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INSTITUTE OF COMPUTER SCIENCE

ACADEMY OF SCIENCES OF THE CZECH REPUBLIC

The numerical solution of the linear problem of
elasticity in the anisotropic nonhomogeneous
material - the method of homogenization

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1 Introduction to the problem

We are interested in the problem of linear elasticity in composite materials. This problem is needed to be solved in many various domains of human activity, for example researching of geodynamical processes in the rock massive or medicine, modelling of fractures etc.

First of all I am going to mention some basic principles and laws of the theory of elasticity, and formulate the general problem of elasticity in the classical and weak form. Next I will describe the method of homogenization of Hook's elasticity coefficients, which are characteristic for concrete material. In practice, the material is generally nonhomogeneous. The destination of the homogenization method is to find the so called homogenized (through a certain average way) coefficients for this type of material. For a numerical solving of homogenization is used the finite element method.

Finally I will show you some types of nonhomogeneous materials and results of homogenization.

2 Formulation of the general problem of elasticity

2.1 Definition of the domain

Let $\Omega \subset \mathbf{R}^3$ be a domain with a Lipschitz-continuous boundary $\Gamma = \Gamma_u \cup \Gamma_\tau \cup R$. Γ_u is a part of the boundary where the resultant shifting U is prescribed, on the Γ_τ surface forces \vec{p} are given and R is a set of the 0 measure which correspond to certain parts of the boundary where a "normal" doesn't exist, for example on the edge of figure. There holds $\Gamma_u \cap \Gamma_\tau = \emptyset$, Γ_u and Γ_τ are empty or opened in Γ . The volume forces described by function \vec{f} work inside of the domain.

We want to find the resultant shifting \vec{u} , the placing of stress $\vec{\tau}$ and deformations $\vec{\epsilon}$ in domain Ω . These quantities are joined by the next mathematical and physical relations.

2.2 Relation for small deformations

Let us consider small deformations, a tensor of small deformations denote e_{ij} . For this holds

$$e_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad i, j = 1, 2, 3. \quad (2.1)$$

2.3 Hook's law

For every point $x \in \Omega$ holds a linear relation between tensors of stress and small deformations:

$$\tau_{ij} = a_{ijkl} e_{kl}, \quad i, j = 1, 2, 3. \quad (2.2)$$

This relation is called *generalized Hook's law*. The material is characterized by Hook's coefficients $a_{ijkl}(x) \in C(\bar{\Omega})$ - generally by functions of point $x \in \Omega$. These coefficients are bounded. The Lipschitz condition holds for them

$$m \leq \frac{a_{ijkl} \xi_{ij} \xi_{kl}}{\|\xi\|^2} \leq M < \infty,$$

where $m, M > 0$ and ξ_{ij} is a symmetric matrix of order 3.

From the symmetry of tensors τ_{ij} and e_{ij} , we obtain the next conditions for Hook's coefficient:

$$a_{ijkl} = a_{jikl} = a_{ijlk} = a_{klij} \quad (2.3)$$

In the equation (2.2) is 81 Hook's coefficients. But from the symmetry equation (2.3) maximum of 21 independent constants $a_{ijkl}(x)$ exist characterized a general material in point x .

Definition 2.3.1 *If constants $a_{ijkl}(x)$ are independent of point $x \in \Omega$, then this type of material will be called **homogeneous**.*

*If constants $a_{ijkl}(x)$ are independent from choice of the system of coordinates, then this type of material will be called **isotropic** in point x (the material has same features in all directions). In the opposite case material is called **anisotropic**.*

If the figure is isotropic, then Hook's law will be form

$$\begin{aligned}\tau_{ii} &= \lambda(e_{11} + e_{22} + e_{33}) + 2\mu e_{ii}, & i = 1, 2, 3, \\ \tau_{ij} &= 2\mu e_{ij}, & i, j = 1, 2, 3, \quad i \neq j,\end{aligned}$$

where $\mu = \mu(x) > 0$ and $\lambda = \lambda(x) \geq 0$ are so called Lamé's coefficients. If the figures are homogeneous in addition, then λ and μ are constants which can be described by Young's elasticity module E and Poisson's constant σ ($0 < \sigma < \frac{1}{2}$):

$$\mu = \frac{E}{2(1 + \sigma)}, \quad \lambda = \frac{2\mu\sigma}{1 - 2\sigma} = \frac{E\sigma}{(1 + \sigma)(1 - 2\sigma)}.$$

