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# WORST SCENARIO METHOD IN HOMOGENIZATION.\* LINEAR CASE

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Abstract. The paper deals with homogenization of a linear elliptic boundary problem with a specific class of uncertain coefficients describing composite materials with periodic structure. Instead of stochastic approach to the problem, we use the worst scenario method due to Hlaváček (method of reliable solution). A few criterion functionals are introduced. We focus on the range of the homogenized coefficients from knowledge of the ranges of individual components in the composite, on the values of generalized gradient in the places where these components change and on the average of homogenized solution in some critical subdomain.

Keywords: homogenization, two-scale convergence, worst-scenario, reliable solution

MSC 2000: 35B27, 35B40, 35J25, 35R05, 49J20

#### 0. Introduction

A lot of mathematical models use data (coefficients of equations, right-hand sides, functions from boundary conditions, etc.), which cannot be easily determined. These data are usually obtained from experimental measurements and from the subsequent numerical solution of the inverse problem. Both of these steps are loaded with errors and therefore we know the data in certain bounds only. From this point of view we speak about problems with uncertain data.

Homogenization is a mathematical method which helps to model the behaviour of composite materials with periodic structure. In such materials it is possible to determine effective parameters from the knowledge of the microstructure. In other words, homogenization means a replacement of the periodically heterogeneous material by

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a homogeneous one which has "equivalent" properties from the macroscopic point of view. The topic is discussed in many papers and monographs (for introduction see e.g. [3], [5], [16], [19]).

In this paper we shall consider a linear elliptic problem with a specific class of uncertain coefficients. Instead of the stochastic approach, the deterministic worst scenario approach introduced by Hlaváček (see [9], [10]) will be used. The main idea consists in defining a suitable functional in the given set of data. This functional can be dependent on both the data and the solution of the model problem and its values are the criterion determining "good" or "bad" data from a certain point of view. This approach seems to be new in homogenization theory.

The paper is organized as follows. After introducing the necessary notation, the model problem is set in Section 2 and its homogenization is presented in Section 3. Section 4 is devoted to the worst scenario method, where some criterion functionals are introduced. Section 5 deals with the finite-dimensional approximation of the given problems. The methods are demonstrated by examples in Section 6. Concluding remarks in Section 7 close the paper.

#### 1. Preliminaries

Throughout the paper, Einstein convention on summation over repeated indices is used. In order to save space, partial derivatives of a function v are also denoted by  $\partial_{x_i}v$ ,  $i=1,\ldots,N$  (similarly the derivatives of higher orders). The symbol  $\nu$  stands for the unit outward normal vector. A sequence of positive parameters  $\{\varepsilon_n\}$  such that  $\varepsilon_n \to 0$  for  $n \to \infty$  is considered. As usual, the subscript n is omitted.

The space of all symmetric real matrices is denoted by  $\mathbb{R}_{\text{sym}}^{N \times N}$  (its dimension is  $\frac{1}{2}N(N+1)$ ). Spaces of continuous functions C,  $C^{\infty}$ , Lebesgue spaces  $L^2$ ,  $L^{\infty}$  and the Sobolev space  $W^{1,2}$  endowed with the usual norms are used.

## 1.1. Y-periodic functions

**Definition 1.1.** Let  $Y = (0;1)^N$  be the unit cube (the so-called unit period). A function  $v \colon \mathbb{R}^N \to \mathbb{R}$  is said to be Y-periodic, if v(y+k) = v(y) for all  $y \in \mathbb{R}^N$ , for all  $k \in \mathbb{Z}^N$ . If the function v has more variables, we say it is Y-periodic in y.

The spaces of Y-periodic functions will be denoted by  $X_{\#}(Y)$ . A function  $v \in X_{\#}(Y)$  is Y-periodic and  $v \in X_{loc}(\mathbb{R}^N)$ , i.e.  $v \in X(Q)$  for every compact subset  $Q \subset \mathbb{R}^N$ . For example, in the case of  $C_{\#}^{\infty}(Y)$ , all derivatives coincide on the opposite sides of  $\partial Y$ . In the case of  $v \in W_{\#}^{1,2}(Y)$ , the traces of the function v coincide almost everywhere on the opposite sides of  $\partial Y$ . The norm in the Banach spaces  $X_{\#}(Y)$  is given by  $\|\cdot\|_{X_{\#}(Y)} = \|\cdot\|_{X(Y)}$ .

**Lemma 1.2.** Let  $v \in W^{1,2}_{\#}(Y)$ . Then

$$\int_{Y} \frac{\partial v}{\partial y_i} \, \mathrm{d}y = 0.$$

Proof. According to the Gauss-Ostrogradski theorem we have

$$\int_{Y} \frac{\partial v}{\partial y_i} \, \mathrm{d}y = \int_{\partial Y} v \nu_i \, \mathrm{d}S = 0,$$

since v is Y-periodic and the normals on the opposite sides of  $\partial Y$  have inverse orientation.

Remark 1.3. The proposition holds even for integrable periodic functions having traces on  $\partial Y$ , where the derivatives are taken in generalized sense defined by functionals giving the values on the elements of the space  $W^{1,2}_{\#}(Y)$ , i.e., if a is an integrable Y-periodic function, then its derivative  $\partial_{y_i} a$  is defined by

$$\int_{Y} \frac{\partial a}{\partial y_{i}} v \, dy = \int_{\partial Y} av \nu_{i} \, dS - \int_{Y} a \frac{\partial v}{\partial y_{i}} \, dy = -\int_{Y} a \frac{\partial v}{\partial y_{i}} \, dy,$$

since the integral over  $\partial Y$  is zero due to the periodicity of both functions and the orientation of normals on the opposite sides. Taking v=1 we have

$$\int_{Y} \frac{\partial a}{\partial y_i} \, 1 \, \mathrm{d}y = -\int_{Y} a \, 0 \, \mathrm{d}y = 0.$$

The spaces of Y-periodic functions with zero mean value are denoted by  $X_{\#0}(Y)$ , i.e.

$$X_{\#0}(Y) = \left\{ v \in X_{\#}(Y) : \int_{Y} v(y) \, \mathrm{d}y = 0 \right\}.$$

**Lemma 1.4.** Let  $v \in W_{\#0}^{1,2}(Y)$ . Then

$$|v|_{W^{1,2}_{\#0}(Y)}\leqslant \|v\|_{W^{1,2}_{\#0}(Y)}\leqslant C|v|_{W^{1,2}_{\#0}(Y)}.$$

Sketch of proof. The first inequality follows directly from the definition of the norm and seminorm, the second inequality is a consequence of Poincaré inequality.

The following spaces of abstract functions are used:

- $C_0^{\infty}[\Omega; C_{\#0}^{\infty}(Y)]$ —the space of functions  $u: \Omega \to C_{\#0}^{\infty}(Y)$  such that the mapping  $x\in\Omega\stackrel{\sim}{\mapsto} u(x)(\cdot)\in C^\infty_{\#0}(Y)$  is infinitely differentiable with compact support in  $\Omega$ ;
- $L^2[\Omega; C_\#(Y)]$ —the space of functions  $u: \Omega \to C_\#(Y)$  which are  $L^2$  integrable
- and  $\|u\|_{L^{2}[\Omega; C_{\#}(Y)]}^{2} = \int_{\Omega} \|u(x)\|_{C_{\#}(Y)}^{2} \, \mathrm{d}x < \infty;$   $L^{2}[\Omega; W_{\#0}^{1,2}(Y)]$ —the space of functions  $u \colon \Omega \to W_{\#0}^{1,2}(Y)$  which are  $L^{2}$  integrable and  $\|u\|_{L^2[\Omega;W^{1,2}_{\#0}(Y)]}^2 = \int_{\Omega} \|u(x)\|_{W^{1,2}_{\#0}(Y)}^2 dx < \infty$ .

Let us remark that every function from these spaces can be identified with a function u(x,y) defined on  $\Omega \times \mathbb{R}^N$  via u(x,y) = u(x)(y). More details can be found e.g. in [13].

## 2. Model Problem

Let us consider a linear elliptic 2nd order problem

(2.1) 
$$-\frac{\partial}{\partial x_i} \left( a_{ij} \frac{\partial u}{\partial x_j} \right) = f \quad \text{in } \Omega,$$

$$u = u_D \quad \text{on } \Gamma_D,$$

$$a_{ij} \frac{\partial u}{\partial x_i} \nu_i = w_N \quad \text{on } \Gamma_N,$$

where  $\Omega$  is a bounded domain with Lipschitz boundary  $\partial \Omega = \bar{\Gamma}_D \cup \bar{\Gamma}_N$  (meas<sub>N-1</sub>  $\Gamma_D >$ 0). This problem describes e.g. stationary heat conduction, electric circuit, diffusion, etc. Let us assume the matrix of coefficients  $A = (a_{ij})_{i,j=1}^N, a_{ij} \in L^{\infty}(\Omega)$ , is symmetric and positive definite, i.e.

$$a_{ij} = a_{ji}, \quad a_{ij}\xi_j\xi_i > 0 \quad \text{for a.a. } x \in \Omega, \ \xi \neq 0.$$

For anisotropic materials in principal directions we have  $a_{ij} = a_{ji} = 0$ ,  $i \neq j$  and for isotropic materials the diagonal elements coincide.

We will consider periodically arranged composite materials which consist of a finite number of homogeneous components. Let us assume the material properties of these components are not known exactly but in certain bounds only. So, in what follows, the coefficients  $a_{ij}$  are periodic piecewise constant functions with uncertain values from the predefined intervals. For the sake of simplicity the other functions (righthand side, boundary values) are considered to be fixed.

Since the coefficients are not continuous, the problem (2.1) cannot be solved in the classical sense—we proceed to a weak formulation. Let us define the space V by

(2.2) 
$$V = \{ v \in W^{1,2}(\Omega) \colon v = 0 \text{ on } \Gamma_D \text{ (in sense of traces)} \}.$$

Then  $W_0^{1,2}(\Omega) \subset V \subset W^{1,2}(\Omega)$  holds. Multiplying formally the equation by an arbitrary function  $v \in V$  and integrating by parts over  $\Omega$  leads to

$$\int_{\Omega} a_{ij} \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} dx = \int_{\Omega} f v dx + \int_{\Gamma_N} w_N v dS,$$

where the Neumann boundary condition and the assumption v=0 on  $\Gamma_D$  were used. Denoting

$$a(u,v) = \int_{\Omega} a_{ij} \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} dx,$$
  
$$b(v) = \int_{\Omega} f v dx + \int_{\Gamma_N} w_N v dS,$$

the weak formulation reads:

(W) Find a function  $u \in W^{1,2}(\Omega)$  such that  $u - u_D \in V$  and the equality

$$a(u, v) = b(v)$$

holds for all functions  $v \in V$ .

The following well-known result on solvability of the problem holds:

**Theorem 2.1.** Let  $f \in L^2(\Omega)$ ,  $u_D \in W^{1,2}(\Omega)$ ,  $w_N \in L^2(\Gamma_N)$  and let there exist  $\alpha > 0$  such that the coefficients  $a_{ij} \in L^{\infty}(\Omega)$  satisfy the ellipticity condition

(2.3) 
$$a_{ij}\xi_i\xi_i \geqslant \alpha|\xi|^2, \quad \forall \xi \in \mathbb{R}^N, \quad a.a. \ x \in \Omega.$$

Then problem (W) has unique solution. Moreover, this solution satisfies the estimate

$$(2.4) ||u||_{W^{1,2}(\Omega)} \leqslant C,$$

where the constant C depends on  $\alpha$ ,  $\Omega$ ,  $\Gamma_N$ ,  $\|u_D\|_{W^{1,2}(\Omega)}$ ,  $\|w_N\|_{L^2(\Gamma_N)}$ ,  $\|a_{ij}\|_{L^\infty(\Omega)}$  and  $\|f\|_{L^2(\Omega)}$ .

