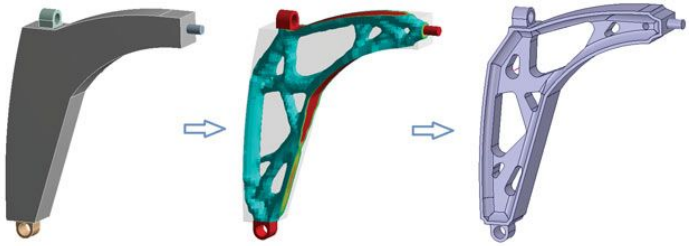
香港中文大學
The Chinese University of Hong Kong

MAEG5160: Design for Additive Manufacturing

Lecture 13: Design with anisotropic materials



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Lecture 13: Design with anisotropic materials

In previous lectures, we have concentrated on the generation of optimal topologies based on the use of *isotropic* materials within the framework of "classical" black-white (or 0-1) structures. Early developments in topology optimization were build around the employment of *composite materials* as an interpolation of void and full material. This was founded on theoretical work that had lead to the understanding that the issue of existence of solutions can be resolved by extending the design space to include relaxed designs, here in the form of composites.

When introducing composites as part of the solution method in topology design one has to deal with a number of aspects of materials science and specifically methods for computing the effective material parameters of composites. Thus *homogenization* is an intrinsic part of topology design together with the area of material science which is concerned with bounds on the properties of composites. The latter deals with the limits on the possible effective material behaviour and directly gives information on the optimal use of local material properties.

What is thus named the *homogenization approach* for topology design constitutes the basis for many studies in topology design. One can here distinguish between the use of the methodology mainly as a tool for interpolation of properties and studies where existence of solutions is a central aspect. One will find that many of the developments previously have a counterpart based on the homogenization method as an interpolation tool. On the other hand, the complete theoretical insight of the existence issue has presently only been gained for problems involving compliance and fundamental frequency optimization.

Design with composite materials is, of course, an important area in its own right. This involves such issues as the optimal choice of orientation of an orthotropic material and especially the optimal layup of laminates. Moreover, one can choose to work with a completely free parametrization of the stiffness tensor in order to find the optimal design where any material can be used. The homogenization method and such aspects of the optimal use of material in a broad sense is the topic of this lecture.

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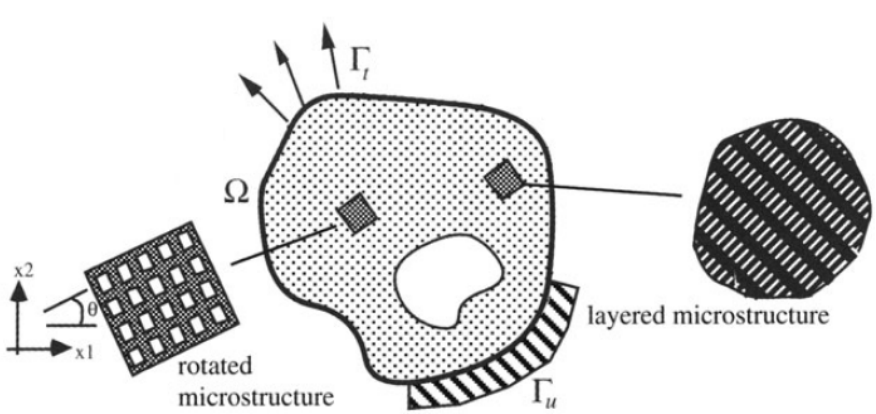

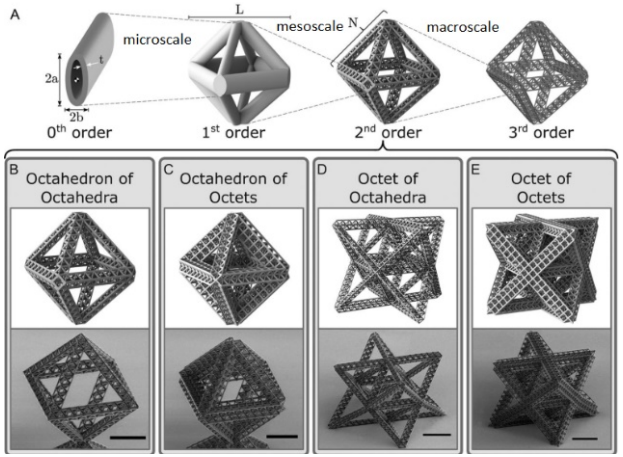

A structure made of materials with micro structure. Notice how the micro structure is rotated by a rotation of the unit cells

1. The homogenization approach

1.1 Parametrization of design

We have already noted that the original 0-1 problem statement of topology design lacks existence of solutions in the continuum setting (the distributed problem). We have hitherto used a *restriction* method to assure existence of solutions. On the other hand, existence studies shows that nonconvergent, minimizing sequences of admissible designs with finer and finer geometrical details that can be found for the original "0-1" problem and that these limits should be interpreted as designs where composites made from the original material (and void) are integral parts of the optimal structure.

