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*M2AN - Modélisation mathématique et analyse numérique*, tome 29, n° 6 (1995), p. 657-686

[http://www.numdam.org/item?id=M2AN\\_1995\\_\\_29\\_6\\_657\\_0](http://www.numdam.org/item?id=M2AN_1995__29_6_657_0)

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## OPTIMUM COMPOSITE MATERIAL DESIGN (\*)

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Communicated by R. TEMAM

Résumé. — *On traite ici le problème d'identification de microstructures : certaines phases à certains pourcentages en volume étant données, comment les mélanger dans une cellule de périodicité, de manière que les constantes effectives du matériau périodique soient les plus proches possibles de valeurs données. On étudie le problème dans le cas de l'équation de conduction linéaire, qui est posé en termes de la théorie du contrôle optimal. On montre l'existence d'une solution ainsi que la convergence d'approximation numérique.*

Abstract. — *The microstructure identification problem is treated: given certain phases in given volume fractions, how to mix them in a periodic cell so that the effective material constants of the periodic composite lie the closest possible to certain prescribed values? The problem is studied for the linear conduction equation. It is stated in terms of optimal control theory; the admissible microgeometries are single inclusion ones. Existence of solution is proved under suitable hypotheses, as well as the convergence of numerical approximations. Numerical examples are presented.*

*In the conduction case, the full characterization of the  $G_\theta$ -closure set (the set of all effective conductivities that result from taking the given phases in the given volume fraction mixed in any feasible microgeometry) is known. One carried out numerical experiments how well can its boundaries be attained using the subclass of single inclusion microgeometries. Results of these experiments are shown as well.*

The concept of composite media not only comes directly from the physical world but also provides a theoretically sound means for relaxation of variational problems — the problem of optimum topology design (see [5], [22], [12], [2] or [14]) in the first rank of importance. It is a classical result of the homogenization theory that composites can be replaced by a macroscopically homogeneous medium whose material constants — the so called *effective constants or effective moduli* — depend on the microgeometry in which the

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(\*) Manuscript received March 10, 94.

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constituent phases form the mixture. The set of all effective constants of mixtures of a given number of phases taken in a given proportion is called the  $G_\theta$ -closure set and its knowledge is essential for the relaxation procedure.

In the case of a scalar linear elliptic partial differential equation (the steady heat transfer equation), the  $G_\theta$ -closure sets are known for mixtures of two phases ; one of the phases may be degenerate, i.e., a void ; see [14], [23], [16]. However, for the case of the system of PDE's of linear elasticity, only a partial information about the  $G_\theta$ -closure sets is available so far ; namely we know how to minimize the complementary energy for a given single macroscopic stress field (see [1]). This is enough for the minimum compliance design of single loaded elastic structures (see [2]) ; however, for the case with multiple loadings as well as for design with other (non-compliance) objective functions, the full knowledge of the  $G_\theta$ -closure set seems inevitable.

But also the scalar case has its difficulties : the construction of extremal microstructures — i.e., those that maximize/minimize the effective energy — is usually a nice theory while practically immanufacturable. So far, the following constructions are known :

**Multiple rank laminates.** The microstructure is a laminate (= layered composite) whose one or both components are again laminates that in turn can consist of laminates, etc. The layered microstructure has the advantage that one can calculate the effective constants analytically. However, the scale levels of the subsequent laminations must be well separated which prohibits practical realization of these microstructures. For an overview cf. [3].

**Coated ellipsoids construction.** This construction is based on the fact that having a medium with the material constants that are equal to those of our desired microstructure, one can insert an ellipsoid of one phase with an ellipsoidal inclusion of the other phase where the ellipsoids have appropriately balanced dimensions, and the effective properties of the medium are not changed upon this insertion. Thus, one fills up the whole body with coated ellipsoids, but using infinitely many length scales, this time not even separated from one another. As a consequence, one cannot manufacture but a rough approximation of such a microstructure. For details see [9].

**Vidgergauz' microstructure.** The only known extremal microstructure that stays on a single length scale is the Vidgergauz' microstructure. It has the form of a properly shaped (oval-like) inclusion of one phase within the matrix of the other phase. The shape of the inclusion is found from the optimality conditions that in this setting have the form that « the inclusions be equally strong », see [24] or [10]. However, the shapes of the inclusion have to be evaluated using elliptic integrals or other non-elementary functions. We note that although it is presented in the elasticity setting, similar results hold for the scalar equation.

The aim of this work is two fold :

**1. Establish a numerical technique for the microstructure identification problem.** We use the optimal control theory to formulate the problem of microstructure identification : given a target matrix of effective moduli, what microstructure has its effective moduli the closest to this target ? — ideally, what microstructure attains the target ? As we are using the classical optimal shape design approach based on the boundary variation technique, the class of admissible microgeometries is restricted to single inclusion ones. We present an approximation of the optimal control problem.

We note that from a different point of view, the problem of microstructure identification has been treated also by O. Sigmund : [20], [21]. That approach works in the linear elasticity setting and uses discrete structures (trusses).

**2. Investigate numerically what parts of the  $G_\theta$ -closure set are covered by the chosen class of microgeometries.** Since the single inclusion microgeometries belong to the « reasonable » (meaning : more or less manufacturable) classes, it is interesting to see how well they manage to cover the full  $G_\theta$ -closure sets. Specifically, in [5] and [22], one uses only sub-optimal microstructures — rectangular inclusions — for relaxation of the optimum shape design problem. We study how big are the differences among the rectangular inclusion composites, the single inclusion composites, and the full  $G_\theta$ -closure sets.

## 1. FORMULATION OF THE IDENTIFICATION PROBLEM

Let us have a body in a plane represented by a domain  $\Omega \subset \mathbb{R}^2$  with the Lipschitz-continuous boundary  $\partial\Omega$ . Let the body be made of two isotropic constituents with different conductivity values  $\alpha I, \beta I$  where  $I$  is the unit tensor and  $0 < \alpha, \beta$ . Let these two phases be distributed in  $\Omega$  making a periodic pattern with the period  $\varepsilon Y$ , where  $Y = ]0, 1[$  is the so called periodic cell and  $\varepsilon > 0$  is a scaling factor. The steady heat transfer in  $\Omega$  is described by the scalar elliptic equation

$$(1.1) \quad - \sum_{i=1}^2 \frac{\partial}{\partial x_i} \left( a^\varepsilon(x) \frac{\partial u}{\partial x_i} \right) = f \quad \text{in } \Omega$$

and by appropriate boundary conditions, say of the Dirichlet type :

$$(1.2) \quad u = 0 \quad \text{on } \partial\Omega .$$

Here  $a^\varepsilon(x) = a(x/\varepsilon)$ ,  $x \in \Omega$ ,  $\varepsilon > 0$ , where  $a : Y \rightarrow \mathbb{R}$  is a piecewise constant function :

$$(1.3) \quad a(y) = \begin{cases} \alpha & \text{if } y \in \omega \\ \beta & \text{if } y \in Y \setminus \omega \end{cases}$$

with  $\omega \subset Y$  being a measurable set. The function, still denoted  $a$ , is extended by periodicity onto the whole of  $\mathbb{R}^2$ . The unique solution of (1.1) together with (1.2) will be denoted by  $u^\varepsilon$ .

It is well known (cf. [4], [6], [13], [17], [19]) that

$$(1.4) \quad u^\varepsilon \rightarrow u^0 \text{ (weakly) in } H_0^1(\Omega) \text{ as } \varepsilon \rightarrow 0 +$$

where  $u^0 \in H_0^1(\Omega)$  is the (unique) solution of the homogenized equation

$$(1.5) \quad - \sum_{i,j=1}^2 \frac{\partial}{\partial x_i} \left( q_{ij} \frac{\partial u^0}{\partial x_j} \right) = f \quad \text{in } \Omega$$

$$u^0 = 0 \quad \text{on } \partial\Omega.$$

The coefficients  $q_{ij}$  are the *homogenized coefficients* or the *effective conductivities* and can be calculated as follows

$$(1.6) \quad q_{ij} = \int_Y a \delta_{ij} dy - \int_Y a \delta_{is} \frac{\partial w^{(j)}}{\partial y_s} dy$$

where  $\delta_{ij}$  is the Kronecker's symbol and  $w^{(j)} \in H_{\text{per}}^1(Y)$  is the solution of the following auxiliary problem on the periodic cell  $Y$ :

$$(1.7) \quad \int_Y a(y) \frac{\partial w^{(j)}}{\partial y_i} \frac{\partial \varphi}{\partial y_i} dy = \int_Y a(y) \frac{\partial \varphi}{\partial y_j} dy \quad \forall \varphi \in H_{\text{per}}^1(Y) \quad \forall j = 1, 2.$$

Here  $H_{\text{per}}^1(Y)$  denotes a subspace of  $H^1(Y)$  containing all functions with equal traces on the opposite sides of  $Y$ . Equivalently,  $H_{\text{per}}^1(Y)$  is a set of all functions whose periodic extensions belong to  $H_{\text{loc}}^1(\mathbb{R}^2)$ . Since the solution of (1.7) is defined uniquely up to an additive constant (see [19]), we pick up those  $w^{(j)}$  that have zero mean value.