## 3. Homogenization

In this section we give a summary of some homogenization results, especially we focus on two-scale convergence approach.

## 3.1. Basic idea

As mentioned in Introduction, homogenization deals with a replacement of the oscillating data by constant ones that approximate the original material in the macroscopic sense. The first homogenization attempts fall into the 19th century, when authors used some averaging methods. Since a universal criterion preferring one method against another one was not available, the authors often approximated the data in different ways.

The homogenization technique went through the biggest development during the 70's of the last century. Babuška proposed a procedure where the model problem is not considered separately but as a one element of a sequence of problems of the same type, where the period ratio decreases, see [2]. Then the limit problem is called the homogenized problem. This idea is straightforward, but it does not say how to determine the homogenized problem. A few concepts were introduced in the past. Besides the asymptotic expansion and local energy methods (see e.g. [3], [8]), G and  $\Gamma$  convergence (see e.g. [4], [7], [20]), two-scale convergence is probably the most powerful tool for homogenization.

Let us proceed to our model problem. Considering the Y-periodic coefficients  $a_{ij}$  we can construct the sequence of coefficients with diminishing period  $\varepsilon$  defined by  $a_{ij}^{\varepsilon}(x) = a_{ij}(x/\varepsilon)$ . This sequence defines a sequence of problems

$$\begin{split} -\frac{\partial}{\partial x_i} \Big( a_{ij}^\varepsilon \frac{\partial u_\varepsilon}{\partial x_j} \Big) &= f &\quad \text{in } \Omega, \\ u_\varepsilon &= u_D &\quad \text{on } \Gamma_D, \\ a_{ij}^\varepsilon \frac{\partial u_\varepsilon}{\partial x_i} \nu_i &= w_N &\quad \text{on } \Gamma_N. \end{split}$$

The weak formulation reads:

$$(W_{\varepsilon})$$
 Find  $u_{\varepsilon} \in W^{1,2}(\Omega)$  such that  $u_{\varepsilon} - u_D \in V$  and

(3.1) 
$$a^{\varepsilon}(u_{\varepsilon}, v) = b(v) \quad \forall v \in V,$$

where

$$a^{\varepsilon}(u,v) = \int_{\Omega} a_{ij}^{\varepsilon} \frac{\partial u}{\partial x_j} \frac{\partial v}{\partial x_i} dx.$$

## 3.2. Two-scale convergence method

Two-scale convergence is a special weak convergence which stands between the usual weak and strong convergence in Lebesgue spaces. It was developed for the homogenization theory in order to simplify the proofs. It overcomes the difficulties resulting from the properties of weakly converging sequences of periodic functions. In such sequences the weak limit does not keep the "information on oscillations" of the original functions. In some cases, the two-scale limit is able to conserve this information and thus, it makes limit procedures possible.

The concept was first introduced by Nguetseng [15] and then developed by Allaire [1] in early 90's. In the case of  $L^2$  the definition reads:

**Definition 3.1.** A sequence  $\{u_{\varepsilon}(x)\}\subset L^2(\Omega)$  is said to be two-scale convergent (denoted  $\stackrel{2-s}{\longrightarrow}$ ) to a function  $u_0(x,y)\in L^2(\Omega\times Y)$  if

(3.2) 
$$\lim_{\varepsilon \to 0} \int_{\Omega} u_{\varepsilon}(x) \psi\left(x, \frac{x}{\varepsilon}\right) dx = \int_{\Omega} \int_{Y} u_{0}(x, y) \psi(x, y) dx dy$$

holds for any test function  $\psi \in L^2[\Omega; C_{\#}(Y)].$ 

This definition is useful in applications due to the following main results.

**Theorem 3.2.** Let  $\{u_{\varepsilon}\}$  be a bounded sequence in  $L^{2}(\Omega)$ . Then there exists a function  $u_{0}(x,y) \in L^{2}(\Omega \times Y)$  such that for an extracted subsequence  $\{u_{\varepsilon'}\}$  we have  $u_{\varepsilon'} \stackrel{2-s}{\rightharpoonup} u_{0}$ .

**Theorem 3.3.** Let  $\{u_{\varepsilon}\}$  be a bounded sequence in  $W^{1,2}(\Omega)$ . Then there exist functions  $u_0(x) \in L^2(\Omega)$ ,  $u_1(x,y) \in L^2[\Omega; W^{1,2}_{\#0}(Y)]$  and an extracted subsequence  $\{\varepsilon'\}$  such that  $u_{\varepsilon'} \rightharpoonup u_0$  in  $W^{1,2}(\Omega)$  and  $\nabla u_{\varepsilon'} \stackrel{2-s}{\rightharpoonup} \nabla u_0 + \nabla_u u_1$ .

Remark 3.4. The test functions from the space  $L^2[\Omega; C_\#(Y)]$  form the so-called admissible test functions. Such functions are Carathéodory which is a sufficient condition for measurability of the composed function  $\psi(x, x/\varepsilon)$ . Moreover, they are regular enough, so that we have

$$\lim_{\varepsilon \to 0} \left\| \psi\left(x, \frac{x}{\varepsilon}\right) \right\|_{L^2(\Omega)} = \|\psi(x, y)\|_{L^2(\Omega \times Y)},$$

$$\left\| \psi\left(x, \frac{x}{\varepsilon}\right) \right\|_{L^2(\Omega)} \leqslant \|\psi(x, y)\|_{L^2[\Omega; C_\#(Y)]}.$$

These two properties are necessary in the proof of the two-scale compactness property (see Theorem 3.2). Elements of the two-scale convergence theory can be found in [1], [11], [13].

Let us apply the previous results to our problem.

**Lemma 3.5.** Let  $a_{ij}$  satisfy condition 2.3 with some  $\alpha > 0$ . Then the sequence of solutions  $\{u_{\varepsilon}\}$  to Problem  $(W_{\varepsilon})$  is bounded in  $W^{1,2}(\Omega)$ , i.e.

$$||u_{\varepsilon}||_{W^{1,2}(\Omega)} \leqslant C$$

holds.

Proof. Since the coefficients  $a_{ij}^{\varepsilon}$  have the same  $L^{\infty}$ -norm (the transformation  $y = x/\varepsilon$  changes the speed of oscillations only, it does not change the norm), the proposition follows immediately and the C is the same constant as in (2.4).

Since the sequence of solutions  $\{u_{\varepsilon}\}$  is bounded in  $W^{1,2}(\Omega)$ , according to Theorem 3.3 there exist functions  $u_0$  and  $u_1$  such that an extracted subsequence  $\{u_{\varepsilon'}\}$  converges weakly to  $u_0$  in  $W^{1,2}(\Omega)$  and  $\{\nabla u_{\varepsilon'}\}$  two-scale converges to  $\nabla u_0 + \nabla_y u_1$ . From the form of the limits one can expect that the solution  $u_{\varepsilon}$  can be expressed as a sum  $u_0(x) + \varepsilon u_1(x, x/\varepsilon)$ .

According to this, in the equality (3.1) we choose the test function in the form  $v_0(x) + \varepsilon v_1(x, x/\varepsilon)$ , where  $v_0 \in C^{\infty}(\Omega)$  ( $v_0 = 0$  on  $\Gamma_D$ ),  $v_1 \in C_0^{\infty}[\Omega; C_{\#0}^{\infty}(Y)]$ , i.e.

$$\int_{\Omega} a_{ij} \left( \frac{x}{\varepsilon} \right) \frac{\partial u_{\varepsilon}}{\partial x_{j}} \left[ \frac{\partial v_{0}}{\partial x_{i}}(x) + \frac{\partial v_{1}}{\partial y_{i}} \left( x, \frac{x}{\varepsilon} \right) + \varepsilon \frac{\partial v_{1}}{\partial x_{i}} \left( x, \frac{x}{\varepsilon} \right) \right] dx 
= \int_{\Omega} f(x) \left[ v_{0}(x) + \varepsilon v_{1} \left( x, \frac{x}{\varepsilon} \right) \right] dx + \int_{\Gamma_{N}} w_{N}(x) \left[ v_{0}(x) + \varepsilon v_{1} \left( x, \frac{x}{\varepsilon} \right) \right] dS.$$

Taking the expression  $a_{ij} \left[ \frac{\partial v_0}{\partial x_i} + \frac{\partial v_1}{\partial y_i} \right]$  as a test function, for  $\varepsilon \to 0$  we can pass to

(3.3) 
$$\int_{\Omega} \int_{Y} a_{ij}(y) \left[ \frac{\partial u_0}{\partial x_j}(x) + \frac{\partial u_1}{\partial y_j}(x,y) \right] \cdot \left[ \frac{\partial v_0}{\partial x_i}(x) + \frac{\partial v_1}{\partial y_i}(x,y) \right] dx dy$$
$$= \int_{\Omega} f(x) v_0(x) dx + \int_{\Gamma_N} w_N(x) v_0(x) dS,$$

which is the integral identity corresponding to the system of equations

$$(3.4) \qquad -\frac{\partial}{\partial y_i} \left( a_{ij}(y) \left[ \frac{\partial u_0}{\partial x_j}(x) + \frac{\partial u_1}{\partial y_j}(x,y) \right] \right) = 0 \quad \text{in } \Omega \times Y,$$

$$-\frac{\partial}{\partial x_i} \left( \int_Y a_{ij}(y) \left[ \frac{\partial u_0}{\partial x_j}(x) + \frac{\partial u_1}{\partial y_j}(x,y) \right] dy \right) = f \quad \text{in } \Omega,$$

$$u_0(x) = u_D \quad \text{on } \Gamma_D,$$

$$\int_Y a_{ij}(y) \left[ \frac{\partial u_0}{\partial x_i}(x) + \frac{\partial u_1}{\partial y_i}(x,y) \right] dy \cdot \nu_j = w_N \quad \text{on } \Gamma_N.$$

This system is called the two-scale homogenized system (the equality (3.3) can be obtained by the following steps: multiplying the first equation by the function  $v_1(x, y)$ ,

multiplying the second equation by the function  $v_0(x)$ , integrating by parts with respect to the appropriate variable, summing both results).

