optimal* for several reasons. First, to define a notion of optimality a proper cost, i.e., a measure of stress, must be defined. There are several possibilities: to take into account the full stress tensor, only its deviatoric part, some scalar criterion like von Mises or Tresca or to consider the maximum value or some  $L^p$  norm. Here we choose the maximum value, in the periodic cell, of the Frobenius norm of the full stress. These stresses are computed by solving the so-called cell problem with periodic boundary condition and imposed averaged or homogenized stress. Second, for manufacturability reasons, we seek a simple periodicity cell, parametrized by just a few parameters. Restricting our search to periodic cells excludes other microstructures, like rank- $n$  laminates, which are known to be optimal for compliance minimization but are unfortunately multi-scale and thus hard to manufacture. We also restrict ourselves to a single hole inside a square cell, which ensures that neighboring cells connect perfectly even if the hole parameters are varying. Finally, for computational efficiency, as well as manufacturability reasons, we limit the number of parameters although, in theory, it could be possible to freely optimize the hole's boundary. Our choice is a super-ellipsoidal hole in a square cell. Clearly other choices of the unit cell would have been possible which could lead to more optimal properties, at the expense of more involved parametrizations. In other words, our choice is a compromise between simplicity and optimality. Note that, if the resulting plane lattices are built horizontally by additive manufacturing techniques, there is no restriction due to our choice of closed holes in terms of overhang constraints or de-powdering after the building process. Although the present paper focuses on 2-d microstructures, the methodology can be extended to the 3-d case. This has already been done for compliance minimization in [16], where the parametrized cell is a type of cubic lattice. For stress minimization, one could imagine a similar microstructure with rounded corners. Furthermore, it is well-known that the optimal shape of a hole for this type of problem depends on the applied load, namely on the averaged or homogenized stress. However, for the sake of simplicity in the optimization process of Part II, we decide to find a periodic microstructure which is independent of the applied stress. Therefore, we apply an averaging process to find a microstructure which is nearly optimal for a whole family of stresses and not merely for one load. On the same token, to reduce the dependence of the microstructure to the imposed stress, we choose to always orientate the unit cell (or similarly the corresponding orthotropic effective Hooke's tensor) with the principal axis of the imposed stress. This orientation is known to be optimal for compliance minimization by a result of Pedersen [22]. Although it is not obvious that it is also optimal for stress minimization, it makes sense from a mechanical point of view. Above all, eliminating the pure shear component of the applied stress, by orientating accordingly the micro-structure, induces a drastic simplification of the optimization process. Of course, in principle it is possible to keep the orientation angle as a design variable and to apply a gradient algorithm for its optimization. We refer to Remark 1 for a discussion on this issue.

There are already some works in shape optimization for stress minimization featuring super-ellipsoidal holes, most notably [23] and [24]. In the former, a level-set representation of the geometry is combined with an XFEM (Extended Finite Element Method) formulation to deal with the sharp interface. Additionally, the optimal micro-structure is solved in terms of the volume fraction and the macroscopic strain. In the latter, the authors used a SIMP-based approach and the goal is to find the optimal semi-axis ratio and corner smoothing parameter to minimize the maximum stress for a micro-structure with a given volume fraction and loaded by a certain macroscopic strain (or stress). Here our goal is different since we want to design an optimal micro-structure which depends only on the volume fraction and on the geometrical variables and not on the applied macroscopic stress.

The paper is organized as follows. Section 2 recalls the necessary results of homogenization in order

to define, not only the homogenized or effective Hooke's law, but also the corrector terms which, upon suitable averaging, yields the stress amplification factors. In Section 3 the super-ellipsoidal hole in a square periodicity cell is precisely defined. In Section 4, some numerical experiments are performed to gain insight on the super-ellipsoidal geometry. Section 5 is our main result where we numerically solve the material design problem of minimizing the maximum stress. Finally, Section 6 is a discussion of the Vigdergauz micro-structure and a comparison with our optimal super-ellipsoidal hole. Finally, let us conclude this introduction by recalling that the proposed super-ellipsoidal hole will be used in Part II of our work [21] to optimize a macroscopic lattice structure for stress minimization.

## 2 Setting of the problem

### 2.1 Stress minimization for classical shapes.

Let us consider a smooth working domain  $D \subset \mathbb{R}^N$  (in practice  $N = 2$  or  $3$ ) and the reference configuration of an elastic body  $\Omega \subset D$ . The part of the boundary of the domain where the shape  $\Omega$  is clamped is denoted by  $\Gamma_D$ , while the part where the surface external force  $g$  is applied is denoted by  $\Gamma_N$ . It is assumed that  $\Gamma_D$  and  $\Gamma_N$  are subsets of  $\partial D$  and are fixed for any  $\Omega \subset D$ . The volumetric external force is denoted by  $f$ . Then, the associated linear elasticity problem is to find the displacement  $u \in H^1(\Omega; \mathbb{R}^N)$  such that

$$\begin{cases} -\operatorname{div}(Ae(u)) = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma_D, \\ Ae(u) \cdot n = g & \text{on } \Gamma_N, \\ Ae(u) \cdot n = 0 & \text{on } \Gamma = \partial\Omega \setminus (\Gamma_D \cup \Gamma_N), \end{cases} \quad (1)$$

where  $A$  corresponds to the elasticity constitutive tensor. The strain tensor is defined as usual by the symmetric gradient  $e(u) = \nabla^s u = (\nabla u + (\nabla u)^T)/2$ . The stress tensor is  $\sigma = Ae(u)$ . Introducing a space  $\mathcal{K}$  of admissible shapes (for example smooth open subsets of  $D$ , the boundary of which contains  $\Gamma_D$  and  $\Gamma_N$ ), the stress minimization problem is defined by

$$\begin{aligned} \min_{\Omega \in \mathcal{K}} \quad & \int_{\Omega} |\sigma|^p dx \\ \text{such that} \quad & \int_{\Omega} dx = V^*, \end{aligned} \quad (2)$$

where  $V^*$  stands for a given target shape volume. The stress are obtained from solving (1) and the exponent is  $p \in [2, \infty)$ . We use in this work the euclidean norm  $|\sigma| = \sqrt{\sigma : \sigma}$ , but other norms (i.e. Von Mises) are also possible. Note that in general, problem (2) is expected to be ill-posed since domains with the same volume but with structure details of smaller length scale may always decrease the cost function [11]. To circumvent this inconvenient, we may relax problem (2) by incorporating composites shapes and by understanding the notion of convergence in a weaker sense, in the sense of homogenization.

### 2.2 Homogenization and correctors

Let us briefly recall how problem (2) can be relaxed by homogenization, as already explained in [14]. We start by some classical results of homogenization theory (see [11] for details). To simplify the analysis, the shape optimization problem is approximated by a two-phase optimal design problem. More precisely, the elasticity tensor  $A$  in (1) is now denoted by  $A_1$  and the void part  $D \setminus \Omega$  is filled with a weak or ersatz material with elasticity tensor  $A_0 \ll A_1$ . The characteristic function of the subdomain occupied by phase  $A_1$  is called  $\chi(x)$  (it takes the value 1 in the phase  $A_1$  and 0 outside).

**H-convergence.** Homogenization theory is concerned with sequences of shapes or two-phase mixtures. Let  $\chi_\epsilon$  be a sequence of characteristic functions in  $L^\infty(D; \{0, 1\})$  and let  $A_\epsilon$  be its corresponding sequence of constitutive tensors, defined by

$$A^\epsilon = (1 - \chi^\epsilon) A_0 + \chi^\epsilon A_1, \quad (3)$$

to which we associate the displacements  $u_\epsilon$  solution of the elasticity problem

$$\begin{cases} -\operatorname{div}(A^\epsilon e(u_\epsilon)) = f & \text{in } D, \\ u_\epsilon = 0 & \text{on } \Gamma_D, \\ A^\epsilon e(u_\epsilon) \cdot n = g & \text{on } \Gamma_N, \\ A^\epsilon e(u_\epsilon) \cdot n = 0 & \text{on } \Gamma = \partial D \setminus (\Gamma_D \cup \Gamma_N), \end{cases} \quad (4)$$

and the corresponding stress tensor  $\sigma^\epsilon = A^\epsilon e(u^\epsilon)$ . Then, the main result of H-convergence theory (see Theorem 1.2.16 of [11]) states that there exists a sub-sequence, still denoted by  $\epsilon$ , a limit material density  $\rho \in L^\infty(D; [0, 1])$  and a limit homogenized tensor  $A^* \in L^\infty(D; \mathbb{R}^{N^4})$ , such that

$$\begin{aligned} \chi^\epsilon &\rightharpoonup \rho && \text{weakly* in } L^\infty(D; [0, 1]), \\ A^\epsilon &\xrightarrow{\text{H}} A^* && \text{in the sense of H-convergence,} \end{aligned} \quad (5)$$

where the H-convergence is defined as the two following convergences

$$\begin{aligned} u^\epsilon &\rightharpoonup u && \text{weakly in } H^1(D; \mathbb{R}^N), \\ \sigma^\epsilon &\rightharpoonup \sigma && \text{weakly in } L^2(D; \mathbb{R}^{N^2}), \end{aligned}$$

where  $\sigma = A^* e(u)$  and  $u$  is the displacement solution of the homogenized elasticity problem

$$\begin{cases} -\operatorname{div}(A^* e(u)) = f & \text{in } D, \\ u = 0 & \text{on } \Gamma_D, \\ A^* e(u) \cdot n = g & \text{on } \Gamma_N, \\ A^* e(u) \cdot n = 0 & \text{on } \Gamma = \partial D \setminus (\Gamma_D \cup \Gamma_N). \end{cases} \quad (6)$$

In (5)  $\rho$  represents the volume fraction of  $A_1$  and  $A^*$  represents the homogenized constitutive tensor, or simply homogenized tensor, of the composite. Because the above results are only weak convergences, it is not possible to prove convergence of the associated sequence of stress objective functions. More precisely, one can only deduce that

$$\liminf_{\epsilon \rightarrow 0} \int_D |\sigma^\epsilon|^p dx \geq \int_D |\sigma|^p dx, \quad (7)$$

where, in most cases, the inequality is strict. To circumvent this limitation and obtain a strong convergence of the stresses, corrector tensors have to be introduced.

**Corrector tensor in homogenization.** According to Lemma 1.3.38 and Theorem 1.3.39 of [11] there exists a sequence of fourth order tensors  $W^\epsilon$ , called correctors, with the following properties

$$\begin{aligned} W^\epsilon &\rightharpoonup I_4 && \text{weakly in } L^2(D; \mathbb{R}^{N^4}), \\ A^\epsilon W^\epsilon &\rightharpoonup A^* && \text{weakly in } L^2(D; \mathbb{R}^{N^4}), \end{aligned} \quad (8)$$

where  $I_4$  is the fourth order identity tensor, and such that

$$\begin{aligned} e(u^\epsilon) - W^\epsilon e(u) &\rightarrow 0 && \text{strongly in } L^1(D; \mathbb{R}^{N^2}), \\ \sigma^\epsilon - A^\epsilon W^\epsilon A^{*-1} \sigma &\rightarrow 0 && \text{strongly in } L^1(D; \mathbb{R}^{N^2}). \end{aligned} \quad (9)$$

In other words, corrector tensors allow us to move from weak to strong convergence of the strains and stresses. If the homogenized displacement  $u$  is smooth enough, the  $L^1$  strong convergence in (9) can be improved in a  $L^2$  strong convergence. Regarding the convergence of the stress  $\sigma_\epsilon$ , following [14], its corrector is called an amplification tensor, defined as

$$P^\epsilon = A^\epsilon W^\epsilon A^{*-1}, \quad (10)$$

which satisfies  $P^\epsilon \rightharpoonup I_4$  weakly in  $L^2(D; \mathbb{R}^{N^4})$  and, in view of equation (9), yields  $\sigma^\epsilon - P^\epsilon \sigma \rightarrow 0$  strongly in  $L^1(D; \mathbb{R}^{N^2})$ .

Unfortunately, to improve (7) and obtain an equality instead of an inequality, a  $L^p$  strong convergence is required which cannot be deduced in full generality for any  $p > 2$ . Therefore, from now on, we shall restrict ourselves to periodic homogenization where the corrector results can be further improved.

### 2.3 Periodic homogenization and correctors

Since H-convergence theory provides no explicit formulae for computing the correctors and amplification tensors, we restrict ourselves to periodic homogenization. The main interest of the periodic case is the availability of such explicit formulae and a better convergence framework which allows us to improve (7) and define a relaxed or homogenized objective function. The main assumption of the periodic setting is that the sequence of characteristic functions  $\chi^\epsilon$  is defined as a periodic function

$$\chi^\epsilon(x) = \chi\left(\frac{x}{\epsilon}\right), \quad (11)$$

where  $\chi(y)$  is a  $Y$ -periodic function, with the unit cube  $Y = (-0.5, 0.5)^N$  and  $\epsilon > 0$  is the (small) period of  $\chi^\epsilon$ . The variable  $y = x/\epsilon$  is called fast variable and is defined in the domain  $Y$ . In the periodic setting, it is not any longer necessary (for technical reasons) to consider a two-phase mixture and, from now on, we come back to the original setting where the ersatz material is void,  $A_0 = 0$ , and the material phase is  $A_1 = A$ . In the unit cell  $Y$ , material  $A$  occupies the subset  $Y_0$  and  $Y \setminus Y_0$  is a hole with boundary  $\Gamma_{int}$ . Thus, the material tensor is defined in  $Y$  by

$$A(y) = \begin{cases} A & y \in Y_0, \\ 0 & y \in Y \setminus Y_0. \end{cases}$$

Periodic homogenization is simpler than the fully general theory of homogenization because the notion of H-convergence can be made more explicit by using two-scale asymptotic expansions (see e.g. [11] for further details). We now recall the main results of interest for our purpose. In particular, correctors, homogenized and amplification tensors can be computed explicitly by solving the so-called cell problems.

**Cell problem.** For given indices  $1 \leq i, j \leq N$ , the cell problem is usually defined as follows: find the periodic solution  $w_{ij}$  of

$$\begin{cases} -\operatorname{div}(A(e_{ij} + e(w_{ij}))) = 0 & \text{in } \mathbb{R}_0^N, \\ A(e_{ij} + e(w_{ij})) \cdot n = 0 & \text{on } \Gamma_{int}, \\ y \mapsto w_{ij}(y) & Y_0 - \text{periodic}, \end{cases} \quad (12)$$

where the tensor  $e_{ij} = \frac{1}{2}(e_i \otimes e_j + e_j \otimes e_i)$  is one element of the canonical basis of symmetric matrices. The solution  $w_{ij}$  is called a corrector function. Equation (12) is posed in the periodic domain  $\mathbb{R}_0^N$  which is obtained by periodic repetition of the cell  $Y_0$  in the full space  $\mathbb{R}^N$ . Note that, because of the periodicity of the solution  $w_{ij}$ , it is enough to solve this equation in a single cell  $Y_0$ . To give a mathematically precise meaning to (12), let us introduce the subspace  $H_{\#}^1(Y_0; \mathbb{R}^N)$  of all functions  $u \in H^1(Y_0; \mathbb{R}^N)$  which are periodic, i.e., with traces equal on opposite sides of the unit cell  $Y_0$ . The cell problem admits the following weak form: find  $w_{ij} \in H_{\#}^1(Y_0; \mathbb{R}^N)$  such that

$$\forall \phi \in H_{\#}^1(Y_0; \mathbb{R}^N) \quad \int_{Y_0} A e(w_{ij}) : e(\phi) + \int_{Y_0} A e_{ij} : e(\phi) = 0, \quad (13)$$

which admits a unique solution up to a rigid body motion (a translation in this case). The correctors yield an explicit formula for the homogenized constitutive tensor as follows

$$A_{ijkl}^* = \int_{Y_0} A(e_{ij} + e(w_{ij})) : e_{kl} dy \quad \forall i, j, k, l \in \{1, \dots, N\}, \quad (14)$$

or equivalently, using the weak form (13),

$$A_{ijkl}^* = \int_{Y_0} A(e_{ij} + e(w_{ij})) : (e_{kl} + e(w_{kl})) dy.$$

The connection with the previous corrector tensor  $W^\epsilon$  defined in (8) is as follows

$$W^\epsilon(x) = W\left(\frac{x}{\epsilon}\right) \quad \text{with} \quad W_{ijkl}(y) = \begin{cases} I_{ijkl}^4 + e(w_{ij})_{kl}(y), & y \in Y_0, \\ 0 & y \in Y \setminus Y_0. \end{cases}$$

Similarly, the previous amplification tensor  $P^\epsilon = A^\epsilon W^\epsilon A^{*-1}$ , defined by (10), reduces to

$$P^\epsilon(x) = P\left(\frac{x}{\epsilon}\right) \quad \text{with} \quad P(y) = \begin{cases} AW(y)A^{*-1} & y \in Y_0, \\ 0 & y \in Y \setminus Y_0. \end{cases}$$

One advantage of the periodic setting is that the strong convergence in (9) can be improved, at least under the assumption that the homogenized solution  $u$  is smooth and that boundary layer effects can be neglected (this is the case for rectangular domains  $D$  for which it is known that boundary layers decay exponentially fast inside the domain [25]). More precisely, under these assumptions, one can prove, for any  $p \geq 1$ ,

$$\sigma^\epsilon - P^\epsilon \sigma \rightarrow 0 \text{ strongly in } L^p(D; \mathbb{R}^{N^2}). \quad (15)$$

This convergence property is crucial to pass to the limit in the objective function and improve (7).

