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Some computational aspects of using extremal material properties in the optimal design of shape, topology and material

by

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In this paper we discuss the optimization of geometry, topology and material of a structure for minimum compliance, reviewing recent work and presenting a number of new numerical results. For topology design, material properties are represented by a composite mixture constructed as a layered medium of a given isotropic material and void while for a more general setting we represent material properties and cost measures in the general form of positive semidefinite constitutive tensors and associated invariants of the tensors, respectively. Analytical forms are presented for the optimized material properties in both cases and it is shown how the analyses for optimization of the material lead to reduced structural optimization problems, for which effective methods for computational solution can be devised.

1. Introduction

Recent work by Bendsøe, Guedes, Haber, Pedersen and Taylor, (Bendsøe et al., 1993), has shown that a generalized approach to structural optimization

encompassing the design of structural material provides for a convenient computational framework for the simultaneous design of shape, topology and material. The general framework means that shape and topology design in dimension three can be treated within a problem statement that has a computational complexity, which apart from the additional size of the problem of analysis, is no more involved than the complexity of the problem in dimension two. The development is restricted to structures comprised of linear elastic material and to small–deformation kinematics and the global design objective is structural compliance under a single loading condition. This is also the framework treated in most studies of topology design using the homogenization modelling (Allaire, Kohn, 1993; Bendsøe, Kikuchi; 1988, Jog, Haber, Bendsøe, 1994), and the analysis of the generalized problem statement can be seen as a natural continuation of this work, where an analytical derivation of the properties of optimal layered materials are used as a basis for setting up a computational scheme for topology design (Allaire, Kohn, 1993; Jog, Haber, Bendsøe, 1994). For completeness of presentation we briefly describe in this paper the layered materials results as well as the results for the free material design formulation. However, for computational methods and results, we concentrate on the generalized formulation.

Optimal design with advanced materials and the closely related field of topology design have been the subject of two recent scientific meetings (Bendsøe, Mota Soares, 1993; Pedersen, 1993) and there is an ongoing intensive research effort within these fields. The problem of optimal rotation of orthotropic materials provides a natural starting point for considerations for a general approach to the concurrent design of material and structure (Pedersen, 1989) and the simultaneous design of material and overall structure has been taken one step further in the recent studies of optimal topology design using homogenization modelling (see, e.g. Allaire, Kohn, 1993; Bendsøe, Diaz, Kikuchi, 1993; Bendsøe, Kikuchi, 1988; Jog, Haber, Bendsøe, 1994; Lipton, 1992; Olhoff, Thomsen, Rasmussen, 1993; Suzuki, Kikuchi, 1991). In this work the structure is assumed to be made up of an arbitrary composition of a strictly limited number of given materials, and for the special case of topology design one of the given materials is void (usually approximated by a very flexible material). The homogenization modelling predicts a ranked set of 'microstructures' or 'structures with microscale variations' as the optimal material distribution and underlines the important relation between the fields of optimal design and materials science (see, e.g. Kohn, 1988 — Lurie, Cherkaev, 1986).

In the optimization problems we consider, the parameters which describe the structure can be divided into the set of parameters defining the local material tensor and the parameter that describes the specific cost of the material and we use that the minimum compliance optimization of a structure with respect to these two sets of parameters can be performed independently. Furthermore, the optimization with respect to the local material tensor parameters can be performed analytically in both the homogenization modelling formulation and the generalized material design formulation. This results in an optimized material

which minimizes the compliance of the applied load. For the layered materials of the homogenization modelling, this material has an effective energy of a non–linear material, while the effective energy for the generalized formulation corresponds to a linear, isotropic, zero–Poisson–ratio material, making the latter approach more tractable to computations. This indicates that this broader form of structural design problem should constitute an effective and general means for studying the optimization of sizes, shape, topology and material selection.

2. General problem formulation

Consider a mechanical element as a body occupying a part of a larger reference domain Ω in $\mathbf{R}^2$ or $\mathbf{R}^3$. Referring to the reference domain Ω we can define an optimal shape design problem as the problem of finding the optimal choice of elasticity tensor $E_{ijkl}(x)$ that is a variable over the domain and which is given a parametrization depending on the design situation at hand. The minimum compliance (maximum global stiffness) problem can for our developments be conveniently written as

$$\max_{\text{design}} \min_{u \in U} \left\{ \int_\Omega W(E,u) d\Omega - l(u) \right\} \tag{1}$$

with $W(E,u) = \frac{1}{2} E_{ijkl}\, \varepsilon_{ij}(u) \varepsilon_{kl}(u)$ and $l(u) = \int_\Omega pud\Omega + \int_{\Gamma_T} tuds$

Here U denotes the space of kinematically admissible displacement fields, p is the body force, t the boundary tractions and $\varepsilon_{ij}(u)$ the linearized strains consistent with small deformation, linear elasticity theory. In the formulation (1) the equilibrium requirement is represented through minimization of the potential energy with respect to deformation and we have used that the measure of compliance equals the negative of twice the value of the potential energy at equilibrium.

Alternatively, we can base our analysis on the principle of minimum complementary energy, so that the problem in terms of stresses has the form:

$$\min_{\text{design}} \quad \min_{\substack{\sigma \\ div\sigma = p \text{ in } \Omega \\ \sigma \cdot n = t \text{ on } \Gamma_T}} \quad \left\{ \int_\Omega \Pi(E,\sigma) d\Omega \right\} \tag{2}$$

with $\Pi(E,\sigma) = \frac{1}{2} E^{-1}_{ijkl}(x) \sigma_{ij} \sigma_{kl}$

For the parametrizations of the rigidity tensors that we will consider in this paper, the tensor E can be chosen independently from point to point of the structures, and the design limitations on E can be divided into pointwise limitations related to the choice of model used to describe E and a global constraint on the resource (volume of material) allocated to the construction of E.