Let us introduce a Hilbert space  $W = V \times L^2[\Omega; W_{\#0}^{1,2}(Y)]$  endowed with the norm<sup>1</sup>

$$\|(v_0, v_1)\|_W = \left[ \int_{\Omega} \left( \sum_{i=1}^N \left[ \frac{\partial v_0}{\partial x_i} \right]^2 \right) dx + \int_{\Omega} \int_{Y} \left( \sum_{i=1}^N \left[ \frac{\partial v_1}{\partial y_i} \right]^2 \right) dx dy \right]^{1/2},$$

where the space V is defined by (2.2). Thanks to the density of smooth functions in W, equality (3.3) holds also for each function  $(v_0, v_1) \in W$ . Thus, Theorem 3.3 makes it possible to pass to two-scale limit in the sequence of the problems  $(W_{\varepsilon})$  to the weak two-scale formulation:

(W2) Find a function  $\mathbf{u}=(u_0,u_1)\in W^{1,2}(\Omega)\times L^2[\Omega;W^{1,2}_{\#0}(Y)]$  such that  $u_0-u_D\in V$  and

$$a_2(\mathbf{u}, \mathbf{v}) = b_2(\mathbf{v}), \quad \forall \, \mathbf{v} = (v_0, v_1) \in W,$$

where

$$a_{2}(\mathbf{u}, \mathbf{v}) = \int_{\Omega} \int_{Y} a_{ij}(y) \left[ \frac{\partial u_{0}}{\partial x_{j}}(x) + \frac{\partial u_{1}}{\partial y_{j}}(x, y) \right] \cdot \left[ \frac{\partial v_{0}}{\partial x_{i}}(x) + \frac{\partial v_{1}}{\partial y_{i}}(x, y) \right] dx dy,$$

$$b_{2}(\mathbf{v}) = \int_{\Omega} f(x) v_{0}(x) dx + \int_{\Gamma_{N}} w_{N}(x) v_{0}(x) dS.$$

**Theorem 3.6.** Problem (W2) has a unique solution  $(u_0, u_1)$ .

Proof. Let us denote  $u_0 = u_0^* + u_D$  and  $\mathbf{u}^* = (u_0^*, u_1)$ ,  $\mathbf{v} = (v_0, v_1)$ . Then (3.3) can be rewritten as

$$a_2(\mathbf{u}^*, \mathbf{v}) = b_2^*(\mathbf{v}),$$

where

$$b_2^*(\mathbf{v}) = \int_{\Omega} f v_0 \, \mathrm{d}x + \int_{\Gamma_N} w_N v_0 \, \mathrm{d}S - \int_{\Omega} \int_Y a_{ij} \frac{\partial u_D}{\partial x_j} \left[ \frac{\partial v_0}{\partial x_i} + \frac{\partial v_1}{\partial y_i} \right] \mathrm{d}x \, \mathrm{d}y.$$

We solve the problem: find  $\mathbf{u}^* \in W$  such that  $a_2(\mathbf{u}^*, \mathbf{v}) = b_2^*(\mathbf{v}), \forall \mathbf{v} \in W$ . Thanks to the property (2.3) and Lemma 1.4 we have

$$\begin{split} a_2(\mathbf{v}, \mathbf{v}) &= \int_{\Omega} \int_Y a_{ij} \left[ \frac{\partial v_0}{\partial x_j} + \frac{\partial v_1}{\partial y_j} \right] \cdot \left[ \frac{\partial v_0}{\partial x_i} + \frac{\partial v_1}{\partial y_i} \right] \mathrm{d}x \, \mathrm{d}y \\ &\geqslant \alpha \sum_{i=1}^N \int_{\Omega} \int_Y \left[ \frac{\partial v_0}{\partial x_i} + \frac{\partial v_1}{\partial y_i} \right]^2 \mathrm{d}x \, \mathrm{d}y \\ &= \alpha \left( \sum_{i=1}^N \int_{\Omega} \left[ \frac{\partial v_0}{\partial x_i} \right]^2 \mathrm{d}x + \sum_{i=1}^N \int_{\Omega} \int_Y \left[ \frac{\partial v_1}{\partial y_i} \right]^2 \mathrm{d}x \, \mathrm{d}y \right) = \alpha \|\mathbf{v}\|_W^2. \end{split}$$

<sup>&</sup>lt;sup>1</sup> In fact, it is a seminorm, but according to Friedrichs inequality and Lemma 1.4 it is equivalent to a norm.

Thus,  $a_2(\mathbf{v}, \mathbf{v})$  is W-elliptic. Since the forms  $a_2(\mathbf{u}, \mathbf{v})$  and  $b_2^*(\mathbf{v})$  are bounded in  $W \times W$  and W, respectively, the assumptions of the Lax-Milgram lemma are fulfilled, which yields the existence and uniqueness of the solution  $(u_0^*, u_1)$ .

Corollary 3.7. The whole sequence  $\{u_{\varepsilon}\}$  converges weakly to  $u_0$  in  $W^{1,2}(\Omega)$  and the whole sequence  $\{\nabla u_{\varepsilon}\}$  two-scale converges to  $\nabla u_0 + \nabla_y u_1$  as  $\varepsilon \to 0$ .

## 3.3. Comparison with the classical approach

Now, let us compare the results introduced above with the classical homogenized problem (see e.g. [3])

(3.5) 
$$-a_{ij}^{0} \frac{\partial^{2} u_{0}}{\partial x_{i} \partial x_{j}} = f \quad \text{in } \Omega,$$

$$u_{0} = u_{D} \quad \text{on } \Gamma_{D},$$

$$a_{ij}^{0} \frac{\partial u_{0}}{\partial x_{j}} \nu_{i} = w_{N} \quad \text{on } \Gamma_{N},$$

where the coefficients  $a_{ij}^0$  are given by the formulas

(3.6) 
$$a_{ij}^{0} = \int_{Y} \left( a_{ij} - a_{ik} \frac{\partial \chi_{j}}{\partial y_{k}} \right) dy$$

and the functions  $\chi_j \in W^{1,2}_{\#0}(Y)$  are Y-periodic solutions of the local problem

$$(3.7) -\frac{\partial}{\partial u_i} \left( a_{ik} \frac{\partial \chi_j}{\partial u_i} \right) = -\frac{\partial a_{ij}}{\partial u_i}.$$

The homogenized matrix  $A_0 = (a_{ij}^0)_{i,j}^N$  has the following properties:

## Theorem 3.10.

- (i) If the matrix  $A = (a_{ij})_{i,j}^N$  is symmetric, then the matrix  $A_0$  is also symmetric.
- (ii) The matrix  $A_0$  satisfies the ellipticity condition

$$a_{ij}^0 \xi_i \xi_i \geqslant \alpha |\xi|^2, \quad \forall \, \xi \in \mathbb{R}^N$$

with the same constant  $\alpha$  as in (2.3).

(iii) If the matrix A is diagonal and the elements are even functions with respect to the planes of symmetry  $y_j = \frac{1}{2}$ , then the matrix  $A_0$  is also diagonal.

The weak formulation of the homogenized problem (3.5) reads:

(WH) Find a function  $u_0 \in W^{1,2}(\Omega)$  such that  $u_0 - u_D \in V$  and

$$a_H(u_0, v) = b_H(v), \quad v \in V,$$

where

$$a_{H}(u,v) = \int_{\Omega} a_{ij}^{0} \frac{\partial u}{\partial x_{j}} \frac{\partial v}{\partial x_{i}} dx,$$
  
$$b_{H}(v) = \int_{\Omega} f v dx + \int_{\Gamma_{N}} w_{N} v dS.$$

The weak formulation of the local problem (3.7) reads:

(WL) Find a function  $\chi_j \in W^{1,2}_{\#0}(Y)$  such that

$$a_L(\chi_j, \mu) = b_L^j(\mu), \quad \forall \, \mu \in W^{1,2}_{\#0}(Y),$$

where

$$a_L(\lambda, \mu) = \int_Y a_{ik} \frac{\partial \lambda}{\partial y_k} \frac{\partial \mu}{\partial y_i} dy,$$
  
$$b_L^j(\mu) = \int_Y a_{ij} \frac{\partial \mu}{\partial y_i} dy.$$

**Lemma 3.11.** The two-scale homogenized problem (3.4) can be separated into a global and local part (3.5)–(3.7) through the relation

(3.8) 
$$u_1(x,y) = -\frac{\partial u_0}{\partial x_j}(x)\chi_j(y).$$

Sketch of proof. The proof is technical—substitution of the expression (3.8) into the system (3.4) and the following averaging with respect to y yields the desired result.

## **Lemma 3.12.** Problem (WL) has a unique solution.

Sketch of proof. The proposition is a consequence of Lemma 3.11 and Theorem 3.6—a direct proof can be obtained by help of the Lax-Milgram lemma and the zero mean value of the right-hand side of (3.7), see Remark 1.3.

The two-scale homogenized problem contains double number of variables but it is of the same type as the original periodic problem. From the numerical point of view, it is obviously better to have the problem separated. Let us remark that the separation to the global and local part is not always possible or can yield too

complicated forms. Here, it is possible due to linearity and relative simplicity of the problem. The main advantage of the two-scale convergence method is the processing in one step, i.e. by the derivation of the homogenized problem we prove also the appropriate convergences of the sequence of solutions.

## 3.4. Correctors

Let us consider the solutions  $u_0$ ,  $u_1$  from Subsection 3.2. The expression  $\varepsilon u_1(x, x/\varepsilon)$  is called the corrector and the function

$$u_{\varepsilon}^{C}(x) = u_{0}(x) + \varepsilon u_{1}\left(x, \frac{x}{\varepsilon}\right)$$

is called the solution with the corrector. According to Lemma 3.1 we have

$$u_{\varepsilon}^{C}(x) = u_{0}(x) - \varepsilon \frac{\partial u_{0}}{\partial x_{j}}(x)\chi_{j}(\frac{x}{\varepsilon}).$$

**Theorem 3.13.** Let  $u_0 \in C^2(\Omega)$ . Then the difference of solutions  $u_{\varepsilon} - u_{\varepsilon}^C$  converges to zero strongly in  $W^{1,2}(\Omega)$  as  $\varepsilon \to 0$ .

Remark 3.14. The solution with the corrector improves the approximation of the original solution  $u_{\varepsilon}$ , but it violates the Dirichlet boundary condition, i.e.  $u_{\varepsilon}^C \neq u_D$  on  $\Gamma_D$ . This can be "repaired" by means of the so-called cut off function; for details and proof of the previous theorem see e.g. [3].

#### 4. Worst scenario method

A deterministic concept of solving the problems with uncertain data was introduced by Hlaváček in [9], [10]. We assume that the main goal of computations is to find the critical values of a certain functional which depends on both the data and the solution of the model problem. This functional is a criterion for "bad" or "good" data and is chosen with respect to the technical requirements; it can represent e.g. the temperature or the heat flow at some crucial places of the material etc. Once the functional is set, we can formulate the appropriate maximization or minimization problem over the set of admissible data. This approach was named the worst scenario method or the reliable solution method. The terms are natural, since the method is looking for the "worst" data even if the probability of their occurrence is small. If such data are too "dangerous" one can proceed with adjusting the technological process to obtain a more secure case—we talk about a "reliable" solution.

Let us remark that the approach mentioned works as an "anti-optimal" control, so we can use the techniques used in optimal design theory.

The general principles of the method are described in [10].

## 4.1. Specification of uncertainties in coefficients

Now, let us specify the uncertainties of the coefficients more precisely. Let the unit cube Y consist of a finite number of disjoint subsets  $Y_k \subset Y$ , k = 1, ..., m and their complement  $Y_0$  in Y. Let us introduce sets  $\mathscr{U}_{ij}^{\mathrm{ad}}$  by

$$\mathscr{U}^{\mathrm{ad}}_{ij} = \{ a \in L^{\infty}_{\#}(Y) \colon a = \mathrm{const.} \ \text{on} \ Y_k, \ a|_{Y_k} \in [C^l_{ij,k}, C^u_{ij,k}], \ k = 0, \dots, m \},$$

where  $C_{ij,k}^l \leq C_{ij,k}^u$  are given constants (lower and upper bounds) such that each combination of functions  $a_{ij} \in \mathcal{U}_{ij}^{\text{ad}}$  satisfies the ellipticity condition (2.3). Natural assumptions are  $C_{ij,k}^l = C_{ji,k}^l$  and  $C_{ij,k}^u = C_{ji,k}^u$ . The set of admissible coefficients is defined by

$$\mathscr{U}^{\text{ad}} = \{ A = (a_{ij})_{i,j=1}^{N} : \ a_{ij} = a_{ji}, \ a_{ij} \in \mathscr{U}^{\text{ad}}_{ij} \}.$$

Overall, Y-periodic coefficients  $a_{ij}$  form a symmetric matrix function  $A \in \mathcal{U}^{\mathrm{ad}}$ , they are constant on every set  $Y_k$  and these constants are from the given intervals.