In the sequel, we shall use the (more explicit) notation

$$\sigma^{\text{loc}}(y) = P(y)\sigma \quad (16)$$

for the microscopic stress in the unit periodicity cell  $Y_0$  created by a constant macroscopic stress  $\sigma$ . In numerical practice, given  $\sigma$ , one first define the macroscopic strain tensor  $e_\sigma = (A^*)^{-1}\sigma$ , then one computes the solution  $w_\sigma(y)$  of the cell problem (12) where  $e_{ij}$  is replaced by  $e_\sigma$  and finally  $\sigma^{\text{loc}}(y) = A(y)e(w_\sigma)(y)$ .

**Homogenized stress norm minimization.** Once all the necessary ingredients of homogenization theory are introduced, one can define the homogenized version of the stress minimization problem. For any given periodic characteristic function  $\chi(y)$  (defining the perforated unit cell  $Y_0$ ), the associated sequence  $\chi^\epsilon$ , defined by (11), satisfies

$$\begin{aligned} \chi^\epsilon &\rightharpoonup \rho = \int_Y \chi(y) dy && \text{weakly* in } L^\infty(D; [0, 1]), \\ A^\epsilon &\xrightarrow{\text{H}} A^* && \text{in the sense of H-convergence,} \end{aligned}$$

where  $A^*$  is given by (14). Furthermore, because of (15), one can replace, up to small remainders,  $\sigma^\epsilon$  by  $P^\epsilon \sigma$ , which yields

$$\lim_{\epsilon \rightarrow 0} \int_D |\sigma^\epsilon|^p dx = \lim_{\epsilon \rightarrow 0} \int_D (P^\epsilon \sigma : P^\epsilon \sigma)^{p/2} dx,$$

where the limit can easily be computed since  $P^\epsilon$  is a periodically oscillating sequence

$$\lim_{\epsilon \rightarrow 0} \int_D (P^\epsilon \sigma : P^\epsilon \sigma)^{p/2} dx = \int_D \int_{Y_0} (P(y)\sigma(x) : P(y)\sigma(x))^{p/2} dy dx.$$

We introduce a notation for this limit

$$\mathcal{P}_p(\sigma) = \int_{Y_0} (P(y)\sigma : P(y)\sigma)^{p/2} dy, \quad (17)$$

which, for  $p$  an even integer, is an homogeneous polynomial of degree  $p$  with respect to the entries of  $\sigma$ . Note that all homogenized quantities, namely  $A^*$ ,  $\rho$  and  $P$  depend solely on the  $Y$ -periodic characteristic function  $\chi$ . Therefore, the periodic homogenized stress minimization problem is

$$\begin{aligned} \min_{\chi} & \int_D \mathcal{P}_p(\sigma) dx \\ \text{such that} & \int_D \rho dx = V^*, \end{aligned} \quad (18)$$

where  $\sigma = A^*e(u)$  is the stress associated to the solution  $u$  of the homogenized problem (6). Problem (18) is a partial relaxation of the original optimization problem (2) because it does not feature all possible composite materials but only those ones obtained by periodic homogenization. In [14] a different partial relaxation was introduced, relying on so-called sequential laminates. In any case,



a full relaxation is not available because the set of all composite materials obtained by a general homogenization process is yet unknown in the elasticity setting.

A crucial remark is to acknowledge the fact that, although periodic homogenization was discussed here only for the case of a purely periodic characteristic function  $\chi(y)$ , it is perfectly legitimate to consider macroscopically modulated periodic functions, like  $\chi(x, y)$ . In other words, the cell problems and the homogenized properties may vary from point to point in the working domain  $D$  and thus depend on  $x$  (this is the strategy followed for example in [16]).

## 2.4 Stress amplification tensor.

The goal of this subsection is to compute the operator  $\mathcal{P}_p$  defined by (17). For simplicity, the exponent  $p$  is assumed to be an even integer. The case  $p = 2$  is the simplest one and, introducing the fourth order tensor

$$\mathbb{P}^{(2)}(y) = P^T(y)P(y) = A^{*-1}W(y)A(y)A(y)W(y)A^{*-1}, \quad (19)$$

it is easily deduced that

$$\mathcal{P}_2(\sigma) = \left( \int_{Y_0} \mathbb{P}^{(2)}(y) dy \right) \sigma : \sigma. \quad (20)$$

The cases  $p > 2$  are much more involved. Indeed, in full generality one expects that

$$\mathcal{P}_p(\sigma) = \mathcal{P}_p^* \cdot \left( \sigma \otimes \cdots \otimes \sigma \right), \quad (21)$$

where  $\mathcal{P}_p^*$  is a  $2p$ -order tensor with entries given by averages of  $p$ -powers of entries of  $\mathbb{P}^{(2)}(y)$ . This tensor  $\mathcal{P}_p^*$  is called the homogenized stress amplification tensor. It is indeed an amplification factor because, in view of (7), it satisfies

$$\mathcal{P}_p(\sigma) \geq |\sigma|^p.$$

To obtain the components of the tensor  $\mathcal{P}_p^*$ , the idea is to rewrite the tensor product (21), or (17), as an integral of a sum of products between  $\mathbb{P}^{(2)}(y)$  and  $\sigma \otimes \sigma$ . From now on we restrict ourselves to the 2-d case, although all formulae below can easily be generalized to the 3-d case, at the expense of heavier notations. Using Voigt notations in 2-d, we have

$$P(y)\sigma : P(y)\sigma = \mathbb{P}^{(2)}(y)\sigma : \sigma = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{12} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{(2)}_{1111} & \mathbb{P}^{(2)}_{1122} & \mathbb{P}^{(2)}_{1112} \\ \mathbb{P}^{(2)}_{1122} & \mathbb{P}^{(2)}_{2222} & \mathbb{P}^{(2)}_{1222} \\ \mathbb{P}^{(2)}_{1112} & \mathbb{P}^{(2)}_{1222} & \mathbb{P}^{(2)}_{1212} \end{bmatrix} \begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \end{bmatrix}, \quad (22)$$

where the components of the tensor  $\mathbb{P}^{(2)}$  are defined by

$$\begin{aligned} \mathbb{P}^{(2)}_{1111} &= P_{1111}^2 + P_{2211}^2 + P_{1211}^2, \\ \mathbb{P}^{(2)}_{2222} &= P_{1122}^2 + P_{1222}^2 + P_{2222}^2, \\ \mathbb{P}^{(2)}_{1212} &= P_{1112}^2 + P_{2212}^2 + P_{1212}^2, \\ \mathbb{P}^{(2)}_{1122} &= P_{1111}P_{1122} + P_{2211}P_{2222} + P_{2212}P_{1222}, \\ \mathbb{P}^{(2)}_{1112} &= P_{1111}P_{1112} + P_{2211}P_{2212} + P_{1211}P_{1212}, \\ \mathbb{P}^{(2)}_{1222} &= P_{1122}P_{1112} + P_{2222}P_{2212} + P_{1222}P_{1212}. \end{aligned}$$

Finally, (22) can be rearranged as a scalar product between 6-th dimensional vectors

$$P(y)\sigma : P(y)\sigma = \begin{bmatrix} \mathbb{P}^{(2)}_{1111} & \mathbb{P}^{(2)}_{2222} & \mathbb{P}^{(2)}_{1212} & 2\mathbb{P}^{(2)}_{1122} & 2\mathbb{P}^{(2)}_{1112} & 2\mathbb{P}^{(2)}_{1222} \end{bmatrix} \begin{bmatrix} \sigma_{11}\sigma_{11} \\ \sigma_{22}\sigma_{22} \\ \sigma_{12}\sigma_{12} \\ \sigma_{22}\sigma_{12} \\ \sigma_{11}\sigma_{12} \\ \sigma_{11}\sigma_{22} \end{bmatrix} = P^{(2)} \cdot \sigma^{(2)}. \quad (23)$$

**Stress norm through multinomials.** Recall the multinomial theorem

$$(x_1 + \dots + x_6)^{p/2} = \sum_{|\alpha|=p/2} \binom{p/2}{\alpha} x^\alpha \quad \text{where} \quad \binom{p/2}{\alpha} = \frac{(p/2)!}{\alpha_1! \dots \alpha_6!},$$

and  $x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \dots x_6^{\alpha_6}$  for  $\alpha \in \mathbb{N}^6$  and  $x \in \mathbb{R}^6$ . Furthermore if  $x = yz$  in the sense that  $x_i = y_i z_i$ ,  $1 \leq i \leq 6$ , we introduce the notation  $y^\alpha \cdot z^\alpha = y_1^{\alpha_1} \dots y_6^{\alpha_6} z_1^{\alpha_1} \dots z_6^{\alpha_6}$ . Using this notation for  $y = P^{(2)}$  and  $z = \sigma^{(2)}$ , the amplification tensor can be written as

$$\mathcal{P}_p(\sigma) = \sum_{|\alpha|=p/2} \binom{p/2}{\alpha} \left( \int_{Y_0} \left( P^{(2)} \right)^\alpha dy \right) \cdot \left( \sigma^{(2)} \right)^\alpha = \mathcal{P}_p^* \cdot \left( \sigma \otimes \dots \otimes \sigma \right), \quad (24)$$

where each entry of  $\sigma \otimes \dots \otimes \sigma$  is homogeneous of degree  $p$ . The entries of  $\mathcal{P}_p^*$  are deduced from (24). In the simplest case of  $p = 2$ , the number of entries is  $N_p = 6$ . However, as the exponent is increased  $p = \{4, 8, 16\}$ , this number increases exponentially  $N_p = \{21, 126, 1287\}$ .

### 3 Super-ellipsoidal holes for stress minimization

Now, the goal is to design a micro-structure parametrized with a small number of variables such that its corresponding amplification tensor  $\mathcal{P}_p^*$  entries are minimized.

#### 3.1 Description of the geometry

For simplicity, in this work we propose a square cell micro-structure with a super-ellipsoidal hole in order to minimize stress concentrations. Although more sophisticated micro-structure could be used, we decided to choose the super-ellipse as a suitable compromise between simplicity and efficiency. On the one hand, this geometry generalizes both the square/rectangle and the circle/ellipse geometries and includes intermediate holes that continuously varies from one to the other. On the other hand, considering a single hole inside a square cell ensures that neighboring cells connect perfectly even if the hole parameters are different. Additionally, the topology is easy to represent via an explicit level-set function which is important for the de-homogenisation procedure (see [16]). By using the super-ellipse geometry, it is possible to conveniently round the corners of the square in order to minimize the maximum stress. On the other hand, for adequate values of the parameters, the super-ellipsoidal hole has some resemblance with the Vigdergauz micro-structure which is proven to be optimal in some cases when minimizing the maximum stress [26] (see Section 6 for more details). Note that some other recent works [23, 24] have also proposed to use super-ellipses in shape optimization.

**Super-ellipse geometry description.** The micro-structure of a unitary square cell  $Y = (-0.5, 0.5)^2$  with a super-ellipsoidal hole may be explicitly described as

$$Y_0 = \{ \psi(y) < 0; \quad \forall y \in Y \},$$

where  $\psi$  is the following level-set function

$$\psi(y) = \left( \frac{y_1}{m_1/2} \right)^q + \left( \frac{y_2}{m_2/2} \right)^q - 1. \quad (25)$$

The super-ellipse is centered at the origin and its semi-axis are  $m_1/2$  and  $m_2/2$ , while the exponent  $q$  can be seen as a smoothing corner parameter. From now on,  $q$  is called the smoothing exponent, restricted to the values  $q \geq 2$ .

**Super-ellipse volume fraction.** Another well-known advantage of a square micro-structure with a super-ellipsoidal hole is that the volume fraction can be explicitly computed by

$$\rho = \int_{Y_0} dy = 1 - c(q)m_1m_2 \quad \text{with} \quad c(q) = \frac{\Gamma\left(1 + \frac{1}{q}\right)^2}{\Gamma\left(1 + \frac{2}{q}\right)}, \quad (26)$$

where  $\Gamma$  is the gamma function.

**Super-ellipsoidal hole examples in a unitary square cell.** A wide range of shapes can be obtained by just changing the parameters of the super-ellipsoidal hole. Examples of particular interest range from small circles or ellipses, which are well known to be optimal for compliance minimization in the limit of small holes [26]), to rectangular holes with one of the semi-axis attaining its maximum value (rank-1 laminate case). These and other examples of the family of micro-structures we are considering in this work are shown in Figure 1.

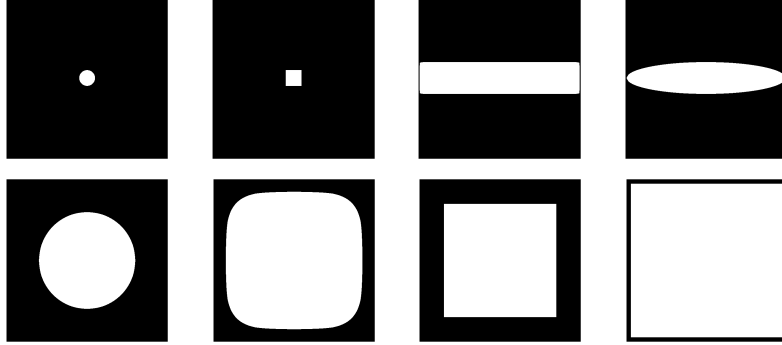


Figure 1: Examples of different super-ellipsoidal holes. From left to right, first line: (i)  $m_1 = m_2 = 0.1$ ;  $q = 2$ ; (ii)  $m_1 = m_2 = 0.1$ ;  $q = 32$ ; (iii)  $m_1 = 0.99$ ;  $m_2 = 0.2$ ;  $q = 32$ ; (iv)  $m_1 = 0.99$ ;  $m_2 = 0.2$ ;  $q = 2$ . Second line: (i)  $m_1 = m_2 = 0.6$ ;  $q = 2$ ; (ii)  $m_1 = m_2 = 0.85$ ;  $q = 4$ ; (iii)  $m_1 = m_2 = 0.7$ ;  $q = 32$ ; (iv)  $m_1 = m_2 = 0.99$ ;  $q = 32$ .