2.4 Classical formulation of the linear problem of elasticity

Let Ω be the domain described in part 2.1. Let's assume $a_{ijkl} \in C^1(\bar{\Omega})$. Let's have functions $f \in [C^1(\Omega)]^3$, $p \in [C(\Gamma_\tau)]^3$ and $U \in [C(\Gamma_u)]^3$. We want to find the vector function $u \in [C^2(\Omega) \cap C^1(\Omega \cup \Gamma_\tau) \cap C(\Omega \cup \Gamma_u)]$, that satisfies

$$\begin{aligned}-\frac{\partial}{\partial x_j} \left(a_{ijkl} \frac{\partial u_k}{\partial x_l} \right) &= f_i, & \forall x \in \Omega, \\ a_{ijkl} \frac{\partial u_k}{\partial x_l} n_j &= p_i & \text{on } \Gamma_\tau, \\ u_i &= U_i & \text{on } \Gamma_u\end{aligned} \tag{2.4}$$

for $i, j, k, l = 1, 2, 3$.

The problem (2.4) can be formulate also by using a tensor of stress τ_{ij} in the following way:

$$\begin{aligned}-\frac{\partial}{\partial x_j} \tau_{ij} &= f_i & \forall x \in \Omega, \\ \tau_{ij} n_j &= p_i & \text{on } \Gamma_\tau, \\ u_i &= U_i & \text{on } \Gamma_u\end{aligned} \tag{2.5}$$

for $i, j = 1, 2, 3$.

2.5 Weak solution

Let Ω be the domain with Lipschitz-continuous boundary and the quadratic form $a_{ijkl}(x) e_{ij} e_{kl}$ be positive-definite, this means that such a constant $a_0 > 0$ exists, making

$$a_{ijkl}(x) e_{ij} e_{kl} > a_0 e_{ij} e_{kl}$$

hold. We assume that between a stress tensor and a tensor of small deformations holds Hook's law (2.2).

Let us define a set (space) of testing functions

$$V = \left\{ \varphi \in [W_2^1(\Omega)]^3 : \varphi = 0 \text{ on } \Gamma_u \text{ "in the sense of traces"} \right\}.$$

If we take any function $v \in V$, multiply equation of balance in (2.5) by it and integrate the obtained equation:

$$\int_{\Omega} \frac{\partial \tau_{ij}}{\partial x_j} v_i dV + \int_{\Omega} f_i v_i dV = 0.$$

By using Green's theorem we obtain

$$-\int_{\Omega} \tau_{ij} e_{ij}(v) dV + \int_{\Gamma} \tau_{ij} n_j v_i dS + \int_{\Omega} f_i v_i dV = 0.$$

According to the choice of space V , the integral over the part of boundary Γ_u is equal to zero. By substituting boundary conditions, we obtain the following relation for finding the weak solution of the problem (2.5).

The weak solution of boundary problem (2.5) is called function $u \in [W_2^1(\Omega)]^3$, which satisfy conditions

$$\begin{aligned} u - U &\in V, \\ \int_{\Omega} \tau_{ij} e_{ij}(v) dV &= \int_{\Gamma_{\tau}} p_i v_i dS + \int_{\Omega} f_i v_i dV \quad \forall v \in V, \end{aligned}$$

where $f \in [L^2(\Omega)]^3$ and $p \in [L^2(\Gamma_{\tau})]^3$.

Proof of the existence of the weak solution is based on Lax-Milgram's lemma. It is necessary to prove that the integral on the left hand side of the equation is continuous with an elliptic form and integrals on the right hand side constitute a continuous linear function. The proof of the solution uniqueness is based on a hypothesis of the existence of two different solutions which satisfy equation (2.5). We can prove that the difference between two solutions must be zero.

3 Homogenization of Hook's coefficients

3.1 The formulation of the linear problem of elasticity for nonhomogeneous anisotropic material

Material usually is nonhomogeneous. It is composed of a homogeneous subdomains, in which each one is characterized by their own coefficients of elasticity a_{ijkl} . For this type of subdomain, coefficients a_{ijkl} are constant. For simplicity assume that these homogeneous subdomain are set up periodically in the material. This kind of material is called *Y-periodic*. One "period Y " contains a group of homogeneous subdomain Y_i (viz. figure). In homogeneous subdomains Y_i coefficients a_{ijkl} are constant and in the entire domain Y , they are functions of variable x . These domains Y make domain Ω .