With this in mind, we rewrite (1) and (2) as:

$$\max_{\substack{\text{variation of cost,}\\ \text{subject to } \int_\Omega \Psi(E)d\Omega = V}} \quad \max_{\substack{\text{local variation of } E,\\ \text{cost } \Psi(E) \text{ given}}} \quad \min_{u \in U} \left\{ \int_\Omega W(E,u)d\Omega - l(u) \right\} \tag{3}$$

$$\min_{\substack{\text{variation of cost,}\\ \text{subject to } \int_\Omega \Psi(E)d\Omega = V}} \quad \min_{\substack{\text{local variation of } E,\\ \text{cost } \Psi(E) \text{ given}}} \quad \min_{\substack{\sigma\\ div\sigma = p \text{ in } \Omega\\ \sigma \cdot n = t \text{ on } \Gamma_T}} \left\{ \int_\Omega \Pi(E,\sigma)d\Omega \right\} \tag{4}$$

and the approach to solving these problems will be to perform the interchange of the two innermost operations (if allowed) to obtain the formulations:

$$\max_{\substack{\text{variation of cost,}\\ \text{subject to } \int_\Omega \Psi(E)d\Omega = V}} \quad \min_{u \in U} \left\{ \int_\Omega \max_{\substack{\text{local variation of } E,\\ \text{cost } \Psi(E) \text{ given}}} [W(E,u)]d\Omega - l(u) \right\} \tag{5}$$

$$\min_{\substack{\text{variation of cost,}\\ \text{subject to } \int_\Omega \Psi(E)d\Omega = V}} \quad \min_{\substack{\sigma\\ div\sigma = p \text{ in } \Omega\\ \sigma \cdot n = t \text{ on } \Gamma_T}} \left\{ \int_\Omega \min_{\substack{\text{local variation of } E,\\ \text{cost } \Psi(E) \text{ given}}} [\Pi(E,\sigma)]d\Omega \right\} \tag{6}$$

where we have used the fact that the energies are non-negative and that the local optimization is a pointwise operation. It is the formulations (5) and (6) which constitute the basis for our developments in the following. Note that the interchange of min-min in the stress formulation (4) is allowed as the constraint sets for the two operators in the min-min problem are given entirely in terms of the variable over which each infimum is sought. Introduction of, for example, stress constraints at the outer design level of problem (2) would destroy this feature. The interchange of the operations in the max-min formulation in displacements is not valid in general, but in the parametrizations we consider this interchange is allowed.

3. Optimal energy expressions for layered materials

In topology design using the homogenization model, the elasticity tensors of the formulations above are restricted to the set of all tensors of composite materials that can be constructed form a given isotropic, linearly elastic material and void. This constitutes a relaxation of the formulation where the tensors are assumed to be of the given material or null, corresponding to a structure being described by the discrete valued design variables of material or void. The relaxation is required to obtain existence of solutions and constitutes a simplification of the problem in the sense that it allows for computations with continuous design variables. It is now well–known that the two–dimensional single load problem can be solved by using a layered medium, with layering at two different micro scales (see, e.g. Allaire, Kohn, 1993; Lipton, 1992; Lurie, Cherkaev, 1986 and

references therein). Such materials have the property that they minimize the complementary energy for a fixed stress field, for all possible composites with a fixed volume fraction of material and void. Similarly, these materials maximize the strain energy for a fixed strain field. These materials are not the only composites that achieve the upper bound on stiffness of a mixture of two materials, but they are convenient composites as the effective material properties can be expressed as fairly simple, explicit rational functions of the layer densities. This is crucial for the developments in the following.

Two densities γ and μ of layers are needed to define the material properties and the total density of the layered material that we use. First, a (first order) layering of the strong and the weak (void) material is constructed, the thicknesses of the strong and weak layers being γ and $(1-\gamma)$, respectively, in the unit cell, [0,1]x$\mathbf{R}$ (see Fig.1). This resulting composite material is then used as one of two components in a new layered material, with layers μ thick of the isotropic, strong material and with layers $(1-\mu)$ thick of the composite just constructed; the layers of this composite material are placed perpendicular to the direction of the new layering. The total density of the strong material in a material point is $\rho = \mu + (1-\mu)\gamma = \mu + \gamma - \mu\gamma$, and the effective material properties are (plane stress):

$$\begin{aligned} &E_{1111} = \frac{\gamma E}{\mu\gamma(1-\nu^2)+(1-\mu)}, \; E_{1122} = \mu\nu E_{1111}, \\ &E_{2222} = \mu E + \mu^2\nu^2 E_{1111}, \; E_{1212} = 0 \end{aligned} \tag{7}$$

Here E is Young's modulus and ν is Poisson's ratio for the base material.

For this specific parametrization of the elasticity tensor E the problems (5) and (6) are:

$$\max_{\substack{\text{density } \rho \\ \int_\Omega \rho d\Omega = V}} \; \min_{v\in U} \left\{ \int_\Omega \max_{\substack{\text{layered} \\ \text{microstructure,} \\ \mu+\gamma-\mu\gamma=\rho}} [W(\rho,E,u)]d\Omega - l(u) \right\} \tag{8}$$

$$\min_{\substack{div\,\sigma=f \\ \sigma\cdot n=t}} \; \min_{\substack{\text{density } \rho \\ \int_\Omega \rho d\Omega = V}} \left\{ \int_\Omega \min_{\substack{\text{layered} \\ \text{microstructure,} \\ \mu+\gamma-\mu\gamma=\rho}} [\Pi(\rho,E,u)]d\Omega \right\} \tag{9}$$

for the displacement and the stress case, respectively. Here we have for the stress based case also interchanged the equilibrium minimization problem and the optimization with respect to the density of material, using the min-min form of this problem. For the displacement formulation the maximization of energy with respect to micro structure can be interchanged with the equilibrium problem (Lipton, 1992), but the interchange of the equilibrium problem and the global design optimization with respect to the bulk density distribution cannot be carried out (Jog, Haber, Bendsøe, 1994; Lipton, 1992).

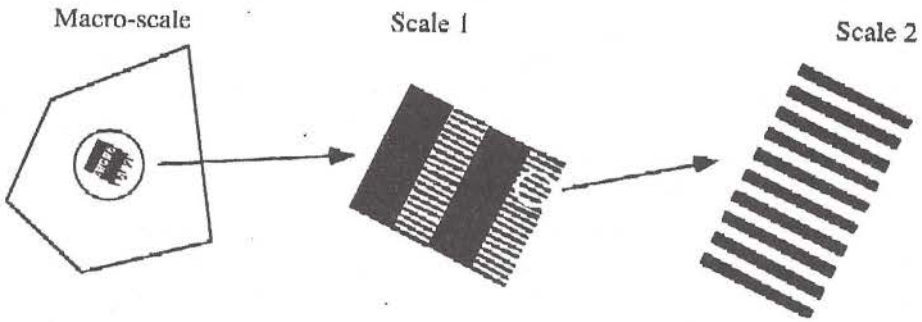

Figure 1. Layered materials. The build–up of a second rank layered material, by successive layering

The problem (2), (9) has been treated in great detail in Allaire, Kohn (1993) where relaxation methods are used directly on the original problem statement. In Jog, Haber, Bendsøe (1994) the results on optimality of layered materials are used to solve analytically the inner problems of (8) and (9) and we briefly outline these results in the following.