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If we decide to work with an *extension* of the design space, the key to assuring the existence of solutions to our basic shape optimization problem with unknown topology is thus the introduction of composite materials constructed from the given isotropic material. The design variable is then the continuous density of the base material in these composites. We immediately note that such a *relaxation* of the problem in itself provides an interpolation for use in computations, as the composites allows for a density of material, i.e., a definition of "grey". Introducing a composite material consisting of an infinite number of infinitely small holes periodically distributed through the base material, the topology problem is consequently transformed to the form of a sizing problem where the sizing variable is the material density ρ. As in SIMP, the on-off nature of the problem is avoided through the introduction of this density, with $\rho = 0$ corresponding to a void, $\rho = 1$ to material and $0 < \rho < 1$ to the porous composite with voids at a micro level. We thus in this situation have a set of admissible E_{ad} stiffness tensors given in the form:

$$
\begin{aligned}
&\text{Geometric variables } \mu, \gamma, \ldots \in L^\infty(\Omega), \text{ angle } \theta \in L^\infty(\Omega) \ , \\
&E_{ijkl}(x) = \tilde{E}_{ijkl}(\mu(x), \gamma(x), \ldots, \theta(x)), \\
&\text{density of material } \rho(x) = \rho(\mu(x), \gamma(x), \ldots) \ , \\
&\int_\Omega \rho(x) \mathrm{d}\Omega \leq V; \ 0 \leq \rho(x) \leq 1, \ x \in \Omega \ ,
\end{aligned}
$$

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where $E_{ijkl}(x)$ are the effective material parameters for the composite. These quantities can be obtained analytically or numerically through a suitable micro mechanical modelling. The composite material will, in general, be anisotropic (or orthotropic) so the angle of rotation (θ) of the directions of orthotropy enters as a design variable, via well-known transformation formulas for frame rotations. Observe that the density of material ρ is, in itself, a function of a number of design variables which describe the geometry of the holes at the micro level and it is these variables that should be optimized. This means that one typically will have more than one design variable per spatial point (or mesh element).

Note that for any material consisting of a given linearly elastic material with microscopic inclusions of void, intermediate values of the density of the base material will provide the structure with strictly less than proportional stiffness. In an optimal structure one could then expect to find p-values of 0 and 1 in large areas. On the contrary, the optimal application of the microstructures (see later) usually results in a very efficient use of intermediate densities of material and the resulting designs have large areas of "grey". One central aspect of this optimal employment of composites is the possibility to adapt to the directions of strain/stress - in a manner of speech, isotropic materials "waste" material also on non-loaded directions.

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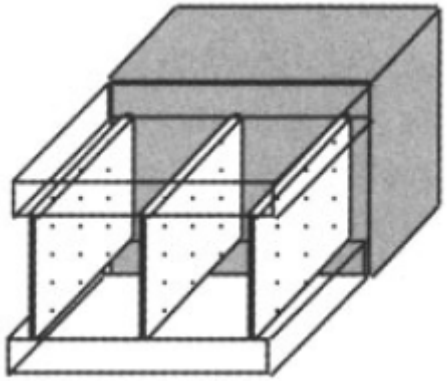
In the initial studies of the homogenization approach, composites consisting of square or rectangular holes in periodically repeated square cells were used for planar problems, and these still play a central role in many applications. Later so-called ranked laminates (layers) have also become popular, both because analytical expressions of their effective properties can be given and because existence of solutions to the minimum compliance problem for both single and multiple load cases in this case can be formally proved (without any additional constraints on the design space).



A 3-dimensional cell of a rank-3 layering, with orthogonal layerings at three different scales. This microstructure is useful for single load problems in 3 dimensions.

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1.2 The homogenization formulas

The "homogenization approach" to topology design of continuum structures as described above relies on the ability to model a material with microstructure, thus allowing for the description of a structure by a density of material. Here one takes an approach where the porous material with microstructure is constructed from a basic unit cell, consisting at a macroscopic level of material and void. The composite, porous medium then consists of infinitely many of such cells, now infinitely small, and repeated periodically through the medium. At this limit, we can also have continuously varying density of material through the structure. The resulting medium can be described by effective, macroscopic material properties which depend on the geometry of the basic cell, and these properties can be computed by invoking the formulas of homogenization theory.

The computation of these effective properties play a key role for the topology optimization. Also, the formulas are central for comparing the different choices of cell structure and they form the basis for the topology design of the materials themselves, where the formulas have already been presented. However, the formulas of homogenization will again be briefly presented here for the case of dimension 2. Suppose that a periodic micro structure is assumed in the neighbourhood of an arbitrary point x of a given linearly elastic structure. The length of periodicity is represented by a parameter δ which is very small and the elasticity tensor E_{ijkl} is given in the form

$$E^{\delta}_{ijkl}(x) = E_{ijkl}(x, \frac{x}{\delta})$$

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where $y \to E_{ijkl}(x,y)$ is Y-periodic, with cell $\mathrm{Y} = [\mathrm{Y}_{1\mathrm{R}}, \mathrm{Y}_{1\mathrm{L}}] \times [\mathrm{Y}_{2\mathrm{R}}, \mathrm{Y}_{2\mathrm{L}}]$ of periodicity. Here x is the macroscopic variation of material parameters, while x/δ gives the microscopic, periodic variations. Now, suppose that the structure is subjected to a macroscopic body force and a macroscopic surface traction. The resulting displacement field $u^\delta(x)$ can then be expanded as

$$u^\delta(x) = u_0(x) + \delta u_1(x, \frac{x}{\delta}) + \ldots\ldots\ldots ,$$

where the leading term $u_0(x)$ is a macroscopic deformation field that is independent of the microscopic variable y. It turns out that this effective displacement field is the macroscopic deformation field that arises due to the applied forces when the stiffness of the structure is assumed given by the effective stiffness tensor

$$E^{\mathbf{H}}_{ijkl}(x) = \frac{1}{|\mathrm{Y}|}\int_{\mathrm{Y}} \left[E_{ijkl}(x,y) - E_{ijpq}(x,y)\frac{\partial \chi^{kl}_p}{\partial y_q} \right] \mathrm{d}y \ . \tag{3.2}$$

Here χ^{kl} is a microscopic displacement field that is given as the Y-periodic solution of the cell-problem (in weak form):

$$\int_{\mathrm{Y}} \left[E_{ijpq}(x,y)\frac{\partial \chi^{kl}_p}{\partial y_q} \right] \frac{\partial \varphi_i}{\partial y_j} \mathrm{d}y = \int_{\mathrm{Y}} E_{ijkl}(x,y)\frac{\partial \varphi_i}{\partial y_j} \mathrm{d}y \ \text{for all} \ \varphi \in U_{\mathrm{Y}} \ , \tag{3.3}$$

where U_{Y} denotes the set of all Y-periodic virtual displacement fields.