The material of domain Ω is given by Hook's coefficients $a_{ijkl}(x)$ as periodic functions with period Y . The result of the homogenization method is finding homogenized coefficients of elasticity a_{ijkl}^0 , which are constant for the entire Ω domain.

Definition 3.1.1 *The function $f(x, y, z)$ will be Y -periodic in variable y , if*

$$f(x, y_1 + k_1\bar{y}_1, y_2 + k_2\bar{y}_2, y_3 + k_3\bar{y}_3, z) = f(x, y_1, y_2, y_3, z)$$

holds for all integers k_1, k_2, k_3 . Let's define the average value

$$M(f) = \int_Y \frac{f(x, y, z)}{\text{meas}(Y)} dV. \quad (3.1)$$

If function $f(y)$ is Y -periodic, then it holds that

$$M\left(\frac{\partial f}{\partial y_j}\right) = 0. \quad (3.2)$$

Let us take new variables $y = \frac{x}{\epsilon}$ and define

$$a_{ijkl}^\epsilon(x) = a_{ijkl}\left(x, \frac{x}{\epsilon}\right) = a_{ijkl}(x, y).$$

The corresponding solution is denoted \vec{u}^ϵ . Then we solve the problem of how to find function \vec{u}^ϵ for $\epsilon > 0$ which satisfies the equation of balance

$$-\frac{\partial}{\partial x_j} \left(a_{ijkl}^\epsilon \frac{\partial u_k^\epsilon}{\partial x_l} \right) = f_i \quad \forall x \in \Omega, \quad (3.3)$$

boundary conditions

$$\begin{aligned} a_{ijkl}^\epsilon \frac{\partial u_k^\epsilon}{\partial x_l} n_j &= p_i && \text{on } \Gamma_\tau, \\ u_i^\epsilon &= U_i && \text{on } \Gamma_u, \end{aligned} \quad (3.4)$$

and Hook's law

$$\tau_{ij}^\epsilon = a_{ijkl}^\epsilon \cdot \epsilon_{kl}^\epsilon(\vec{u}^\epsilon). \quad (3.5)$$

3.2 The converting of the problem with periodic Hook's coefficients to the problem with a homogenized coefficient

Let us consider $\epsilon \rightarrow 0^+$. Functions a_{ijkl}^ϵ intensively change their function values on the interval Y likewise function \vec{u}^ϵ . But the function \vec{u}^ϵ is not periodical. Let's find it in Taylor's form in point $\frac{x}{\epsilon}$, it means for one constant ϵ :

$$\vec{u}^\epsilon(x) = \vec{u}\left(x, \frac{x}{\epsilon}\right) + \epsilon \vec{u}^1\left(x, \frac{x}{\epsilon}\right) + \epsilon^2 \vec{u}^2\left(x, \frac{x}{\epsilon}\right), \quad (3.6)$$

where functions $\vec{u}^i\left(x, \frac{x}{\epsilon}\right) = \vec{u}^i(x, y)$ are periodic in y on interval Y and are independent of ϵ . The dependence of function $\vec{u}(x, y)$ on ϵ is only given by multiples ϵ and ϵ^2 . The general relation holds for derivation of composite function

$$\frac{df\left(x, \frac{x}{\epsilon}\right)}{dx_j} = \frac{\partial f\left(x, \frac{x}{\epsilon}\right)}{\partial x_j} + \frac{1}{\epsilon} \frac{\partial f\left(x, \frac{x}{\epsilon}\right)}{\partial y_j}.$$

Now we arrange the boundary problem (3.3, 3.4) in the following way:

1. The function $\vec{u}^\epsilon(x, y)$ in the boundary problem (3.3, 3.4) is a function of two variables. For this we express its derivations with the help of a given relation for the derivation of a composite function of two variables.
2. We use Taylor's form (3.6) as a substitute to the arranged boundary problem

$$\vec{u}^\epsilon = \vec{u}^\epsilon + \epsilon \cdot \vec{u}^1 + \epsilon^2 \cdot \vec{u}^2.$$