In what follows, we are going to write  $q_{ij}(\omega)$  in order to stress the dependence of  $q_{ij}$  on the shape  $\omega$ . We will analyze this dependence in detail. To this end we introduce a class  $\mathcal{O}$  of admissible inclusions. We require that  $\omega \in \mathcal{O}$  be a subdomain of  $Y$  and that  $\text{meas } \omega = \theta_\alpha$  where  $0 < \theta_\alpha < 1$  is the concentration of the phase  $\alpha$ .

For the optimal control approach that we are going to apply, it is necessary to ensure *compactness* of the class  $\mathcal{O}$ , in the sense of convergence of characteristic functions in the  $L^2(Y)$ -norm. This means that for any  $\{\omega_n\}_{n \rightarrow \infty} \subset \mathcal{O}$ , there exists a subsequence  $\{\omega_{n'}\} \subset \{\omega_n\}$  and an element  $\omega \in \mathcal{O}$  such that

$$(1.8) \quad \chi(\omega_{n'}) \rightarrow \chi(\omega) \text{ in } L^2(Y) \text{ as } n' \rightarrow \infty$$

where  $\chi(\omega)$  denotes the characteristic function of the domain  $\omega$ . We will use the symbol  $\omega_n \rightarrow \omega$  to denote the convergence of domains in the above sense.

Since we are going to apply the optimal shape design approach, we impose the following conditions :

(i)  $\bar{C} \subset \omega \subset \bar{D}$  for some  $C, D$  being non-empty subdomains of  $Y$  ;

(ii)  $\exists \bar{\varepsilon} > 0$  such that any element  $\omega \in \mathcal{O}$  possesses the  $\bar{\varepsilon}$ -cone property ; and define

$$(1.9) \quad \mathcal{O} := \{ \omega \subset Y \mid \omega \text{ satisfies (i) and (ii), meas } \omega = \theta_\alpha \} .$$

Let us mention that the requirement (ii) already guarantees the compactness (1.8) — see [18]. Indeed, the system  $\mathcal{O}$  is compact with respect to the topology given by the Hausdorff distance, i.e., we can extract a subsequence  $\{\omega_{n'}\} \subset \{\omega_n\}_{n \rightarrow \infty}$  that converges to certain  $\omega \in \mathcal{O}$  in the Hausdorff metrics and that

$$(1.10) \quad \chi(\omega_{n'}) \rightarrow \chi(\omega) \text{ in } L^\infty \text{ weak } \star .$$

Now it is readily seen that (1.8) holds true as well.

LEMMA 1.1 (**Continuity**). *Let  $\omega_n \rightarrow \omega$ ,  $\omega_n, \omega \in \mathcal{O}$ . Then*

$$(1.11) \quad q_{ij}(\omega_n) \rightarrow q_{ij}(\omega) \text{ as } n \rightarrow \infty, \quad i, j = 1, 2 .$$

*Proof:* Denote

$$(1.12) \quad a_n(y) = \alpha \chi(\omega_n) + \beta(1 - \chi(\omega_n))$$

$$a(y) = \alpha \chi(\omega) + \beta(1 - \chi(\omega)) .$$

Then  $a_n \rightarrow a$  in  $L^2(Y)$  as follows from (1.8). From (1.7) we see that

$$(1.13) \quad w^{(j)}(\omega_n) \rightarrow w^{(j)}(\omega) \text{ in } H^1(Y) \text{ as } n \rightarrow \infty \quad j = 1, 2$$

and consequently (1.11) holds. □

Let  $\mathbb{S}$  denote the set of  $2 \times 2$  symmetric positive definite matrices and let  $J: \mathbb{S} \rightarrow \mathbb{R}$  be a *lower semicontinuous* cost functional :

$$(1.14) \quad A_n \rightarrow A \text{ in } \mathbb{S} \Rightarrow \liminf_{n \rightarrow \infty} J(A_n) \geq J(A).$$

We denote  $\mathcal{F}(\omega) = J(A(\omega))$  where  $A(\omega) = (q_{ij}(\omega))_{i,j=1}^2$  is the homogenized conductivity tensor corresponding to the particular choice of  $\omega \in \mathcal{O}$ .

Finally, define the problem

$$(\mathbb{P}) \quad \begin{cases} \text{Find } \omega^* \in \mathcal{O} \text{ such that} \\ \mathcal{F}(\omega^*) = \inf_{\omega \in \mathcal{O}} \mathcal{F}(\omega) \end{cases}$$

Using classical compactness arguments, it is easy to prove

**THEOREM 1.2 (Existence).** *The problem  $(\mathbb{P})$  has at least one solution  $\omega^*$ .*

Here we present two typical examples of cost functionals that satisfy the lower semicontinuity (1.14) (more : these are continuous). Namely

$$(1.15) \quad J(A) = \sum_{i,j=1}^2 (A_{ij} - C_{ij})^2, \quad C_{ij} \in \mathbb{R}, \quad A \in \mathbb{S}$$

$$(1.16) \quad J(A) = \sum_{i=1}^2 (\lambda_i(A) - \mu_i)^2, \quad \mu_i \in \mathbb{R}, \quad A \in \mathbb{S}$$

where  $C_{ij}$  are prescribed values of the target effective conductivity matrix or  $\mu_i$  are prescribed values of the target principal conductivities.  $\lambda_i(A)$  denotes the  $i$ -th eigenvalue of  $A$ .

## 2. APPROXIMATION OF THE IDENTIFICATION PROBLEM

The aim of this part is to describe the discretization of the problem  $(\mathbb{P})$  introduced in previous section and to study the convergence properties of discrete models. We start with discretization of the state problem (1.7).

Let  $\{V_h\}$ ,  $V_h \subset H_{\text{per}}^1(Y)$  be a family of finite-dimensional subspaces of  $H_{\text{per}}^1(Y)$ , for which  $\dim V_h = n(h) \rightarrow \infty$  as  $h \rightarrow 0+$ , and that have the following approximation property :

$$(2.1) \quad \forall v \in H_{\text{per}}^1(Y) \exists \{v_h\}, v_h \in V_h \text{ such that } v_h \rightarrow v \text{ in } H^1(Y).$$

*Remark 2.1:* In practice, the finite element method will be used for construction of the spaces  $V_h$ . Then the symbol  $h$  is related to the norm of partition  $\mathcal{T}_h$  of the domain into finite elements.

For any  $H > 0$ , let  $\mathcal{O}_H$  be a system of measurable subsets  $\omega_H$  of  $Y$  that are uniquely defined by a finite number of parameters  $\Phi_i$ ,  $i = 1, \dots, m(H)$  where  $m(H) \rightarrow \infty$  as  $H \rightarrow 0+$  and that satisfy  $|\text{meas } \omega_H - \theta_\alpha| \leq \eta(H)$  where  $\eta(H) \rightarrow 0+$  when  $H \rightarrow 0+$ .

*Example 2.1:* Let  $\{\mathcal{T}_h\}_{h \rightarrow 0+}$  be a regular family of partitions of  $\bar{Y}$ . For any  $h > 0$ , let  $\{T_i\}$  be a system of all finite elements  $T_i$  belonging to  $\mathcal{T}_h$ . With any  $\omega \in \mathcal{O}$  we associate the subset  $\omega_H$ , defined as follows:

$$(2.2) \quad \omega_H := \cup \{T_i \in \mathcal{T}_h \mid \text{meas}(T_i \cap \omega) \neq 0\}.$$

The system  $\mathcal{O}_H$  will contain all such sets  $\omega_H$ .

In this case, the parameters  $\Phi_i$  can be identified with centers of gravity of  $T_i$ , for instance. Moreover,  $\mathcal{O}_H$  contains a finite number of  $\omega_H$ 's.  $\square$

*Example 2.2:* This example will be used in subsequent sections when dealing with practical applications. Let  $\mathcal{O}$  be a family of domains introduced in (1.9). In addition, let all  $\omega \in \mathcal{O}$  be star-shaped with respect to the center of the square  $Y$ . Boundaries of such domains can be described in the polar coordinate system, as follows.

For any  $\omega \in \mathcal{O}$  there exists a function  $r : [0 ; 2\pi] \rightarrow ]0, \sqrt{2}/2[$  such that  $r(0) = r(2\pi)$  and

$$(2.3) \quad \partial\omega = \{(x(\varphi), y(\varphi)) \mid \varphi \in [0 ; 2\pi[ \}$$

where

$$(2.4) \quad x(\varphi) = \frac{1}{2} + r(\varphi) \cos \varphi$$

$$y(\varphi) = \frac{1}{2} + r(\varphi) \sin \varphi.$$

Any domain  $\omega$  will be approximated by a sequence of regular polygonal domains  $\{\omega_H\}_{H=\frac{1}{m}, m \rightarrow \infty}$ . Every  $\omega_H$  is a polygon with vertices  $N_1, \dots, N_m$ :

$$(2.5) \quad N_i = (x(\varphi_i), y(\varphi_i)) \quad \text{where} \quad \varphi_i = \frac{2\pi i}{m}$$

so the division of the angle interval is uniform. In this case, the parameters  $\Phi_i$  will be identified with the radii  $r(\varphi_i)$ .