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With $y^{11} = (y_1, 0)$, $y^{12} = (y_2, 0)$, $y^{21} = (0, y_1)$ and $y^{22} = (0, y_2)$, the variational form for the definition of the effective properties is:

$$E^H_{ijkl}(x) = \min_{\varphi \in U_Y} \frac{1}{|\mathrm{Y}|} a_{\mathrm{Y}}(y^{ij} - \varphi, y^{kl} - \varphi) \ ,$$

while the form of the equations (3.2) and (3.3) in compact notation is

$$E^H_{ijkl}(x) = \frac{1}{|\mathrm{Y}|} a_{\mathrm{Y}}(y^{ij} - \chi^{ij}, y^{kl} - \chi^{kl}) \ ,$$

$$a_{\mathrm{Y}}(y^{ij} - \chi^{ij}, \varphi) = 0 \quad \text{for all } \varphi \in U_{\mathrm{Y}} \ .$$

From Equations (3.2) and (3.3) we see that the effective moduli for plane problems can be computed by solving three analysis problems for the unit cell Y. For most geometries this has to be done numerically using finite element methods or, as can be advantageous, by use of boundary element methods or spectral methods. For use in a design context the homogenization process should be implemented as an easy-to-use pre-processor. Equations (3.2) and (3.3) hold for mixtures of linearly, elastic materials and for materials with voids. Figure below shows the variation of the effective moduli for a material consisting of square cells with square holes.

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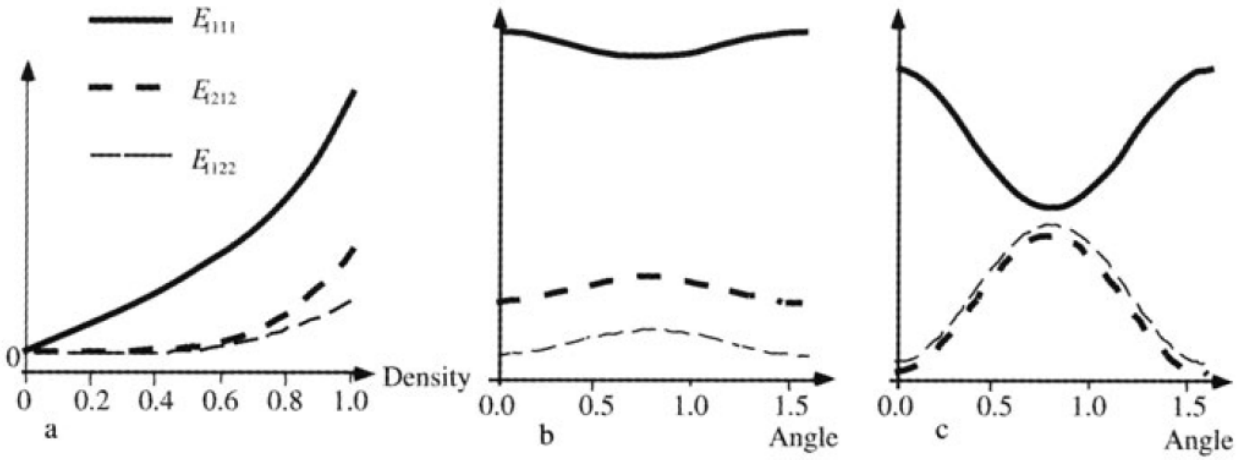

The dependence of the effective material properties of a periodic composite with square holes in square cells on the size of hole and the angle of rotation of the cell. a): The effective properties in a frame aligned with the directions of the sides of the cell. Dependence on material density *p.* The dependence on cell rotation (seen from a fixed frame), b) for a small sized hole with density of material in the cell of 0.91 and c) for a large sized hole with density of material 0.36.

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It is important here to underline that the use of homogenized material coefficients is consistent with a basic property of the minimum compliance problem. To this end, consider a minimizing sequence of designs in the set of 0-1 designs and assume that this sequence of designs consists of micro cells given by a scaling parameter $\delta>0$. In the limit of $\delta \rightarrow 0$, the sequence of designs has a response governed by the homogenized coefficients. It is a fundamental property of the homogenization process that the displacements $u^{\delta}(x)$ of the sequence of designs will converge *weakly* to the displacement $U_0(x)$ of the homogenized design. As the compliance functional is a weakly continuous functional of the displacements this implies the convergence of the compliance values. We can thus conclude that inclusion of homogenized materials in the design formulation does not provide for a jump in performance, but rather provides (some) closure of the design space. Moreover, at the same time we achieve a design description by continuous variables, and can avoid the recourse to any additional interpolation scheme.

We remark that *layered materials have analytical expressions for the effective moduli and this is a distinct advantage for optimization*. For other types of micro voids the effective moduli have to be computed numerically for a number of dimensions of the voids in the unit cell, and for other values of densities the effective moduli can be interpolated using for example Legendre polynomials or splines; this gives an easy method for computing design derivatives as well. Note that the interpolation only needs to be carried out for different values of Poisson's ratio, as Young's modulus enters as a scaling factor.