3. We compare coefficients with the same power of ϵ .

After providing the first part let us denote it by operators

$$\begin{aligned} (A^\epsilon u^\epsilon)_i &= -\frac{\partial}{\partial x_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial x_l} \right), \\ (A^0 u^\epsilon)_i &= -\frac{\partial}{\partial y_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial y_l} \right), \\ (A^1 u^\epsilon)_i &= -\frac{\partial}{\partial y_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial x_l} \right) - \frac{\partial}{\partial x_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial y_l} \right), \\ (A^2 u^\epsilon)_i &= -\frac{\partial}{\partial x_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial x_l} \right) \end{aligned}$$

and the equation of balance (3.3) let us write in the form

$$\epsilon^{-2} (A^0 u^\epsilon)_i + \epsilon^{-1} (A^1 u^\epsilon)_i + (A^2 u^\epsilon)_i = f_i$$

or

$$-\frac{\partial}{\partial x_j} \left(a_{ijkl} \frac{\partial u_k^\epsilon}{\partial x_l} \right) = (A^\epsilon u^\epsilon)_i = (\epsilon^{-2} A^0 + \epsilon^{-1} A^1 + A^2)_i u_i^\epsilon = f_i. \quad (3.7)$$

After comparing, we obtain these equations:

1. from the equation of balance (3.3):

$$A^0 u^0 = 0 \quad \text{in } \Omega \times Y, \quad (3.8)$$

$$A^0 u^1 + A^1 u^0 = 0 \quad \text{in } \Omega \times Y, \quad (3.9)$$

$$A^0 u^2 + A^1 u^1 + A^2 u^0 = f \quad \text{in } \Omega \times Y, \quad (3.10)$$

$$A^1 u^2 + A^2 u^1 = 0 \quad \text{in } \Omega \times Y, \quad (3.11)$$

$$A^2 u^2 = 0 \quad \text{in } \Omega \times Y, \quad (3.12)$$

2. from the first boundary condition (3.4):

$$a_{ijkl}(y) \frac{\partial u_k^0(x, y)}{\partial y_l} n_j(x) = 0 \quad \text{on } \Gamma_\tau \times Y, \quad (3.13)$$

$$a_{ijkl}(y) \left(\frac{\partial u_k^1(x, y)}{\partial y_l} + \frac{\partial u_k^0(x, y)}{\partial x_l} \right) n_j(x) = p_i \quad \text{on } \Gamma_\tau \times Y, \quad (3.14)$$

$$a_{ijkl}(y) \left(\frac{\partial u_k^2(x, y)}{\partial y_l} + \frac{\partial u_k^1(x, y)}{\partial x_l} \right) n_j(x) = 0 \quad \text{on } \Gamma_\tau \times Y, \quad (3.15)$$

$$a_{ijkl}(y) \frac{\partial u_k^2(x, y)}{\partial x_l} n_j(x) = 0 \quad \text{on } \Gamma_\tau \times Y, \quad (3.16)$$

3. from the second boundary condition (3.4):

$$u_i^0 = U_i \quad \text{on } \Gamma_u \times Y \quad (3.17)$$

$$u_i^1 = 0 \quad \text{on } \Gamma_u \times Y \quad (3.18)$$

$$u_i^2 = 0 \quad \text{on } \Gamma_u \times Y \quad (3.19)$$

Equations (3.12,3.16,3.19) give a boundary problem which has the solution $u_i^2 = 0$. This solution is not interesting from a physical point of view (no forces work, initial and resultant shifting are zero).

We can prove the following lemma:

Lemma 3.2.1 *Let $f \in [L_{per}^2(Y)]^3$. The equation $A^0 u = f$ has a solution $u \in [W_{per}^{1,2}(Y)]^3$ if and only if $M(f) = 0$. This solution is unique except for an additive constant.*

Thus the solution u^0 of the equation (3.8) is independent of the variable y ($u^0 = u^0(x)$), because the identity

$$-\frac{\partial}{\partial y_j} \left(a_{ijkl}(y) \frac{\partial u_k^0}{\partial y_l} \right) = 0$$

holds and the function u^0 must be independent of y in order to satisfy this equation. From equation (3.9) we obtain

$$A^0 u^1 = -A^1 u^0 = \frac{\partial}{\partial y_j} \left(a_{ijkl}(y) \frac{\partial u_k^0(x)}{\partial x_l} \right). \quad (3.20)$$

This equation has the solution from a space of $[W_{per}^{1,2}(Y)]^3$ at every point x . We will find the solution of whole equation in the form

$$u_g^1(x, y) = -\chi_g^{kl}(y) \frac{\partial u_k^0(x)}{\partial x_l} + \tilde{u}_g(x), \quad (3.21)$$

where $\chi \in [W_{per}^{1,2}(Y)]^3$. The form of solution follows directly from the relation (3.20).