**Limit cases.** Special attention must be paid to the limit cases of super-ellipsoidal holes. Certainly, the micro-structure rigidity becomes singular when the super-ellipsoidal hole touches the square cell boundary, more specifically when  $m_i \rightarrow 1$  for  $i = 1$  or  $2$ . Since we are interested in optimal micro-structure, there is no restriction in introducing bounds on the geometrical parameters,  $m_{L_i} \leq m_i \leq m_{U_i}$ . From now on, we take in all the examples  $m_{L_i} = 0$  and  $m_{U_i} = 0.99$ . This upper bound will ensure the invertibility of the stiffness matrix in the corresponding macroscopic problem [21]. Furthermore, with such a bound the perforated cells are always properly meshed. In this work we use the Mmg library, which is available in [27] and fully described in [28].

**Super-ellipse parametrization.** To minimize the number of cell parameters, we decide to choose the "best" smoothing exponent  $q$  for every value of the parameters  $m_1$  and  $m_2$ . This optimal value of  $q$  is given by an optimization process described below. Special care is required because this optimization has a tendency to minimize the volume and not to properly round the corners of the super-ellipse. Thus, a volume fraction constraint has to be enforced when solving the optimization problem. See section 5.1 for more details. Then, we replace variables  $(m_1, m_2)$  by the semi-axis ratio  $\xi$  and the volume fraction  $\rho$ . Those variables are defined by

$$\xi = \arctan(m_1/m_2) \quad \text{and} \quad \rho = 1 - c(q)m_1m_2. \quad (27)$$

Using the *arctan* function allows us to bound the domain of the semi-axis parameter  $\xi$ . Alternatively, the converse relations are:

$$m_1 = \sqrt{\frac{1 - \rho}{c(q) \tan(\xi)}} \quad \text{and} \quad m_2 = \sqrt{\frac{(1 - \rho) \tan(\xi)}{c(q)}}. \quad (28)$$

Additionally, note that the upper bound on  $m_i$  implies the following non-linear bounds

$$\xi_{\min}(\rho, q) = \xi_2(m_{U_2}, q, \rho) \leq \xi \leq \xi_1(m_{U_1}, q, \rho) = \xi_{\max}(\rho, q),$$

where the functions  $\xi_1$  and  $\xi_2$  are defined as

$$\xi_1(m_1, q, \rho) = \arctan\left(\frac{m_1 c(q)}{1 - \rho}\right) \quad \text{and} \quad \xi_2(m_2, q, \rho) = \arctan\left(\frac{1 - \rho}{m_2 c(q)}\right). \quad (29)$$

Thus, for a given smoothing exponent  $q$ , the ranges of the semi-axis and volume fraction are  $\xi \in [\xi_{\min}(\rho, q), \xi_{\max}(\rho, q)]$  and  $\rho \in [\rho_{\min}(q), 1]$  where  $\rho_{\min}(q) = 1 - c(q)m_{U_1}m_{U_2}$ . We call this set the admissible space

$$\mathcal{V}_{ad}(q) = \left\{ (\xi, \rho) \mid \xi \in [\xi_{\min}(\rho, q), \xi_{\max}(\rho, q)] \quad \text{and} \quad \rho \in [\rho_{\min}(q), 1] \right\}. \quad (30)$$

Note that the admissible space  $\mathcal{V}_{ad}(q = 2)$  for an elliptic hole cannot achieve a complete void in the unit cell structure since the minimal volume fraction is about  $\rho_{\min}(q = 2) \sim 0.2$ . Instead, the admissible space  $\mathcal{V}_{ad}(q = 32)$  for an almost rectangular hole achieves  $\rho_{\min}(q = 32) \sim 0.02$ . In particular,  $q = 32$  provide the most elongated holes and the lowest volume fraction micro-structures. This has a strong impact on most of the topology optimization problems since usually one of the objectives is to reduce the volume of the structure. Note that the largest admissible space is precisely the one for almost rectangular holes,  $\mathcal{V}_{ad}(q = 32)$ . In Figure 2 are precisely plotted the admissible space for almost rectangular holes  $\mathcal{V}_{ad}(q = 32)$  and for elliptic holes  $\mathcal{V}_{ad}(q = 2)$ .

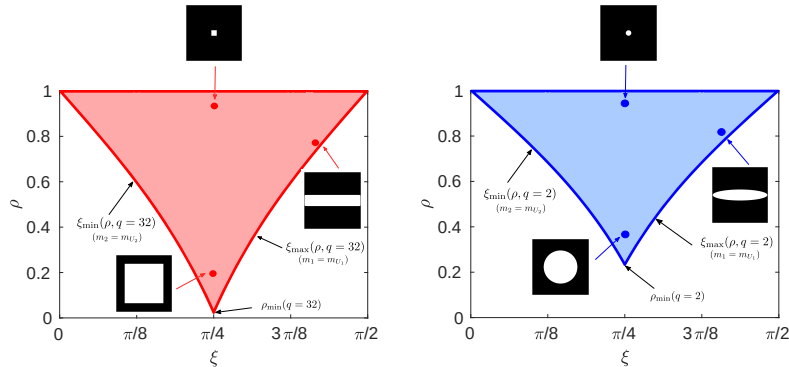


Figure 2: Admissible design space  $\mathcal{V}_{ad}(q)$ . Clearly, the almost rectangular case  $\mathcal{V}_{ad}(q = 32)$  (left image) is larger than the ellipsoidal case  $\mathcal{V}_{ad}(q = 2)$  (right image). Note that the rectangular admissible design  $\mathcal{V}_{ad}(q = 32)$  is larger than the ellipsoidal one  $\mathcal{V}_{ad}(q = 2)$ .

Note that in this parametrization no orientation of the hole is considered. This is because, according to the optimization strategy of [16], the orientation of the entire square cell will be optimized in the macroscopic topology optimization problem. More details will be given in Part II [21].

### 3.2 Mesh-size dependency

Certainly, mesh-size effects may appear when minimizing any measure of the stress. It is well-known that the stress values may tend to infinity at some points (for example, corners) as the mesh-size tends to zero. Since the super-ellipsoidal hole looks like a rectangular hole when the smoothing exponent  $q$  goes to infinity, there may be very large point-wise values of the stress in such a case. In Figure 3 we plot the microscopic stress  $\sigma_{11}^{\text{loc}}(y)$ , defined by (16), for a uniaxial horizontal stress tensor  $\sigma_{11} = 1$ ,  $\sigma_{22} = 0$  and  $\sigma_{12} = 0$ . Indeed for a rectangular hole, the maximum stress diverges when refining the mesh, as expected. On the contrary, for a rounded corner (corresponding to  $q = 4$ ), the maximum stress remains bounded under mesh refinement. For simplicity, in this work, we use a high quality conformal mesh (provided by the open-source software Mmg [28]) to properly describe the perforated cell. We found that it was accurate for evaluating the maximum stress. Other different numerical techniques like filtering [24] or the use of XFEM formulation [23] are also possible. All our numerical results are obtained with a similar mesh size, fine enough to capture the round corners. In this section, as well as in the entire paper, we consider an isotropic elasticity tensor  $A = 2\mu I_4 + (\kappa - \mu)I_2 \otimes I_2$  where  $I_4$  and  $I_2$  correspond to the fourth and second order identity tensors. The shear and bulk modulus in 2-d are defined by  $\mu = \frac{E}{2(1+\nu)}$  and  $\kappa = \frac{E}{2(1-\nu)}$  and the values of the Young modulus and Poisson ratio are taken as  $E = 1$  and  $\nu = 1/3$ .

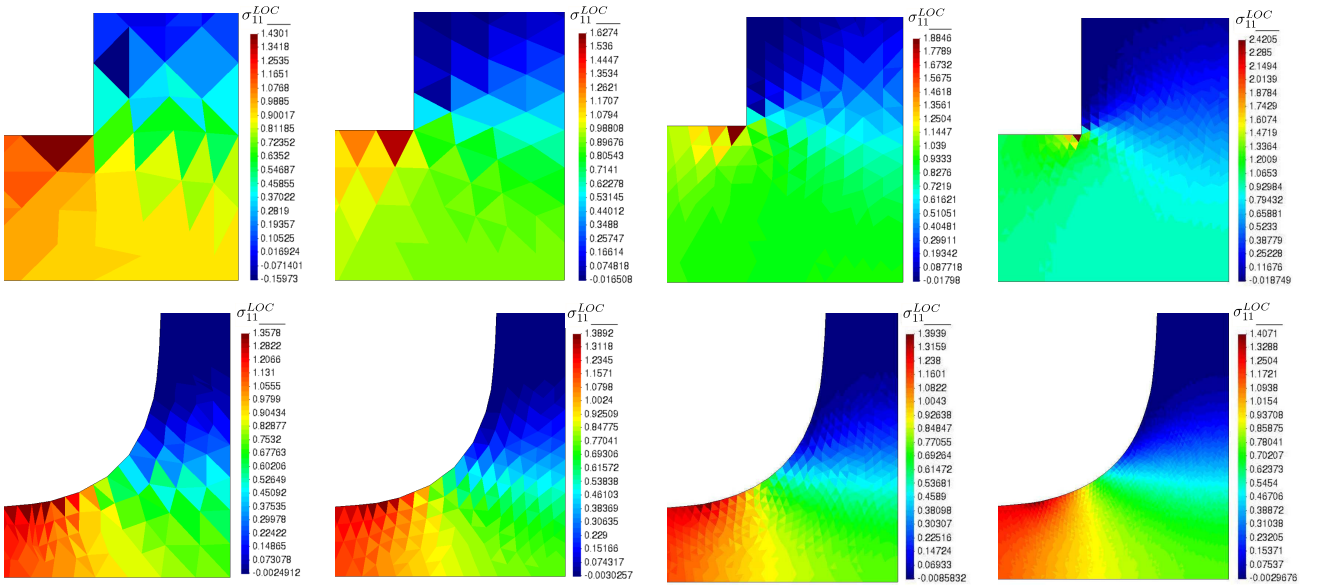


Figure 3: Mesh convergence of the microscopic stress  $\sigma_{11}^{\text{loc}}(y)$  when applying a macroscopic stress load  $\sigma_{11} = 1$ ,  $\sigma_{22} = 0$  and  $\sigma_{12} = 0$  to a square micro-structure with a rectangular and a super-ellipsoidal hole ( $q = 4$ ). The mesh sizes are  $h \in \{0.1, 0.05, 0.0025, 0.00125\}$ .

## 4 Numerical Experiments

In order to get some insight and understand the nature of the problem, we conduct in this section two different numerical experiments. In the first experiment, we study the homogenized and amplification factor for  $p = 2$  when considering rectangular or ellipsoidal holes. In the second experiment, we move towards larger stress exponents  $p \geq 2$ , but this time for different intermediate super-ellipsoidal holes. For simplicity, we only show here a brief summary of the numerical experiments. A detailed and more exhaustive study is reported in the supplementary material of this work [29].

### 4.1 First numerical experiment: $p = 2$ or rectangular and ellipsoidal holes

We compare the homogenized tensors, as well as the stress amplification tensors with  $p = 2$ , for the two simplest cases: rectangular and ellipsoidal holes. Note that the symmetry of the rectangular and ellipsoidal holes provides orthotropic homogenized fourth order tensors.

**Homogenized tensor.** In Figure 4, we show all the homogenized tensor entries for both the rectangular and ellipsoidal holes in the admissible design space  $\mathcal{V}_{ad}(q)$ . Note that comparing in the space  $(\xi, \rho)$  rather than in the space  $(m_1, m_2)$  allow us to compare holes with the same volume fraction. For a full comparison in the space  $(m_1, m_2)$ , see the first experiment in the supplementary material [29]. We first observe in Figure 4 that both entries  $A_{1122}$  and  $A_{1212}$  monotonically increases with the volume fraction  $\rho$ . For a given volume fraction  $\rho$ , the larger values of  $A_{1122}$  and  $A_{1212}$  are obtained at symmetric holes ( $\xi = \pi/4$ ). Alternatively, the entries  $A_{1111}$  and  $A_{2222}$  clearly increases with the design variables  $m_1$  and  $m_2$  rather than with the volume fraction  $\rho$  (see the supplementary material [29]). We also see that, for a fixed volume fraction  $\rho$ , the more horizontally elongated the hole (like a rank-1 laminate, with  $\xi \rightarrow \xi_{UB}$ ), the larger the component  $A_{1111}$ . A similar result holds for  $A_{2222}$  with vertical holes.

**Amplification tensor.** The influence of considering rectangular or ellipsoidal holes on the stress norm may be easily identified through the amplifier entries. Since some amplifier entries may blow up to infinity for small volume fractions, for clarity purposes in Figure 5, the inverse of the stress amplification tensor  $\mathbb{P}_2^{-1}$  is plotted in the admissible design spaces  $\mathcal{V}_{ad}(q = 2)$  and  $\mathcal{V}_{ad}(q = 32)$ . Note that since  $\mathbb{P}_2 \geq \mathbb{I}$  in the sense of fourth order tensor, its inverse is bounded from above. In Figure 5, we observe that the component  $(\mathbb{P}_2^{-1})_{1122}$  has a concave dependency with  $\rho$  and has a maximum value

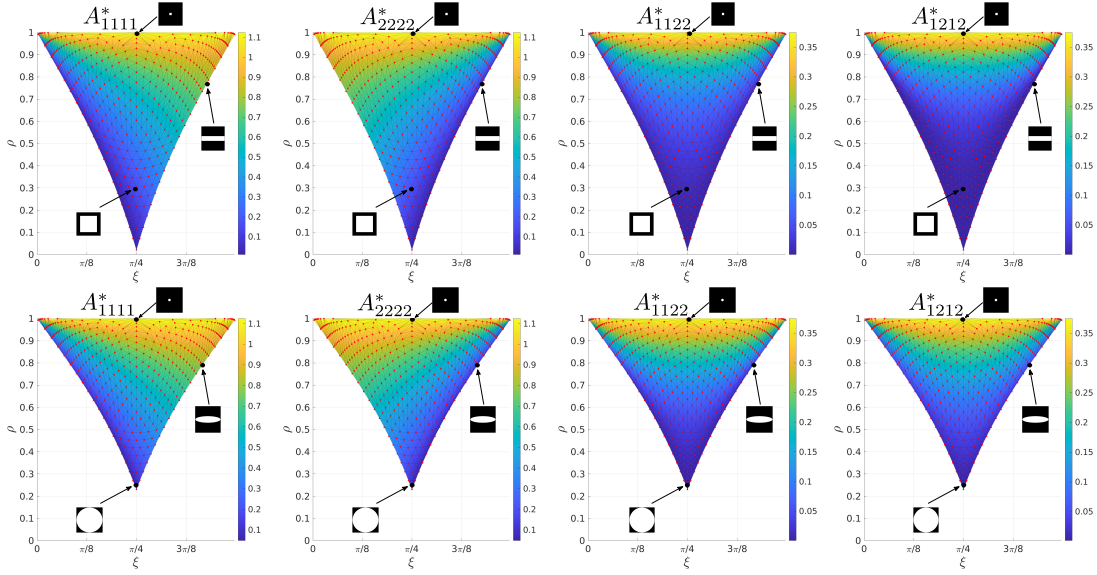


Figure 4: Entries of the homogenized tensor  $A^*$  for all possible rectangular (top line) and ellipsoidal (bottom line) holes.