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Layered material We now consider a layered material (cf., scale 2 of Fig. 3.2 rotated 90°) with layers directed along the y_2-direction and repeated periodically along the y_1-axis. The unit cell is $[0,1] \times \mathbf{R}$, and it is clear that the unit cell fields χ^{kl} are independent of the variable y_2. Also note that in Equation (3.2), the term involving the cell deformation field χ^{kl} is of the form $E_{ijpq}(x,y)\frac{\partial \chi_p^{kl}}{\partial y_q}$, so an explicit expression for χ^{kl} is not needed. Using periodicity and appropriate test functions and assuming that the direction of the layering coalesces with the directions of orthotropy of the materials involved, the only non-zero elements E_{1111}, E_{2222}, $E_{1212}(= E_{1221} = E_{2121} = E_{2112})$, $E_{1122}(= E_{2211})$ of the tensor E_{ijkl} can be calculated as shown in Appendix 5.4. Specifically, for a layering of two isotropic materials with the same Poisson ratio ν, with different Young's moduli E^+ and E^- and with layer thicknesses γ and $(1-\gamma)$, respectively, the layering formulas (in plane stress) reduce to the following simple expressions:

$$E^H_{1111} = I_1,\ E^H_{2222} = I_2 + \nu^2 I_1,\ E^H_{1212} = \frac{1-\nu}{2} I_1,\ E^H_{1122} = \nu I_1\ ,$$

$$I_1 = \frac{1}{1-\nu^2}\frac{E^+E^-}{\gamma E^- + (1-\gamma)E^+},\ I_2 = \gamma E^+ + (1-\gamma)E^-\ .$$

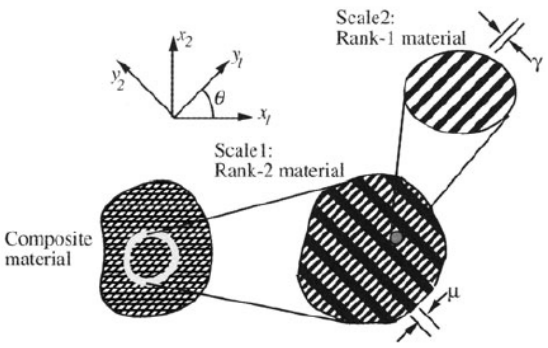

Figure 3.2

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It has been noted earlier that layered materials (so-called rank-N layered materials) play an important role as a class of composites for use in the homogenization approach. Such materials are created by successive layering of one material with composites already constructed. For example, the construction of a rank-2 layering is as follows. First, a (first order) layering of the strong and the weak material (void in the following) is constructed (see scale 2 of Fig. 3.2). This resulting composite material is then used as one of two components in a new layered material, with layers of the isotropic, strong material and of the composite just constructed; the layers of this composite material are placed at an angle to the direction of the new layering. The effective material properties of the resulting material can be computed by recursive use of the effective material parameters for a layering and the moduli are computed as the material is constructed, bottom up. The rank-N construction is analogous, and just includes more steps. For a rank-2 layering of material and void, with *perpendicular* layerings and with primary layerings of density μ in the 2-direction and the secondary layer of density γ in direction 1 (as in Fig. 3.2), the resulting material properties are:

$$E^H_{1111} = \frac{\gamma E}{\mu\gamma(1-\nu^2)+(1-\mu)}, \quad E^H_{1122} = \mu\nu E^H_{1111},$$
$$E^H_{2222} = \mu E + \mu^2\nu^2 E^H_{1111}, \quad E^H_{1212} = 0\ ,$$

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where E is Young's modulus and ν is Poisson's ratio of the base material. Also,the total density of the strong material in the unit cells of this rank-2 layered material is

$$\rho = \mu + (1-\mu)\gamma = \mu + \gamma - \mu\gamma \ .$$

The importance of the layered materials not only hinges on the analytical formulas for the effective material parameters. Of equal significance, studies on bounds on the effective material properties of composite mixtures made of two isotropic materials have shown that for elasticity the stiffest (or softest) material for a single load or multiple load problem can be obtained by a layered medium, with layering at several microscales. For single load problems the stiffest material consists of orthogonal layers, with no more than 2 layers for dimension 2 and no more than 3 layers for dimension 3. For multiple load problems the stiffest material (for the weighted average formulation) consists of layers that are not necessarily orthogonal, up to 3 for dimension 2 and up to 6 for dimension 3. The rank-2 materials are not the only composites which in 2-D achieves the upper bound on stiffness of a mixture of two materials. The layered materials are thus not special in the sense of being uniquely optimal, but they are special in the sense that their effective material properties can be expressed analytically.

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Parametrization by moments

The formulas presented above become very cumbersome if one employs rank-N layerings with many non-perpendicular layers. In this case it is more convenient to work with the so-called *moment* formulation for the effective material properties.

It turns out that the full range of effective material properties for *all* rank-N layerings in 2-D can be described by just 5 parameters (see Appendix 5.4). These are the bulk density ρ of material together with four moments (m_1, m_2, m_3, m_4) that are parameters of the form

$$\left.\begin{aligned} m_1 &= \textstyle\sum_{r=1}^{m} \mu_r \cos(2\theta^r),\ m_2 = \sum_{r=1}^{m} \mu_r \cos(4\theta^r)\ , \\ m_3 &= \textstyle\sum_{r=1}^{m} \mu_r \sin(2\theta^r),\ m_4 = \sum_{r=1}^{m} \mu_r \sin(4\theta^r)\ , \end{aligned}\right\} \text{ with } \sum_{r=1}^{m} \mu_r = 1\ .$$