On contrary to the previous example, here the family  $\mathcal{O}_H$  contains infinitely many elements.  $\square$



Let  $V_h$  and  $\omega_H \in \mathcal{O}_H$  be given. We are looking for a function  $w_h^{(j)} \in V_h$  such that

$$(2.6) \quad \int_Y a_H(y) \frac{\partial w_h^{(j)}}{\partial y_i} \frac{\partial \varphi_h}{\partial y_i} dy = \int_Y a_H(y) \frac{\partial \varphi_h}{\partial y_j} dy \quad \forall \varphi_h \in V_h, \quad j = 1, 2$$

where the coefficient field is

$$(2.7) \quad a_H(y) = \begin{cases} \alpha & \text{if } y \in \omega_H \\ \beta & \text{if } y \in Y \setminus \omega_H. \end{cases}$$

Having these  $w_h^{(j)}$ , we get the approximate homogenized coefficients  $q_{ij,h}(\omega_H)$  from

$$(2.8) \quad q_{ij,h}(\omega_H) = \int_Y a_H \delta_{ij} dy - \int_Y a_H \delta_{is} \frac{\partial w_h^{(j)}}{\partial y_s} dy.$$

Analogously to the continuous case, we shall take the solutions  $w_h^{(j)}$  of (2.6) that satisfy the additional zero-mean-value condition.

Let  $J_h : \mathbb{S} \rightarrow \mathbb{R}$  be an approximation of the cost functional  $J$ . The approximation of the problem  $(\mathbb{P})$  then reads :

$$(\mathbb{P}_{hH}) \quad \begin{cases} \text{Find } \omega_H^* \in \mathcal{O}_H \text{ such that} \\ \mathcal{J}_h(\omega_H^*) = \inf_{\omega_H \in \mathcal{O}_H} \mathcal{J}_h(\omega_H) \end{cases}$$

where  $\mathcal{J}_h(\omega_H) = J(A_h(\omega_H))$ ,  $A_h(\omega_H) = (q_{ij,h}(\omega_H))_{i,j=1}^2$ .

In order to guarantee the existence of at least one solution of  $(\mathbb{P}_{hH})$ , we shall assume

$$(2.9) \quad \text{For any } H > 0, \text{ the family } \mathcal{O}_H \text{ is compact in the sense of (1.8)}$$

$$(2.10) \quad J_h \text{ is lower semicontinuous in the sense of (1.14) .}$$

Then the following holds.

**THEOREM 2.1 (Existence) :** *Let (2.9) and (2.10) be satisfied. Then  $(\mathbb{P}_{hH})$  has at least one solution.*

*Proof is the same as that of Theorem 1.2.  $\square$*

In the sequel, we shall study the mutual relation between  $(\mathbb{P})$  and  $(\mathbb{P}_{hH})$  when  $h, H \rightarrow 0 +$ . To this end we need the following additional assumptions :

The system  $\{\mathcal{O}_H\}$ ,  $H \rightarrow 0+$  is compact in the following sense : for any  $\{\omega_H\}$ ,  $\omega_H \in \mathcal{O}_H$  there exists a subsequence  $\{\omega_{H'}\}_{H' \rightarrow 0+}$  and an element  $\omega \in \mathcal{O}$  such that

$$(2.11) \quad \omega_{H'} \rightarrow \omega \text{ as } H' \rightarrow 0+ .$$

For any  $\omega \in \mathcal{O}$  there exists a sequence  $\{\omega_H\}$ ,  $\omega_H \in \mathcal{O}_H$  such that

$$(2.12) \quad \omega_H \rightarrow \omega \text{ as } H \rightarrow 0+ .$$

If  $A_h$ ,  $A \in \mathbb{S}$ ,  $A_h \rightarrow A$ , then

$$(2.13) \quad \lim_{h \rightarrow 0+} J_h(A_h) = J(A) .$$

Let us remark that the set convergences in (2.11) and (2.12) are taken in the sense introduced in Section 1. Finally, we also assume that  $h \rightarrow 0+$  whenever  $H \rightarrow 0+$ , and vice versa.

We start by proving the following auxiliary

LEMMA 2.2 : Let  $\omega_H \rightarrow \omega$ ,  $\omega_H \in \mathcal{O}_H$ ,  $\omega \in \mathcal{O}$  and (2.1) be satisfied. Then

$$(2.14) \quad q_{ij,h}(\omega_H) \rightarrow q_{ij}(\omega) \text{ as } h, H \rightarrow 0+ \quad \forall i, j = 1, 2 .$$

*Proof:* The problem (2.6) admits a unique solution among zero-mean-value functions. The sequence  $\{w_h^{(j)}\}$  is bounded in the  $H^1(Y)$ -norm by virtue of the Poincaré's inequality. Thus, there exists a subsequence  $\{w_{h'}^{(j)}\} \subset \{w_h^{(j)}\}$  and an element  $w^{(j)} \in H_{\text{per}}^1(Y)$  with zero mean value, such that

$$(2.15) \quad w_{h'}^{(j)} \rightharpoonup w^{(j)} \text{ in } H^1(Y) .$$

Next,  $a_H \rightarrow a$  in the  $L^2(Y)$ -norm and  $a$  is in the form (1.3). This, together with (2.1) and (2.15), yields that  $w^{(j)}$  solves (1.7). Under the assumption of zero mean value of the solutions, (1.7) has a unique solution and consequently, the whole sequence  $\{w_h^{(j)}\}$  tends weakly to  $w^{(j)}$ . It is readily seen that  $\{w_h^{(j)}\}$  tends strongly to  $w^{(j)}$  in  $H^1(Y)$ . Passing to the limit with  $h'$ ,  $H \rightarrow 0+$  and making use of (2.15), we get (2.14).  $\square$

The main result of this section is the following

**THEOREM 2.3 (Convergence):** *Let (2.1) and (2.9)-(2.13) hold. Let  $\omega_H^* \in \mathcal{O}_H$  be a solution of  $(\mathbb{P}_{hH})$  and  $q_{ij,h}(\omega_H^*)$  the approximation of the homogenized coefficients. Then there exist: a subsequence  $\{\omega_{H'}\} \subset \{\omega_H\}$  and a subsequence  $\{q_{ij,h}(\omega_{H'})\} \subset \{q_{ij,h}(\omega_H^*)\}$ , an element  $\omega^* \in \mathcal{O}$  and real numbers  $q_{ij}$ ,  $i, j = 1, 2$  such that*

$$(2.16) \quad \omega_{H'}^* \rightarrow \omega^*$$

$$(2.17) \quad q_{ij,h}(\omega_{H'}^*) \rightarrow q_{ij}$$

as  $h, H' \rightarrow 0 +$ . Moreover,  $\omega^*$  solves  $(\mathbb{P})$  and  $q_{ij} = q_{ij}(\omega^*)$  are the corresponding homogenized coefficients.

*Proof:* The existence of a subsequence  $\{\omega_{H'}^*\}$  satisfying (2.16) follows from (2.11). The convergence (2.17) results from Lemma 1.1. All what remains to show is the fact that  $\omega^*$  solves  $(\mathbb{P})$ .

To accomplish this, let  $\bar{\omega} \in \mathcal{O}$  be arbitrary. By (2.12), there exists a sequence  $\{\bar{\omega}_H\}$ ,  $\bar{\omega}_H \in \mathcal{O}_H$  such that

$$(2.18) \quad \bar{\omega}_H \rightarrow \bar{\omega}, \quad H \rightarrow 0 +$$

and at the same time

$$(2.19) \quad q_{ij,h}(\bar{\omega}_H) \rightarrow q_{ij}(\bar{\omega}), \quad i, j = 1, 2$$

as again follows from Lemma 2.2. The definition of  $(\mathbb{P}_{hH})$  yields :

$$(2.20) \quad \mathcal{F}_h(\omega_{H'}^*) \leq \mathcal{F}_h(\bar{\omega}_{H'}) .$$

Now, letting  $h, H' \rightarrow 0 +$  in (2.20), we arrive at the assertion of the theorem when we make use of (2.18), (2.19) and (2.14). □

*Example 2.3:* Let  $\mathcal{O}$  be given by (1.9). For any  $H = \frac{1}{m}$ ,  $m$  integer, we define  $\mathcal{O}_H$  as the set of those  $\omega_H$  that satisfy :

$$(2.21) \quad \omega_H \text{ is a regular polygonal domain in the sense of Example 2.2, the vertices } N_i \in \bar{D} \setminus C \text{ for } i = 0, \dots, m ;$$

$$(2.22) \quad \exists \kappa \in ]0, 1[ \text{ and } \exists c > 0 \text{ such that } |\text{meas } \omega_H - \theta_\alpha| \leq cH^\kappa ;$$

$$(2.23) \quad \text{All interior vertex angles are greater than some } \varepsilon > 0 \text{ which is independent of } H .$$

Then the system  $\{\mathcal{O}_H\}_{H \rightarrow 0+}$  satisfies (2.11) and (2.12). Indeed, let  $\{\omega_H\}_{H \rightarrow 0+}$ ,  $\omega_H \in \mathcal{O}_H$ , be an arbitrary sequence. Due to (2.23), all  $\omega_H$  possess the  $\tilde{\varepsilon}$ -cone property. Then there exist a subsequence  $\{\omega_{H'}\} \subset \{\omega_H\}$  and an element  $\omega$  such that

$$(2.24) \quad \omega_{H'} \rightarrow \omega \text{ as } H' \rightarrow 0+ .$$

The domain  $\omega$  will possess the  $\tilde{\varepsilon}$ -cone property as well, it will be  $\text{meas } \omega = \theta_\alpha$  (because of (2.22)) and  $\bar{C} \subset \omega \subset \bar{D}$ . Consequently,  $\omega \in \mathcal{O}$ .