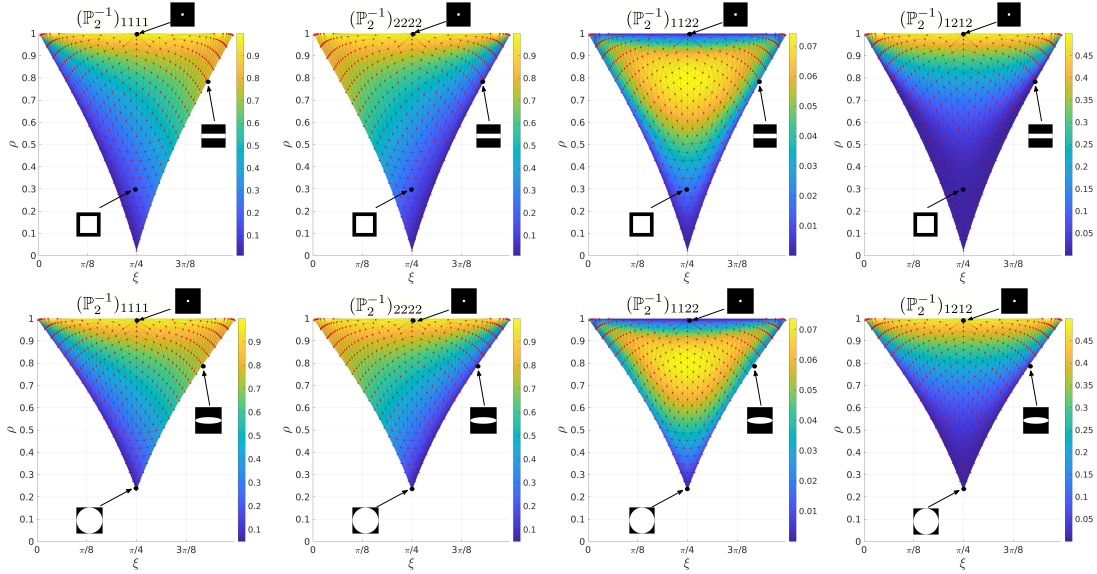


Figure 5: Inverse of amplification tensor  $\mathbb{P}_2$  for all possible rectangular (top line) and ellipsoidal (bottom line) holes.

around  $\rho \sim 0.8$ . The component  $(\mathbb{P}_2^{-1})_{1212}$  increases monotonically with  $\rho$  and depends weakly on  $\xi$ . Symmetric holes have larger  $(\mathbb{P}_2^{-1})_{1212}$ . Alternatively, as reported in the supplementary material [29], the  $(\mathbb{P}_2^{-1})_{1111}$  and  $(\mathbb{P}_2^{-1})_{2222}$  depends mainly on the  $m_1$  and  $m_2$  variables directly. For a given volume fraction  $\rho$ , we also see that the larger values of  $(\mathbb{P}_2^{-1})_{1111}$  is when considering horizontally elongated holes (like rank-1 laminates). We also observe that the variation of the amplification entries with  $(\xi, \rho)$  variables for rectangular and ellipsoidal holes are similar. However their values are considerably different. In general, we observe that for small holes ellipsoidal and rectangular holes behave similar and for large holes rectangular holes are preferred, specially for elongated ones ( $m_1 \rightarrow 1$  or  $m_2 \rightarrow 1$ ). A quantitative and exhaustive comparison is reported in the supplementary material [29].

## 4.2 Second numerical experiment: $p \geq 2$

In this second numerical experiment, we move to general super-ellipses ( $2 \leq q \leq 32$ ) and consider stress norm exponents  $p \geq 2$ .

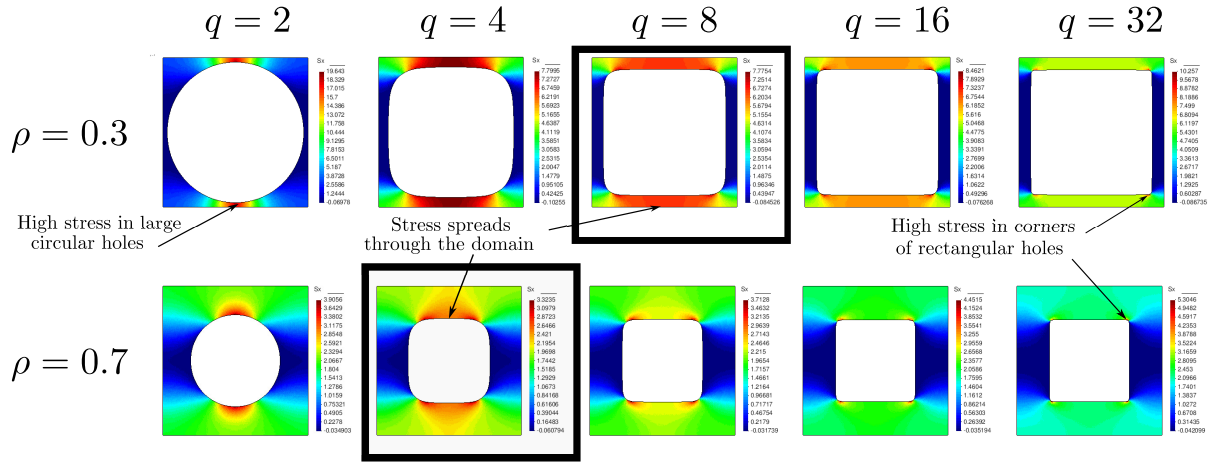


Figure 6: Plot of the local stress field  $\sigma_{11}^{\text{loc}}(y)$  for an uni-axial horizontal macroscopic stress tensor  $\sigma = [1 \ 0 \ 0]$ . In each row, the case with lowest maximum value of the stress is inscribed in a black box. Rectangular holes with smoothed corners are preferred for large holes. More rounded (ellipsoidal) holes are preferred for intermediate holes.

**Maximum stress norm.** First, we study the maximum stress norm for symmetric ( $m_1 = m_2$ ) representative super-ellipses for two different volume fraction. The idea is to observe the influence of the smoothing exponent parameter  $q$  in the maximum stress norm. In Figure 6, we show the  $\sigma_{11}^{\text{loc}}(y)$  component when the cell is loaded with a macroscopic stress  $\sigma = [1 \ 0 \ 0]$ . We observe that circles ( $q = 2$ ) and rectangles ( $q = 32$ ) are far from optimal. Circular holes suffers from imposing areas with very small thickness which entails large stress concentrations. Alternatively, squares suffers from imposing infinite curvature in the corners which entails also large stress values. Super-ellipsoidal holes have usually smaller maximum stress when considering intermediate smoothing exponent  $q$  values. For example, for  $\rho = 0.3$ , the optimal exponent is around  $q = 8$  and for  $\rho = 0.7$  is  $q = 4$ . In Figure 6, the optimal values are inscribed in a black box. Roughly speaking, optimal exponents evidenced that large stresses are more spatially distributed (larger red areas in Figure 6). See the second experiment of the supplementary material [29] for a more exhaustive study with smaller volume fraction  $\rho$  and different macroscopic stress. This representative example evidenced the importance of selecting an optimal smoothing parameter  $q$  for minimizing the maximum stress norm.

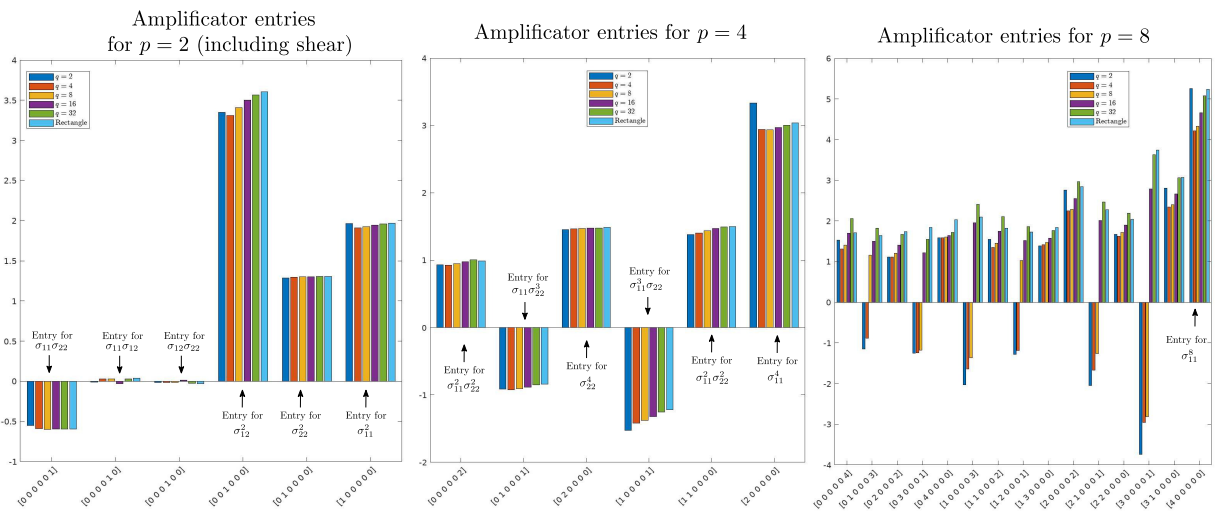


Figure 7: Entries of the stress amplification tensor  $\mathcal{P}_p$  for intermediate elongated super-ellipsoidal holes with  $2m_1 = m_2$  and  $\rho = 0.7$ . While the case  $p = 2$  includes the shear components, the three other figures do not consider shear terms. For example, the case  $[1 \ 1 \ 0 \ 0 \ 0 \ 2]$  represents the amplification entry that corresponds to  $(\sigma_{11}\sigma_{11})^1(\sigma_{22}\sigma_{22})^1(\sigma_{12}\sigma_{12})^0(\sigma_{22}\sigma_{12})^0(\sigma_{11}\sigma_{12})^0(\sigma_{11}\sigma_{22})^2 = \sigma_{11}^4\sigma_{22}^4$ .

**Amplification tensor entries.** Now we study the influence of using different super-ellipsoidal holes on the stress norm with an increasing sequence of stress norm exponent  $p$ . More specifically, we analyse the values of the amplifier entries for  $p = 2$ ,  $p = 4$  and  $p = 8$ . In the left image of Figure 7, we plot all the amplifier entries with  $p = 2$ . We observe that the shear components are the largest ones. This is not a surprise and we recall that in Part II [21], following [16], we align the micro-structure with the principal stresses and consequently shear entries become irrelevant. Thus, for simplicity, in the middle and left images of Figure 7, we plot no shear components. In Figure 7, we observe an exponential increase of the number of amplifier entries when increasing the stress norm exponent  $p$ . We also see that, after shear effects, the larger entries (for this elongated super-ellipsoidal hole) come from pure traction cases. We recall that the amplifier entries are identified through the monomial terms. For example the case [1 1 0 0 2] in the horizontal axis of the right image in Figure 7 represents the amplifier entry that corresponds to  $(\sigma_{11}\sigma_{11})^1(\sigma_{22}\sigma_{22})^1(\sigma_{12}\sigma_{12})^0(\sigma_{22}\sigma_{12})^0(\sigma_{11}\sigma_{12})^0(\sigma_{11}\sigma_{22})^2 = \sigma_{11}^4\sigma_{22}^4$ . A more exhaustive study is also reported in the second experiment of the the supplementary material [29]. We clearly observe that intermediate smoothing exponent  $q$  entails smaller values of the amplifier entries. Specially, as we increase the stress norm exponent  $p$ . This means again that rectangular and ellipsoidal holes are not optimal and confirms the need of optimizing the smoothing exponent  $q$  for minimizing the stress norm.

### 4.3 Outcome from numerical experiments

After these two numerical experiments, the following conclusions are in order.

- (i) For large size holes: rectangles (with rounded corners) are preferred (see Figure 6).
- (ii) For medium size and elongated ( $\xi \rightarrow \xi_{UB}$  or  $\xi \rightarrow \xi_{LB}$ ) holes, rectangles (with rounded corners) are also preferred (see supplementary material [29]).
- (iii) For medium size symmetric holes ( $\xi \sim \pi/4$ ), circular and super-ellipsoidal holes with small smoothing exponent  $q$  behaves better than rectangular holes (see Figure 6).
- (iv) For small holes, rectangular and ellipsoidal holes behave similar (see Figure 7 and supplementary material [29]).
- (v) The optimal smoothing exponent depends clearly on the applied macroscopic stress.
- (vi) The numerical results also suggest that, in most of the situations, intermediate values of  $q$  are better than 2 or 32, i.e. pure ellipsoidal or rectangular holes.

All these outcomes are a guide for the following optimization of the exponent  $q$  of the super-ellipsoidal hole.

## 5 Optimal micro-structure for stress minimization

This optimal design problem is decomposed in three steps. In a first step, for a given applied macroscopic stress  $\sigma$ , a given volume fraction  $\rho$  and a given semi-axis ratio  $\xi$ , the smoothing exponent  $q$  is optimized for minimizing the maximum local stress by solving the optimization problem (33). Note that, since the macroscopic stress is aligned with the microstructure and its amplitude is irrelevant in linearized elasticity, this stress is parametrized by a single scalar parameter  $\phi$  in (35). The optimal smoothing exponent  $q^* = q^*(\xi, \rho, \phi)$  thus depends on three quantities ( $\xi, \rho, \phi$ ). In a second step, the optimal exponent  $q^*$  is averaged with respect to  $\phi$ , the stress parameter. The average is not uniform but weighted with a bias in terms of  $\xi$ . It is expected that the macroscopic optimization of Part II will favor holes which are more elongated in the direction of the largest principal stress. Indeed, such an optimal behaviour is precisely quantified for rank-2 laminates in 2-d compliance minimization [11]. Here, for stress minimization we propose a kernel to average  $q^*(\xi, \rho, \phi)$  with respect to  $\phi$  with more emphasis on values which are more likely to appear for a given  $\xi$ . Finally, in a third step, the resulting average optimal exponent  $q_N(\xi, \rho)$  is approximated by a simple analytic formula, obtained by a least-square problem. In other words, this three-step process delivers a family of *nearly optimal* microstructures depending on solely two parameters: their volume fraction  $\rho$  and an anisotropy parameter  $\xi$  (semi-axis



ratio). They do not depend on the applied stress but they have been designed to be quite optimal for macroscopic stresses which are likely to appear in the macroscopic optimization of Part II.

## 5.1 Optimization problem

The results of Section 4 outlined that the optimal smoothing exponent  $q$  for minimizing the maximum stress depends on many parameters. Let us now systematize the insight obtained from these numerical experiments by solving the following optimization problem: given a semi-axis ratio  $\xi$ , a volume fraction  $\rho$  and a given loading macroscopic stress  $\sigma$ , find the optimal smoothing exponent and the semi-axis parameters  $(q^*, m_1, m_2) \in \mathcal{U}_{ad}$  which minimize

$$\min_{(m_1, m_2, q) \in \mathcal{U}_{ad}} \max_{y \in Y_0} \left\{ |\sigma^{\text{loc}}(y)|^2 = P(y)\sigma : P(y)\sigma \right\}, \quad (31)$$

where  $\sigma^{\text{loc}}(y)$ , which depends on  $(\sigma, m_1, m_2, q)$ , is the microscopic stress defined by (16) for a constant macroscopic stress  $\sigma$  (its precise computation is explained in Section 2.3). The space of admissible smoothing exponent  $q$  and semi-axis parameters  $m_i$  is defined as

$$\mathcal{U}_{ad} = \left\{ q \in \mathcal{Q}, m_1 \in \mathcal{M}_1, m_2 \in \mathcal{M}_2, \arctan\left(\frac{m_1}{m_2}\right) = \xi \quad \text{and} \quad 1 - c(q)m_1m_2 = \rho, \forall (\xi, \rho) \in \mathcal{V}_{ad}(q) \right\},$$

where  $\mathcal{Q} = [q_{\min}, q_{\max}]$ ,  $\mathcal{M}_i = [m_{L_i}, m_{U_i}]$  and  $\mathcal{V}_{ad}(q)$  is defined by (30). We recall that the dependency of the cost with respect to the design variables comes from the definition of the cell  $Y_0$  as

$$Y_0 = \{y \in Y; \quad \psi(y, m_1, m_2, q) < 0\}, \quad (32)$$

where  $\psi(y, m_1, m_2, q)$  is the level-set that defines the super-ellipsoidal hole (see Section 3.1). Although problem (31) features three independent variables, its two constraints on  $\rho$  and  $\xi$  allow us to compute explicitly  $m_1$  and  $m_2$ , for a given  $q$ . Therefore, in the end (31) becomes the following one variable minimization problem

$$\min_{q \in \mathcal{Q}_m} \max_{y \in Y_0} \left\{ |\sigma^{\text{loc}}(y)|^2 = P(y)\sigma : P(y)\sigma \right\}, \quad (33)$$

where the admissible space is defined as  $\mathcal{Q}_m = [q_{LB}, q_{UB}]$ . The values  $q_{LB}, q_{UB}$  are obtained taking into account that  $m_i \in \mathcal{M}_i = [m_{L_i}, m_{U_i}]$  by solving

$$\begin{aligned} c(q_{LB}) - \max \left( \frac{(1-\rho)}{m_{L_1} \tan(\xi)}, \frac{(1-\rho) \tan(\xi)}{m_{L_2}}, c(q_{\min}) \right) &= 0, \\ c(q_{UB}) - \min \left( \frac{(1-\rho)}{m_{U_1} \tan(\xi)}, \frac{(1-\rho) \tan(\xi)}{m_{U_2}}, c(q_{\max}) \right) &= 0, \end{aligned} \quad (34)$$

for all  $(\xi, \rho) \in \mathcal{V}_{ad}(q)$  where  $c(q)$  is the function defined in (26) for computing the volume fraction. Since  $c(q)$  is an increasing monotone function, we obtain the values of the bounds  $q_{LB}$  and  $q_{UB}$  by solving equation (34) with a simple bisection method. Concerning the stress  $\sigma$  in (33), we recall that in this approach, the micro-structure is aligned according to the principal stress, avoiding shear effects.