In terms of these moments and the density ρ, the effective compliance tensor can for example be written as (in plane stress and for layerings of material and void)

$$C^H = C^+ + \frac{(1-\rho)}{\rho E}[D]^{-1}\ ,$$

where the entries of the tensor D are

$$\begin{aligned} D_{1111} &= \tfrac{1}{8}(3 + m_2 - 4m_1)\ , \quad D_{2222} = \tfrac{1}{8}(3 + m_2 + 4m_1)\ , \\ D_{1122} &= D_{2211} = \tfrac{1}{8}(1 - m_2)\ , \\ D_{1112} &= D_{1121} = D_{2111} = \tfrac{1}{8}(m_3 - m_4)\ , \\ D_{1222} &= D_{2221} = D_{2122} = D_{2212} = \tfrac{1}{8}(m_3 + m_4)\ , \\ D_{1212} &= D_{1221} = D_{2112} = D_{2121} = \tfrac{1}{8}(1 - m_2)\ . \end{aligned}$$

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When considering all possible layer combinations as well as layer directions, the tensor C^H will be parametrized by (m_1, m_2, m_3, m_4) belonging to the convex set $\mathcal{M}$ given as

$$\mathcal{M} = \left\{ \mathbf{m} \in \mathbf{R}^4 \middle| \begin{array}{l} m_1^2 + m_3^2 \leq 1,\ -1 \leq m_2 \leq 1, \\ 2m_1^2(1 - m_2) + 2m_3^2(1 + m_2) + \\ +(m_2^2 + m_4^2) - 4m_1 m_3 m_4 \leq 1 \end{array} \right\} .$$

This convex set also encompasses the material tensors of rank-2 and rank-3 layerings. However, compared to a rank-3 layering described by 2 relative densities and 3 directions of layerings, by introduction of the *moments* (m1 m2, m3, m4) there is one less variable to worry about. If optimization is carried out using these moments one may wish to recover a composite from the optimal moments - it turns out that for any given set of moments, a composite with at most three layers can be can be constructed analytically. For 3-D a parametrization in terms of moments can also be given. Here one has to work with 15 moments and a characterization of the set of moments in terms of matrix-inequalities.

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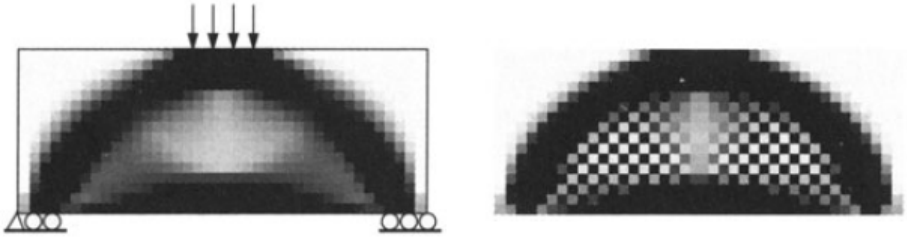
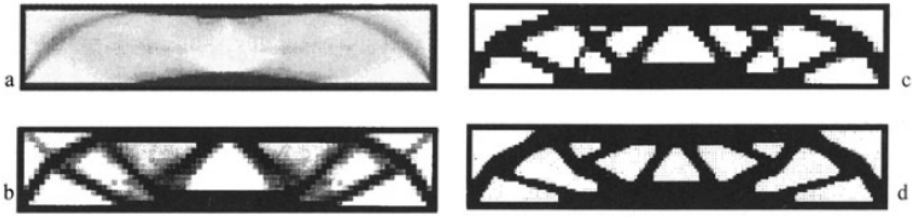
1.3 Implementation of the homogenization approach

The homogenization approach to design of a structure with composites can be implemented using the same flow of computations as for the material distribution method with isotropic materials. However, two additional aspects have to be considered. *First, a database of material properties as functions of the design variables should be generated, with one set of data for each allowed value of Poisson ratio. For layered materials no database is required, only a suitable subroutine. Second, the optimization routine should also cater for angles of rotations of the unit cells. Finally, the implementation should be able to remove checkerboard patterns as these also appear in this setting.*

The homogenization approach has been used as the basis for many design studies. Compared to use of for example SIMP, the homogenization approach requires additional design variables to describe the structure. On the other hand, one always works with microstructures of a given type, giving a direct physical understanding and in many cases a formal framework for computing the behaviour for intermediate densities when more involved physical situations are involved.



Optimal design using a rank-2 material. Left: The optimal design using an element wise constant density function and a 8-node displacement model. Right: The unstable checkerboard solution obtained when using a 4-node displacement model



Optimal design using a rank-2 material strain energy density with penalties on intermediate densities and on perimeter. a) shows the density distribution for the unpenalized case. In b) intermediate densities are penalized. In c) and d) intermediate densities and perimeter are penalized, with d) being a fine mesh variant of c)

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In many cases the homogenization approach is actually used as a basis for computing black and white designs, and the extended design space that encompasses composites is not employed to obtain information about the optimal micro-scale use of material as well. Also, to obtain such “classical” designs, explicit penalties on the density is typically needed to steer the design to a 0-1 format; in some circumstances neglecting the rotation angle of the cells in the composite constitutes a sufficient penalization that results in such designs. For compliance design it is also known that the use of such sub-optimal microstructures consisting of square holes in square cells give rise to rather well defined designs consisting almost entirely of areas with material or no material and very little area with intermediate density of material, i.e. very little composite material. This favours the use of this micro geometry for obtaining 0-1 designs and the success of the material distribution method in applications would probably never have come about if such sub-optimal microstructures had not been used in the initial numerical studies of the method (this was before the optimality of the layered materials had been proven).