Let  $\omega \in \mathcal{O}$  be given. Then the piecewise linear Lagrange interpolations of its boundary  $\partial\omega$  at nodes  $N_i$  define the sequence  $\{\omega_H\}$ , satisfying (2.21)-(2.23). Moreover  $\partial\omega_H \rightrightarrows \partial\omega$  (the uniform convergence). Hence  $\omega_H \rightarrow \omega$ .  $\square$

### 3. A RELIABLE METHOD FOR COMPUTING HOMOGENIZED COEFFICIENTS

There is a reliable way of calculating the homogenized coefficients using both primal and dual formulations of the problem (1.7); for a thorough description we refer to the paper [7]. The method yields the result together with a reliable, *a posteriori* error estimate.

The homogenization formulae can be written also in a different way — as a variational principle of minimum local potential energy :

$$(3.1) \quad \xi_i q_{ij} \xi_j = \inf_{w \in H_{\text{per}}^1(Y)} \int_Y a(y) \left( \xi_k + \frac{\partial w}{\partial y_k} \right) \left( \xi_k + \frac{\partial w}{\partial y_k} \right) dy .$$

From this it was observed that the homogenized coefficients are of the nature of energy. If we solve the problem (3.1) by a conforming Ritz numerical method (based e.g. on the Finite Elements), we are sure that the numerical energies converge to the exact value *from above*.

On the other hand, there is a dual formulation to (3.1), known as the minimum local complementary energy principle :

$$(3.2) \quad \xi_i r_{ij} \xi_j = \inf_{u \in U} \int_Y (a(y))^{-1} (\xi_k + u_k) (\xi_k + u_k) dy$$

where  $(r_{ij})$  is the inverse of  $(q_{ij})$ . The space  $U$  of equilibrium fluxes contains all periodic divergence-free vector fields with zero mean value :

$$(3.3) \quad U = \left\{ u \in H_{\text{per}}^{\text{div}^0}(Y; \mathbb{R}^n) \mid \int_Y u dy = 0 \right\}$$

In 2-D, the space of the periodic divergence-free functions with zero mean value is generated by the *curl* operator from the space of periodic stream functions (for proof see [7]). If we do the substitution, (3.2) reads

$$(3.4) \quad \xi_i r_{ij} \xi_j = \inf_{\psi \in H_{\text{per}}^1(Y)} \int_Y (a(y))^{-1} \left( \xi_k + \frac{\partial \psi}{\partial y_k} \right) \left( \xi_k + \frac{\partial \psi}{\partial y_k} \right) dy.$$

The numerical solutions of (3.2) will converge again from above, causing the dual  $q_{ij}$ 's to converge *from below*. This yields two sided bounds on the exact value of the homogenized coefficients and if the average of these bounds is taken as our numerical solution, the norm of the difference of the bounds estimates the maximum numerical error. This is *reliable*.

The actual solution technique is a bit more complicated: along with the finite element method error also an error due to the use of an iterative linear system solver enters the game. Nonetheless, also this has the nice property that the numerical results stay on one side (above/below) of the exact values. A  $p$ -type finite element method was used.

For the optimization it is convenient to know to what extent it is safe to rely upon the solution of the state problem.

#### 4. THE DESIGN SENSITIVITY ANALYSIS

Theorem 2.3 asserts that under some hypotheses the solution to the micro-geometry identification problem can be approximated numerically. Majority of numerical optimization algorithms requires that the user supplies a procedure to evaluate the objective function value and the constraint function values and a procedure that computes gradients of the objective function and of the constraint functions. This section deals with the evaluation of the gradients.

We use the material derivative method. Let our current geometry be  $\omega$ . We introduce a « velocity » field  $V \in W_0^{1,\infty}(Y; \mathbb{R}^n)$  and study how the homogenized coefficients change if we map the square  $Y$  onto itself by a mapping  $F_t = I + tV$  where the « time »  $t > 0$  diminishes. By  $\omega_t$  we denote  $F_t(\omega)$  — the perturbed image of  $\omega$ .

If we use the test function  $w^{(i)}$  in (1.7), the homogenized coefficients formula can be cast as

$$(4.1) \quad q_{ij} = \int_Y a(y) \delta_{ij} dy - \int_Y a(y) \frac{\partial w^{(i)}}{\partial y_k} \frac{\partial w^{(j)}}{\partial y_k} dy.$$

In the sequel we state the terms for the calculation of  $q_{ij}(\omega_t)$ , and then we evaluate the Gateaux differential

$$(4.2) \quad \dot{q}_{ij}(\omega) = \left. \frac{d}{dt} q_{ij}(\omega_t) \right|_{t=0}.$$

We use the substitution theorem for the first term in (4.1) :

$$(4.3) \quad \int_Y a_t(y) \delta_{ij} dy = \int_Y a(y) \delta_{ij} I_t dy$$

where  $I_t = \det \nabla F_t$  and  $a_t(y)$  equals either  $\alpha$  (for  $y \in \omega_t$ ) or  $\beta$  (for  $y \in \mathcal{N}\omega_t$ ). Thus

$$(4.4) \quad \int_Y a_t(y) \delta_{ij} dy - \int_Y a(y) \delta_{ij} dy = t \int_Y a(y) \delta_{ij} \operatorname{div} V dy + o(t).$$

In the treatment of the second term in (4.1) we first have to calculate the derivative of the state problem solutions  $w^{(j)}$ . We have

$$(4.5) \quad \int_Y a_t(y) (\nabla w_t^{(j)}, \nabla \varphi) dy = \int_Y a_t(y) (e_j, \nabla \varphi) dy$$

or, after substitution,

$$(4.6) \quad \int_Y a(y) ((\nabla F_t^{-1})^T \nabla w_t^{(j)}, (\nabla F_t^{-1})^T \nabla \varphi) I_t dy = \\ = \int_Y a(y) (e_j, (\nabla F_t^{-1})^T \nabla \varphi) I_t dy.$$

The first-order terms in the difference of (1.7) from (4.6) are the following :

$$(4.7) \quad \int_Y a(y) (\nabla \dot{w}^{(j)}, \nabla \varphi) dy + \int_Y a(y) (\nabla w^{(j)}, \nabla \varphi) \operatorname{div} V dy - \\ - \int_Y a(y) ((\nabla V)^T \nabla w^{(j)}, \nabla \varphi) dy - \int_Y a(y) (\nabla w^{(j)}, (\nabla V)^T \nabla \varphi) dy \\ = - \int_Y a(y) (e_j, (\nabla V)^T \nabla \varphi) dy + \int_Y a(y) (e_j, \nabla \varphi) \operatorname{div} V dy$$

where  $\dot{w}^{(j)} = \left. \frac{d}{dt} w_t^{(j)} \right|_{t=0}$ .

If we introduce matrices  $\mathcal{A} = (\operatorname{div} V) I - \nabla V - (\nabla V)^T$  and  $\mathcal{B} = (\operatorname{div} V) I - \nabla V$ , we can rewrite (4.7) as

$$(4.8) \quad \int_Y a(y) (\nabla \dot{w}^{(j)}, \nabla \varphi) dy = \int_Y a(y) (\mathcal{B} e_j, \nabla \varphi) dy - \\ - \int_Y a(y) (\mathcal{A} \nabla w^{(j)}, \nabla \varphi) dy$$

which is the equation for the derivative  $\dot{w}^{(j)}$ .