**Remark 1** *The orientation of the unit cell is considered as a macroscopic design variable which will be used in the macroscopic optimization problem of Part II [21]. Based on Pedersen work [22] for compliance minimization, the orientation is updated during the optimization process by aligning the unit cell with the principal stress axis, see [16], [17] for example. This is an optimal choice for compliance minimization but not necessarily for stress minimization. However, our numerical experience is that applying Pedersen orientation rule guarantees in almost all cases a decrease of the objective function and is thus a very efficient scheme because of its low computational cost.*

Therefore, in the optimization of the smoothing exponent  $q$ , we do not consider shear stress, namely we assume  $\sigma_{12} = 0$ . Additionally, note that since this work is limited to linear elasticity, the macroscopic stress norm plays no role. This would not be the case for non-linear elasticity. Consequently  $\sigma$  is parametrized (in Voigt notation) just by the stress angle  $\phi$  as

$$\sigma = [\sigma_{11} = \sin(\phi) \quad \sigma_{22} = \cos(\phi) \quad \sigma_{12} = 0]. \quad (35)$$

Solving the optimization problem (33) provides the optimal smoothing exponent  $q^*(\xi, \rho, \phi)$ . Since the objective function in (33) is a maximum value and thus is non-differentiable, we solve the optimization problem (33) with the standard successive parabolic interpolation algorithm combined with a golden section search [30]. In full generality the stress angle  $\phi$  is defined in  $[0, 2\pi]$  (with implicit periodicity condition), but changing  $\phi$  in  $\phi + \pi$  simply amounts to change the sign of  $\sigma$ , which leaves invariant the objective function in (31) and (33). Therefore, the stress angle is limited to the  $[0, \pi]$  interval and

$$q^*(\xi, \rho, \phi) = q^*(\xi, \rho, \varphi(\phi))$$

where  $\varphi$  is defined as

$$\varphi(\phi) = \begin{cases} \phi & 0 \leq \phi \leq \pi, \\ \phi - \pi & \pi \leq \phi \leq 2\pi. \end{cases} \quad (36)$$

Thus, in practice, instead of  $q^*(\xi, \rho, \phi)$ , we directly compute  $q^*(\xi, \rho, \varphi)$ . To do so, we solve problem (33) by sampling the admissible space  $\mathcal{V}_{ad}(q)$  with 400 points. Instead of uniformly sampling  $\mathcal{V}_{ad}(q)$ , we uniformly discretize  $m_1 \in [m_{L_1}, m_{U_1}]$  and  $m_2 \in [m_{L_2}, m_{U_2}]$  with 20 points and we use equations (27) (with  $q = 32$ ) to obtain the 400  $(\xi, \rho)$  sample points. The following bounds are set:  $m_{L_1} = m_{L_2} = 0.01$ ,  $m_{U_1} = m_{U_2} = 0.99$ ,  $q_{\min} = 2$  and  $q_{\max} = 32$ . The cell  $Y_0$  is discretised with an unstructured triangular mesh of typical size  $h = 0.01$ . As an example, Figure 8a displays the convergence of the cost in (33) for  $\xi = \pi/4$  ( $m_1 = m_2$ ),  $\rho = 0.15$  and  $\phi = \pi/4$  ( $\sigma_{11} = \sigma_{22}$ ) and the optimal super-ellipsoidal hole. Our experience is that in all cases, the algorithm converges in roughly  $20 \sim 30$  iterations.

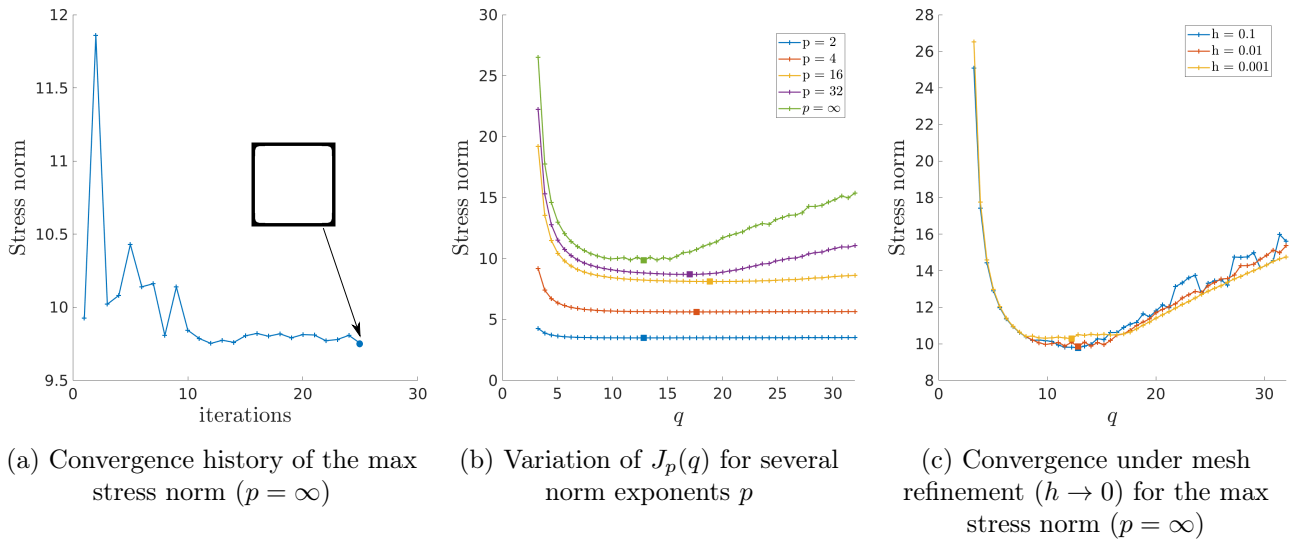


Figure 8: Optimization of the stress norm  $J_p(q)$  for  $\xi = \pi/4$  ( $m_1 = m_2$ ),  $\rho = 0.15$  and  $\phi = \pi/4$  ( $\sigma_{11} = \sigma_{22}$ ). In (b) the optimal super-ellipsoid exponent  $q^*$  is indicated with a square dot.

Remark that exchanging  $\phi$  with  $\pi/2 - \phi$  amounts to rotate the stress tensor by  $\pi/2$  (or exchanging the roles of  $\sigma_{11}$  and  $\sigma_{22}$ ). Since the super-ellipsoidal hole has cubic symmetry, rotating it by  $\pi/2$  is equivalent to exchanging the roles of the semi-axis values  $m_1$  and  $m_2$ , namely exchanging  $\xi$  with  $\pi/2 - \xi$ . Therefore, we deduce  $q^*(\xi, \rho, \phi) = q^*(\pi/2 - \xi, \rho, \pi/2 - \phi)$ , which halves the amount of computations to obtain the optimal exponent  $q^*$ . In total, we optimized (in parallel) 400 types of microstructures for 40 load stress angle  $\phi$  values (uniformly distributed). In total, we solved 16000 cases and each optimization problem has taken around 100 seconds of computation.

**Variation of the optimal super-ellipsoidal exponent  $q$  with the norm exponent  $p$ .** Although in problem (33) we considered the  $p = \infty$  norm, other choices of  $p$  are also possible. For a general  $p \geq 2$ , the stress norm is defined as

$$J_p(q) = \left( \int_{Y_0} |\sigma^{\text{loc}}(y)|^p \right)^{1/p}. \quad (37)$$

The variation of the stress norm with the optimal smoothing exponent  $q$  for different values of  $p$  is precisely represented in Figure 8b. The square markers shown in Figure 8b point the minimum value of the stress norm  $J_p(q)$ . We observe that in this case, for all norm exponent  $p$  the optimal holes are neither an ellipsoidal nor a rectangular hole but a super-ellipsoidal hole with an exponent  $q$  in the range (12; 18). Additionally, the optimal value  $q^*$  of the super-ellipsoidal exponent does not vary monotonically with the norm exponent  $p$ . Note also that for small values of  $p$ ,  $J_p(q)$  is almost flat. Thus, for small  $p$ , the optimal value of  $q$  is not very relevant since any other value of  $q$  will give similar values of  $J_p(q)$ . Most importantly, the stress norm  $J_p(q)$  has larger variations with respect to  $q$  for higher values of the norm exponent  $p$ . Thus, for large values of  $p$ , which is in general the case of interest, the optimization process with respect to  $q$  becomes crucial. This example shows that considering  $p = \infty$  for designing the optimal super-ellipsoidal hole is an appropriate choice. Note that for large norm exponent  $p$ , some oscillations appear in the graph of  $J_p(q)$ : they are due to numerical discretization errors as explained in the next paragraph.

**Convergence under mesh refinement of the optimal super-ellipsoidal exponent.** Another aspect to consider when minimizing the stress norm is the mesh size  $h$ , specially for large values of  $p$ . In Figure 8c the maximum stress norm  $J_\infty(q)$  is plotted for different mesh sizes. As expected, the value of  $J_\infty(q)$  strongly depends on  $h$  for large values of  $q$  but is well computed for smaller values, say  $q \leq 20$ . However, it turns out that in this situation the optimal exponent  $q^*$  does not depend much on the mesh size  $h$ . Even better, the function  $J_\infty(q)$  is rather flat around its minimal value which implies that a small error in the choice of the optimal smoothing exponent  $q^*$  entails merely a small change in the max stress norm. However, in other situations where the  $J_\infty(q)$  is flat almost everywhere, the mesh discretization plays, as we will see, an important role on choosing the optimal  $q^*$ . Prompted by these observations, in all our computations, we use  $h = 0.01$ .

## 5.2 Averaging with respect to stress values

The optimal exponent  $q^*(\xi, \rho, \sigma)$  clearly depends not only on the geometrical parameters  $(\xi, \rho)$  but also on the applied macroscopic stress  $\sigma$ . Recall that  $\sigma$  is parametrized by a stress angle  $\phi$  in (35). In this work, one of the goals is precisely to obtain a parametrized optimal geometry independent of the applied stress. This requirement is made for simplicity or for manufacturing reasons, as explained in [16] or [17]. The idea of the optimal design strategy in Part II [21] of our work is to use a simple parametrized family of unit cells, thus independent of the stress tensor. For that purpose, the optimal smoothing exponent  $q^*(\xi, \rho, \sigma)$  has to be averaged in terms of the stress. This averaging process should not be uniform and must take into account that the resulting cells  $Y_0$  will be used in an optimal design process. More precisely, the macroscopic structural optimization of Part II will favor some values of  $(\xi, \rho)$  for given stress  $\sigma$ . For example, it is well known that for compliance minimization the thickness of the "walls" of the micro-structure should be proportional to the stress that it has to sustain in its direction. This is rigorously proved for rank-2 laminates in 2-d [11] and it is a numerical evidence for rectangular holes in a square cell [31]. Note that this fact is different from the optimal orientation of orthotropic materials [22] which is already taken into account by taking  $\sigma_{12} = 0$ . Intuitively, the macroscopic optimization algorithm will tend to propose large/elongated rectangular holes when dealing with pure traction stresses and more symmetric holes when dealing with more hydrostatic loads.

Therefore, it is likely that micro-structures which have a semi-axis ratio  $m_1/m_2$  will be favored by the structural optimization process at places where the stress tensor ratio  $|\sigma_{11}|/|\sigma_{22}|$  has similar values. Note that the ratio  $\sigma_{11}/\sigma_{22}$  may be positive or negative, so its absolute value is close to  $m_1/m_2$  if  $\phi \sim \xi$  or  $\phi \sim \pi - \xi$ . In other words, the average of  $q^*(\xi, \rho, \phi)$  is performed with a non-uniform weight in terms of  $\phi$ , which is proportional to how close is the ratio of the principal stresses with the semi-axis ratio  $\xi$  and  $\pi - \xi$ . Then, we propose to compute the averaged optimal smoothing exponent as follows

$$q_N(\xi, \rho) = \frac{1}{2} \int_0^{2\pi} P(\phi - \xi) q^*(\xi, \rho, \varphi(\phi)) d\phi + \frac{1}{2} \int_0^{2\pi} P(\phi - (\pi - \xi)) q^*(\xi, \rho, \varphi(\phi)) d\phi, \quad (38)$$

where  $P(\phi)$  is the Gaussian probability function, with parameter  $s > 0$  (in the sequel  $s = 0.1$ ), defined

by

$$P(\phi) = \frac{1}{\sqrt{2\pi}s^2} \exp^{-\frac{\phi^2}{2s^2}}.$$

In (38) it is implicitly assumed that the functions of  $\phi$  are  $2\pi$ -periodic. In particular, the symmetry property (36) is used to define  $\varphi(\phi)$  and thus the optimal smoothing exponent is well defined for  $\phi \in [0, 2\pi]$  although it has been explicitly computed only for  $\varphi \in [0, \pi]$ . The fast decrease of the Gaussian probability function, due to the small value of parameter  $s$ , allows us to truncate  $P(\phi)$  to 0 when  $|\phi| \geq \pi/8$ , without any loss of accuracy. Similarly, the standard deviation of the optimal smoothing exponent is defined as

$$\begin{aligned} s_q(\xi, \rho) &= \frac{1}{2} \int_0^{2\pi} P(\phi - \xi) |q^*(\rho, \xi, \varphi(\phi)) - q_N(\rho, \xi)|^2 d\phi \\ &+ \frac{1}{2} \int_0^{2\pi} P(\phi - (\pi - \xi)) |q^*(\rho, \xi, \varphi(\phi)) - q_N(\rho, \xi)|^2 d\phi. \end{aligned} \quad (39)$$

In Figure 9, we plot in blue some optimal smoothing exponent  $q^*$  for different sample points  $(\xi, \rho)$  of the admissible design space  $\mathcal{V}_{ad}(q)$  and in black the mean value  $q_N$  computed according to (38). We also plot the micro-structure with the optimal super-ellipsoidal hole for different stress angles  $\phi$  and its corresponding macroscopic stress load. In red, the Gaussian probability function centered on  $\xi$  and  $\pi - \xi$  is displayed.