On the other hand, one of the main interest in using composites in the design formulation is to see how this can influence the effectiveness of a structure, and ultimately, to understand what constitutes the best structure. That composites have a big part to play in such design studies can be seen when computing minimum compliance designs with layered materials where the result usually consists of large areas of intermediate densities ("grey“ areas of composite).

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1.4 Conditions of optimality for compliance optimization - rotations and densities

In the following we shall derive the necessary conditions of optimality for the *minimum compliance design* problem that employs *composite* materials in the parametrization of design. For this design formulation there are now *two* distinct types of design variables. First, the composite material is an anisotropic (normally orthotropic) material for which the *angle of rotation* of the unit cell is an important unconstrained design variable, and second, the *sizes describing the unit cells* constitute a different type of variables which are globally constrained through the volume constraint. For the latter, the derivation of the conditions of optimality follows directly from the developments, so we will here concentrate on the problem for the directions of orthotropy.

Optimal rotation of orthotropic materials

The composites with cell symmetry described in the preceding sections are orthotropic, and the angle of rotation of the material axes of this material will influence the value of the compliance of the structure. It turns out that the optimal rotation can be found analytically and this is of great importance for computations and it is interesting in its own right. Thus the optimal rotation of an orthotropic material is not only of importance for the present setting, but is equally significant in the design of composite structures, laminates, etc. For this reason we will here derive the conditions of optimality for material rotations in plane stress/strain problems (i.e. 2-D).

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Assume an orthotropic material as given. Then in the frame of reference given by the material axes of this material we have a stress-strain relation

$$\sigma_{ij} = E_{ijkl}\varepsilon_{kl}$$

with E_{1111}, E_{2222}, E_{1122}, E_{1212} being the only non-zero components of the stiffness tensor E_{ijkl}. We assume that $E_{1111} \geq E_{2222}$, and assume that a given set ε_{ij}^k, $k = 1, \ldots, M$, of strain fields for a number of load cases are specified. With compliance design in mind, we see from the formulations (1.6) and (1.34) of the minimum compliance problem that our interest is to maximize the weighted sum of a number of strain energy densities:

$$W = \frac{1}{2}\sum_{k=1}^{M} w^k \left[E_{1111}{\varepsilon_{11}^k}^2 + E_{2222}{\varepsilon_{22}^k}^2 + 2E_{1122}\varepsilon_{11}^k\varepsilon_{22}^k + 4E_{1212}{\varepsilon_{12}^k}^2\right] .$$

$$[c] = \begin{bmatrix} c_{1111} & c_{1122} & c_{1133} & c_{1123} & c_{1131} & c_{1112} \\ c_{2211} & c_{2222} & c_{2233} & c_{2223} & c_{2231} & c_{2212} \\ c_{3311} & c_{3322} & c_{3333} & c_{3323} & c_{3331} & c_{3312} \\ c_{2311} & c_{2322} & c_{2333} & c_{2323} & c_{2331} & c_{2312} \\ c_{3111} & c_{3122} & c_{3133} & c_{3123} & c_{3131} & c_{3112} \\ c_{1211} & c_{1222} & c_{1233} & c_{1223} & c_{1231} & c_{1212} \end{bmatrix} \equiv \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}$$

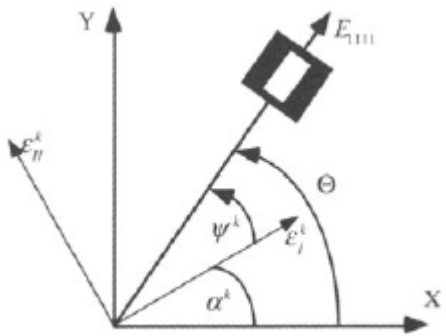
We now express the strains in terms of the principal strains ε_I^k, ε_{II}^k, where we choose $|\varepsilon_I^k| \geq |\varepsilon_{II}^k|$ for convenience:

$$\varepsilon_{11}^k = \frac{1}{2}\left[(\varepsilon_I^k + \varepsilon_{II}^k) + (\varepsilon_I^k - \varepsilon_{II}^k)\cos 2\psi^k\right] ,$$

$$\varepsilon_{22}^k = \frac{1}{2}\left[(\varepsilon_I^k + \varepsilon_{II}^k) - (\varepsilon_I^k - \varepsilon_{II}^k)\cos 2\psi^k\right] ,$$

$$\varepsilon_{12}^k = -\frac{1}{2}(\varepsilon_I^k - \varepsilon_{II}^k)\sin 2\psi^k .$$

Here ψ^k is the angle of rotation of the material frame relative to the frame of the k'th principal strains. We are interested in the angle Θ of rotation of the material relative to a chosen frame of reference which maximizes the function W. Each angle ψ^k is thus written as $\psi^k = \Theta - \alpha^k$, where α^k is the angle of rotation of the k'th strain field



The definition of angles of rotation of material and principal strain axes

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Inserting the expressions for the strains expressed in terms of the reference principal strains into the equation for W and differentiating, we get the condition of stationarity as:

$$\sum_{k=1}^{M} w^k \left[A^k \sin 2(\Theta - \alpha^k) + B^k \sin 2(\Theta - \alpha^k) \cos 2(\Theta - \alpha^k) \right] = 0 \ ,$$

$$A^k = (\varepsilon_I^{k\,2} - \varepsilon_{II}^{k\,2})(E_{1111} - E_{2222}) \ ,$$

$$B^k = (\varepsilon_I^k - \varepsilon_{II}^k)^2 (E_{2222} + E_{1111} - 2E_{1122} - 4E_{1212}) \ .$$