Now, we turn our attention to the homogenized coefficients formula (4.1). Taking into account what we already did, its second term has the following derivative :

$$(4.9) \quad \int_Y a(y) (\mathcal{A} \nabla w^{(i)}, \nabla w^{(j)}) dy + \\ + \int_Y a(y) (\nabla \dot{w}^{(i)}, \nabla w^{(j)}) dy + \int_Y a(y) (\nabla w^{(i)}, \nabla \dot{w}^{(j)}) dy .$$

Next, we choose  $w^{(i)}$  as a test function in (4.8). This will give us the third term of (4.9). At last, when we write  $i$  instead  $j$  in (4.8) and choose  $w^{(j)}$  as the test function, we get the second term of (4.9). We were able to eliminate the state problem solution derivatives ; we arrive (together with (4.4)) at the formula

$$(4.10) \quad \dot{q}_{ij} = \int_Y a(y) \delta_{ij} \operatorname{div} V dy + \int_Y a(y) (\mathcal{A} \nabla w^{(i)}, \nabla w^{(j)}) dy - \\ - \int_Y a(y) (\mathcal{B} e_i, \nabla w^{(j)}) dy - \int_Y a(y) (\mathcal{B} e_j, \nabla w^{(i)}) dy .$$

This formula is convenient for the numerical work as well, since it contains volume integrals only. Moreover, any error estimate on  $w$  will imply an estimate of the error in  $\dot{q}_{ij}$ .

## 5. IMPLEMENTATION OF THE IDENTIFICATION PROBLEM

The reliable method from Section 3, the design sensitivity analysis procedure from Section 4 and the design approach presented in Example 2.3 were implemented in a computer code.

The class  $\mathcal{O}$  was restricted to star-shaped, single inclusion geometries. Shapes of the inclusions are parametrized by a polar function around the center

of the cell. We restricted ourselves to center-symmetric inclusions : this somewhat decreased the design ambiguity involved in the effective coefficient values. The justifying argument is that starting from a center-symmetric inclusion, we could get a non-symmetric one later in the optimization process only as a result of numerical imprecisions.

We take

$$(5.1) \quad \omega(r) = \left\{ \left( \frac{1}{2} + \rho \cos \varphi, \frac{1}{2} + \rho \sin \varphi \right) \mid |\rho| < r(\varphi), \varphi \in [0; \pi[ \right\}$$

$$(5.2) \quad \mathcal{O} = \{ \omega(r) \mid r \in C_{\text{per}}^{0,1}[0; \pi], \bar{q} \leq r \leq \bar{r}, |r'| \leq L \text{ a.e.} \}$$

where  $\bar{r}$  expresses the shape of the rectangle of side  $1 - \bar{q}$ . We note that in the examples shown in this paper, we confined the inclusions inside a square 98 % the size of the cell, i.e., we take  $\bar{q} = 0.02$ . This value seems to be a good compromise : on the one hand, it allows for reasonably good identification, on the other hand, the state problems can be solved with a reasonable accuracy (the relative error is typically of the order  $10^{-3}$ ).

The symbol  $L > 0$  in (5.2) is a Lipschitz constant that bounds oscillations of the boundary. This ensures the  $\bar{\varepsilon}$ -cone property and hence the compactness of the family. In the numerical realization, we left this constraint out, since it is included implicitly for each fixed  $H$  ; it is only in the limit passage that this causes problems.

The cost function (1.15) that supports full identification of the desired coefficients  $C_{ij}$  was used. The identification of eigenvalues by (1.16) (i.e. of the tensor up to a rotation) may lead to a non-smooth optimization problem which hasn't been tried out yet. Nevertheless, restricting ourselves to tensors represented by diagonal matrices, one can use the cost functional (1.15) for identification of the corresponding eigenvalues.

In the discrete form, polygonal approximations of the contact curve were taken. The nodes of the approximation  $N_i$  (= vertices of the polygon) were distributed equally over the angle interval  $[0; \pi]$ .

The reliable  $p$ -type finite element solution procedure described in Section 3 performs well even with coarse finite element meshes. The mesh was constructed in the following way : in the inclusion, the triangles are given by the following vertices : the center of the cell and by the nodes  $N_i$  and  $N_{i+1}$  that are control nodes for the shape of the inclusion. In the matrix, we formed quadrilaterals  $N_i B_i B_{i+1} N_{i+1}$  where  $B_i$  is the intersection of the radius of the node  $N_i$  with the boundary of the cell. These quadrilaterals were divided up to two triangles ; always the choice that yields better shaped triangles is taken.

The design variables were the distances of the nodes  $N_i$  from the center of the cell. In our numerical procedure it is unfeasible that the inclusions expanded up to the boundary of the cell, for the following reasons :

- There always is a layer of finite elements around the inclusion. The state problem gets ill conditioned if this layer is compressed too much.



- The possible remedy to the above objection, to leave the finite element layer out if it gets too thin, would introduce a non-differentiability to the cost functional.

- This would imply a great difficulty in the design sensitivity analysis : we would have two boundaries that can possibly coincide and yet we want to move each of them independently.

A general SQP optimization package <sup>(2)</sup> was employed, and a sensitivity analysis routine calculates the gradient of the cost function with respect to the design variables as described in Section 4. The optimization terminates when the norm of the gradient of the Lagrangian is below a fixed constant. The computer code then generates the result presentation form.

### 5.1. Description of the presentation form

The computer code generates an Encapsulated PostScript file that presents the numerically identified microstructure and its data. The phases are assigned different shades of gray ; as a rule the more conductive phase is the darker one. There are two panels and a legend in the presentation form. On the left panel, we show the phase arrangement in a  $4 \times 4$  array of periodic cells. This illustrates the whole composite. On the right panel, there is a detailed view of the periodic cell.

Finally, the legend contains basic data about the composite, with the following meaning of the symbols : in the **Phases** part, we present the constituent phases :  $\theta$  is the phase concentration and  $A$  its conductivity. In the **Target** section,  $C$  is the desired target of the identification. Then comes the **Result** part where we read :

$A$  : the effective conductivity of the presented microstructure ;

$e$  : the relative error of the calculation of the effective conductivity, see Section 3 ;

$i$  : the iteration count of the last SQP iteration ; and

$f$  : value of the cost function (1.15).

There are two ways of writing a tensor. If it is isotropic, it is written as a multiple of  $I$  — of the identity tensor. If the tensor is not isotropic (in the conduction context every material is orthotropic), we write  $\text{diag}(\lambda_1, \lambda_2)$  for the eigenvalues of the tensor. In the case the eigendirections do not coalign

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<sup>(2)</sup> The NLPQLD package by K. Schittkowski. The permission to use this package is gratefully acknowledged.

with the coordinate axes, we append a rot ( $\phi$ ) term to give the angle from the  $e_1$  axis to the eigendirection corresponding to  $\lambda_1$  -measured counterclockwise.

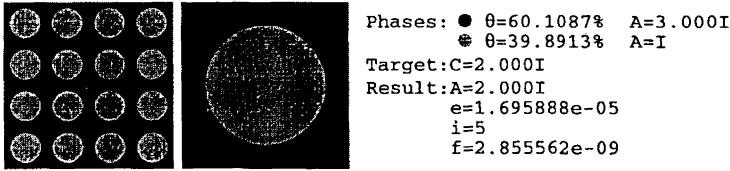


Figure 1. — Identification of a target without the volume constraint. The target belongs to the  $G$ -set. A perfect identification.

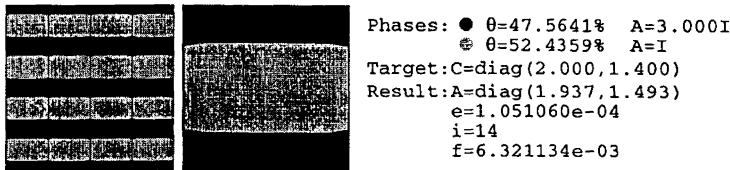


Figure 2. — Identification of a target without the volume constraint. The target lies outside the  $G$ -set. The effective moduli are the closest possible to the target.

## 5.2. Examples of the numerical microstructure identification

Figures 1 and 2 present two identifications *without* the volume constraint  $\text{meas } \omega = \theta_\alpha$ . Letting the volume fractions of the phases free, we can study the  $G$ -closure set :

$$G := \cup \{G_\theta | 0 \leq \theta \leq 1\}$$

i.e., the set of effective moduli of all composites made from the given phases. The target on figure 1 lies in the  $G$ -closure set, and it was identified very well. The target on figure 2 lies outside the  $G$ -closure set, and therefore the identification did its best : the numerical effective moduli lie as close to the boundary of the  $G$ -closure as the numerical approximation permits.

There is more interest in identifications *with* the volume constraint, or equivalently, in  $G_\theta$ -closure studies. On figures 3-5, we present identifications of targets that lie inside, above and below the  $G_\theta$ -closure set, respectively.

We should always check whether the cost function values are not in the range where only a tiny change of homogenized coefficients (within the error estimate) would cause dramatic changes of the cost function value. In the

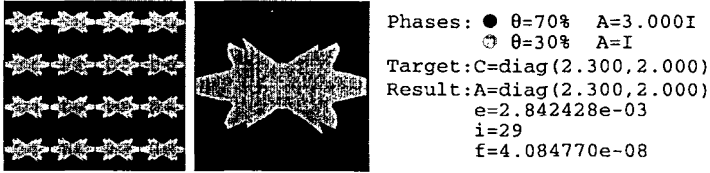


Figure 3. — Identification of a target with the volume constraint. The target belongs to the  $G_\theta$ -closure set.