Further we substitute this solution to the (3.20) and arrange it to the form

$$\frac{\partial}{\partial y_j} \left[a_{ijgh}(y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \right] = 0. \quad (3.22)$$

The equation (3.10) has the solution from a space of $[W_{per}^{1,2}(Y)]^3$ (it follows from lemma) if and only if

$$M \left(A^0 u^2 + A^1 u^1 + A^2 u^0 - f \right) = 0.$$

But we know that $u^2 = 0$, so we can write

$$M \left(A^1 u^1 + A^2 u^0 - f \right) = 0.$$

Now we substitute solution (3.21) and after arranging it we obtain

$$M \left[\frac{\partial}{\partial y_j} a_{ijgh} \left(\delta_{gk} \delta_{hl} - \frac{\partial \chi_g^{kl}(y)}{\partial y_h} \right) \frac{\partial u_k^0}{\partial x_l} + f_i \right] = 0. \quad (3.23)$$

Let us denote that

$$a_{ijkl}^0 = M \left[\frac{\partial}{\partial y_j} a_{ijgh} \left(\delta_{gk} \delta_{hl} - \frac{\partial \chi_g^{kl}(y)}{\partial y_h} \right) \right]. \quad (3.24)$$

The equation (3.23) we can then describe in the form

$$\frac{\partial}{\partial x_j} \left(a_{ijkl}^0 \frac{\partial u_k^0}{\partial x_l} \right) + f_i = 0.$$

From equation (3.13) we obtain

$$a_{ijkl}^0 \frac{\partial u_k^0}{\partial x_l} n_j = p_i \quad \text{on } \Gamma_\tau.$$

Definition 3.2.2 *The problem*

$$\frac{\partial}{\partial x_j} \left(a_{ijkl}^0 \frac{\partial u_k^0}{\partial x_l} \right) + f_i = 0 \quad \text{in } \Omega, \quad (3.25)$$

$$\begin{aligned} a_{ijkl}^0 \frac{\partial u_k^0}{\partial x_l} n_j &= p_i && \text{on } \Gamma_\tau, \\ u_i^0 &= U_i && \text{on } \Gamma_u \end{aligned} \quad (3.26)$$

for $i = 1, 2, 3$, where coefficients a_{ijkl}^0 are of the form (3.24) and functions $\chi \in [W_{per}^{1,2}(Y)]^3$ satisfy equations (3.22), is called the problem homogenized in consideration to the original problem. For functions χ^{kl} symmetry $\chi^{kl} = \chi^{lk}$ holds.

We changed the problem with periodic coefficients of elasticity a_{ijkl}^ϵ to the problem with constant (homogenized) coefficients a_{ijkl}^0 . For homogenized coefficients the condition of symmetry holds and they are bounded, this mean that

$$\begin{aligned} a_{ijkl}^0 &= a_{klij}^0 = a_{jikl}^0 = a_{ijlk}^0, \\ m &\leq \frac{a_{ijkl}^0 \xi_{ij} \xi_{kl}}{\|\xi\|^2} \leq M < +\infty \end{aligned}$$

for any symmetric matrix $\xi_{ij} \in R^3$ and positive constants m, M .

3.3 The introduction of functions $\tilde{\chi}^{kl}$

We must know the derivations of functions χ^{kl} in order to compute homogenized coefficients a_{ijkl}^0 . Then we compute homogenized coefficients by numerical integration from equation (3.24). We know that functions χ^{kl} are unique in space $[W_{per}^{1,2}(Y)]^3$ except that an additive constant and the relation

$$\frac{\partial}{\partial y_j} \left[a_{ijgh} (y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \right] = 0$$

holds. Let us multiply this relation by any function $\varphi_i \in [W_{per}^{1,2}(Y)]^3$ and integrate:

$$\int_Y \frac{\partial}{\partial y_j} \left[a_{ijgh} (y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \right] \varphi_i dV = 0 \quad \forall \varphi \in [W_{per}^{1,2}(Y)]^3. \quad (3.27)$$

Let Y_i be subdomains of interval Y in the sense that there are given various materials. Let's denote a_{ijkl}^m functions a_{ijkl}^0 in subdomain Y_m . The number of materials is n . After multiplying (3.27) for individual subintervals Y_i , we obtain

$$\sum_{m=1}^n \int_{Y_m} \frac{\partial}{\partial y_j} \left[a_{ijgh}^m (y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \right] \varphi_i dV = 0.$$