Stationarity is thus achieved if the following fourth order polynomial in $\sin 2\Theta$ is zero:

$$P(\sin 2\Theta) = a_4 \sin^4 2\Theta + a_3 \sin^3 2\Theta + a_2 \sin^2 \Theta + a_1 \sin 2\Theta + a_0 \ ,$$

$$a_4 = z_3^2 + z_4^2 \ , \ a_3 = 2z_1 z_4 - 2z_3 z_2 \ ,$$

$$a_2 = z_1^2 + z_2^2 - z_3^2 - z_4^2 \ , \ a_1 = z_2 z_3 - 2z_1 z_4, \ \ a_0 = \frac{z_3^2}{4} - z_1^2 \ ,$$

$$z_1 = \sum_{k=1}^{M} w^k A^k \sin 2\alpha^k \ , \ z_2 = \sum_{k=1}^{M} w^k A^k \cos 2\alpha^k \ ,$$

$$z_3 = 2 \sum_{k=1}^{M} w^k B^k \sin 4\alpha^k \ , \ z_4 = 2 \sum_{k=1}^{M} w^k B^k \cos 4\alpha^k \ .$$

The energy W is periodic so there exist at least two real roots of P. Also, as the order of P is four, the roots of P can be given analytically. The actual minimizer of the compliance is found by evaluating W for the four or eight stationary rotations. This feature is of great importance for the numerical implementation of the homogenization approach for optimal topology design, as the iterative optimization of a periodic function with several local minima and maxima is very likely to give the wrong result. Also, the analytical derivation of the optimal angles saves considerably in computational time.

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For the single load case we can express directly the stationary angle ψ (using the principal strain axes as the reference system):

$$\sin 2\psi = 0\ , \quad \text{or} \quad \cos 2\psi = -\gamma, \text{ with } \gamma = \frac{\alpha}{\beta}\frac{\varepsilon_I + \varepsilon_{II}}{\varepsilon_I - \varepsilon_{II}}, \text{ and}$$

$$\alpha = (E_{1111} - E_{2222}) \geq 0\ , \quad \beta = (E_{2222} + E_{1111} - 2E_{1122} - 4E_{1212})\ .$$

Inserting these values in the second variation of W with respect to ψ (Pedersen 1989), it can be seen that the maximizing ψ (i.e. the compliance minimizer) depends on the sign of the parameter β. The parameter β is a measure of the shear stiffness of the orthotropic material. For low shear stiffness, that is, $\beta \geq 0$, the globally minimal compliance is achieved for $\psi = 0$,

i.e. the intuitive result that the numerically largest principal strain is aligned with the stiffer material axis; also, from the stress-strain relation, we see that in this case these axes are aligned with the axes of principal stresses. The materials used in topology design (as described in Sect. 3.1.1) are weak in shear , i.e., $\beta \geq 0$. For certain (engineering) laminates with ply-angle $\pm\phi$, $22,5° \leq \phi \leq 45°$, we can have the situation of high shear stiffness, i.e. $\beta \leq 0$ (Pedersen 1989). In this case, $\cos 2\psi = -\gamma$ is the global minimum for compliance as long as $-1 < \gamma < 0$ (γ has the sign of β), and for $\gamma \leq -1$, $\psi = 0$ is again the global minimum. Note that a similar analysis can be carried out based on given stresses (here the complementary energy should be minimized,

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For three dimensional elasticity we have three angles of rotations possible for the axes of orthotropy (e.g. using Euler angles) and the expressions above for first variations with respect to angles become much more complicated. For the materials used for design, it is possible to show stationarity of the alignment of material axes, principal strain axes and principal stress axes. The full answer to the 3-D cases is still open.

For the materials involving multi-layered media (the rank-N laminates or layerings) the result on the optimal rotation follows by alternative means from the studies on optimal bounds on effective moduli of materials. For these materials it is thus proven that for the single load case, the optimal rotation of the material is consistent with an alignment of the layerings with the principal stresses/strains and this holds in dimension two *and* three.

We remark here that the problem of optimal design of the spatially varying angle of rotation of a fixed orthotropic material is not, in itself, well-posed in general. Relaxation is needed for this case also, as the introduction of for example layered materials consisting of the orthotropic material at various rotations extends the range of available materials.

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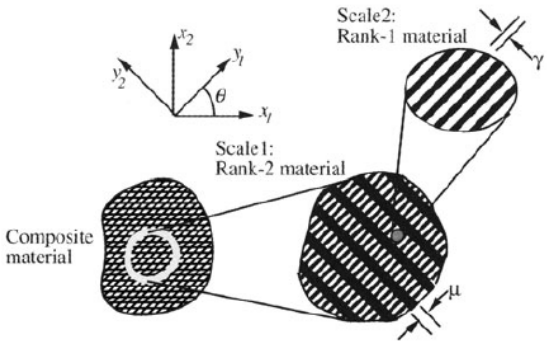
Optimality conditions for density The conditions of optimality for the density parameters describing the stiffness of a composite can be derived exactly along the lines of Sect. 1.2.1. For the problems at hand we note that the tensor E_{ijkl} now depends on geometric quantities which define the microstructure. For a square, 1 by 1, micro cell with a *rectangular* hole of dimension $(1-\mu)$ times $(1-\gamma)$ the density of material is given as $\rho = \mu+\gamma-\mu\gamma$ and the constraints on the design variables μ, γ are

$$\int_\Omega (\mu + \gamma - \mu\gamma)(x)\mathrm{d}\Omega = V, \quad 0 \le \mu(x) \le 1\ ,\ 0 \le \gamma(x) \le 1\ .$$