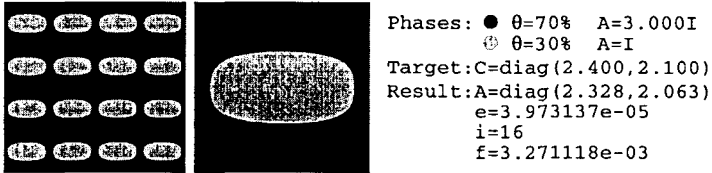


Figure 4. — Identification of a target with the volume constraint. The target lies above the  $G_\theta$ -closure set, or equivalently, there is too little of the more conductive phase. The identification matches projection of the target onto the  $G_\theta$ -set.

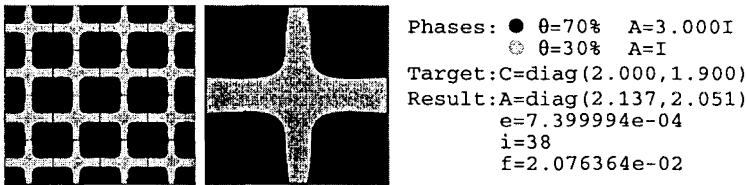


Figure 5. — Identification of a target with the volume constraint. The target lies below the  $G_\theta$ -closure set, or equivalently, there is too much of the more conductive phase. The identification again matches projection of the target onto the  $G_\theta$ -set.

examples presented here a reasonable limit of the cost value is about  $10^{-7}$ ; below this limit the success in identification is to the greatest extent a numerical coincidence. However, for practical purposes this accuracy is more than enough.

## 6. NUMERICAL STUDIES OF THE $G_\theta$ -CLOSURE SETS

### 6.1. Optimal bounds on the effective moduli

Let us have two phases with conductivities  $A, B \in \mathbb{S}$ ; let both  $A$  and  $B$  be positive definite. Let us take the set of effective conductivities  $H \in \mathbb{S}$  of all

composites where we mix the two phases  $A$  and  $B$  in volume fractions  $\theta_A$  and  $\theta_B$ , respectively; we assume  $\theta_A, \theta_B \geq 0$  and  $\theta_A + \theta_B = 1$ . The set of all these  $H$  is the  $G_\theta$ -closure where we take  $\theta = \theta_A$ .

If we have a composite of effective conductivity  $H \in G_\theta$ , then the same composite rotated by an arbitrary rotation tensor  $R$  (i.e., an orthogonal tensor with positive determinant) has the effective conductivity  $R^T H R$  which clearly also belongs to  $G_\theta$ . Then we see that the  $G_\theta$  set is rotation invariant and that in fact only the eigenvalues of  $H$  carry substantial information. These eigenvalues, called the *effective moduli*, are denoted  $\lambda_1$  and  $\lambda_2$ . From now on, we take the  $G_\theta$  set as a subset of the plane of the eigenvalues. We will not distinguish between the two of them, so the set will necessarily be symmetric with respect to the isotropy axis  $\lambda_1 = \lambda_2$ .

For a composite made of two isotropic phases with conductivities  $\alpha I$  and  $\beta I$  taken in volume fractions  $\theta_\alpha$  and  $\theta_\beta$ , the following elementary bounds hold true:

$$(EB) \quad h \leq \lambda_i \leq m \quad \text{for } i = 1, 2$$

where  $m$  and  $h$  denote the arithmetic and harmonic means, respectively:

$$m = \theta_\alpha \alpha + \theta_\beta \beta$$

$$h = (\theta_\alpha \alpha^{-1} + \theta_\beta \beta^{-1})^{-1}.$$

The elementary bounds are readily seen from the variational principles (3.1)-(3.2) if one tries zero as a test function. We note that the point of maximum anisotropy  $(m, h)$  (or  $(h, m)$ , equivalently) is realized by the layered composite (= laminate): the conductivity is maximum ( $m$ ) in the direction of the layers and minimum in the direction orthogonal to the layers ( $h$ ). Analytical formulas are available for conductivity of a layered composite with arbitrary (including anisotropic) phases; in the case of isotropic phases we easily see the result from the physical situation of resistors in parallel and in series.

The elementary bounds (EB) are necessary but not sufficient: there are points, e.g.  $(m, m)$  and  $(h, h)$  that satisfy the bounds and yet cannot be realized by any microstructure. A finer approach is necessary, one has to estimate the two eigenvalues together. Using the Hashin-Shtrikman variational principle, one can derive the following inequalities satisfied by the effective moduli  $\lambda_1, \lambda_2$ :

$$(LB) \quad \sum_{i=1}^2 \frac{1}{\lambda_i - \alpha} \leq \frac{1}{m - \alpha} + \frac{1}{h - \alpha}$$

$$(UB) \quad \sum_{i=1}^2 \frac{1}{\beta - \lambda_i} \leq \frac{1}{\beta - m} + \frac{1}{\beta - h}$$

where we assume  $0 \leq \alpha < \beta$ . It is easy to check that any effective moduli  $(\lambda_1, \lambda_2)$  that satisfy these bounds, satisfy also the elementary bounds. However, here it can be proved that any homogenized conductivity tensor with eigenvalues that satisfy the bounds (LB) and (UB) is attained by a microstructure, and consequently, the  $G_\theta$ -closure set is fully characterized by these bounds. This is the reason for calling the bounds *optimal*.

On figures 6 and 7, the curves of the « lenses » correspond to the  $G_\theta$ -closure sets for the case  $\alpha = 1$  and  $\beta = 3$ ;  $\theta_\beta$  is 10 % through 90 % in the steps by 10 %.

Perforated composites — mixtures of a phase and a void — are usually treated by the limit passage  $\alpha \rightarrow 0+$ . In the practice, the inclusion is taken to be filled with a relatively poorly conducting phase. We studied also this case and it turned out to be sufficient to take  $\alpha = 0.001$  and  $\beta = 1$ . The  $G_\theta$ -closure sets are the « fatter », the smaller the ratio  $\frac{\alpha}{\beta}$ . In the limit, the lower bound (LB) degenerates and a  $G_\theta$ -closure set is given just by the upper bound (UB) and by the condition of non-negativity of  $\lambda_1$  and  $\lambda_2$ . On figure 16 we show the upper boundaries of the  $G_\theta$ -closure sets, again for  $\theta_\beta = 10\%, \dots, 90\%$ .

There is a vast literature about optimal bounds on the effective moduli of composites; we won't list but a few references: [15], [8], [23], [17] or for an overview [11].

## 6.2. Numerical $G_\theta$ -closure identification procedure

We studied the case of two isotropic phases with conductivities  $I$  and  $3I$ . We are going to call the phase  $\alpha = 1$  *weaker* and the phase  $\beta = 3$  *stronger*. If the domain  $\omega$  represents the inclusion, then the rest  $\mathcal{Y} \setminus \omega$  is called the *matrix* of the composite.

The single inclusion microgeometry offers the following two ways of arranging the phases in the cell:

**The strong arrangement:** Strong matrix and weak inclusion.

**The weak arrangement:** Weak matrix and strong inclusion.

We took volume fraction  $\theta_\beta = 10\%, 20\%, \dots, 90\%$  and picked up targets on the boundaries of the  $G_\theta$ -closure sets; the effective moduli of the composites on the upper boundary (= maximum energy microstructures) are those that satisfy (UB) as an equality, and the effective moduli on the lower boundary (= minimum energy microstructures) are those that saturate (LB).

We used 32 design variables, i.e., the polygonal inclusions had 64 vertices. Such polygons already approximate sufficiently well inclusions with smooth boundaries. For each of the targets we performed two numerical identifications: once for the strong arrangement of the cell and the other time for the weak one. We observed that the strong arrangement yield effective moduli that

were somewhat higher than those of the weak arrangement. Therefore, it is a good idea to use strong matrix composites for identification of targets on the upper boundary of the  $G_\theta$ -closure set and weak matrix composites for identifying the lower boundary.

Figure 6 shows the targets as well as the effective moduli of the results of the numerical identifications where we used strong matrix composites for the targets on the upper boundaries of the  $G_\theta$ -closure sets and weak matrix composite for targets on the lower boundaries, i.e., if we follow the above recommendation. For comparison, figure 7 presents the identification results for the other choice, i.e. when we use weak matrix for the upper boundary and strong matrix for the lower one.