Remark 4.1. The ellipticity condition  $\xi A \xi^T \ge \alpha |\xi|^2$  is equivalent to positive definiteness of the quadratic form  $\xi A \xi^T$ , i.e.

$$\xi A \xi^T \geqslant \alpha |\xi|^2 \ \forall \, A \in \mathscr{U}^{\mathrm{ad}} \Longleftrightarrow \xi A \xi^T > 0 \ \forall \, A \in \mathscr{U}^{\mathrm{ad}}.$$

In the case of symmetric interval matrices, a sufficient condition for positive definiteness of the forms  $\xi A \xi^T$  was introduced by Rohn, see [18]. For our purposes it can be formulated in the following way:

Each quadratic form  $\xi A \xi^T$ ,  $A \in \mathcal{U}^{ad}$ , is positive definite, if

$$\lambda_{\min} \Big( \frac{1}{2} [C^l_{(k)} + C^u_{(k)}] \Big) - \varrho \Big( \frac{1}{2} [C^u_{(k)} - C^l_{(k)}] \Big) > 0,$$

where  $C_{(k)}^l = (C_{ij,k}^l)_{i,j=1}^N$ ,  $C_{(k)}^u = (C_{ij,k}^u)_{i,j=1}^N$ , k = 0, ..., m, are matrices of lower and upper bounds,  $\lambda_{\min}(M)$  ( $\varrho(M)$ ) is the minimal eigenvalue (the spectral radius, respectively) of the matrix M.

## 4.2. Choice of the criterion functionals

Here, a few criteria will be set. The existence of a solution of the corresponding maximization problems will be proved.

Homogenized coefficients. The first problem deals with the "badness" of the homogenized coefficients. A natural question is: do the extremal values of the original discontinuous coefficients attain also the extremal (maximal or minimal) values of the homogenized coefficients? Therefore, for this problem the criterion functionals  $\Phi_{ij}$  are defined by formulas (3.6), i.e.

(4.1) 
$$\Phi_{ij}(A,\chi) = \int_{Y} \left( a_{ij} - a_{ik} \frac{\partial \chi_j}{\partial y_k} \right) dy,$$

where  $\chi = (\chi_1, \dots, \chi_N)$  is the unique solution of the local problem (WL). The appropriate maximization (minimization) problem reads:

(P1) Find 
$$\bar{A} \in \mathcal{U}^{\mathrm{ad}}$$
 ( $\underline{A} \in \mathcal{U}^{\mathrm{ad}}$ ) such that

$$(4.2) \Phi_{ij}(\bar{A}, \chi(\bar{A})) \geqslant \Phi_{ij}(A, \chi(A)) \forall A \in \mathscr{U}^{\mathrm{ad}},$$

$$(\Phi_{ij}(\underline{A}, \chi(\underline{A})) \leqslant \Phi_{ij}(A, \chi(A)) \forall A \in \mathscr{U}^{\mathrm{ad}}, \text{ respectively}.$$

**Lemma 4.2.** The set  $\mathscr{U}^{\mathrm{ad}}$  is compact in  $L^{\infty}_{\#}[Y; \mathbb{R}^{N \times N}_{\mathrm{sym}}]$  (the space of all symmetric essentially bounded periodic matrix functions).

Proof. The proposition follows from the fact that the set  $\mathscr{U}^{\mathrm{ad}}$  is represented by a closed bounded subset of a finite dimensional space. Indeed, every  $\mathscr{U}^{\mathrm{ad}}_{ij}$  can be represented by the cartesian product of (m+1) closed intervals, and thus  $\mathscr{U}^{\mathrm{ad}}$  is the cartesian product of  $\frac{1}{2}(m+1)N(N+1)$  closed intervals, which is a closed bounded set in  $\mathbb{R}^{(m+1)N(N+1)/2}$ .

**Lemma 4.3.** Let  $A_n \in \mathcal{U}^{ad}$  and  $A_n \to A$  in  $\mathcal{U}^{ad}$ . Then  $\chi_j(A_n) \to \chi_j(A)$  in  $W^{1,2}_{\#0}(Y)$ .

Proof. First, we prove that functions  $\chi_j(A)$  are bounded in  $W^{1,2}_{\#0}(Y)$  for each  $A \in \mathscr{U}^{\mathrm{ad}}$ . Lemma 1.4, the ellipticity condition (2.3), (WL) and the Cauchy-Schwarz inequality yield

$$\frac{\alpha}{C^2} \|\chi_j\|_{W^{1,2}_{\#0}(Y)}^2 \leqslant \alpha |\chi_j|_{W^{1,2}_{\#0}(Y)}^2 \leqslant a_L(\chi_j, \chi_j) = b_L^j(\chi_j)$$

$$\leqslant \max_i \|a_{ij}\|_{L^{\infty}_{\#}(Y)} \sqrt{N} |\chi_j|_{W^{1,2}_{\#0}(Y)} \leqslant \max_i \|a_{ij}\|_{L^{\infty}_{\#}(Y)} \sqrt{N} \|\chi_j\|_{W^{1,2}_{\#0}(Y)}.$$

Since  $\max_{i} \|a_{ij}\|_{L^{\infty}_{\#}(Y)} \leq \max\{\max_{i,k} |C^{u}_{ij,k}|, \max_{i,k} |C^{l}_{ij,k}|\} = \tilde{C}, \forall a_{ij} \in \mathscr{U}^{\mathrm{ad}}_{ij}$ , we have

$$\|\chi_j\|_{W^{1,2}_{\#0}(Y)} \leqslant \frac{C^2 \sqrt{N}\tilde{C}}{\alpha} \quad \forall A \in \mathscr{U}^{\mathrm{ad}}.$$

Let us denote  $\chi_j^n \equiv \chi_j(A_n)$  and  $\chi_j \equiv \chi_j(A)$ . According to (WL) for all  $\mu \in W_{\#_0}^{1,2}(Y)$  we have

$$\int_{Y} \left( a_{ik}^{n} \frac{\partial \chi_{j}^{n}}{\partial y_{k}} - a_{ik} \frac{\partial \chi_{j}}{\partial y_{k}} \right) \frac{\partial \mu}{\partial y_{i}} \, \mathrm{d}y = \int_{Y} (a_{ij}^{n} - a_{ij}) \frac{\partial \mu}{\partial y_{i}} \, \mathrm{d}y.$$

In the equality let us put

$$\mu \equiv \chi_1^n - \chi_1.$$

Then

$$\int_{Y} a_{ik}^{n} \left( \frac{\partial \chi_{1}^{n}}{\partial y_{k}} - \frac{\partial \chi_{1}}{\partial y_{k}} \right) \left( \frac{\partial \chi_{1}^{n}}{\partial y_{i}} - \frac{\partial \chi_{1}}{\partial y_{i}} \right) dy + \int_{Y} (a_{ik}^{n} - a_{ik}) \frac{\partial \chi_{1}}{\partial y_{k}} \left( \frac{\partial \chi_{1}^{n}}{\partial y_{i}} - \frac{\partial \chi_{1}}{\partial y_{i}} \right) dy 
= \int_{Y} (a_{i1}^{n} - a_{i1}) \left( \frac{\partial \chi^{n_{1}}}{\partial y_{i}} - \frac{\partial \chi_{1}}{\partial y_{i}} \right) dy.$$

Lemma 1.4 and the ellipticity condition yield

$$\frac{\alpha}{C^2} \|\chi^{n_1} - \chi_1\|_{W^{1,2}_{\#0}(Y)}^2 + \int_Y (a_{ik}^n - a_{ik}) \frac{\partial \chi_1}{\partial y_k} \left( \frac{\partial \chi_1^n}{\partial y_i} - \frac{\partial \chi_1}{\partial y_i} \right) dy$$

$$\leqslant \int_Y (a_{i1}^n - a_{i1}) \left( \frac{\partial \chi_1^n}{\partial y_i} - \frac{\partial \chi_1}{\partial y_i} \right) dy.$$

Both integrals converge to zero, since  $a_{i1}^n \to a_{i1}$  in  $L_\#^\infty(Y)$  and the derivatives  $\partial_{y_i} \chi_1^n$ ,  $\partial_{y_i} \chi_1$  are bounded in  $L_\#^2(Y)$  for each  $n \in \mathbb{N}$ . Thus

$$\|\chi_1^n - \chi_1\|_{W_{\#_0}^{1,2}(Y)}^2 \longrightarrow 0$$

holds, which is the desired result for j=1. Similarly one can proceed with convergence for  $\chi_2, \ldots, \chi_N$ .

**Theorem 4.4.** Problem (P1) has a solution.

Proof. Let  $\{A_n\}\subset \mathscr{U}^{\mathrm{ad}}$  be a maximizing sequence of the functional  $\Phi_{ij}(A,\chi(A))$ , i.e.

(4.3) 
$$\lim_{n \to \infty} \Phi_{ij}(A_n, \chi(A_n)) = \sup_{A \in \mathcal{U}^{\text{ad}}} \Phi_{ij}(A, \chi(A)).$$

Due to Lemma 4.2 there exists an element  $\bar{A}$  and an extracted subsequence  $A_{n'} \to \bar{A}$  in  $\mathscr{U}^{\mathrm{ad}}$ . Lemma 4.3 yields  $\chi_j(A_{n'}) \to \chi_j(\bar{A})$  in  $W^{1,2}_{\#0}(Y)$ . Since both the convergences are strong, we obviously have

$$\lim_{n'\to\infty} \Phi_{ij}(A_{n'},\chi(A_{n'})) = \Phi_{ij}(\bar{A},\chi(\bar{A})).$$

Together with relation (4.3) we have

$$\Phi_{ij}(\bar{A},\chi(\bar{A})) = \sup_{A \in \mathscr{U}^{\mathrm{ad}}} \Phi_{ij}(A,\chi(A)).$$

The existence of the minimizing element can be obtained analogously.

Generalized gradient (heat flow). The second problem deals with auxiliary functions  $\chi_j$ . According to Subsection 3.4, these functions play the essential role in the so-called solution with the corrector  $u_{\varepsilon}^C$ . For a sufficiently smooth homogenized solution  $u_0$  the strong convergence  $\|u_{\varepsilon} - u_{\varepsilon}^C\|_{W^{1,2}(\Omega)} \to 0$  holds. In other words, the function  $u_{\varepsilon}^C$  approximates not the only values  $u_{\varepsilon}$ , but also the derivatives  $\partial_{x_i}u_{\varepsilon}$ . In technical applications the so-called generalized gradient of the solution (it can represent e.g. heat flow in the coordinate directions) plays an important role. Since the coefficients  $a_{ij}$  are bounded in  $L_{\#}^{\infty}(Y)$ , also the convergence

$$\left\| a_{ij}^{\varepsilon} \frac{\partial u_{\varepsilon}}{\partial x_{j}} - a_{ij}^{\varepsilon} \frac{\partial u_{\varepsilon}^{C}}{\partial x_{j}} \right\|_{L^{2}(\Omega)} \to 0 \quad \text{as } \varepsilon \to 0$$

holds. Thus, for  $\varepsilon$  small enough, the expression  $a_{ij}^{\varepsilon} \partial_{x_j} u_{\varepsilon}^C$  represents a reasonable approximation of the generalized gradient  $a_{ij}^{\varepsilon} \partial_{x_j} u_{\varepsilon}$ . We have

$$a_{ij}^{\varepsilon} \frac{\partial u_{\varepsilon}^{C}}{\partial x_{j}} = a_{ij} \left(\frac{x}{\varepsilon}\right) \frac{\partial}{\partial x_{j}} \left(u_{0}(x) - \varepsilon \chi_{k} \left(\frac{x}{\varepsilon}\right) \frac{\partial u_{0}}{\partial x_{k}}(x)\right)$$

$$= a_{ij} \left(\frac{x}{\varepsilon}\right) \left[\frac{\partial u_{0}}{\partial x_{j}}(x) - \varepsilon \frac{\partial \chi_{k}}{\partial x_{j}} \left(\frac{x}{\varepsilon}\right) \frac{\partial u_{0}}{\partial x_{k}}(x) \frac{1}{\varepsilon} - \varepsilon \chi_{k} \left(\frac{x}{\varepsilon}\right) \frac{\partial^{2} u_{0}}{\partial x_{k} \partial x_{j}}(x)\right].$$