This relation also holds for the rank-2 layered material with layers of density μ and γ. For the present setting the optimality criterion update derived in Sect. 1.2.1 then has the format:

$$\mu_{K+1} = \begin{cases} \max\{(1-\zeta)\mu_K, 0\} \text{ if } \mu_K B_K^\eta \le \max\{(1-\zeta)\mu_K, 0\}\ , \\ \mu_K B_K^\eta \text{ if } \max\{(1-\zeta)\mu_K, 0\} \le \mu_K B_K^\eta \le \min\{(1+\zeta)\mu_K, 1\}\ , \\ \min\{(1+\zeta)\mu_K, 1\} \text{ if } \min\{(1+\zeta)\mu_K, 1\} \le \mu_K B_K^\eta\ , \end{cases}$$

$$\gamma_{K+1} = \begin{cases} \max\{(1-\zeta)\gamma_K, 0\} \text{ if } \gamma_K E_K^\eta \le \max\{(1-\zeta)\gamma_K, 0\}\ , \\ \gamma_K E_K^\eta \text{ if } \max\{(1-\zeta)\gamma_K, 0\} \le \gamma_K E_K^\eta \le \min\{(1+\zeta)\gamma_K, 1\}\ , \\ \min\{(1+\zeta)\gamma_K, 1\} \text{ if } \min\{(1+\zeta)\gamma_K, 1\} \le \gamma_K E_K^\eta\ . \end{cases}$$

Here μ_K, γ_K denotes the variables at iteration step K , and B, E are

$$B_K = [\Lambda_K(1-\gamma_K)]^{-1} \sum_{k=1}^{M} w^k \frac{\partial E_{ijpq}}{\partial \mu}(\mu_K, \gamma_K)\varepsilon_{ij}(u_K^k)\varepsilon_{pg}(u_K^k)\ ,$$

$$E_K = [\Lambda_K(1-\mu_K)]^{-1} \sum_{k=1}^{M} w^k \frac{\partial E_{ijpq}}{\partial \gamma}(\mu_K, \gamma_K)\varepsilon_{ij}(u_K^k)\varepsilon_{pg}(u_K^k)\ .$$

Also here, Λ is a Lagrange multiplier that should be adjusted in an inner iteration loop in order to satisfy the active volume constraint.

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A hierarchical solution procedure for anisotropic material

The problem separation described above naturally leads one to consider a different computational implementation as compared to the procedure described previously. Such an implementation can for example work with problem in the displacements and density only. We accordingly consider the solution as given, either through an analytical or a computational procedure. Then it has exactly the format of the compliance problem dealt with the SIMP model, that is, the compliance is a function of the density and is given by the solution of a minimum potential energy problem. This problem can then be solved for example by an optimality criterion method or by MMA. Here one needs sensitivity information of the compliance, i.e., derivative information for the equilibrium problem, which is given by the derivative of the optimized strain energy W with respect to the density. For an analytically derived optimal strain energy functional this derivative is straightforward to obtain, while for a computationally derived optimal strain energy functional this derivative is given simply as the Lagrange multiplier for the volume constraint of problem, i.e., the derivative is given directly from the computation of the optimal energy. The equilibrium problem is in general a non-linear problem, so the equilibrium problem requires an inner iteration loop at this point, but computational experience has shown that, as the optimization over the bulk density is in itself iterative, only one (or a few) equilibrium iterations need to be used for each design update.

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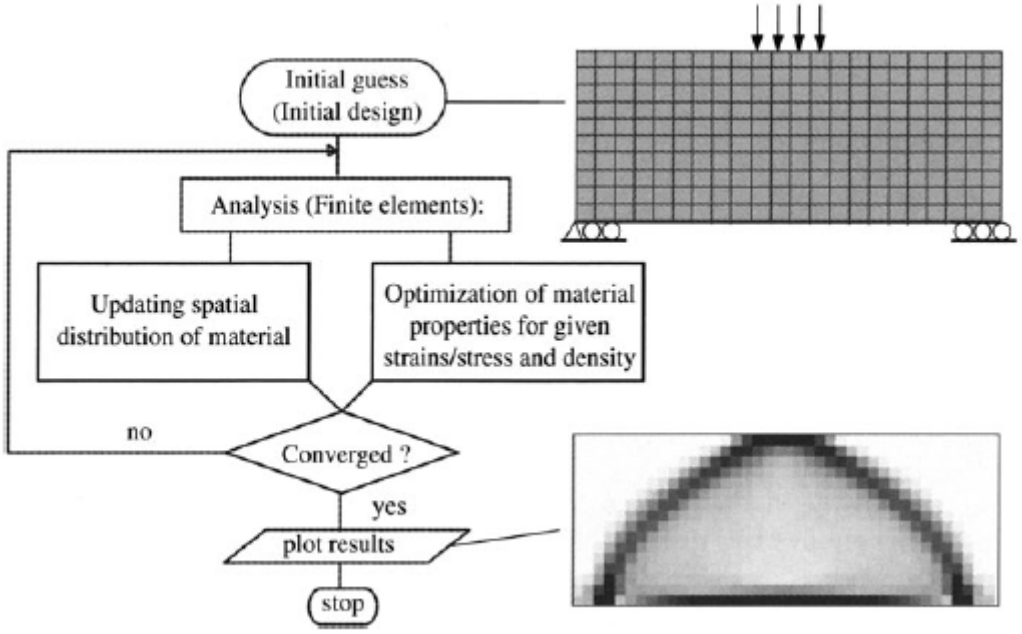
One of the advantages of the computational program just described is that the main flow of the procedure is *independent* of the modelling of the material used for the description of design. This latter information is added as an external module. This feature makes it possible to generate flexible procedures, where the material model can be changed easily.



Optimal design using a hierarchical approach. The resulting structure is here a low volume solution to the problem

Thank you for your attention