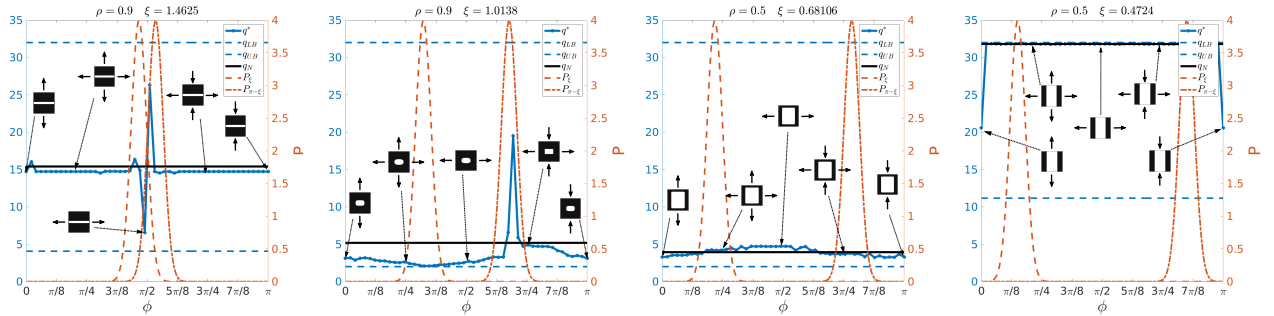


Figure 9: In blue: optimal smoothing exponent  $q^*(\xi, \rho, \phi)$  for different super-ellipsoidal holes as a function of the stress angle  $\phi$ . In red: Gaussian probability functions to average the optimal smoothing exponent according to (38). In black: averaged optimal smoothing exponent  $q_N(\xi, \rho)$ .

In the left image of Figure 9, which corresponds to a small horizontal and elongated super-ellipsoidal hole, we observe that the optimal smoothing exponent is almost constant (around a value of 15) for all stress cases, except for a strong oscillation near  $\phi = \pi/2$ , which corresponds to a horizontal traction stress load case. This is because, as can be seen in Figure 8b, for  $\phi \sim \pi/2$  the stress norm  $J_\infty(q)$  is almost flat with respect to the smoothing exponent  $q$  and consequently the mesh discretization artificially determines the optimal smoothing exponent. The weighted mean value  $q_N(\xi, \rho)$  of the smoothing exponent, from now on called averaged smoothing exponent, is the horizontal black line, which is clearly very close to the blue curve of the optimal smoothing exponent  $q^*(\xi, \rho, \phi)$ .

In the second left image of Figure 9, which corresponds to a small and quite symmetric super-ellipsoidal hole, the optimal smoothing exponent is again roughly constant, except for one peak around  $\phi \sim (\pi - \xi)$ , and its averaged value is smaller than the previous one for the horizontal hole. Again, this is due to the flatness of the stress norm function with respect to the smoothing exponent. In this case, the standard deviation is larger.

In the third and fourth left images of Figure 9, which correspond to two large super-ellipsoidal holes, one symmetric and the other vertical, the optimal smoothing exponent is almost constant for all stress angles. Its value is small for the first case and large for the second one. Thus, in both cases, the mean value  $q_N(\xi, \rho)$  is a very accurate approximation (small standard deviation). Overall, we may conclude that: (i) elongated ( $|\xi - \pi/4| \gg 1$ ) super-ellipsoidal holes entail large value of the optimal smoothing exponent  $q^*$ , while on the contrary quite symmetric ( $|\xi - \pi/4| \ll 1$ ) super-ellipsoidal holes yield small values of  $q^*$ ; (ii) the optimal smoothing exponent  $q^*$  depends weakly on the macroscopic

stress load in the sense that it is almost constant except for one peak or oscillation; (iii) even when the standard deviation of the optimal smoothing exponent  $q^*$  is large, the stress norm of the mean value  $J_\infty(q_N)$  is very similar to the stress norm of the optimal exponent  $J_\infty(q^*)$  because the stress norm function  $J_\infty(q)$  is very flat. Consequently, averaging (non-uniformly) the optimal smoothing exponent  $q^*$  in terms of the macroscopic stress load is a suitable and reasonable simplification.

### 5.3 Regularized smoothing exponent for the super-ellipsoidal hole

**Behaviour of the averaged smoothing exponent.** After solving the optimization problem (33), delivering the optimal smoothing exponent  $q^*(\xi, \rho, \sigma)$ , the weighted average, presented in (38), is applied to get the averaged smoothing exponent  $q_N(\xi, \rho)$ . We now investigate the behaviour of  $q_N(\xi, \rho)$  with respect to its variables. The first row of Figure 10 displays the standard deviation of  $q_N$ , the averaged smoothing exponent  $q_N$  and its regularization  $q_A$  in the  $(\xi, \rho)$ -plane. Note that these three plots are symmetric with respect to the vertical line  $\xi = \pi/4$  because  $\tan(\pi/2 - \xi) = 1/\tan(\xi)$ , which amounts to exchange  $m_1$  and  $m_2$ , i.e. to rotate by  $\pi/2$  the microstructure. The second row of Figure 10 displays the same quantities in the  $(m_1, m_2)$ -plane. Recall that (28) relates  $m_1$  and  $m_2$  with  $(q_N, \xi, \rho)$ . In Figure 10b is plotted the averaged smoothing exponent  $q_N(\xi, \rho)$ . We first observe that for extreme

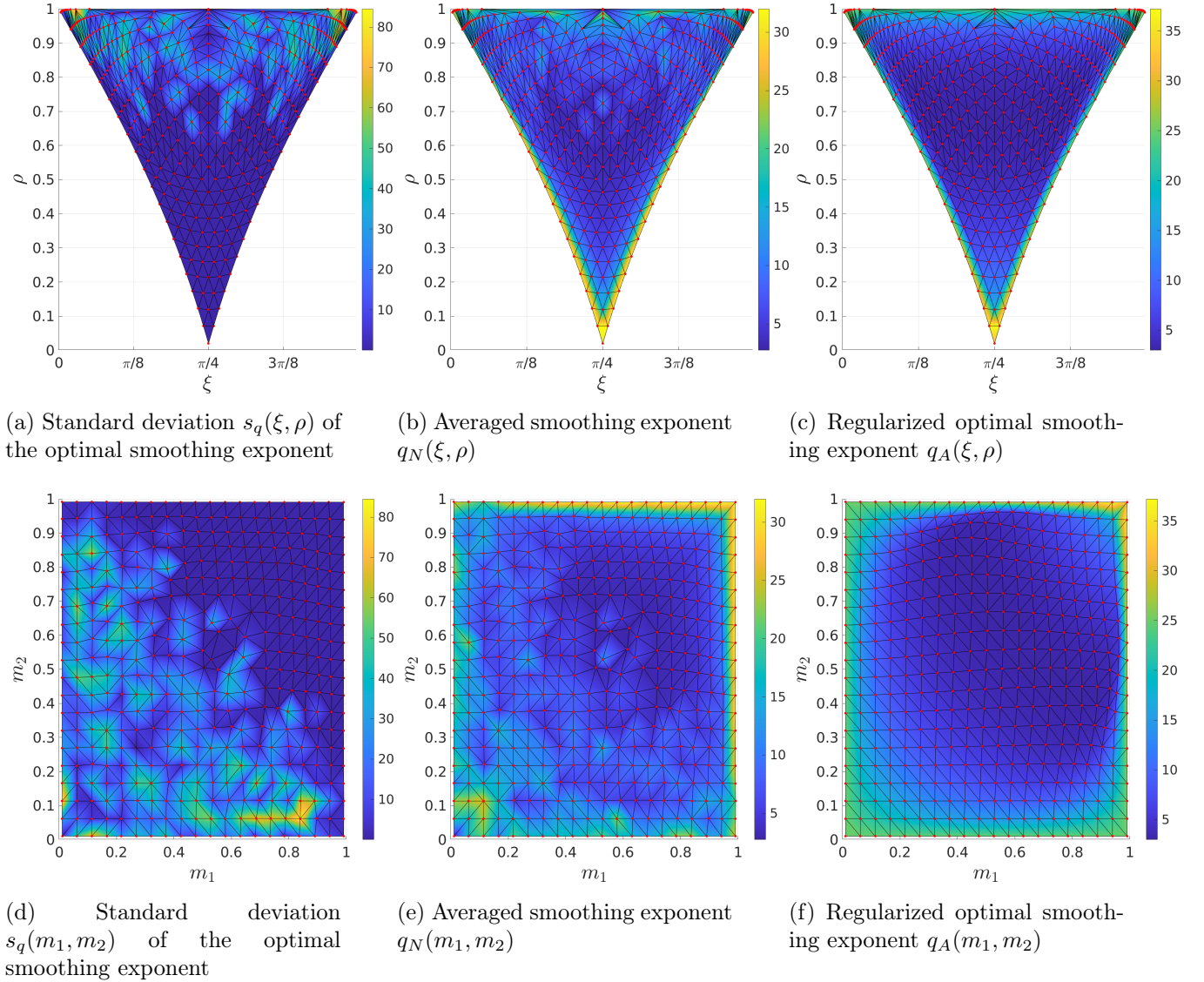


Figure 10: Averaged smoothing exponent and its regularization.

values of the semi-axis,  $\xi \rightarrow \xi_{LB}(\rho)$  or  $\xi \rightarrow \xi_{UB}(\rho)$  (see their precise definitions in (5.3) below), namely for very elongated holes, the value of  $q_N$  is very large and thus the averaged super-ellipsoidal holes are

rectangular holes (with slightly rounded corners). The dependency of  $q_N$  with the size of the hole for quite symmetric holes ( $\xi$  close to  $\pi/4$ ) features three different regimes. When the hole is very large (small  $\rho$ ), rectangular holes with rounded corners are preferred (large  $q_N$ ). For intermediate size holes ( $\rho \sim [0.2, 0.9]$ ), rounded holes (small  $q_N$ ) are preferred. For very small holes (large  $\rho$ ), although some oscillations appear, rectangular holes with rounded corners (large  $q_N$ ) seems to be preferred.

In Figure 10a the standard deviation  $s_q(\xi, \rho)$  is displayed, allowing to quantify the averaging of the optimal smoothing exponent  $q^*$ . Clearly, the averaged value  $q_N$  is a significantly accurate representation of the optimal smoothing exponent  $q^*$  for a large range of super-ellipsoidal sizes ( $\rho \in [\rho_{min}, 0.7]$ ). For small super-ellipsoidal holes ( $\rho \in [0.7, 1]$ ), especially when they are elongated ( $\xi \rightarrow \xi_{LB}$  or  $\xi \rightarrow \xi_{UB}$ ), the optimal smoothing exponent significantly varies when considering different stress load cases. However, the experiments showed us that these oscillations have a limited impact since the stress norm function  $J_\infty(q)$  is flat in these situations.

**Regularization by an analytical expression.** To simplify and regularize the behaviour of the averaged smoothing exponent  $q_N(\xi, \rho)$  (shown in Figure 10b), we propose an analytic expression to approximate and regularize  $q_N$ . There are many possible ways for regularizing  $q_N$  but, after some trial and error, we choose the following procedure. First, recall that, for given  $\rho$ , the semi-axis ratio  $\xi$  varies in the range  $(\xi_{LB}(\rho); \xi_{UB}(\rho))$ , which is defined by

$$\begin{aligned}\xi_{LB}(\rho) &= \max\left(\xi_1(m_{L_1}, q_{min}, \rho), \xi_2(m_{U_2}, q_{max}, \rho)\right), \\ \xi_{UB}(\rho) &= \min\left(\xi_1(m_{U_1}, q_{max}, \rho), \xi_2(m_{L_2}, q_{min}, \rho)\right).\end{aligned}$$

where the functions  $\xi_1$  and  $\xi_2$  are already introduced in (29). Since  $q_N(\xi, \rho)$  is symmetric with respect to the vertical line  $\xi = \pi/4$ , its regularization  $q_A(\xi, \rho)$  is built to have the same symmetry. It is defined as a combination of two approximations,  $q_{\xi_{\pi/4}}(\rho)$  which approximates  $q_N(\pi/4, \rho)$ , and  $q_{\xi_{UB}}(\rho)$  which approximates  $q_N(\xi_{UB}(\rho), \rho)$  (and by symmetry also  $q_N(\xi_{LB}(\rho), \rho)$ ), namely

$$q_A(\xi, \rho) = (1 - \xi_A(\xi, \rho)^\alpha) q_{\xi_{\pi/4}}(\rho) + \xi_A(\xi, \rho)^\alpha q_{\xi_{UB}}(\rho),$$

where  $\alpha > 0$  is a parameter to be chosen and  $0 \leq \xi_A(\xi, \rho) \leq 1$  is defined as a rescaled version of  $\xi$  by

$$\xi_A(\xi, \rho) = \frac{|\xi - \pi/4|}{\xi_{UB}(\rho) - \pi/4}.$$

The upper bound approximation  $q_{\xi_{UB}}(\rho)$  is defined as a combination of the values of the averaged smoothing exponent in  $\rho_{min}$  and  $\rho_{max}$ . Denoting  $q_{\rho_{min}} = q_N(\xi_{UB}(\rho_{min}), \rho_{min})$  and  $q_{\rho_{max}} = q_N(\xi_{UB}(\rho_{max}), \rho_{max})$ , we introduce

$$q_{\xi_{UB}}(\rho) = \left(1 - \rho_A(\rho)^\beta\right) q_{\rho_{min}} + \rho_A(\rho)^\beta q_{\rho_{max}},$$

where  $\beta > 0$  is a parameter to be chosen and  $0 \leq \rho_A(\rho) \leq 1$  is defined as

$$\rho_A(\rho) = \frac{\rho - \rho_{min}}{\rho_{max} - \rho_{min}} \quad \text{with} \quad \rho_{min} = 0.0199, \quad \rho_{max} = 0.9999.$$

The approximation  $q_{\xi_{\pi/4}}(\rho)$  for  $\xi = \pi/4$  is defined by

$$q_{\xi_{\pi/4}}(\rho) = \frac{A\rho^2 + B\rho + C}{D\rho^2 + E\rho + 1},$$

where the constants  $A, B, C, D$  and  $E$  are determined by imposing the equality  $q_{\xi_{\pi/4}}(\rho) = q_N(\pi/4, \rho)$  at  $\rho_{min} = 0.0199$ ,  $\rho_{max} = 0.9999$ ,  $\rho_s = 0.2$  and at the minimum point  $\rho_m$  of  $q_{\xi_{\pi/4}}(\rho)$ . In view of the values of  $q_N(\xi, \rho)$  in Figure 10b, we impose that  $q_{\xi_{\pi/4}}(\rho_{min}) = 32$ ,  $q_{\xi_{\pi/4}}(\rho_{max}) = 25$ ,  $q_{\xi_{\pi/4}}(\rho_m) = 3$ . The other parameters,  $\alpha = 20.252$ ,  $\beta = 0.543$ ,  $\rho_m = 0.649$  and  $q_{\rho_s} := q_{\xi_{\pi/4}}(\rho) = 11.779$ , are obtained by solving the least square problem

$$\min_{\alpha, \beta, \rho_m, q_{\rho_s}} e_r = \frac{\|q_N - q_A(\alpha, \beta, \rho_m, q_{\rho_s})\|^2}{\|q_N\|^2} \quad \text{with} \quad \|q\|^2 = \int_{\rho_{min}}^{\rho_{max}} \int_{\xi_{LB}(\rho)}^{\xi_{UB}(\rho)} q(\xi, \rho)^2 d\xi d\rho.$$

The relative error at the solution is  $e_r = 0.082$ . The optimal values of the constants are  $A \approx 52.8$ ,  $B \approx -82.0$ ,  $C \approx 37.4$ ,  $D \approx -6.8$ ,  $E = 6.2$ . The regularized smoothing exponent  $q_A$  in terms of  $(\xi, \rho)$  and  $(m_1, m_2)$  is depicted in Figures 10c and 10f: it is quite close to the averaged smoothing exponent  $q_N$  (which is computed numerically) but with less oscillations, as could be expected. Figure 11 displays a cross section, along the vertical line  $\xi = \pi/4$ , of the two exponents  $q_A$  and  $q_N$ , as functions of  $\rho$ . From now on, we use the analytical smoothing exponent  $q_A$ , instead of  $q_N$ , for computing the optimal

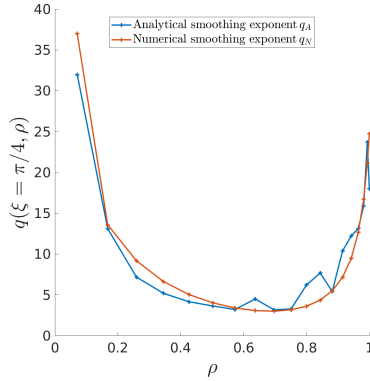


Figure 11: Analytical smoothing exponent  $q_A(\xi = \pi/4, \rho)$  and averaged smoothing exponent  $q_N(\xi = \pi/4, \rho)$ .

super-ellipsoidal holes.