Let us neglect the expression  $\varepsilon \chi_k(x/\varepsilon) \partial^2_{x_k x_j} u_0(x)$  and let us introduce a vector **w** having components

$$w_i = a_{ij}(y) \left[ \frac{\partial u_0}{\partial x_i}(x) - \frac{\partial \chi_k}{\partial x_i}(y) \frac{\partial u_0}{\partial x_k}(x) \right].$$

We see that the expression contains local functions  $a_{ij}$ ,  $\partial_{x_j}\chi_k$  and global functions  $\partial_{x_k}u_0$ . Let us eliminate the influence of the global functions by the constrained condition  $|\nabla u_0(x)| = 1$ . It is natural, since then the vector function  $\mathbf{w}$  plays the role of the generalized gradient under the assumption of the unit vector of derivatives  $\partial_{x_i}u_0$ . In other words,  $\mathbf{w}$  does not depend on a position in the domain  $\Omega$ , but it does on the microstructure only. Since we are interested in maximal (critical) values of the generalized gradient (heat flow), we define the criterion functional  $\Phi$  in the following way:

(4.4) 
$$\Phi(A,\chi(A)) = \frac{1}{|\tilde{Y}|} \left[ \int_{\tilde{Y}} \sum_{i=1}^{N} [\overline{w}_i(A,\chi(A))]^2 \, \mathrm{d}y \right]^{1/2},$$

where

$$\overline{w}_i = \max_{|\nabla u_0| = 1} w_i$$

and  $\tilde{Y}$  is a suitably chosen subset of the basic period Y (usually at the places of a "sharp change" of the composite components, where the values of the derivatives are high). Functions  $w_i$  are linear in the variables  $\partial_{x_k}u_0$  of the type  $\sum_{i=1}^N b_k^{(i)}\xi_k$ . By the method of Lagrange multipliers one can observe that this linear function has the maximal value  $\sqrt{b_1^2 + \ldots + b_N^2}$  and the minimal value  $-\sqrt{b_1^2 + \ldots + b_N^2}$  on the set  $|\xi| = 1$ . Thus,

$$\sum_{i=1}^{N} \overline{w}_{i}^{2} = \sum_{i=1}^{N} \left\{ \left[ a_{i1} \left( 1 - \frac{\partial \chi_{1}}{\partial y_{1}} \right) - a_{i2} \frac{\partial \chi_{1}}{\partial y_{2}} - a_{i3} \frac{\partial \chi_{1}}{\partial y_{3}} - \dots - a_{iN} \frac{\partial \chi_{1}}{\partial y_{N}} \right]^{2} + \left[ -a_{i1} \frac{\partial \chi_{2}}{\partial y_{1}} + a_{i2} \left( 1 - \frac{\partial \chi_{2}}{\partial y_{2}} \right) - a_{i3} \frac{\partial \chi_{2}}{\partial y_{3}} - \dots - a_{iN} \frac{\partial \chi_{2}}{\partial y_{N}} \right]^{2}$$

$$\vdots$$

$$+ \left[ -a_{i1} \frac{\partial \chi_{N}}{\partial y_{1}} - a_{i2} \frac{\partial \chi_{N}}{\partial y_{2}} - a_{i3} \frac{\partial \chi_{N}}{\partial y_{3}} - \dots + a_{iN} \left( 1 - \frac{\partial \chi_{N}}{\partial y_{N}} \right) \right]^{2} \right\}.$$

Remark 4.5. Obviously, the "smooth" gradient  $\nabla u_0$  does not affect the values of the generalized gradient  $\mathbf{w}$  so strongly as the rapidly oscillating gradient  $\nabla \chi_j^{\varepsilon}$ . Thus, we eliminate its influence to get the microstructure description only (in the variable y). Since we find the maximal values on the set  $|\nabla u_0| = 1$ , we get an upper estimate of  $\mathbf{w}$  for a.a.  $x \in \Omega$ .

The elimination by the constrained condition  $|\nabla u_0| = 1$  is carried out for each component  $w_i$  separately. It would be more natural to use this constrained condition for the (squared) length of the gradient  $|\mathbf{w}|^2$ . However, it would lead to a much more complicated form.

The corresponding maximization problem reads:

(P2) Find  $\bar{A} \in \mathcal{U}^{\mathrm{ad}}$  such that

$$\Phi(\bar{A}, \chi(\bar{A})) \geqslant \Phi(A, \chi(A)) \quad \forall A \in \mathscr{U}^{\mathrm{ad}}.$$

**Theorem 4.6.** Problem (P2) has a solution.

Proof. Let  $\{A_n\}$  be a maximizing sequence of a functional  $\Phi$ , i.e.

(4.5) 
$$\lim_{n \to \infty} \Phi(A_n, \chi(A_n)) = \sup_{A \in \mathscr{U}^{\mathrm{ad}}} \Phi(A, \chi(A)).$$

Due to compactness of  $\mathscr{U}^{\mathrm{ad}}$  there exists  $\bar{A} \in \mathscr{U}^{\mathrm{ad}}$  and a subsequence such that  $A_{n'} \to \bar{A}$  in  $\mathscr{U}^{\mathrm{ad}}$ . According to Lemma 4.3 we also have  $\chi_j^{n'} \equiv \chi_j(A_{n'}) \to \bar{\chi}_j \equiv \chi_j(\bar{A})$  in  $W_{\#0}^{1,2}(Y)$ . The integrand of the functional  $\Phi$  can be transcribed as a sum of three

function types:  $b^2$ ,  $b\partial_{y_k}\mu$ ,  $b^2(\partial_{y_k}\mu)^2$ , where b corresponds to the coefficients  $a_{ij}$  and  $\partial_{y_k}\mu$  corresponds to the derivatives  $\partial_{y_j}\chi_i$ . Thus,  $b_{n'}\to \bar{b}$  in  $L^\infty_\#(Y)$  and  $\partial_{y_k}\mu^{n'}\to \partial_{y_k}\bar{\mu}$  in  $L^2_\#(Y)$ . The convergence  $b_{n'}\to \bar{b}$  in  $L^2_\#(Y)$  holds, since  $L^\infty_\#(Y)\subset L^2_\#(Y)$ . Further,

$$\begin{split} \left| \int_{Y} \left( b_{n'} \frac{\partial \mu_{n'}}{\partial y_{k}} - \bar{b} \frac{\partial \bar{\mu}}{\partial y_{k}} \right) \mathrm{d}y \right| &= \left| \int_{Y} (b_{n'} - \bar{b}) \frac{\partial \mu_{n'}}{\partial y_{k}} \, \mathrm{d}y + \int_{Y} \bar{b} \left( \frac{\partial \mu_{n'}}{\partial y_{k}} - \frac{\partial \bar{\mu}}{\partial y_{k}} \right) \mathrm{d}y \right| \\ &\leqslant \| b_{n'} - \bar{b} \|_{L_{\#}^{2}(Y)} \left\| \frac{\partial \mu_{n'}}{\partial y_{k}} \right\|_{L_{\#}^{2}(Y)} \\ &+ \| \bar{b} \|_{L_{\#}^{2}(Y)} \left\| \frac{\partial \mu_{n'}}{\partial y_{k}} - \frac{\partial \bar{\mu}}{\partial y_{k}} \right\|_{L_{\#}^{2}(Y)} \longrightarrow 0. \end{split}$$

In a similar way we can show that

$$\int_{Y} \left[ b_{n'}^{2} \left( \frac{\partial \mu_{n'}}{\partial y_{k}} \right)^{2} - \bar{b}^{2} \left( \frac{\partial \bar{\mu}}{\partial y_{k}} \right)^{2} \right] dy \to 0.$$

Altogether,

$$\lim_{n'\to\infty} \Phi(A_{n'}, \chi(A_{n'})) = \Phi(\bar{A}, \chi(\bar{A})).$$

According to (4.5),  $\bar{A}$  is the maximizing element.

**Homogenized solution**  $u_0$ . Now, let us define the functional  $\Phi$  by the relation

(4.6) 
$$\Phi(u_0(A_0(A,\chi(A)))) = \frac{1}{|\tilde{\Omega}|} \int_{\tilde{\Omega}} u_0(A_0(A,\chi(A))) dx,$$

where  $A_0$  is the matrix of the homogenized coefficients defined by (3.6) and  $u_0$  is the solution of problem (WH). It represents the average value of the homogenized solution  $u_0$  on a subdomain  $\tilde{\Omega} \subset \Omega$ . Thus, the question is, how the matrix of coefficients A influences homogenized solution  $u_0$  (temperature) at some (critical) places of material.

(P3) Find  $\bar{A} \in \mathcal{U}^{\mathrm{ad}}$  such that

$$\Phi(u_0(A_0(\bar{A},\chi(\bar{A})))) \geqslant \Phi(u_0(A_0(A,\chi(A)))) \quad \forall A \in \mathscr{U}^{\mathrm{ad}}.$$

**Lemma 4.7.** Let  $A_n \to A$  in  $\mathscr{U}^{\mathrm{ad}}$ . Then  $A_0(A_n,\chi(A_n)) \to A_0(A,\chi(A))$  in  $\mathbb{R}^{N \times N}_{\mathrm{sym}}$ .

Proof. Let us denote  $\chi_j^n \equiv \chi_j(A_n)$ . Since  $A_n \to A$  in  $\mathscr{U}^{\mathrm{ad}}$ , Lemma 4.3 yields  $\chi_j^n \to \chi_j \equiv \chi_j(A)$  in  $W_{\#0}^{1,2}(Y)$ . Thus,

$$a_{ij}^{0,n} = \int_{Y} \left( a_{ij}^{n} - a_{ik}^{n} \frac{\partial \chi_{j}^{n}}{\partial y_{k}} \right) dy = \int_{Y} a_{ij}^{n} dy - \int_{Y} a_{ik} \frac{\partial \chi_{j}^{n}}{\partial y_{k}} dy - \int_{Y} \left( a_{ik}^{n} - a_{ik} \right) \frac{\partial \chi_{j}^{n}}{\partial y_{k}} dy$$

$$\longrightarrow \int_{Y} \left( a_{ij} - a_{ik} \frac{\partial \chi_{j}}{\partial y_{k}} \right) dy = a_{ij}^{0}.$$

Overall,  $A_0^n \to A_0$  in  $\mathbb{R}_{\text{sym}}^{N \times N}$ .

**Theorem 4.8.** Problem (P3) has a solution.

Proof. Let  $\{A_n\}$  be a maximizing sequence of the functional  $\Phi$ , i.e.

$$\lim_{n\to\infty} \Phi(u_0(A_0(A_n,\chi(A_n)))) = \sup_{A \subset \mathscr{Y}_{\mathrm{ad}}} \Phi(u_0(A_0(A,\chi(A)))).$$

Since  $\mathscr{U}^{\mathrm{ad}}$  is compact, there exists an element  $\bar{A}$  and a subsequence  $\{A_{n'}\}$  such that  $A_{n'} \to \bar{A}$  in  $\mathscr{U}^{\mathrm{ad}}$ . Thanks to Lemma 4.7 one can verify that  $u_0(A_0(A_{n'},\chi(A_{n'}))) \to u_0(A_0(\bar{A},\chi(\bar{A})))$  in  $W^{1,2}(\Omega)$  (in a similar way as in Lemma 4.3). Thanks to continuity of the functional  $\Phi$ , we have

$$\lim_{n' \to \infty} \Phi(u_0(A_0(A_{n'}, \chi(A_{n'})))) = \Phi(u_0(A_0(\bar{A}, \chi(\bar{A})))).$$

Thus,  $\bar{A}$  is the maximizing element.