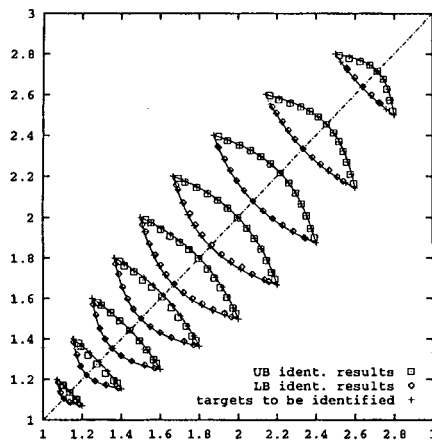


Figure 6. — Identification of the boundaries of the  $G_\theta$ -closure set.  $\alpha = 1$ ,  $\beta = 3$ . The good choice of the composites — stronger matrix, weaker inclusion for the upper branch and stronger inclusion, weaker matrix for the lower one.

Figure 8 shows the detailed view of the volume fraction case  $\theta_\beta = 40\%$  which is quite representative. Figures 9-15 present some of the numerically computed microstructures ; the first half of each of these figures shows the better choice of the composite arrangement while the second part (the worse choice) is shown for comparison purposes. Figure 9 shows identification of the most conductive isotropic target and up to figure 12, the targets move along the upper boundary of the  $G_\theta$ -closure set away from the isotropy axis  $\lambda_1 = \lambda_2$ , toward the most anisotropic target. The target in the corner of the  $G_\theta$  set is attained by a layered composite and its effective moduli can be calculated by hand :  $\lambda_1 = m$ ,  $\lambda_2 = h$ , or vice versa. This point satisfies both (UB) and (LB) as equalities. Then the targets switch to the lower boundary ; on figures 13-15 the targets move back from the corner of the « lens » towards the lowest isotropic conductivity.

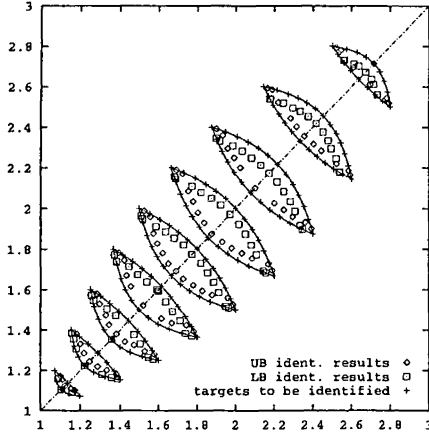


Figure 7. — Identification of the boundaries of the  $G_0$ -closure set.  $\alpha = 1$ ,  $\beta = 3$ . The worse choice of the composites — weaker matrix, stronger inclusion for the upper branch and weaker inclusion, stronger matrix for the lower one.

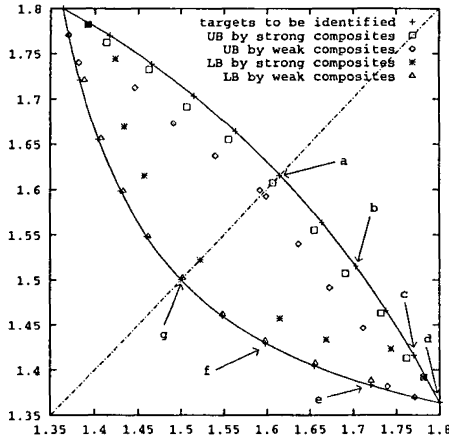


Figure 8. — Detailed view of the volume fraction case  $\theta_\beta = 40\%$ . Both the good and the worse choices of the cell arrangements are shown here. The numerically calculated microstructures for the targets indicated by points  $a - g$  will be shown on subsequent figures.

Figure 16 shows identifications of targets on the upper boundaries of the  $G_0$ -closure sets in the case  $\alpha = 0.001$  and  $\beta = 1$ , i.e., for the approximation

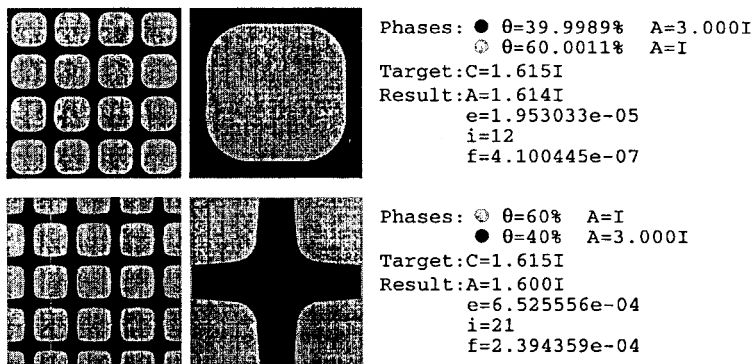


Figure 9. — Case a on figure 8 : the most conductive isotropic target.

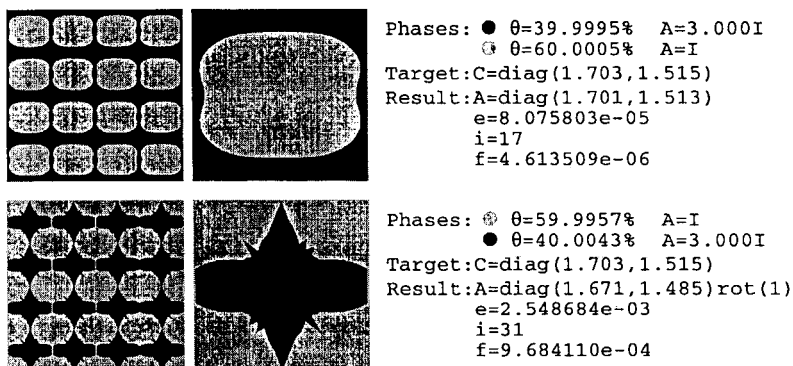


Figure 10. — Case b on figure 8 : an upper branch target with a slight anisotropy.

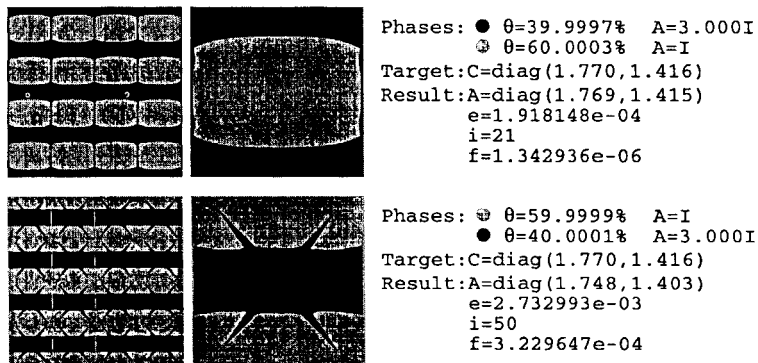


Figure 11. — Case c on figure 8 : a more anisotropic upper branch target.



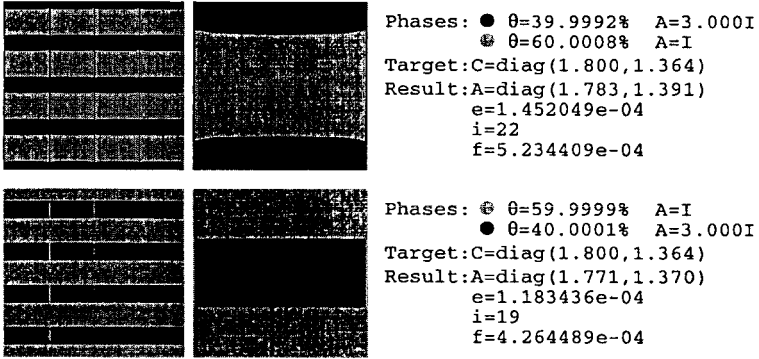


Figure 12. — Case d on figure 8 : the most anisotropic target.

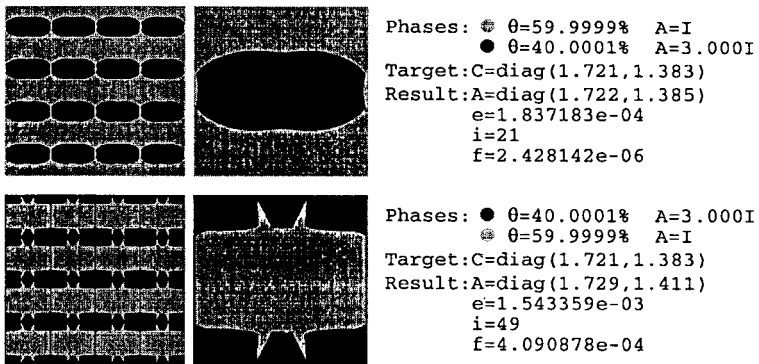


Figure 13. — Case e on figure 8 : a more anisotropic lower branch target.

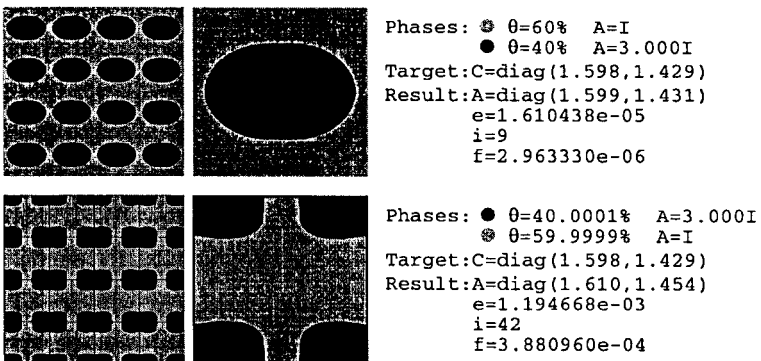


Figure 14. — Case f on figure 8 : a slightly anisotropic lower branch target.