**Some optimal micro-structures.** For a more visual description of the proposed optimal micro-structures, we plot in Figure 12 some of them. As observed in the numerical experiments, they range from circular and ellipsoidal holes (for small holes) to some limit cases (large square, elongated rectangular holes).

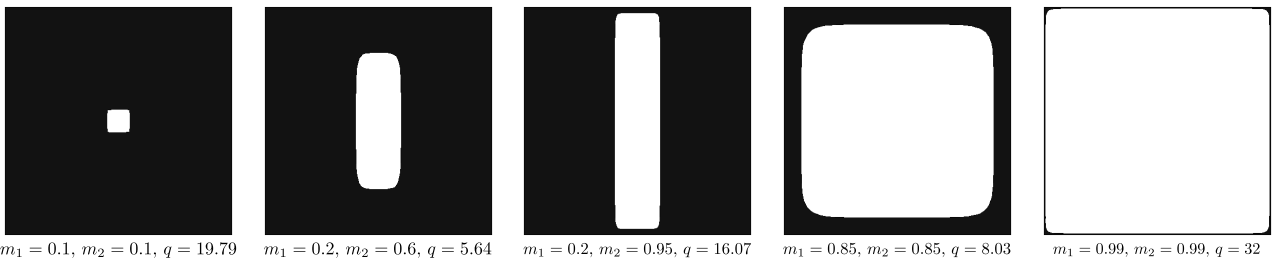


Figure 12: Some optimal super-ellipsoidal holes that minimize the maximum stress norm  $J_\infty$ .

## 5.4 Homogenized and amplification tensors for optimal super-ellipsoidal holes

Once optimal super-ellipsoidal holes have been obtained by the process just described and based on maximal stress minimization, it is time to exhibit their homogenized properties.

**Homogenized tensor  $A^*$ .** In Figure 13, the entries of the homogenized tensor are plotted for the super-ellipsoidal hole with smoothing exponent  $q_A(\xi, \rho)$ . Note that for the exponent  $q_A$ , the range of the admissible values of parameters  $(\xi, \rho)$  is identical to the admissible design space for rectangular holes  $\mathcal{V}_{ad}^R$ . This means that when solving the macroscopic stress minimization problem, detailed in Part II [21], (almost) void micro-structure could be considered. Due to horizontal and vertical symmetry, the entries  $A_{1112}^*$  and  $A_{2212}^*$  are zero and therefore are not displayed in Figure 13. The entries  $A_{1111}^*$  and  $A_{2222}^*$  strongly (and monotonically) depends on  $m_1$  and  $m_2$  respectively. Instead, the entries  $A_{1122}^*$  and  $A_{1212}^*$  strongly (and monotonically) depends on the volume fraction  $\rho$ . Again for a fix volume fraction  $\rho$ , elongated horizontal holes ( $m_1 \rightarrow 1$ ), this is of the rank-1 nature, exhibit large values of the entry  $A_{1111}^*$ . The same for  $A_{2222}^*$  with vertical elongated holes.

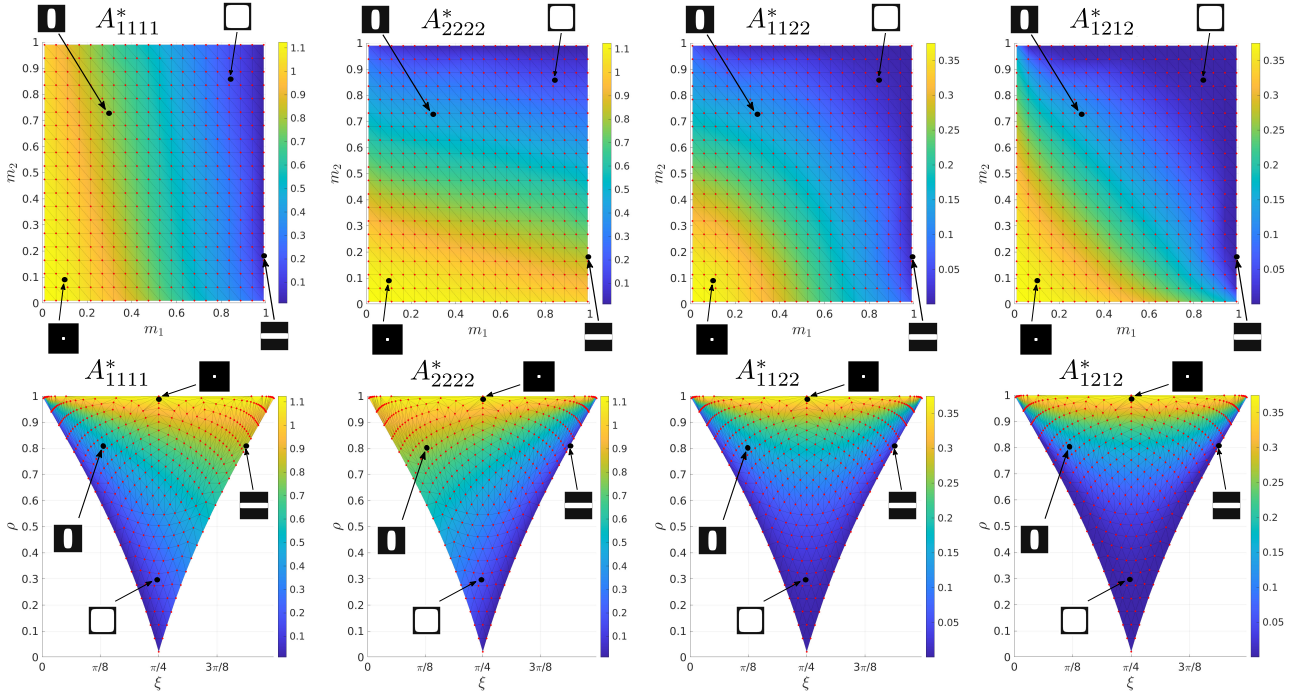


Figure 13: Entries of the homogenized tensor  $A^*$  for the super-ellipsoidal hole with smoothing exponent  $q_A(\xi, \rho)$ .

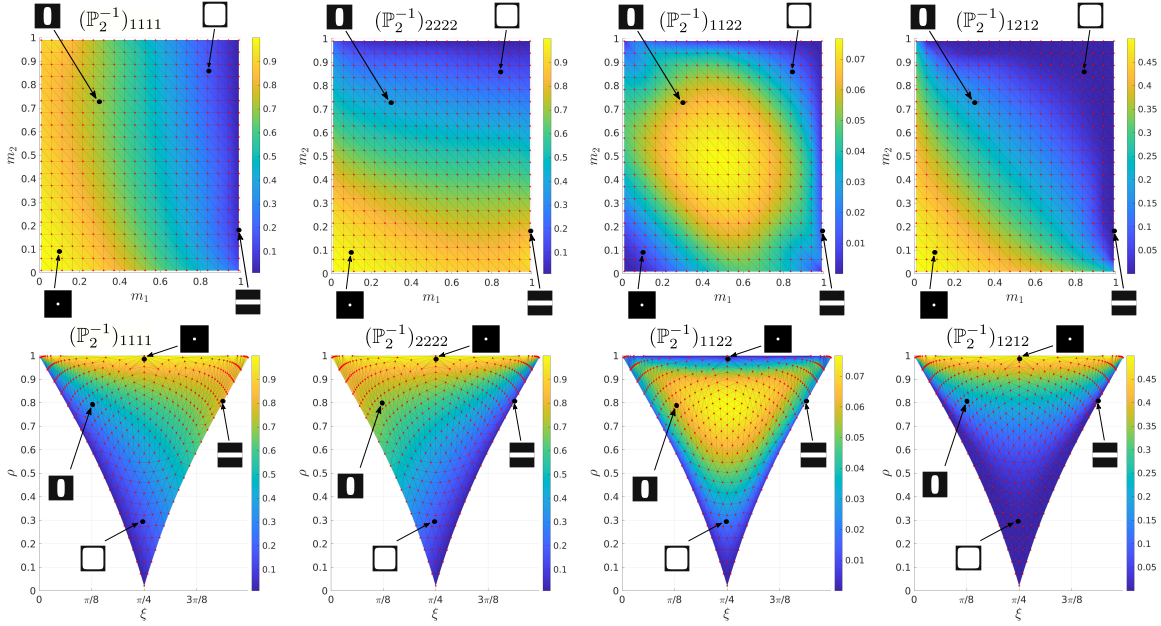


Figure 14: Inverse of the amplification tensor for the super-ellipsoidal hole with smoothing exponent  $q_A(\xi, \rho)$ .

**Amplification tensor with  $p = 2$ .** In Figure 14 is plotted the inverse of the amplification tensor (in the case  $p = 2$ ) for the super-ellipsoidal hole with smoothing exponent  $q_A(\xi, \rho)$ . We observe the strong dependency of  $(\mathbb{P}_2^{-1})_{1111}$  with respect to  $m_1$  and that of  $(\mathbb{P}_2^{-1})_{2222}$  with  $m_2$ . The entry  $(\mathbb{P}_2^{-1})_{1122}$  has a maximum in  $\xi = \pi/4$  (symmetric hole) and  $\rho = 0.8$ , while  $(\mathbb{P}_2^{-1})_{1212}$  is monotonically increasing with the volume fraction  $\rho$ .

## 5.5 Comparing optimal super-ellipsoidal holes with rectangular holes

To quantify the gain obtained by the optimization process, we compare the optimal super-ellipsoidal hole (featuring the smoothing exponent  $q_A(\xi, \rho)$ ) with a rectangular hole (or almost rectangular with



$q = 32$ ) in terms of rigidity and stress norm.

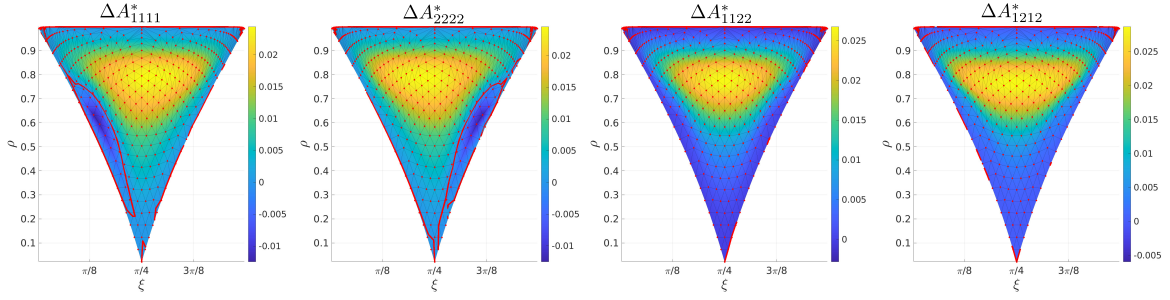


Figure 15: Difference of the homogenized tensors between the optimal super-ellipsoidal and rectangular holes.

**Homogenized tensor  $A^*$ .** In Figure 15, we plot the difference, denoted by  $\Delta A^*$ , of the homogenized tensors between the micro-structures with an optimal super-ellipsoidal hole and a rectangular hole. Where  $\Delta A^*$  is positive, optimal super-ellipsoidal holes outperforms rectangular holes in terms of rigidity and vice-versa. The zero level-set line,  $\Delta A^* = 0$ , is depicted in red to clearly distinguish both positive and negative regions. We observe that in almost all situations, the optimal super-ellipsoidal hole outperforms, in terms of rigidity, the rectangular hole. The maximum gain in terms of rigidity occurs for symmetric holes  $\xi = \pi/4$  ( $m_1 = m_2$ ) and volume fractions around  $\rho = 0.8$ . We recall that the limits  $\xi \rightarrow \xi_{UB}$  and  $\xi \rightarrow \xi_{LB}$  corresponds to the limit cases  $m_1 \rightarrow 1$  and  $m_2 \rightarrow 1$ , namely very elongated holes in the horizontal or vertical direction, respectively. Those very elongated holes behave like rank-1 laminates. Note that in the elongated horizontal limit case  $\xi \rightarrow \xi_{UB}$  (or  $m_1 \rightarrow 1$ ), the optimal super-ellipsoidal hole behaves as the rectangular hole in terms of stiffness in the horizontal direction: see  $\Delta A_{1111}^*$  when  $\xi \rightarrow \xi_{UB}$ . Of course, a symmetric situation occurs for vertically elongated holes ( $\xi \rightarrow \xi_{LB}$  or  $m_2 \rightarrow 1$ ) when looking at  $\Delta A_{2222}^*$ .

**Amplification tensor.** In Figure 16, we plot the difference, denoted by  $\Delta \mathbb{P}_2^{-1}$ , of the inverse amplification tensors between the micro-structures with an optimal super-ellipsoidal hole and a rectangular hole. Where  $\Delta \mathbb{P}_2^{-1}$  is positive, optimal super-ellipsoidal holes outperforms rectangular holes since they have a lower stress amplification tensor and vice-versa. Clearly, the gain is more marked for the entries  $(\mathbb{P}_2^{-1})_{1111}$  and  $(\mathbb{P}_2^{-1})_{2222}$  than for  $(\mathbb{P}_2^{-1})_{1122}$  and  $(\mathbb{P}_2^{-1})_{1212}$  where the differences are of the order of  $10^{-3}$ . According to Figure 16, the super-ellipsoidal hole outperforms the rectangular hole in most cases. However, there is a small zone where the rectangular hole outperforms the super-ellipsoidal hole. To understand this result, we analyse in more detail the difference of the  $(\mathbb{P}_2^{-1})_{1111}$  entry (symmetric analysis for  $(\mathbb{P}_2^{-1})_{2222}$ ) in the following four cases:

- **Medium size symmetric holes** ( $\rho \in [0.2, 0.8]$ ,  $\xi \sim \pi/4$ ): in this case the optimal super-ellipsoidal hole is clearly better than the rectangular hole because it amplifies less the stress  $\sigma_{11}^{\text{loc}}(y)$  when loading with an uni-axial horizontal macroscopic stress tensor  $\sigma = [1 \ 0 \ 0]$ . This is because, the high stress are caused here only by the corners of the hole, which for the optimal smoothing exponent case have been optimally rounded.
- **Small and large size holes** ( $\rho \in [0.8, \rho_{\max}]$  and  $\rho \in [\rho_{\min}, 0.2]$ ): the behaviours of the optimal super-ellipsoidal hole and of the rectangular hole are very similar.
- **Medium size horizontally elongated holes** ( $\rho \in [0.2, 0.8]$ ,  $\xi \rightarrow \xi_{UB}$ ): again for this type of microstructure, which is like a rank-1 laminate, the behaviours of the optimal super-ellipsoidal hole and of the rectangular hole are very similar.
- **Medium size vertically elongated holes** ( $\rho \in [0.2, 0.8]$ ,  $\xi \rightarrow \xi_{LB}$ ): we observe that the rectangular hole amplifies less the stress norm (with  $p = 2$ ). The reason for this lower performance of the optimal super-ellipsoidal hole is clear. In such a case, high stresses have two distinct origins:

they are created by the corners of the hole but also by the thin horizontal ligaments which separate the hole from the top and bottom boundary of the cell. See third image of Figure 12. Optimal super-ellipsoidal holes smooth the corners at the cost of reducing the thickness of these thin bars. Since the high stresses occupy a larger zone in these thin bars than around the corners, and because these stresses are averaged by the  $p = 2$  norm to obtain the value of  $\mathbb{P}_2$ , it turns out that rectangular holes have a smaller stress norm despite their square corners. If we had compared the stress amplification tensor  $\mathbb{P}_p$  for a much larger exponent  $p > 2$ , the optimal super-ellipsoidal hole would have superseded the rectangular hole. Eventually, it is worth noticing that, in the further process of macroscopic optimization (using the methodology proposed in [16]), the present case of a very elongated vertical hole loaded with an uni-axial horizontal macroscopic stress is very unlikely to be optimal and should not appear in practice.