## 5. Finite dimensional approximation of the problem

This section deals with the approximate solutions of the problems mentioned in the previous section. The situation is simplified due to the fact that the set  $\mathscr{U}^{\mathrm{ad}}$  can be represented by a closed bounded subset of a finite-dimensional subspace—thus, we do not carry out the approximation of this set.

Let  $W_{\#0,h}^{1,2}(Y)$  be a finite-dimensional subspace of  $W_{\#0}^{1,2}(Y)$ . The Galerkin approximation of the problem (WL) from Subsection 3.3 reads:

 $(\mathrm{WL}_h)$  Find a function  $\chi_i^h \in W^{1,2}_{\#0,h}(Y)$  such that

(5.1) 
$$a_L(\chi_j^h, \mu_h) = b_L^j(\mu_h), \quad \forall \, \mu_h \in W_{\#0,h}^{1,2}(Y).$$

**Theorem 5.1.** There exists a unique solution  $\chi_j^h$  of the Galerkin approximation (WL<sub>h</sub>). Moreover, there exists a sequence of subspaces  $\{W_{\#0,h}^{1,2}(Y)\}$  such that the sequence of approximate solutions  $\{\chi_j^h\}$  converges to  $\chi_j$  strongly in  $W_{\#0}^{1,2}(Y)$  as  $h \to 0+$ .

Sketch of proof. Taking a suitable base in the space  $W^{1,2}_{\#0,h}(Y)$ , the equality (5.1) yields a system of linear algebraic equations. Since the bilinear form  $a_L(\chi_j,\mu)$  is an elliptic bounded form on  $W^{1,2}_{\#0}(Y)\times W^{1,2}_{\#0}(Y)$  and  $b^j_L(\mu)$  is a bounded linear form on  $W^{1,2}_{\#0}(Y)$ , the above mentioned system has a unique solution. The space  $W^{1,2}_{\#0}(Y)$  is a Hilbert separable space and thus there exists a sequence of finite-dimensional subspaces which approximates<sup>2</sup> this space. By this property we can easily obtain the strong convergence of  $\chi^h_j$  to the exact solution  $\chi_j$  in  $W^{1,2}_{\#0}(Y)$ .  $\square$ 

The approximation of the problem (P1) from Subsection 4.2 reads:

(P1<sub>h</sub>) Find 
$$\bar{A}_h \in \mathcal{U}^{\mathrm{ad}}$$
 ( $\underline{A}_h \in \mathcal{U}^{\mathrm{ad}}$ ) such that

$$\Phi_{ij}(\bar{A}_h, \chi_h(\bar{A}_h)) \geqslant \Phi_{ij}(A, \chi_h(A)) \quad \forall A \in \mathscr{U}^{\mathrm{ad}}, 
(\Phi(\underline{A}_h, \chi_h(\underline{A}_h)) \leqslant \Phi(A, \chi_h(A)) \quad \forall A \in \mathscr{U}^{\mathrm{ad}}, \text{ respectively},$$

where the functionals  $\Phi_{ij}$  are defined by the relation (4.1).

**Theorem 5.2.** Problem  $(P1_h)$  has a solution.

The above statement can be proved in the same way as Theorem 4.4.

**Lemma 5.3.** Let  $\{\bar{A}_h\}$ ,  $h \to 0+$ , be a sequence of approximate solutions of problems  $(P1_h)$  such that  $\bar{A}_h \to A$  in  $\mathscr{U}^{\mathrm{ad}}$ , let  $\chi_j^h$   $(\chi_j)$  be the solution of problem  $(\mathrm{WL}_h)$   $((\mathrm{WL})$ , respectively) and let  $\{W_{\#0,h}^{1,2}(Y)\}$  approximate  $W_{\#0}^{1,2}(Y)$ . Then  $\chi_j^h(\bar{A}_h) \to \chi_j(A)$  in  $W_{\#0}^{1,2}(Y)$  as  $h \to 0+$ .

Proof. For a fixed h we have

$$\|\chi_j^h(\bar{A}_h) - \chi_j(A)\|_{W_{\#0}^{1,2}(Y)} \leq \|\chi_j^h(\bar{A}_h) - \chi_j^h(A)\|_{W_{\#0}^{1,2}(Y)} + \|\chi_j^h(A) - \chi_j(A)\|_{W_{\#0}^{1,2}(Y)}.$$

Convergence of the first term on the right-hand side can be proved in the same way as Lemma 4.3, i.e., taking  $\mu_h \equiv \chi_1^h(\bar{A}_h) - \chi_1^h(A)$  as a test function, the definition

<sup>&</sup>lt;sup>2</sup> We say that a sequence of finite-dimensional subspaces  $\{V_h\}$  approximates the space V if for each element  $v \in V$  there exists a sequence  $\{v_h\}$ ,  $v_h \in V_h$  such that  $||v_h - v||_V \to 0$  as  $h \to 0+$ .

of  $(WL_h)$  yields

$$\int_{Y} \left( \bar{a}_{ik}^{h} \frac{\partial \chi_{1}^{h}}{\partial y_{k}} (\bar{A}_{h}) - a_{ik} \frac{\partial \chi_{1}^{h}}{\partial y_{k}} (A) \right) \left( \frac{\partial \chi_{1}^{h}}{\partial y_{i}} (\bar{A}_{h}) - \frac{\partial \chi_{1}^{h}}{\partial y_{i}} (A) \right) dy$$

$$= \int_{Y} \left( \bar{a}_{i1}^{h} - a_{i1} \right) \left( \frac{\partial \chi_{1}^{h}}{\partial y_{i}} (\bar{A}_{h}) - \frac{\partial \chi_{1}^{h}}{\partial y_{i}} (A) \right) dy.$$

Using the ellipticity condition (2.3) and Lemma 1.4, we get

$$\frac{\alpha}{C^2} \|\chi_1^h(\bar{A}_h) - \chi_1^h(A)\|_{W_{\#0}^{1,2}(Y)}^2 + \int_Y (\bar{a}_{ik}^h - a_{ik}) \frac{\partial \chi_1}{\partial y_k} (A) \left( \frac{\partial \chi_1^h}{\partial y_i} (\bar{A}_h) - \frac{\partial \chi_1}{\partial y_i} (A) \right) dy$$

$$\leqslant \int_Y (\bar{a}_{i1}^h - a_{i1}) \left( \frac{\partial \chi_1^h}{\partial y_i} (\bar{A}_h) - \frac{\partial \chi_1}{\partial y_i} (A) \right) dy.$$

Since all derivatives are bounded in  $L^2_{\#}(Y)$ , the integrals obviously converge to zero as  $h \to 0+$ . Thus,

$$\|\chi_1^h(\bar{A}_h) - \chi_1^h(A)\|_{W_{\#_0}^{1,2}(Y)}^2 \to 0.$$

Theorem 5.1 yields the convergence  $\|\chi_j^h(A) - \chi_j(A)\|_{W^{1,2}_{\mu_0}(Y)} \to 0.$ 

**Theorem 5.4.** Let  $\{\bar{A}_h\}$  ( $\{\underline{A}_h\}$ ) be a sequence of solutions of problems (P1<sub>h</sub>), let  $\bar{A}$  ( $\underline{A}$ ) be a solution of problem (P1) and let the sequence of finite-dimensional subspaces  $\{W_{\#0,h}^{1,2}(Y)\}$  approximate the space  $W_{\#0}^{1,2}(Y)$ . Then there exists an extracted subsequence  $\{\bar{A}_{h'}\}$  ( $\{\underline{A}_{h'}\}$ ) such that

$$\Phi_{ij}(\bar{A}_{h'},\chi_{h'}(\bar{A}_{h'})) \to \Phi_{ij}(\bar{A},\chi(\bar{A}))$$
 as  $h \to 0+$ ,  
 $(\Phi_{ij}(\underline{A}_{h'},\chi_{h'}(\underline{A}_{h'})) \to \Phi_{ij}(\underline{A},\chi(\underline{A}))$  as  $h \to 0+$ , respectively).

Proof. By definition we have

(5.2) 
$$\Phi_{ij}(\bar{A}_h, \chi_h(\bar{A}_h)) \geqslant \Phi_{ij}(A, \chi_h(A)) \quad \forall A \in \mathscr{U}^{\mathrm{ad}}.$$

Since  $\mathscr{U}^{\mathrm{ad}}$  is compact, there exists an element  $\tilde{A} \in \mathscr{U}^{\mathrm{ad}}$  and an extracted subsequence  $\{\bar{A}_{h'}\}$  such that  $\bar{A}_{h'} \to \tilde{A}$  in  $\mathscr{U}^{\mathrm{ad}}$  as  $h' \to 0$ . Using Lemma 5.3 and Theorem 5.1 we can pass to the limit on both sides of the inequality (5.2):

$$\lim_{h\to 0+} \Phi_{ij}(\bar{A}_{h'},\chi_{h'}(\bar{A}_{h'})) = \Phi_{ij}(\tilde{A},\chi(\tilde{A})) \geqslant \Phi_{ij}(A,\chi(A)).$$

Thus  $\tilde{A}$  is a maximizing element. Since  $\bar{A}$  is also a maximizing element, we have  $\Phi_{ij}(\tilde{A},\chi(\tilde{A})) = \Phi_{ij}(\bar{A},\chi(\bar{A}))$ , which is the desired result. The minimizing element can be obtained analogously.

Remark 5.5. Generally,  $\tilde{A} \neq \bar{A}$ , since the uniqueness of  $\bar{A}_h$  ( $\bar{A}$ ) of the problem (P1<sub>h</sub>) ((P1), respectively) is not guaranteed.

The approximation of problem (P2) reads:

 $(P2_h)$  Find  $\bar{A}_h \in \mathcal{U}^{ad}$  such that

$$\Phi(\bar{A}_h, \chi_h(\bar{A}_h)) \geqslant \Phi(A, \chi_h(A)) \quad \forall A \in \mathscr{U}^{\mathrm{ad}},$$

where  $\chi_h$  is the solution of the problem (WL<sub>h</sub>) and the functional  $\Phi$  is defined by the relation (4.4).

**Theorem 5.6.** Problem  $(P2_h)$  has a solution.

Proof of this theorem can be obtained in the same way as in Theorem 4.6.

**Theorem 5.7.** Let  $\{\bar{A}_h\}$  be a sequence of solutions of problems  $(P2_h)$ , let  $\bar{A}$  be a solution of problem (P2) and let the sequence of finite-dimensional subspaces  $\{W_{\#0,h}^{1,2}(Y)\}$  approximate the space  $W_{\#0}^{1,2}(Y)$ . Then there exists a subsequence  $\{\bar{A}_{h'}\}$  such that

$$\Phi(\bar{A}_{h'}, \chi_{h'}(\bar{A}_{h'})) \to \Phi(\bar{A}, \chi(\bar{A}))$$
 as  $h \to 0 + ...$ 

Proof. In the proof one can follow the same steps as in the proof of Theorem 5.4.

In the case of problem (P3) we have:

(WH<sub>h</sub>) Find  $u_0^h \in W_h^{1,2}(\Omega)$  such that  $u_0^h - u_D \in V_h \subset V$  and

$$a_H(u_0^h, v_h) = b_H(v_h), \quad \forall v_h \in V_h.$$

**Theorem 5.8.** Problem (WH<sub>h</sub>) has a unique solution. Moreover, there exists a sequence of finite-dimensional subspaces  $\{V_h\}$  such that the sequence of approximate solutions  $\{u_0^h\}$  converges to the solution  $u_0$  strongly in  $W^{1,2}(\Omega)$  as  $h \to 0+$ .

Proof is standard, based on the Lax-Milgram lemma. The existence of a sequence of finite-dimensional subspaces that approximates the space V is ensured by separability of V.