3.1. The stress case

With the principal stresses denoted by σ_I, σ_{II} the inner optimization in (9) requires co–alignment of the layerings with the principal stress directions (cf. Pedersen, 1989) and the subsequent optimization with respect to layer densities results in an extremal complementary energy of the form:

$$\begin{aligned}
&\Pi_1 = \frac{1}{2E\rho}\left[\sigma_I^2 + \sigma_{II}^2 - 2(1-\rho+\rho\nu)\sigma_I\sigma_{II}\right] \text{ if } \sigma_I\sigma_{II} > 0;\\
&\Pi_1 = \frac{1}{2E\rho}\left[\sigma_I^2 + \sigma_{II}^2 + 2(1-\rho-\rho\nu)\sigma_I\sigma_{II}\right] \text{ if } \sigma_I\sigma_{II} < 0;\\
&\Pi_1 = \frac{\sigma_I^2}{2E\rho} \text{ if } \sigma_{II} = 0;\ \Pi_1 = \frac{\sigma_{II}^2}{2E\rho} \text{ if } \sigma_I = 0.
\end{aligned} \tag{10}$$

Here the first two expressions correspond to the stationary points of optimization with respect to the layer densities μ and γ and represent the optimized energy of a layered material with two layers. The latter two expressions for the optimal energy are obtained if $\sigma_I\sigma_{II} = 0$, in which case we have a region with a unidirectional, single layering or a solid region corresponding to $\mu = 0$, $\gamma = \rho$ or $\mu = \rho$, $\gamma = 0$.

Finally, for the second inner problem of (9), we minimize with respect to the bulk density ρ. With $\lambda \geq 0$ denoting a Lagrange multiplier for the volume constraint we get that the optimal bulk density is $\rho = |\sigma_I| + |\sigma_{II}|/\sqrt{2\lambda E}$.

Taking into consideration that the optimal bulk density should satisfy the volume constraint, the expressions for the complementary strain energy density corresponding to the optimal densities are:

$$\text{if } \frac{|\sigma_I| + |\sigma_{II}|}{\sqrt{2E\lambda(\sigma_I, \sigma_{II})}} \leq 1 :$$

$$\begin{cases} \Pi_2(\sigma) = \dfrac{1}{2E}\left\{\sqrt{2E\lambda(\sigma_I, \sigma_{II})}(|\sigma_I| + |\sigma_{II}|) + 2(1-\nu)\sigma_I\sigma_{II}\right\}, \\ \text{if } \sigma_I\sigma_{II} \leq 0 \\ \Pi_2(\sigma) = \dfrac{1}{2E}\left\{\sqrt{2E\lambda(\sigma_I, \sigma_{II})}(|\sigma_I| + |\sigma_{II}|) - 2(1+\nu)\sigma_I\sigma_{II}\right\}, \\ \text{if } \sigma_I\sigma_{II} \geq 0 \end{cases} \tag{11}$$

$$\text{if } \frac{|\sigma_I| + |\sigma_{II}|}{\sqrt{2E\lambda(\sigma_I, \sigma_{II})}} \geq 1 :$$

$$\Pi_2(\sigma) = \frac{1}{2E}\left\{|\sigma_I|^2 + |\sigma_{II}|^2 + 2\nu|\sigma_I||\sigma_{II}|\right\}.$$

By the procedure described above we have thus reduced the stress based problem to a non–linear, non-smooth elasticity problem with a complementary energy functional given by (11).

3.2. The strain case

With the principal stresses denoted by ε_I, ε_{II}, with $|\varepsilon_I| \geq |\varepsilon_{II}|$, the inner optimization in (8) results in the extremal strain energy of the form:

$$\text{For } \frac{\varepsilon_I + \varepsilon_{II}}{(1-\nu)\varepsilon_I} < \rho < 1 :$$
$$W_1(\rho, \varepsilon) = \frac{E}{2(1-\nu)(2-\rho+\nu\rho)}\left[\varepsilon_I^2 + \varepsilon_{II}^2 + 2(1-\rho+\rho\nu)\varepsilon_I\varepsilon_{II}\right]; \tag{12a}$$

$$\text{For } \frac{\varepsilon_I - \varepsilon_{II}}{(1+\nu)\varepsilon_I} < \rho < 1 :$$
$$W_1(\rho, \varepsilon) = \frac{E}{2(1+\nu)(2-\rho-\nu\rho)}\left[\varepsilon_I^2 + \varepsilon_{II}^2 - 2(1-\rho-\rho\nu)\varepsilon_I\varepsilon_{II}\right]; \tag{12b}$$

$$\text{For } 0 \leq \rho \leq \frac{\varepsilon_I + \varepsilon_{II}}{(1-\nu)\varepsilon_I} \text{ or } 0 \leq \rho \leq \frac{\varepsilon_I - \varepsilon_{II}}{(1+\nu)\varepsilon_I} :$$
$$W_1(\rho, \varepsilon) = \frac{\rho E\varepsilon_I^2}{2} \text{ if } |\varepsilon_I| \geq |\varepsilon_{II}|; \tag{12c}$$
$$W_1(\rho, \varepsilon) = \frac{\rho E\varepsilon_{II}^2}{2} \text{ if } |\varepsilon_I| \leq |\varepsilon_{II}|.$$

Here (12c) holds for regions with single layers where the optimized material is non–linear while (12a) and (12b) are for regions with 2 layers and here the optimized effective energy corresponds to the energy of an isotropic, linearly elastic material. This material has the same stiffness matrix as the optimal material obtained in the stress case. In all cases, the layers are coaligned with the principal strains.