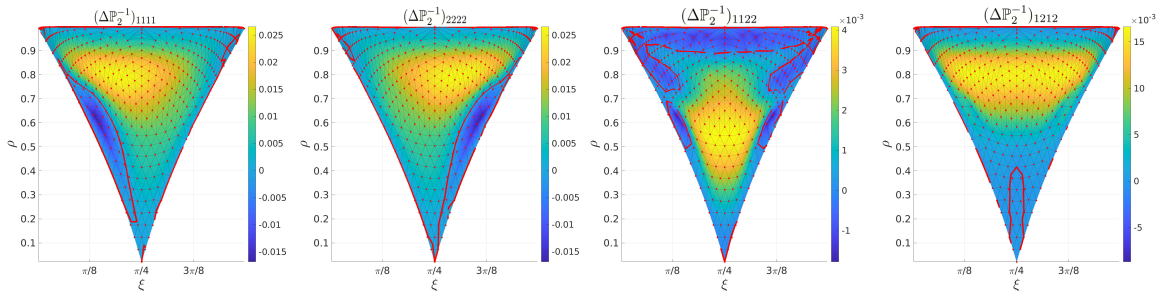


Figure 16: Difference of the inverse amplification tensors between the optimal super-ellipsoidal and rectangular holes.

## 6 Relation with the Vigdergauz micro-structure

For minimizing the stress concentration, we proposed a super-ellipsoidal hole with an optimal smoothing exponent. There is another well-known periodic micro-structure which is known to be optimal for stress distribution which is the so-called Vigdergauz micro-structure [32]. More precisely, for a macroscopic stress tensor with same sign principal stresses, the Vigdergauz micro-structure is the most rigid one for compliance minimization and is also minimizing the maximal stress norm in the cell [33]. In particular, the boundary of the hole is equi-stressed and [33] proposed an implicit expression of the boundary of the Vigdergauz micro-structure in terms of the macroscopic strains (or macroscopic stress) and the volume fraction (apart from the material properties). More recently, Liu et al. proposed in work [34] an alternative expression in terms of the volume fraction and another (non-intuitive) geometrical variable. The goal of this section is to numerically compare our micro-structure featuring a super-ellipsoidal hole with the Vigdergauz micro-structure. The conclusion is that they are very similar and the differences between their shapes is negligible in practice.

Therefore, we favor super-ellipsoidal holes because the Vigdergauz micro-structures have a very complex parametrization which is not easy to handle numerically. In fact, it is not explicit and depends on elliptic integrals and requires finding zeros of non-linear equations. This makes the super-ellipsoidal hole more convenient in terms of simplicity and computational cost.

**Level-set description of Vigdergauz micro-structure.** Let us first provide a description of the Vigdergauz micro-structure through the zero value of a level-set function. Early work [33] described the Vigdergauz micro-structure in terms of the macroscopic strain and volume fraction (and material) parameters. In [34], the Vigdergauz micro-structure is described by a symmetry (non-intuitive) parameter  $r$  and the volume fraction  $\rho$ . Here, we slightly modify the parametrization of the last work by using the semi-axis ratio  $\xi$  instead and the volume fraction parameter  $\rho$ , as we did for computing the optimal super-ellipsoidal hole. In both works [33] and [34], a parametric description of the curve is provided. However, this is not enough for representing the micro-structure in terms of the zero value of a level-set function which is in general more appropriate in a topology optimization framework. In this

work, we provide such implicit description of the micro-structure and its corresponding level-set. In the unit square cell  $Y$  with coordinates  $(y_1, y_2)$ , the level-set function of the Vigdergauz micro-structure is defined as

$$\psi_v(y_1, y_2) = \begin{cases} \psi_0 & \text{if } |y_1| \leq \frac{m_1}{2} \quad \text{and} \quad |y_2| \leq \frac{m_2}{2}, \\ c_0 & \text{otherwise,} \end{cases} \quad (40)$$

with the function  $\psi_0(y_1, y_2)$  defined by

$$\psi_0(y_1, y_2) = (1 - y_{p_1}^2)(1 - y_{p_2}^2) - R.$$

The fact that  $\psi_v$  is not continuous at the boundary of the inner rectangle  $(-m_1/2, m_1/2) \times (-m_2/2, m_2/2)$  does not matter here since only its sign is important. Thus, the value of  $c_0 < 0$  can be taken arbitrarily but negative. In this work, we take  $c_0 = -|\psi_0|$ . The coordinates  $y_{p_1}$  and  $y_{p_2}$  are computed as

$$y_{p_1} = F^{-1}\left(\frac{y_1 f_1}{m_1/2}, r_1\right) \quad \text{and} \quad y_{p_2} = F^{-1}\left(\frac{y_2 f_2}{m_2/2}, r_2\right)$$

and the parameters  $f_1 = F(\sqrt{1-R}, r_1)$  and  $f_2 = F(\sqrt{1-R}, r_2)$ , where  $R = (1-r_1)(1-r_2)/(r_1 r_2)$ . The function  $F(t, k)$  is the incomplete elliptic integral of first kind defined by

$$F(t, k) = \int_0^t \frac{dx}{\sqrt{(1-x^2)(1-kx^2)}}$$

and  $F^{-1}(t, k)$  is the Jacobi elliptic function, precisely defined as the inverse of  $t \rightarrow F(t, k)$ . Both functions are implemented in almost all numerical software packages. The semi-axis parameters  $m_1$  and  $m_2$  of the Vigdergauz micro-structures can be expressed only in terms of  $r_1$  and  $r_2$  as

$$m_1 = \frac{1-t_2}{1-t_1 t_2} s_1 \quad \text{and} \quad m_2 = \frac{1-t_1}{1-t_1 t_2} s_2$$

where the parameters  $t_1, t_2, s_1$  and  $s_2$  are given by

$$\begin{aligned} t_1 &= \frac{F(1, 1-r_1)}{F(1, r_1)}, & s_1 &= \frac{f_1}{F(1, r_1)}, \\ t_2 &= \frac{F(1, 1-r_2)}{F(1, r_2)}, & s_2 &= \frac{f_2}{F(1, r_2)}. \end{aligned}$$

Knowing the values of the parameters  $r_1$  and  $r_2$ , we can explicitly compute the level-set function (40). Such values are determined by imposing a priori given values for the semi-axis ratio  $\xi$  and volume fraction  $\rho$ . This is done by solving the following two non-linear equations

$$\tan(\xi) = \frac{m_1}{m_2} = \frac{1-t_2}{1-t_1} \frac{s_1}{s_2}, \quad (41)$$

$$\rho = 1 - \frac{t_1(1-t_2) + t_2(1-t_1)}{(1-t_1 t_2)}, \quad (42)$$

with  $r_1$  and  $r_2$  as unknowns, which are bounded by  $0 < r_1 < 1$  and  $0 < r_2 < 1$ . Note that all variables that appear in (42) depend only on  $r_1$  and  $r_2$ . In this work, we used two nested bisection loops to solve these two non-linear equations. In Figure 17, some examples of the Vigdergauz micro-structures are plotted which look reasonably similar to square micro-structures with a super-ellipsoidal hole.

**Closest super-ellipsoidal hole.** From the previous analysis the level-set function of the Vigdergauz micro-structure  $\psi_v(\xi, \rho)$ , defined by (40), is precisely parametrized by the semi-axis ratio  $\xi$  and the volume fraction  $\rho$ . Recall that the level-set function of the super-ellipse  $\psi_s(q, \xi, \rho)$ , defined in (25), was characterized in terms of the volume fraction  $\rho$ , the semi-axis ratio  $\xi$  and the smoothing parameter  $q$  through equation 28. Thus, our goal is to find the best  $q$  such that both micro-structures are as close as possible in the following sense. The difference between two characteristic functions is measured

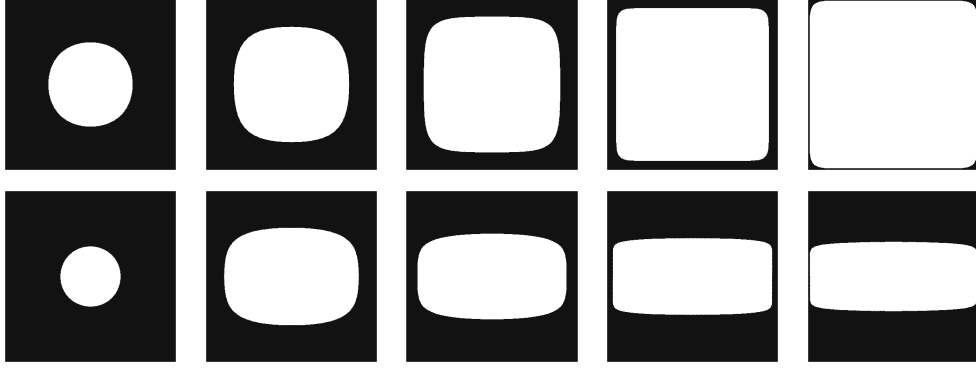


Figure 17: Vigdergauz micro-structures examples

with the  $L^1$  norm which represents the volume of the difference set. For numerical reasons we rely on a smoothed version of the characteristic function which is defined by the zero level-set. We use a standard discrete (with compact support) kernel filter for the smoothing, which was introduced in [35] and is denoted by  $P_1 : L^\infty(Y, \{0, 1\}) \rightarrow L^\infty(Y, [0, 1])$  where  $Y$  is the micro-structure cell domain. Thus, the optimization problem to solve is

$$\min_{q \in [q_{\min}, q_{\max}]} \int_Y |\rho_s(\xi, \rho, q) - \rho_v(\xi, \rho)| \quad (43)$$

where the densities functions  $\rho_s(\xi, \rho, q)$  and  $\rho_v(\xi, \rho)$  are defined as

$$\rho_s(\xi, \rho, q) = P_1(\chi_s(\xi, \rho, q)) \quad \text{and} \quad \rho_v(\xi, \rho) = P_1(\chi_v(\xi, \rho)).$$

Thus, they are the smoothed versions of the characteristic functions

$$\chi_s(\xi, \rho, q) = \begin{cases} 0 & \text{if } \psi_s(\xi, \rho, q) > 0 \\ 1 & \text{if } \psi_s(\xi, \rho, q) \leq 0 \end{cases} \quad \text{and} \quad \chi_v(\xi, \rho) = \begin{cases} 0 & \text{if } \psi_v(\xi, \rho) > 0, \\ 1 & \text{if } \psi_v(\xi, \rho) \leq 0. \end{cases}$$

Since problem (43) is a minimization problem with respect the sole variable  $q$ , we use again a successive parabolic interpolation algorithm combined with a golden section search [30]. In Figure 18, some

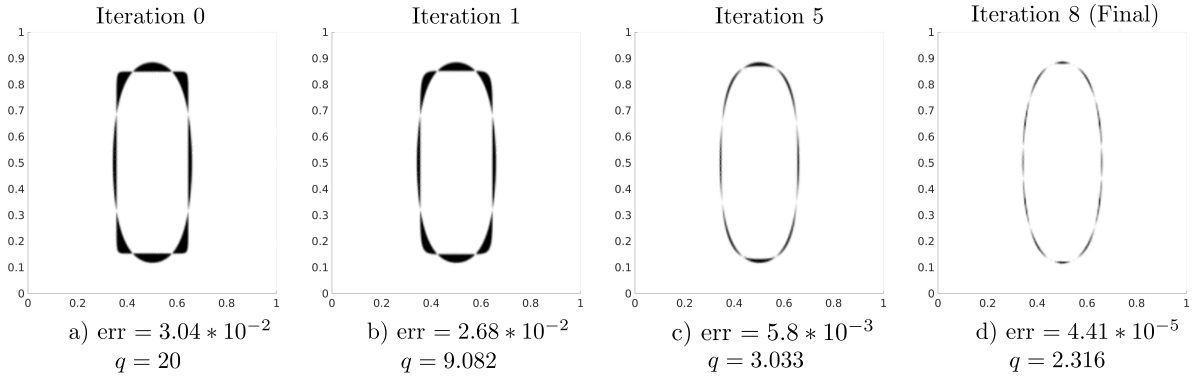


Figure 18: Symmetric difference between a Vigdergauz micro-structures and a square micro-structure with a super-ellipsoidal hole (from left to right, improving value of the exponent  $q$ , from 20 to 2.316). The relative error of the densities is given as  $\text{err} = \frac{\int_Y |\rho_s - \rho_v|}{\int_Y |\rho_v|}$ .

intermediate and the final iterations of the optimization problem (with  $q_{\min} = 2$  and  $q_{\max} = 32$ ) are shown for the hole  $\xi = \pi/8$  ( $m_2 = 2.41m_1$ ) and  $\rho = 0.8$ . A triangular mesh with 102400 P1 finite elements with a total of 51521 nodes is used. Clearly, one can observe in Figure 18 that the Vigdergauz micro-structure is approximated by a super-ellipsoidal hole with a very high accuracy (negligible error). This experiment justifies the use of a super-ellipsoidal hole instead of the Vigdergauz micro-structure when minimizing the maximum stress since we can obtain similar results but with much more simplicity.

## 7 Conclusion

This is the first part of a work devoted to the optimization of lattice structures for stress minimization. This first part focused on the design of a family of 2-d parametrized periodicity cell which are nearly optimal for local stress minimization. These parametrized cells will be used in the second part [21] for optimizing the macroscopic lattice structures, by using a de-homogenization technique, as presented in [16] for compliance minimization.

We proposed in this work to optimize a square cell with a super-ellipsoidal hole. On the one hand, it is rich enough to generalize the standard rectangular and ellipsoidal holes and on the other hand it is simple enough to be explicitly described and further used in the de-homogenization method of Part II [21].

Before optimizing the micro-structure, two numerical experiments were performed to gain insight in the design process. First, we compared rectangular and ellipsoidal holes in terms of effective properties, as well as amplification tensors, which take into account the local increase of the stress, compared to the macroscopic stress, due to the micro-structure. Second, the amplification factors were computed for various values of the exponent  $p$  when the stress is evaluated with an  $L^p$  norm. They confirm that neither rectangles, nor ellipses are always optimal and that super-ellipses are a good compromise.

Our main result is the optimization of the exponent  $q$ , defining the super-ellipse for minimizing the maximum local stress when solving a periodic cell problem, loaded by a given macroscopic stress. For each stress load (aligned with the hole), each volume fraction and each semi-axis ratio, an optimal super-ellipse exponent  $q$  has been found. Since the goal is to design a micro-structure which depends only on geometric parameters and not on the applied stress, these optimal super-ellipse exponents were averaged with respect to the applied stress with a bias towards stresses which are more likely to appear in the macroscopic optimization of Part II. Then, for simplicity and further use, we proposed an analytical formula for approximating the optimal averaged exponent in terms of the geometrical parameters of the super-ellipsoidal hole. We observed a clear reduction of the stress norm (through the amplifier tensor) of the proposed optimal super-ellipsoidal hole with respect of the rectangular hole. As a final check of our results, we compared the optimal super-ellipsoidal hole with the Vigdergauz micro-structure, which is known to be optimal for minimizing the maximum stress in some cases, but is not simple enough for a systematic use in numerical computations. We numerically checked that the Vigdergauz micro-structure can be approximated by an optimal super-ellipsoidal hole with high accuracy.

**Acknowledgements.** This work is partially supported by the SOFIA project, funded by Bpifrance (Banque Publique d'Investissement). This work has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 833092.

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