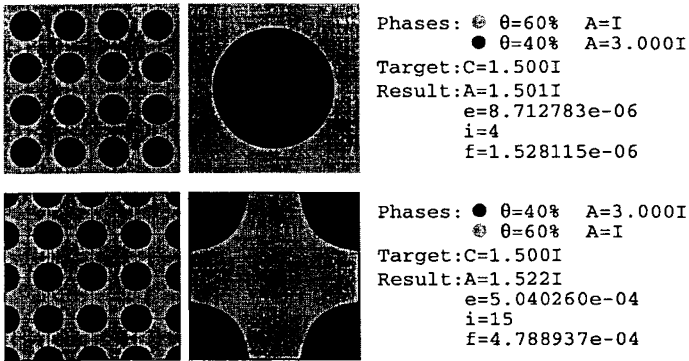


Figure 15. — Case g on figure 8 : the least conductive isotropic target.

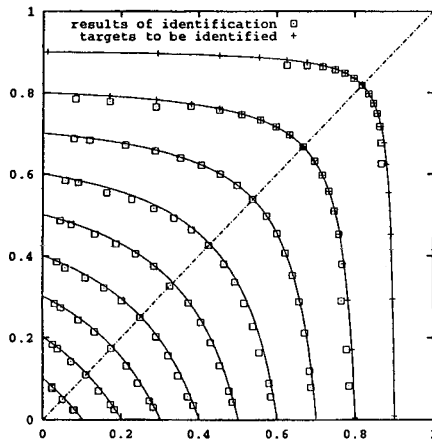


Figure 16. — Simulation of perforated composites. Identification of the upper boundaries of the  $G_0$ -closure sets.  $\alpha = 0.001$ ,  $\beta = 1$ .

to perforated composites. We note that the only meaningful choice of the cell arrangement is the strong one ; it is obvious that an insulator remains inconducive if one inserts only isolated inclusions of a conductor.

### 6.3. Rectangular inclusion composites

Consider now a subclass of the single inclusion composites ; assume inclusions of rectangular shape only. There are only two parameters describing the shape of the inclusion : its width and height. In the  $G_0$ - closure studies,

the area of the inclusion is constrained to a constant, and consequently, only one free parameter is left, namely the aspect ratio of the rectangle. Then there was no need to do identification, it was sufficient to perform plain calculations of the effective moduli.

On figure 17 we show the results for the case of two phases  $\alpha = 1$  and  $\beta = 3$ . Here the curve that is closer to the upper boundary is generated by

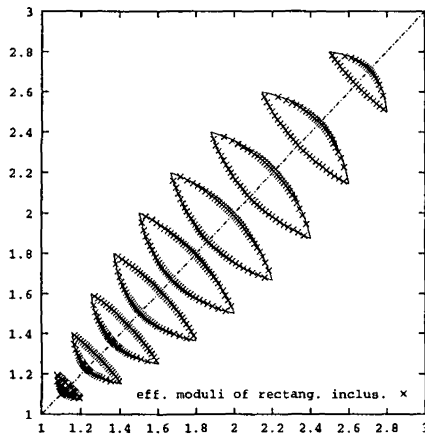


Figure 17. — Effective moduli of the rectangular inclusion composites.  $\alpha = 1$ ,  $\beta = 3$ .

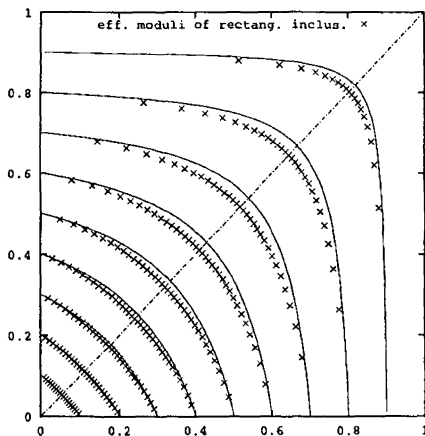


Figure 18. — Effective moduli of the rectangular inclusion composites with (nearly) void in the inclusion.  $\alpha = 0.001$ ,  $\beta = 1$ .

strong matrix composites, while the curve by the lower boundary is a result of the weak arrangement of the cell. On figure 18 we show the results for the nearly insulating inclusions :  $\alpha = 0.001$  and  $\beta = 1$ . Only strong matrix composites were used.

#### 6.4. Comments on the results

The identification performs well unless one requires too strong anisotropy. In the strongly anisotropic case, it would be natural for the inclusions to interconnect and make a layered composite. However, it is a limitation of our numerical procedure that the inclusions cannot do this. On figure 12, instead of laminates that would be the most appropriate microstructure, we see an almost rectangular inclusion composite with longer edge of maximum possible length.

Another consequence of the limitations of our numerical approach is that the effective moduli of the composite follow the conductivity of the matrix more than that of the inclusion. We have seen this already in Section 6.1 in the context of rank-2 laminates : the simple laminate of  $\alpha I$  and  $\beta I$  being layered with the stronger phase gives a composite whose effective moduli saturate the upper bound (UB), while layering with the weaker phase leads to saturation of the lower bound (LB). Also the numerical examples confirm that the conductivity of the matrix is decisive. The reason is that in the periodic array, the matrix is a connected set while the inclusions are isolated.

If we make the choice that is less convenient (the strong arrangement for the lower bound and the weak arrangement for the upper one), we observe a more or less pronounced tendency of the inclusion to form « crosses » that would — if allowed — interconnect to a frame in the periodic array while the original matrix would be driven out into corners of the cell. So, if the inclusions had enough freedom, the roles of the two phases would completely interchange. The difference between such a microstructure and the one obtained from the more appropriate choice would be just a translation by vector  $(\pm \frac{1}{2}, \pm \frac{1}{2})$ .

However, not all results are oval-shaped inclusions. The main cause of the oscillatory shape on figure 10, again for the less convenient arrangement of the cell, is numerical instability. With a penalization that would favorize smoother designs, the identification could be led to an oval-shaped inclusion as in most other cases. However, the numerical instability makes the identification procedure take the way towards an alternative extremal microstructure — the rank-2 laminate. Of course, the ability of the single inclusion shapes to mimic the lamination on two levels is very poor ; on the other hand, it is surprising how good a job the reliable  $p$ -finite element method did, in this both physically and numerically ill-conditioned case. The case on the second subfigure in

figure 11 is also interesting : we see that at a certain stage of the optimization, the shape of the inclusion was oscillatory, but it could return to a generally smooth shape with only slight residuals of the oscillations.

The oval shapes of the inclusions from our numerical identifications are very similar to those Vidjergauz obtained analytically. There is a hope that Vidjergauz' approach could be used in the (simpler) conduction setting and that the optimality condition « the flux over the phase interface be uniform » would lead to an optimality condition for the interface curve. However, this is to be done in the future.

Figures 17 and 18 demonstrate that rectangular inclusion composites are sub-optimal. The curves of the effective moduli and the boundaries of the  $G_\theta$ -closure sets are close but they do not coincide — with the only exception of layered composites in the corners of the  $G_\theta$ -closure sets. Comparison of figure 6 to figure 17 and of figure 16 to figure 18 reveals that also in the numerical approximation, the well arranged single inclusion composites are substantially closer to the boundaries of the  $G_\theta$ -closure sets than the rectangular inclusion composites.

## 7. CONCLUSIONS

The microstructure identification problem is well posed and can be treated by means of optimal control theory.

In the numerical realization, the suggested procedure performed well. However, there are certain limitations that are due to the classical optimal shape design technique and that are difficult to overcome within that framework. Perhaps implementation of the fictitious domain method into Example 2.3 could show a possible way.

The true interest in the microstructure identification task would be for the problem of elasticity. An analog of the reliable method for the effective Hooke's law is under intensive work.

The numerical studies of the  $G_\theta$ -closure set seem to be a method that could yield ideas on how to give its characterization. This would be very desirable in the elasticity case.

In the context of optimum shape design, the single inclusion composites will make better relaxation (closer to the quasiconvex envelope) than the composites with rectangular inclusion. We could imagine a numerical shape optimization procedure that would make use of our code to construct the best composite on-line. Another possibility would be to do precomputing.

The use of the reliable method that yields an *a posteriori* error estimate for solution of the state problem is the basis for robustness of the identification procedure.

As far as linear behaviour is the main point of interest, our numerical implementation provides a ready-to-use means for designing real composites.

**Acknowledgement.** — This work was supported by grant 201/94/1863 of the Grant Agency of Czech Republic.

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