3.3. The limiting case of Michell's structural continua

The theory of layout of Michell frames and its extensions to flexural systems is the classical approach to topology and layout design of structures (Hemp, 1973; Michell, 1904; Rozvany, 1976, 1989). Computational experiments have shown that for small volumes of available material ($V <<$ volume of Ω) the homogenization method predicts structures that resemble truss-type layouts and Michell continua type layouts (Suzuki, Kikuchi, 1991). The structural continua of a Michell frame consist of two mutually orthogonal fields of tension/compression only members that are directed along the principal strain directions of a strain field and the total amount of material used is described by two independent densities of material, constrained to satisfy some volume constraint. The frame is described by a specific strain energy of the form:

$$W = \frac{E}{2}\left[\alpha\varepsilon_I^2 + \beta\varepsilon_{II}^2\right] \tag{13}$$

where α, ε_I and β, ε_{II} are the densities and corresponding principal strains in the two directions of the continua.

The Michell frame is usually considered as a limiting case for low densities of material, where the interaction of thin members in a planar frame can be ignored. Thus we are in the limiting situation where the layers in a layered material become 'thin' as compared to the cell size of the problem. This can be modelled by letting the density of material tend to zero in an asymptotic expansion. Clearly, taking the limit of zero density of material requires a rescaling of the loads and tractions also, in order to make the limit well posed. We thus introduce a scaling parameter ξ that will make the layer densities small by a rescaling in accordance to a length rescaling by a factor of ξ. The rescaled densities are:

$$\mu_1 = \xi^2\mu; \quad \gamma_1 = \xi^2\gamma; \quad \rho_1 = \xi^2\rho. \tag{14}$$

Using the rescaled densities together with an expansion of the stresses and strains in the expressions for the optimized energies described above, taking only the terms of zero order in ξ and requiring that the energies remain finite in the limit of $\xi \to 0$, it can be seen that the required rescaling of stresses and strains are $\xi\sigma_{ij}$ and $\frac{1}{\xi}\varepsilon_{ij}$, respectively. The optimized energies become

$$\Pi_1^M = \frac{1}{2E\rho}(|\sigma_I| + |\sigma_{II}|)^2 \tag{15}$$

$$W_1^M = \frac{\rho E\varepsilon_I^2}{2} \tag{16}$$

in all cases (we maintain the ordering $|\varepsilon_I| \geq |\varepsilon_{II}|$). Here, the strain energy corresponds to the energy written above, after optimization over the design

variables α and β. As above, we can for the stress based problem continue with an optimization over ρ, subject to the volume constraint. This results in the stress based problem reduced to the form

$$\min_{\substack{\sigma \\ div\sigma=p, \sigma\cdot n=t}} \left\{ \int_\Omega (|\sigma_I| + |\sigma_{II}|) d\Omega \right\} \tag{17}$$

which is the classical Michell problem formulated in stresses. Here the specific reference to the volume constraint is not present, as the Lagrange multiplier for this constraint only enters as a scaling parameter, which has no influence on the form of the optimal solution. The problem corresponds to a layout problem, where the cost of carrying the principal stresses is minimized over all statically admissible stress fields.

We note that one can also arrive at the strain based energy expression by considering the original strain energy expression and performing the optimization over layer densities after taking the limit of $\xi \to 0$. Also, the limit for the stress based case can be performed by considering the limit of an infinitely large Lagrange multiplier λ for the volume constraint (i.e. small density) (Allaire, Kohn, 1993).

4. The optimal energy expression for general materials

The problem we will now consider is the problem (1) in its most general form, that is, we take the minimization over all positive, semi–definite rigidity tensors E_{ijkl} and use the integral over the domain of some invariant $\Psi(E_{ijkl})$ of the rigidity tensor as the measure of cost. For physical reasons, the possible rigidity tensors in this design formulation are restricted to the set of positive semi–definite, symmetric 4-tensors. In the homogenization method of topology design, the total volume of material, defined at the micro level, provides a natural cost function for optimization problem formulations, but there is no such apparent cost function for the general material design formulation we consider here. Instead, we use certain invariants of the stiffness tensor as the measure of cost, thus ensuring that the optimal design solutions are not influenced by the choice of reference frame. Moreover, we can express cost and energy in any frame that is suitable for our formulation, a feature that is crucial for the developments.

In this paper we choose the following two invariants as examples of local cost, described by the specific cost functions ρ_A, ρ_B defined as,

$$\text{Case A:} \quad \rho_A = E_{ijij} \; ; \qquad \text{Case B:} \quad \rho_B^2 = E_{ijkl} E_{ijkl} \tag{18}$$

i.e., measures of the trace and the square of the Frobenius norm of the 4-tensor

E, respectively. The two problems we will consider are thus:

$$\text{Case A:} \quad \max_{\substack{\text{density } \rho \\ 0<\rho_{\min}\le\rho_A\le\rho_{\max}<\infty \\ \int_\Omega \rho d\Omega \le V}} \max_{\substack{\text{rigidity } E\ge 0 \\ E_{ijij}=\rho}} \min_{u\in U} \left\{ \int_\Omega W(\rho, E, u) d\Omega - l(u) \right\} \tag{19}$$

$$\text{Case B:} \quad \max_{\substack{\text{density } \rho \\ 0<\rho_{\min}\le\rho\le\rho_{\max}<\infty \\ \int_\Omega \rho^2 d\Omega \le V}} \max_{\substack{\text{rigidity } E\ge 0 \\ E_{ijkl}E_{ijkl}=\rho^2}} \min_{u\in U} \left\{ \int_\Omega W(\rho, E, u) d\Omega - l(u) \right\} \tag{20}$$

The cost constraints, linear in Case A and quadratic in Case B, are convex in both cases. In (19) and (20) we have introduced upper (and lower bounds) on the cost densities in order to ensure that the problem be well posed. The generalized problem as described here has, in a discretized formulation, been studied numerically by Ringertz (Ringertz, 1993). These investigations are based on the use of an interior point algorithm, with a logarithmic barrier function employed for converting the constraint $E > 0$ to a convex constraint, and all entries of E are used as design variables. In the developments to follow, we show that an analytical optimization can reduce the number of free design variables in problems (19) and (20) from 6 in dimension two and 21 in dimension three to only **one** in both dimensions (actually in any dimension).