The approximation of problem (P3) reads:

 $(P3_{s,h})$  Find  $\bar{A}_{s,h} \in \mathscr{U}^{ad}$  such that

$$\Phi(u_0^h(A_0(\bar{A}_{s,h},\chi_s(\bar{A}_{s,h})))) \geqslant \Phi(u_0^h(A_0(A,\chi_s(A)))) \quad \forall \, A \in \mathscr{U}^{\mathrm{ad}},$$

where  $u_0^h$  is the approximate solution of problem (WH<sub>h</sub>),  $\chi_s$  is the approximate solution of problem (WL<sub>s</sub>) and the functional  $\Phi$  is defined by the relation (4.6).

**Theorem 5.9.** Problem  $(P3_{s,h})$  has a solution.

Proof. In the proof one can follow the same steps as in the proof of Theorem 4.8.

**Theorem 5.10.** Let  $\{\bar{A}_{s,h}\}$ ,  $s \to 0+$ ,  $h \to 0+$  be a sequence of solutions of problems  $(P3_{s,h})$ , let  $\bar{A}$  be a solution of problem (P3), let a sequence of finite-dimensional subspaces  $\{W_{\#0,s}^{1,2}(Y)\}$  approximate the space  $W_{\#0}^{1,2}(Y)$  and let a sequence of finite-dimensional subspaces  $\{V_h\}$  approximate the space V. Then there exists a subsequence  $\{\bar{A}_{s',h'}\}$  such that

$$\Phi(u_0^{h'}(A_0(\bar{A}_{s',h'},\chi_{s'}(\bar{A}_{s',h'})))) \to \Phi(u_0(A_0(\bar{A},\chi(\bar{A}))))$$
 as  $s' \to 0+$ ,  $h' \to 0+$ .

Sketch of proof. The proof follows the following steps:

- i) Due to compactness of  $\mathscr{U}^{\mathrm{ad}}$ , there exists an element  $\tilde{A}$  and a subsequence  $(s',h') \to (0+,0+)$  such that  $\bar{A}_{s',h'} \to \tilde{A}$  in  $\mathscr{U}^{\mathrm{ad}}$ .
- ii) The convergence  $\chi_{s'}(\bar{A}_{s',h'}) \to \chi(\tilde{A})$  in  $W^{1,2}_{\#0}(Y)$  can be verified in a similar way as in Lemma 5.3.
- iii) Steps i) and ii) yield the convergence  $A_0(\bar{A}_{s',h'},\chi_{s'}(\bar{A}_{s',h'})) \to A_0(\tilde{A},\chi(\tilde{A}))$  in  $\mathbb{R}^{N\times N}_{\mathrm{sym}}$ .
- iv) The convergence  $u_0^{h'}(A_0(\bar{A}_{s',h'},\chi_{s'}(\bar{A}_{s',h'}))) \rightarrow u_0(A_0(\tilde{A},\chi(\tilde{A})))$  in  $W^{1,2}(\Omega)$  holds (analogy to Lemma 5.3).
- v) Step iv) immediately yields

$$\Phi(u_0^{h'}(A_0(\bar{A}_{s',h'},\chi_{s'}(\bar{A}_{s',h'})))) \to \Phi(u_0(A_0(\tilde{A},\chi(\tilde{A})))).$$

Thus,  $\tilde{A}$  is a maximizing element and

$$\Phi(u_0(A_0(\tilde{A}, \chi(\tilde{A})))) = \Phi(u_0(A_0(\bar{A}, \chi(\bar{A})))).$$

## 6. Numerical experiments

In this section we show a few 2D examples demonstrating the above considerations. Let us emphasize that the input parameters are not real, they have an illustrative character only.

## 6.1. Methods of computations

All of the algorithms were programmed under MATLAB environment with help of PDE toolbox and NAG toolbox routine E04JAF.

Solutions  $\chi_1$ ,  $\chi_2$ . These functions are found by the finite element method (with linear triangular elements). The algorithm is slightly modified for requirements of a periodic solution. The periodic boundary condition involves that the values of functions  $\chi_1$ ,  $\chi_2$  must be almost everywhere the same on the opposite sides of Y. This means the triangulation nodes correspond on the opposite sides, i.e. they lie on the same levels and have the same prescribed values. This correspondence can be ensured by the same numbering of the two opposite nodes. For a while the position of the solution is not "fixed" and thus the system of linear equations contains a linearly dependent row—so, we add the condition of zero mean value of the functions  $\chi_1$ ,  $\chi_2$  into the stiffness matrix.

Homogenized coefficients and generalized gradient. These values are obtained by numerical integration.

**Homogenized solution**  $u_0$ . Homogenized solution  $u_0$  was computed by the finite element method (with linear triangular elements). In this case the MATLAB routine called assemple included in PDE toolbox was used, see [17].

Finding maximum (or minimum) of a functional. Since the matrix of coefficients A can be represented by 3(m+1) values (m is the number of subsets of period Y, see Subsection 4.1), finding maximum (or minimum) of a functional reduces to finding the extremes of a 3(m+1) variable function in a compact set. These extremes are obtained by use of the NAG E04JAF iterative process based on the Quasi-Newton method, which suitably approximates the Hess matrix of the second order derivatives from the function values, see [14]. Since the more detailed description is not available, we omit it here. Let us only remark that the algorithm does not involve the strict compliance of the conditions which guarantee the existence of extremes (namely the continuity of the second order derivatives of the objective function).

## 6.2. Examples

For the sake of brevity we will not write the subscript h (or s) for the approximately computed functions  $\bar{A}$ ,  $\underline{A}$ ,  $\chi$ ,  $u_0$ .

**Homogenized coefficients.** Here, we deal with problem (P1) from Subsection 4.2. For the plane case, criterion functionals are in the form

$$\begin{split} &\Phi_{11} = \int_{Y} \left( a_{11} - a_{11} \frac{\partial \chi_{1}}{\partial y_{1}} - a_{12} \frac{\partial \chi_{1}}{\partial y_{2}} \right) \mathrm{d}y, \\ &\Phi_{12} = \Phi_{21} = \int_{Y} \left( a_{12} - a_{11} \frac{\partial \chi_{2}}{\partial y_{1}} - a_{12} \frac{\partial \chi_{2}}{\partial y_{2}} \right) \mathrm{d}y, \\ &\Phi_{22} = \int_{Y} \left( a_{22} - a_{21} \frac{\partial \chi_{2}}{\partial y_{1}} - a_{22} \frac{\partial \chi_{2}}{\partial y_{2}} \right) \mathrm{d}y. \end{split}$$

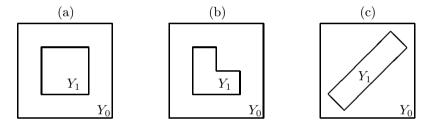


Figure 1. Ordering on the basic period.

Example 1. First, let us consider the simplest situation, when the composite consists of two isotropic components according to Fig. 1 (a), i.e.  $a_{11} = a_{22}$ ,  $a_{12} = a_{21} = 0$ . Since the components are symmetric with respect to axes  $y_1 = \frac{1}{2}$ ,  $y_2 = \frac{1}{2}$ , we have also  $a_{12}^0 = a_{21}^0 = 0$ . Let us choose the values of coefficients in intervals  $a_{11}|_{Y_0} \in [90; 110]$ ,  $a_{11}|_{Y_1} \in [190; 210]$ . Thus, we maximize (or minimize) just one functional  $\Phi_{11} = \Phi_{22}$ .

$$\begin{split} \bar{A} &= \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}, \quad \text{where } \ \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases} \\ \underline{A} &= \begin{pmatrix} \underline{a}_{11} & 0 \\ 0 & \underline{a}_{22} \end{pmatrix}, \quad \text{where } \ \underline{a}_{11} = \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \\ \Phi_{11}(\bar{A}, \chi(\bar{A})) &= \Phi_{22}(\bar{A}, \chi(\bar{A})) = 128.811, \quad \Phi_{11}(\underline{A}, \chi(\underline{A})) = \Phi_{22}(\underline{A}, \chi(\underline{A})) = 107.851. \end{split}$$

We can see that the critical values of the matrix A appear on the boundaries of given intervals. It corresponds to the image of the linear problem—higher values of particular components imply higher values of the homogenized coefficient.

Example 2. In the second example, let us consider a two-component composite with isotropic properties again, but with a different geometric shape according to Fig. 1(b). The coefficients are from the same intervals as in Example 1. Since functions  $a_{11} = a_{22}$  are not symmetric on Y, the coefficients  $a_{12}^0 = a_{21}^0$  given by the functional  $\Phi_{12}$  will be also nonzero. For the functionals  $\Phi_{11} = \Phi_{22}$  we get

$$\bar{A} = \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}, \quad \text{where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases}$$

$$\underline{A} = \begin{pmatrix} \underline{a}_{11} & 0, \\ 0 & \underline{a}_{22}, \end{pmatrix}, \text{ where } \underline{a}_{11} = \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases}$$

$$\Phi_{11}(\bar{A}, \chi(\bar{A})) = \Phi_{22}(\bar{A}, \chi(\bar{A})) = 130.629, \ \Phi_{11}(\underline{A}, \chi(\underline{A})) = \Phi_{22}(\underline{A}, \chi(\underline{A})) = 109.658.$$

For the functional  $\Phi_{12}$  we have

$$\begin{split} \bar{A} &= \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}, \quad \text{where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases} \\ \underline{A} &= \begin{pmatrix} \underline{a}_{11} & 0 \\ 0 & \underline{a}_{22} \end{pmatrix}, \quad \text{where } \underline{a}_{11} = \underline{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \\ \Phi_{12}(\bar{A}, \chi(\bar{A})) = 0.902, \quad \Phi_{12}(\underline{A}, \chi(\underline{A})) = 0.429. \end{split}$$

For the functionals  $\Phi_{12} = \Phi_{21}$  we got critical values on the opposite sides of intervals, but we can see that the influence of the non-diagonal homogenized coefficients is small.

Example 3. In this experiment the situation is further generalized. Let us consider that one component is isotropic, while the other is anisotropic described by non-diagonal coefficients, too. Moreover, the shape of the subdomain  $Y_1$  strengthens these "non-diagonal properties", see Fig. 1 (c). The coefficients are described by intervals:  $a_{11}|_{Y_0} = a_{22}|_{Y_0} \in [90; 110]$ ,  $a_{12}|_{Y_0} = a_{21}|_{Y_0} = 0$ ,  $a_{11}|_{Y_1} = a_{22}|_{Y_1} \in [190; 210]$ ,  $a_{12}|_{Y_1} = a_{21}|_{Y_1} \in [165; 185]$ . For the functional  $\Phi_{11} = \Phi_{22}$  we get

$$\begin{split} \bar{A} &= \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix}, \text{ where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases} \quad \bar{a}_{12} = \bar{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 165 & \text{on } Y_1, \end{cases} \\ \underline{A} &= \begin{pmatrix} \underline{a}_{11} & \underline{a}_{12} \\ \underline{a}_{21} & \underline{a}_{22} \end{pmatrix}, \text{ where } \underline{a}_{11} = \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \quad \underline{a}_{12} = \underline{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 185 & \text{on } Y_1, \end{cases} \\ \Phi_{11}(\bar{A}, \chi(\bar{A})) = \Phi_{22}(\bar{A}, \chi(\bar{A})) = 120.288, \quad \Phi_{11}(\underline{A}, \chi(\underline{A})) = \Phi_{22}(\underline{A}, \chi(\underline{A})) = 88.856. \end{split}$$

As regards the functional  $\Phi_{12} = \Phi_{21}$  we have

$$\bar{A} = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix}, \text{ where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \quad \bar{a}_{12} = \bar{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 185 & \text{on } Y_1, \end{cases}$$

$$\underline{A} = \begin{pmatrix} \underline{a}_{11} & \underline{a}_{12} \\ \underline{a}_{21} & \underline{a}_{22} \end{pmatrix}, \text{ where } \underline{a}_{11} = \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases} \quad \underline{a}_{12} = \underline{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 165 & \text{on } Y_1, \end{cases}$$

$$\Phi_{12}(\bar{A}, \chi(\bar{A})) = 48.776, \quad \Phi_{12}(\underline{A}, \chi(\underline{A})) = 29.135.$$

While two values in the critical matrix  $\bar{A}$  (and  $\underline{A}$ ) are on the lower (and upper) ends of appropriate intervals, one value appears on the opposite end.