In order to analyse (19) and (20) we move the pointwise maximization over the elasticity tensor to the inside of the equilibrium problem, as indicated in section 2. For the trace cost, one can use a saddle point argument to substantiate this operation, and for both problems, the validity of the operation can be verified by fairly straightforward arguments, based on the form of the optimized inner problem (Bendsøe et al., 1993). The interchange results in the sub–problems,

$$\text{Case A:} \quad \max_{\substack{\text{rigidity } E\ge 0 \\ E_{ijij}=\rho}} W(\rho, E, u) \tag{21}$$

$$\text{Case B:} \quad \max_{\substack{\text{rigidity } E\ge 0 \\ E_{ijkl}E_{ijkl}=\rho^2}} W(\rho, E, u) \tag{22}$$

Here, the term $(E_{ijkl}\varepsilon_{kl})\varepsilon_{ij}$ (an inner product) is maximal if $E_{ijkl}\varepsilon_{kl}$ is proportional to ε_{ij}, i.e. if ε is an eigentensor for the rigidity tensor E. Moreover, in view of (18) and from the requirement that E is positive semi–definite, it follows that ε is the only eigentensor for the optimal E with non–zero eigenvalue, and this eigenvalue must be equal to ρ in both case A and case B. Thus, the strain energy density for the optimal material has the general expression,

$$W_1 = \frac{1}{2}\rho\varepsilon_{ij}\varepsilon_{ij} \tag{23}$$

for the strains in any frame, corresponding to an isotropic, linear hyper–elastic effective medium. However, as we shall see, the optimized *material* for any fixed strain ε is orthotropic for all dimensions N.

The short development above gives the optimized energy but not directly the expressions for the rigidity tensor in the Cartesian tensor basis. For this (in dimension 3), we write ε in terms of the principal strains $\varepsilon_K, K = 1, 2, 3$. In the frame of reference given by the principal strains, the stiffness tensor is written in matrix form as:

$$E = X^T \begin{pmatrix} \rho & 0 & 0 & & \\ 0 & 0 & 0 & 0_{3\times 3} & \\ 0 & 0 & 0 & & \\ & & & & \\ & 0_{3\times 3} & & 0_{3\times 3} & \end{pmatrix} X \tag{24}$$

where X is an orthogonal transformation from the Cartesian tensor basis to an orthonormal basis of tensors where the first basis tensor is ε. Using the notation $\varepsilon_P = (\varepsilon_I, \varepsilon_{II}, \varepsilon_{III})$, $\|\varepsilon_P\|^2 = \varepsilon_I^2 + \varepsilon_{II}^2 + \varepsilon_{III}^2$ the resulting rigidity matrix is,

$$E = \begin{pmatrix} E_{3\times 3} & 0_{3\times 3} \\ 0_{3\times 3} & 0_{3\times 3} \end{pmatrix} \tag{25}$$

with the sub–matrix $E_{3\times 3}$ given by

$$E_{3\times 3} = \frac{\rho}{\|\varepsilon_P\|^2} \varepsilon_P \varepsilon_P^T \tag{26}$$

Note that the specific cost function ρ can be expressed as $\rho = E_{iiii}$ for both case A and case B.

The optimal material is at each point an orthotropic material, which is co–aligned with the principal strain axes. Also, note that the material rigidity tensor has only one non–zero eigenvalue. Thus, the extremization of the strain energy density results in a material which is at the utmost limit of feasibility for satisfying the positivity constraints $E \geq 0$, and the material can only carry strain fields which are direct rescalings of the given strain field for which the optimization was undertaken. This underlines the true optimal nature of the material. Such behaviour of extremized materials is also evident in the homogenization method for topology design with one given material, as described above, but there we have only one zero eigenvalue corresponding to vanishing shear stiffness (in dimension 2). The restriction used in the homogenization approach that the composite material should be constructed from some specified elastic material is thus a penalty that is evident in the form of optimized strain energies.

Having thus obtained the optimized strain energy density we can now state the resulting problems,

$$\text{Case A:} \quad \begin{aligned} &\max_{\text{density } \rho} \min_{u \in U} \left\{ \frac{1}{2} \int_\Omega \rho \varepsilon_{ij} \varepsilon_{ij} d\Omega - l(u) \right\} \\ &\text{subject to:} \\ &0 < \rho_{\min} \leq \rho \leq \rho_{\max}, \quad \int_\Omega \rho d\Omega \leq V \end{aligned} \tag{27}$$

$$\text{Case B:} \quad \begin{aligned} &\max_{\text{density } \rho} \min_{u \in U} \left\{ \frac{1}{2} \int_\Omega \rho \varepsilon_{ij} \varepsilon_{ij} d\Omega - l(u) \right\} \\ &\text{subject to:} \\ &0 < \rho_{\min} \leq \rho \leq \rho_{\max}, \quad \int_\Omega \rho^2 d\Omega \leq V \end{aligned} \tag{28}$$

The reduced problem for Case A is exactly equivalent to a variable–thickness design problem for a sheet made of an isotropic zero–Poisson–ratio material, with the density ρ playing the role of the thickness of the sheet. Case B is a similar problem, but with a rather unusual convex cost that favours intermediate densities. The reduced problems have a very simple form and have been studied in great detail (Céa, Malanowski, 1970; Rossow, Taylor, 1973; Taylor, 1969). The problem of variable thickness sheet design is one of the few examples of distributed parameter design for which regularization is not needed. In fact, the existence of optimal solutions in $L^\infty(\Omega)$ (with the weak* topology) can be proved by a fairly straightforward development, which generalizes to both case A and B (Bendsøe et al., 1993; Céa, Malanowski, 1970). Moreover, a finite element discretization of the variable thickness sheet design problems is of the same form as the equivalent problem for trusses and thus a numerical optimization can make use of the very efficient optimization algorithms devised for truss problems (Bendsøe, Ben–Tal, Zowe, 1994).

The reduced problems (27) and (28) formulated above are again saddle point problems. The common objective function is concave in the cost density and convex in the displacements. Also, the cost density is constrained to a compact set of $L^\infty(\Omega)$ (with the weak* topology) and the objective is semi–continuous with respect to this topology as well as the topology of the displacements. This assures the existence of a saddle value of problems (27) and (28) and we can find the optimal compliance values by solving:

$$\text{Case A:} \quad \begin{aligned} &\min_{u \in U} \left\{ \frac{1}{2} \Phi_A(\varepsilon) - l(u) \right\}, \quad \text{where} \\ &\Phi_A(\varepsilon) = \max_{\substack{\text{density } \rho \\ 0 < \rho_{\min} \leq \rho \leq \rho_{\max} \\ \int_\Omega \rho d\Omega \leq V}} \int_\Omega \rho \varepsilon_{ij} \varepsilon_{ij} d\Omega \end{aligned} \tag{29}$$

$$\text{Case B:} \qquad \begin{array}{l} \min\limits_{u\in U}\left\{\dfrac{1}{2}\Phi_B(\varepsilon)-l(u)\right\}, \quad \text{where} \\ \Phi_B(\varepsilon)=\max\limits_{\substack{\text{density } \rho \\ 0<\rho_{\min}\le\rho\le\rho_{\max} \\ \int_\Omega \rho^2 d\Omega\le V}} \displaystyle\int_\Omega \rho\varepsilon_{ij}\varepsilon_{ij}d\Omega \end{array} \tag{30}$$

Here we can derive analytically the solution to the convex inner problems. Introducing a Lagrange multiplier λ for the cost constraints, this optimization results in the following optimized potential energies:

$$\Phi_A(\varepsilon)=\min_{\lambda\ge 0}\left\{\int_\Omega \max\left\{\rho_{\min}(\varepsilon_{ij}\varepsilon_{ij}-\lambda),\rho_{\max}(\varepsilon_{ij}\varepsilon_{ij}-\lambda)\right\}d\Omega+\lambda V\right\} \tag{31}$$

$$\begin{array}{l} \Phi_B(\varepsilon)=\displaystyle\int_\Omega \rho\varepsilon_{ij}\varepsilon_{ij}d\Omega, \text{ where} \\ \rho=\begin{cases} \rho_{\min} & \text{if} \quad \rho_{\min}>\frac{1}{2\lambda}\varepsilon_{ij}\varepsilon_{ij} \\ \frac{1}{2\lambda}\varepsilon_{ij}\varepsilon_{ij} & \text{if} \quad \rho_{\min}\le\frac{1}{2\lambda}\varepsilon_{ij}\varepsilon_{ij}\le\rho_{\max} \\ \rho_{\max} & \text{if} \quad \rho_{\max}<\frac{1}{2\lambda}\varepsilon_{ij}\varepsilon_{ij} \end{cases} \\ \text{with } \lambda \text{ determined by} \\ \displaystyle\int_\Omega \rho^2 d\Omega=V \end{array} \tag{32}$$

This implies that the design variables can be removed entirely from the problem, and the resulting problems are non–linear and non–smooth, convex analysis problems.

We end this section by remarking that the procedure described above can be performed for the stress based case as well. The resulting problems are, as expected:

$$\text{Case A:} \qquad \min_{\substack{\text{density } \rho \\ 0<\rho_{\min}\le\rho\le\rho_{\max} \\ \int_\Omega \rho d\Omega\le V}} \ \min_{\substack{div\sigma=f \\ \sigma\cdot n=t}} \left\{\frac{1}{2}\int_\Omega \frac{1}{\rho}\sigma_{ij}\sigma_{ij}d\Omega\right\} \tag{33}$$

$$\text{Case B:} \qquad \min_{\substack{\text{density } \rho \\ 0<\rho_{\min}\le\rho\le\rho_{\max} \\ \int_\Omega \rho^2 d\Omega\le V}} \ \min_{\substack{div\sigma=f \\ \sigma\cdot n=t}} \left\{\frac{1}{2}\int_\Omega \frac{1}{\rho}\sigma_{ij}\sigma_{ij}d\Omega\right\} \tag{34}$$

where the optimal cost density can be found from expressions similar to (32) above.

5. Numerical implementation

The developments above show that the analytical derivation of the optimal material properties for a minimum compliance design problem in the strain

based formulation gives rise to a problem of the form ($q = 1$ or 2)

$$\max_{\substack{\text{density } \rho \\ \int_\Omega \rho^q d\Omega = V}} \min_{u \in U} \left\{ \int_\Omega W_1(\rho, \varepsilon(u)) d\Omega - l(u) \right\} \tag{35}$$

We concentrate our discussion of possible computational schemes to the displacements based formulation which is compatible with the popular finite element stiffness method. For this case, a conceptual optimality criterion algorithm for solving (35) is (Bendsøe, Diaz, Kikuchi, 1993; Jog, Haber, Bendsøe, 1994; Rozvany, 1989):

k - th iteration step:

1. For ρ_k fixed, solve the equilibrium problem

$$\min_{u \in U} \left\{ \int_\Omega W_1(\rho_k, \varepsilon(u)) d\Omega - l(u) \right\},$$

with solution u_k

2. Update density by

$$\rho_{k+1} = \max \left\{ \rho_{\min}, \min \left\{ \left[\frac{1}{\lambda_k} \frac{1}{q \rho_k^{q-1}} \frac{\partial W_1}{\partial \rho}(\rho_k, \varepsilon(u_k)) \right]^\eta \rho_k, \rho_{\max} \right\} \right\}$$

with λ_k determined by the constraint

$$\int_\Omega \rho_{k+1}^q d\Omega = V \tag{36}$$

The design update in step 2. of (36) is an optimality criteria based update where a scalar Lagrange multiplier for the volume constraint has to be determined in an inner iteration loop. This multiplier is uniquely determined by the volume constraint and its value should be determined by a Golden Section method or a Newton procedure. With the latter approach in mind we note that the function

$$F(\lambda) = \int_\Omega \max \left\{ \rho_{\min}, \min \left\{ \left[\frac{1}{\lambda} \frac{\partial W_1}{\partial \rho}(\rho, \varepsilon(u)) \right]^\eta \rho, \rho_{\max} \right\} \right\} d\Omega \tag{37}$$

is a continuous, decreasing function, which is differentiable except at most a countable set of points. In any discretization of the domain, there will be at most a finite set of non–differentiable points and the computation of the directional derivative is straightforward. Note that we have introduced in the design update formula a tuning parameter η, which should be adjusted in order to obtain convergence and stability of the algorithm. For the linear cost constraint 0.8 is a suitable choice for this parameter, while 0.4 is a suitable choice in the case of the quadratic cost measure. This has been found by experiments. Note that for the density update we have to compute the derivative of the strain energy with respect to the density. For the generalized materials this derivative is just the

specific (with respect to density) strain energy, while for the homogenization method this derivative is given by the expression

$$\text{For } \tfrac{\varepsilon_I+\varepsilon_{II}}{(1-\nu)\varepsilon_I} < \rho < 1: \quad \tfrac{\partial W_1}{\partial \rho} = \tfrac{E}{2}\left[\tfrac{\varepsilon_I-\varepsilon_{II}}{(2-\rho+\nu\rho)}\right]^2; \tag{38a}$$