Example 4. Let us consider the same situation as in the previous example according to Fig. 1 (c), but moreover, let us assume that the material of the part  $Y_0$  is also anisotropic. Coefficients are prescribed in the following way:  $a_{11}|_{Y_0} = a_{22}|_{Y_0} \in [90;110], \ a_{12}|_{Y_0} = a_{21}|_{Y_0} \in [65;85], \ a_{11}|_{Y_1} = a_{22}|_{Y_1} \in [190;210], \ a_{12}|_{Y_1} = a_{21}|_{Y_1} \in [165;185].$  For the functionals  $\Phi_{11} = \Phi_{22}$  we get

$$\bar{A} = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix},$$
where  $\bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases}$   $\bar{a}_{12} = \bar{a}_{21} = \begin{cases} 79.950 & \text{on } Y_0, \\ 165 & \text{on } Y_1, \end{cases}$ 

$$\underline{A} = \begin{pmatrix} \underline{a}_{11} & \underline{a}_{12} \\ \underline{a}_{21} & \underline{a}_{22} \end{pmatrix},$$
where  $\underline{a}_{11} = \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases}$   $\underline{a}_{12} = \underline{a}_{21} = \begin{cases} 85 & \text{on } Y_0, \\ 165 & \text{on } Y_1, \end{cases}$ 

$$\Phi_{11}(\bar{A}, \chi(\bar{A})) = \Phi_{22}(\bar{A}, \chi(\bar{A})) = 128.830, \quad \Phi_{11}(\underline{A}, \chi(\underline{A})) = \Phi_{22}(\underline{A}, \chi(\underline{A})) = 107.040$$

and for the functional  $\Phi_{12} = \Phi_{21}$ 

$$\begin{split} \bar{A} &= \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix}, \\ \text{where } \bar{a}_{11} &= \bar{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases}, \quad \bar{a}_{12} &= \bar{a}_{21} = \begin{cases} 85 & \text{on } Y_0, \\ 185 & \text{on } Y_1, \end{cases} \\ \underline{A} &= \begin{pmatrix} \underline{a}_{11} & \underline{a}_{12} \\ \underline{a}_{21} & \underline{a}_{22} \end{pmatrix}, \\ \text{where } \underline{a}_{11} &= \underline{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 209.882 & \text{on } Y_1, \end{cases} \quad \underline{a}_{12} &= \underline{a}_{21} = \begin{cases} 65 & \text{on } Y_0, \\ 165 & \text{on } Y_1, \end{cases} \\ \Phi_{12}(\bar{A}, \chi(\bar{A})) &= 102.691, \quad \Phi_{12}(\underline{A}, \chi(\underline{A})) = 82.078. \end{split}$$

In this case, where the description of the material properties is more complicated, we get the values  $a_{12}$  also inside the admissible intervals.

**Generalized gradient.** For the plane case, the functional  $\Phi$  from problem (P2) (see Subsection 4.2) is in the form

$$\Phi = \frac{1}{|\tilde{Y}|} \left( \int_{\tilde{Y}} \left\{ \left[ a_{11} \left( 1 - \frac{\partial \chi_1}{\partial y_1} \right) - a_{12} \frac{\partial \chi_1}{\partial y_2} \right]^2 + \left[ -a_{11} \frac{\partial \chi_2}{\partial y_1} + a_{12} \left( 1 - \frac{\partial \chi_2}{\partial y_2} \right) \right]^2 + \left[ a_{21} \left( 1 - \frac{\partial \chi_1}{\partial y_1} \right) - a_{22} \frac{\partial \chi_1}{\partial y_2} \right]^2 + \left[ -a_{21} \frac{\partial \chi_2}{\partial y_1} + a_{22} \left( 1 - \frac{\partial \chi_2}{\partial y_2} \right) \right]^2 \right\} dy \right)^{1/2}.$$

Example 5. Let us consider the situation according to Fig. 2(a) with the same range of coefficients as in Example 1. The maximizing matrix of the coefficients is

$$\bar{A} = \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}$$
, where  $\bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases}$   
 $\Phi(\bar{A}, \chi(\bar{A})) = 4691.420.$ 

Similarly to Example 1, the maximizing values are on the upper boundaries of intervals determining the set  $\mathcal{U}^{\mathrm{ad}}$ . This result was not expected. In the case of a functional which represents the size of the derivatives of functions in a certain sense (e.g. the size of the gradients of these functions), we would get the values on the opposite sides. Intuitively, a "higher jump" in values should cause "higher" values of derivatives. However, numerical experiments do not confirm this property and thus, it is not suitable to think of functions  $\chi_1$ ,  $\chi_2$  separately.

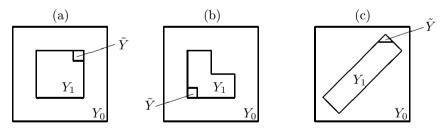


Figure 2. Choice of the subdomain Y.

Example 6. In this example let us take the arrangement in the composite according to Fig. 2(b) and the range of values as in Example 2. The critical values are

$$\bar{A} = \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}, \text{ where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 210 & \text{on } Y_1, \end{cases}$$

$$\Phi(\bar{A}, \chi(\bar{A})) = 4760.215.$$

The subdomain  $\tilde{Y}$  is situated into the left bottom corner of the set  $Y_1$  because the gradient has its peak in that corner. Since the other corners are closer to each other, the corresponding peaks are not so high. Therefore, the values of the generalized gradient are more uniformly distributed there.

Example 7. This example models the situation according to Fig. 2(c) and the tolerance of the coefficients is the same as in Example 3. The maximizing matrix is

$$\begin{split} \bar{A} = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix}, & \text{where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 110 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \\ \bar{a}_{12} = \bar{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 185 & \text{on } Y_1, \end{cases} \\ \Phi(\bar{A}, \chi(\bar{A})) = 5668.581. \end{split}$$

Similarly to Example 3, we get one value in the matrix  $\bar{A}$  on the side opposite to the other values.

**Homogenized solution**  $u_0$ . The following two examples correspond to Fig. 3. The shape of the domain  $\Omega$  is a rectangle with sides whose ratio is 2:1. Three heat sources are placed in the body corresponding to the subdomains  $\Omega_1$ ,  $\Omega_2$  and  $\Omega_3$ . They have the prescribed value  $f_1 = f_2 = f_3 = 3000$ .

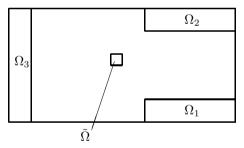


Figure 3. "Macroscopic problem."

Approximately in the center of the domain  $\Omega$  the test subdomain  $\tilde{\Omega}$  is placed. The Neumann condition  $\partial_{\nu}u_0 = 0$  is prescribed on parts of boundary  $\partial\Omega \cap \partial\Omega_1$ ,  $\partial\Omega \cap \partial\Omega_2$  and  $\partial\Omega \cap \partial\Omega_3$  (the sources are isolated). On the rest of the boundary, the Dirichlet condition  $u_0 = 0$  is given. This model problem was inspired by the example shown in [6]. Let us recall that the functional  $\Phi$  is in the form

$$\Phi(u_0(A_0(A,\chi(A)))) = \frac{1}{|\tilde{\Omega}|} \int_{\tilde{\Omega}} u_0(A_0(A,\chi(A))) dx.$$

Example 8. The microstructure and the range of coefficients is given in the same way as in Example 1 (see Fig. 1(a)). Then, the matrix  $\bar{A}$  maximizing the

functional  $\Phi$  has values

$$\begin{split} \bar{A} = \begin{pmatrix} \bar{a}_{11} & 0 \\ 0 & \bar{a}_{22} \end{pmatrix}, \quad \text{where } \ \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \\ \Phi(u_0(A_0(\bar{A},\chi(\bar{A})))) = 4.605. \end{split}$$

Example 9. In this example, the ranges of coefficients are set in the same way as in Example 3 (components are arranged according to Fig. 1(c)). The maximizing matrix  $\bar{A}$  is

$$\begin{split} \bar{A} = \begin{pmatrix} \bar{a}_{11} & \bar{a}_{12} \\ \bar{a}_{21} & \bar{a}_{22} \end{pmatrix}, & \text{where } \bar{a}_{11} = \bar{a}_{22} = \begin{cases} 90 & \text{on } Y_0, \\ 190 & \text{on } Y_1, \end{cases} \\ \bar{a}_{12} = \bar{a}_{21} = \begin{cases} 0 & \text{on } Y_0, \\ 185 & \text{on } Y_1, \end{cases} \\ \Phi(u_0(A_0(\bar{A}, \chi(\bar{A})))) = 6.361. \end{split}$$

We can see that the results of two previous examples are "inverse" to the results of Examples 1 and 3—for instance, Example 8 deals with a composite formed by isotropic materials and the result can be interpreted—"higher values of the homogenized coefficient imply lower values of average temperature on the test domain  $\tilde{\Omega}$ ".

## 7. Conclusion

We have dealt with homogenization of linear elliptic problems with periodically oscillating coefficients that models the behaviour of periodically organized composite materials. The material constants of the components determining the coefficients are not prescribed exactly, but in certain bounds only. These uncertainties were treated by the worst scenario method. The method requires to set a criterion determining "bad" and "good" coefficients in a given set. This criterion is described by a functional. The choice of the functionals was discussed in Section 4. The method was demonstrated on several examples.

The paper proves that the method can be applied in the homogenization theory. By a suitable choice of the criterion functional we can solve a wide range of problems. Here we focused on deducing the tolerance of the effective parameters in the composite material from the knowledge of tolerances of the particular components, further on the behaviour of the generalized gradient at the crucial places of "sharp" changes of materials and on the average value of the homogenized solution in a test subdomain. The experiments suggest that in the case of isotropic materials, the functionals have a monotone behaviour. However, this characteristic gets lost in the case of anisotropic materials. Let us emphasize that the resulting value of functionals is influenced by many parameters—a number of components in the composite,

their shape, arrangement and the relative ratio on the unit period Y, the coefficients describing the properties of these components and their range. It is probable that a suitable combination of the factors mentioned yields more critical values inside the intervals determining the original set of coefficients  $a_{ij}$ .

From both the mathematical and the technical point of view an extension to the following steps is interesting:

- (i) A sensitive analysis with respect to input parameters with help of the gradient of the criterion functional.
- (ii) Use of functionals that combine more than one aspect, for example, a functional that represents the balance between temperature and heat flow. It deals with the so-called multiobjective optimization methods. The construction of the appropriate functionals is described e.g. in [12]. A certain compromise between the particular criteria is the result.
- (iii) The extension to homogenization of the system of linear equations

$$\begin{split} -\frac{\partial}{\partial x_j} \Big( a_{ijkl} \frac{\partial u_k}{\partial x_l} \Big) &= f_i & \text{in } \Omega, \\ u_i &= u_D^i & \text{on } \Gamma_D, \\ a_{ijkl} \frac{\partial u_k}{\partial x_l} \nu_j &= w_N^i & \text{on } \Gamma_N, \end{split}$$

where i = 1, 2, 3. These problems are meaningful mainly in linear elasticity theory (see [8]).

(iv) Nonlinear problems—the above mentioned methods can be applied to various nonlinear problems, but the form of the homogenized problem is usually not favourable from numerical point of view. This is due to impossibility of a separation to a local and global part in the two-scale homogenized system.

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