$$\text{For } \tfrac{\varepsilon_I-\varepsilon_{II}}{(1+\nu)\varepsilon_I} < \rho < 1: \quad \tfrac{\partial W_1}{\partial \rho} = \tfrac{E}{2}\left[\tfrac{\varepsilon_I+\varepsilon_{II}}{(2-\rho-\nu\rho)}\right]^2; \tag{38b}$$

$$\begin{aligned}&\text{For } 0 \le \rho \le \tfrac{\varepsilon_I+\varepsilon_{II}}{(1-\nu)\varepsilon_I} \text{ or } 0 \le \rho \le \tfrac{\varepsilon_I-\varepsilon_{II}}{(1+\nu)\varepsilon_I}:\\ &\tfrac{\partial W_1}{\partial \rho} = \tfrac{E\varepsilon_I^2}{2} \text{ if } |\varepsilon_I| \ge |\varepsilon_{II}|;\ \tfrac{\partial W_1}{\partial \rho} = \tfrac{E\varepsilon_{II}^2}{2} \text{ if } |\varepsilon_I| \le |\varepsilon_{II}|.\end{aligned} \tag{38c}$$

The equilibrium problem in (36) is in the homogenization modelling case a non–linear problem, so the equilibrium problem requires an inner iteration loop at this point. The problem of analysis is actually linear in the solid regions and in regions governed by equations (12a) and (12b), while it is non–linear in the regions governed by equations (12c). In the latter regions an isotropic secant stiffness matrix can be used, so that in the computations all regions are described by isotropic stiffness matrices. Computational experience (Jog, Haber, Bendsøe, 1994) 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. For the case of a generalized material design, the equilibrium problem simplifies, as we in this case have a linear equilibrium problem for a structure made of a linearly elastic isotropic zero–Poisson–ratio material.

Note that for both types of problems we can thus use equilibrium solvers that can handle isotropic materials only, even though the design problem is in essence precisely seeking the distribution of an orthotropic material. It is the use of the optimal energy functionals that causes this and it makes it fairly simple to implement these design problems using commercial finite element packages. For the generalized materials approach, the variation of the density ρ can be simulated through a variation in the Young's modulus of the isotropic zero–Poisson–ratio material, while for the homogenization approach the density dependence of the stiffness can be simulated through a variation of Young's modulus as well as the Poisson ratio of an isotropic material.

In order to reveal the structure of the discretized versions of the problems (27) and (28) for the generalized material design, we introduce the approximations:

$$\begin{aligned}&u = u_k Y_k,\ k = 1, \ldots\ldots, N\\ &\rho = \rho_i\, \Xi_i,\ i = 1, \ldots\ldots, M\end{aligned} \tag{39}$$

of the displacement field u and the density field ρ, with non–negative basis functions Ξ_i for ρ. We can then write discretizations of problems (27) and (28),

$$
\begin{aligned}
&\max_t \min_u \left\{ \frac{1}{2} \sum_{i=1}^{M} t_i u^T \boldsymbol{A}_i u - p^T u \right\} \\
&\text{subject to:} \\
&0 < t_{\min} \leq t_{\min}^i \leq t_i \leq t_{\max}^i < \infty, \ i = 1, \ldots, M \\
&\text{and} \quad \begin{cases} \text{for Case A: } \displaystyle\sum_{i=1}^{M} b_i t_i = V \\ \text{for Case B: } \displaystyle\sum_{i=1}^{M} c_i t_i^2 = V \end{cases}
\end{aligned} \tag{40}
$$

Here $\boldsymbol{A} = \sum_{i=1}^{M} t_i \, \boldsymbol{A}_i$ is the stiffness matrix and

$$
\begin{aligned}
&t_i = \rho_i, \ b_i = \int_\Omega \Xi_i \, d\Omega > 0, \ c_i = \int_\Omega \Xi_i^2 \, d\Omega > 0, \\
&(\boldsymbol{A}_i)_{kl} = \int_\Omega \Xi_i \varepsilon_{pq}(Y_k) \varepsilon_{pq}(Y_l) \, d\Omega, \ \boldsymbol{A}_i \geq 0 \\
&p_k = l(Y_k)
\end{aligned} \tag{41}
$$

For element–wise constant approximations of the density, t_i and $\boldsymbol{A}_i$ are the specific element density and the specific element stiffness matrix, respectively. The problem (40) is a convex problem in the t's only, after solving for the displacements u. This fact follows easily as the inner equilibrium problem is a minimization over a set of linear functions in t, the result of which is a concave function. This property is of course of importance when considering algorithms for the problem at hand.

The optimality criterion method described above is an efficient method for solving problem (35) for both the homogenization and the generalized material design situation. For the latter case, alternative and efficient methods can be obtained by restating problem (40) in the form:

$$
\begin{aligned}
&\min_t p^T u \\
&\text{subject to:} \\
&\sum_{i=1}^{M} t_i \boldsymbol{A}_i u = p^T u \\
&0 < t_{\min} \leq t_{\min}^i \leq t_i \leq t_{\max}^i < \infty, \ i = 1, \ldots, M \\
&\text{and} \quad \begin{cases} \text{for Case A: } \displaystyle\sum_{i=1}^{M} b_i t_i = V \\ \text{for Case B: } \displaystyle\sum_{i=1}^{M} c_i t_i^2 = V \end{cases}
\end{aligned} \tag{42}
$$

which lends itself to the application of interior point algorithms as described in detail in references Bendsøe, Ben–Tal, Zowe (1994), Ringertz (1993). For

example, the use of a logarithmic barrier function method has proved useful in these works. Note that for efficiency, sparse matrix techniques have been employed. A different class of specialized algorithms have appeared that work with the discretized version of the displacements only problem (29) (Bendsøe, Ben–Tal, Zowe, 1994) and again sparse techniques have been employed for these algorithms. Extensions of these methods to the quadratic cost constraint for case B are currently under development.

6. Examples

In order to exemplify the type of results that arise from the above optimal design formulation using generalized material behaviour we include some numerical results for some 2-dimensional plane stress design problems seen in the literature (Bendsøe, Diaz, Kikuchi, 1993; Jog, Haber, Bendsøe, 1994; Olhoff, Bendsøe, Rasmussen, 1991; Olhoff, Thomsen, Rasmussen, 1993), covering both case A and case B. The results were generated using a Q4 or a Q8 finite element approximation of the displacement field and an element–wise constant approximation of the density field. The optimality criterion method was used for the design optimization. In some figures we show the result obtained in terms of the optimal moduli given by equations (23) and we show the spatial variation of the three non–zero moduli, as well as the co–aligned principal directions of material and strains. For some examples we only show the variation of the cost density ρ, but only in cases where topology is the main issue so that this variable is the main variable of interest. Note that the cost density ρ has in reality little direct physical meaning, as the structures generated are supposed to be built of an optimized, orthotropic material. Thus, in the figures black areas indicate regions where the density of cost is at the maximum level allowed in the formulation and do not signify solid regions; even the black areas consist of the optimized, orthotropic material that can only carry the applied load. However, as is evident from the figures, the cost density ρ gives perfectly applicable shapes and topologies as needed in a preliminary design stage.

It is evident from the numerical results that for practical purposes the use of the trace cost (case A) is to be preferred as the square of the Frobenius norm cost has a tendency to spread the material more over the design area. This is to be expected as this cost constraint in a sense gives preference to intermediate density values. From a computational point of view the Frobenius cost constraint is to be favoured as only a moderate number (approx. 10 to 20) of iteration steps of the optimality criterion algorithm (36) are needed to obtain satisfaction of the Kuhn–Tucker conditions, while the linear trace cost problems typically require up to at least 100 iterations for convergence. It is thus recommended that even trace cost problems are solved using the Frobenius cost problem as a pre–processor for generating good starting designs.

Note that a discretization using a Q4 finite element approximation of the

displacement field and an element–wise constant approximation of the density field is less prone to develop the unstable checkerboard patterns reported for implementations of the homogenization approach for this type of approximation (Bendsøe, Diaz, Kikuchi, 1993; Jog, Haber, Bendsøe, 1994). However, mild checkerboard patterns are visible in some of the present examples. As suggested in reference Jog, Haber, Bendsøe (1994) for the homogenization modelling we tried to increase the degrees of freedom for the displacements and our experiments confirms the conclusion of that reference that the unstable checkerboard patterns can be avoided by using a Q8 finite element approximation of the displacement field and an element wise constant approximation of the density field. However, this feature is not well understood at this time. An alternative to the use of Q8 displacement elements is to use Q4 elements together with a filter which projects the density values of four adjacent elements onto checkerboard free density distributions (Bendsøe, Diaz, Kikuchi, 1993). This method can be considered as an equivalent to using a Q8 element for the displacements together with a three degree of freedom per element discretization of the density field.

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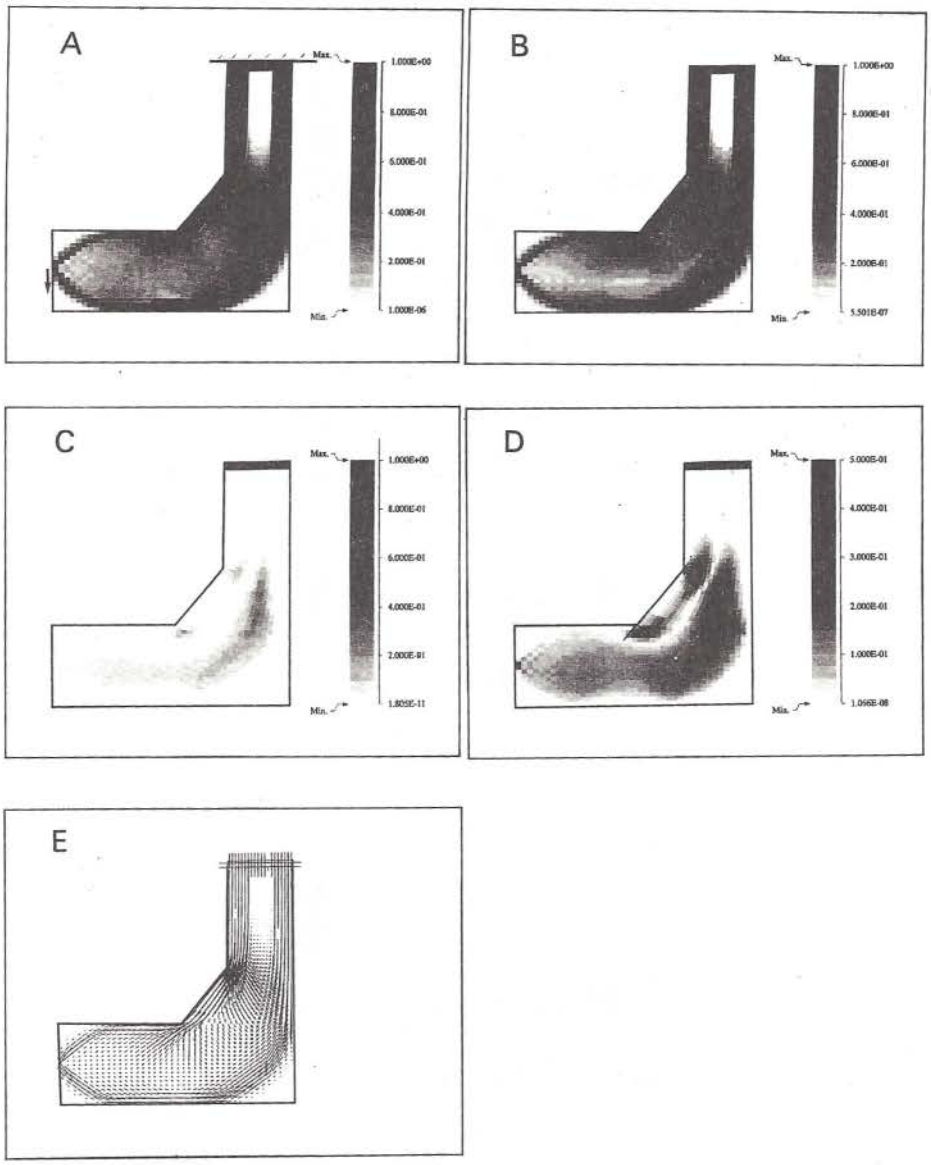

Figure 2. Transmitting a force around a corner. The upper part at the support is considered as fixed (see also Olhoff, Thomsen, Rasmussen, 1993). An example of optimal design of material and structure using the trace cost and Q4 elements for displacements. **A:** Distribution of cost. **B:** Distribution of E_{1111}. **C:** Distribution of E_{2222}. **D:** Distribution of $|E_{1122}|$. **E:** Directions and sizes of principal strains.

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