Now we arrange this relation for n -th subinterval Y_n by using Green's formula. Let's consider two various subdomains Y_p, Y_r . Their outer normals are different in the

direction of vectors at the meeting point and also on the opposite sides of subdomains. Thus members containing normals n (that mean integrals over the boundary ∂Y_n) will make a disturbance in resultant sum. The relation (3.22) can be rewritten into the form

$$\int_{Y_n} a_{ijgh}^n(y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \frac{\partial \varphi_i}{\partial y_j} dV = 0 \quad \forall \varphi \in [W_{per}^{1,2}(Y)]^3. \quad (3.28)$$

For every couple of subdomains Y_p, Y_r at every point of the conjunction of their closure, the relation

$$a_{ijgh}^p(y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) = a_{ijgh}^r(y) \left(\frac{\partial \chi_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \quad (3.29)$$

holds. But this formulation isn't suitable for numerical solving, problems are caused by their discretization. Equations (3.29) hold some points of the given mesh only. But for each one order we have a different number of points and also a different number of equations. The matrix of the system of equations obtained by discretization of problem (3.28) will generally not be in the square form. This problem can be solved theoretically by the choice of special mesh for all further ordering so that the number of equations is equal to the number of unknown parameters. But then finding out of the regularity of that matrix is very difficult. Therefore we will solve the following problem:

$$\int_Y \frac{\partial}{\partial y_j} \left[a_{ijgh}(y) \left(\frac{\partial \tilde{\chi}_g^{kl}(y)}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \right] \varphi_i dV = 0 \quad \forall \varphi \in [W_{per}^{1,2}(Y)]^3, \quad (3.30)$$

where $\tilde{\chi}^{kl}$ will be a suitable approximation of χ^{kl} . When we arrange it by using Green's formula, we obtain

$$\int_Y a_{ijgh} \left(\frac{\partial \tilde{\chi}_g^{kl}}{\partial y_h} - \delta_{gk} \delta_{hl} \right) \frac{\partial \varphi_i}{\partial y_j} dV = 0 \quad \forall \varphi \in [W_{per}^{1,2}(Y)]^3. \quad (3.31)$$

This problem only has one solution $\tilde{\chi}^{kl} \in [W_{per}^{1,2}(Y)]^3$. The proof is based on Lax-Milgram's lemma.

3.4 The computing of functions $\tilde{\chi}^{kl}$

We will compute functions $\tilde{\chi}^{kl}$ from the equation (3.31). Functions φ^n are taken from any base B of a certain subspace $[W_{per}^{1,2}(Y)]^3$ with a finite dimension. We look for the function $\tilde{\chi}^{kl}$ in form

$$\tilde{\chi}^{kl} = \sum_{\varphi^i \in B} \alpha_i^{kl} \varphi^i.$$

Unknown coefficients α_i^{kl} are computed from the system of linear equations

$$A\alpha_i^{kl} = b^{kl}, \quad (3.32)$$

that we obtain by using a finite element method (FEM). The matrix A and the vector of right hand sides b^{kl} have the following form:

$$(A)_{m,n} = \int_Y a_{ijgh} \frac{\partial \varphi_g^m}{\partial y_h} \frac{\partial \varphi_i^n}{\partial y_j} dV,$$

$$(b^{kl})_n = \int_Y a_{ijkl} \frac{\partial \varphi_i^n}{\partial y_j} dV \quad \text{for fixed } k, l.$$

The matrix A is the Gram's matrix, it is regular, symmetric and positive-definite.

3.5 The setting of matrix A and vector b^{kl} by FEM

To access homogenized coefficients a_{ijkl}^0 we must solve as the first the system (3.32) and compute functions $\tilde{\chi}^{kl}$ by using computed functions α^{kl} . The system of linear equations will be solved numerically, but first we must set matrix A and vector b^{kl} by using the following process.

The approximation of the domain

The domain $Y \subset R^3$ is splitting into a system of smaller cubes. Now we perform the *triangulation* of the domain. We split every cube into six tetrahedrons, which are called *finite elements*. The triangulation of the entire domain must be regular, that means any two tetrahedrons have either an empty conjunction or a common apex, common a whole edge or whole face. The regularity is guaranteed in the case of six tetrahedrons in cube. We raise the mesh of tetrahedrons $\{V_p \mid p \in N\}$, which approximates the given domain. We assume that functions a_{ijkl}^0 are constant for every element (tetrahedron).

The choice of the basis space and basis functions

Now we return to the triangulation by using tetrahedrons. To every apex (in the system of tetrahedrons), which is not on boundary of domain Y , we add three basis functions from the basis space $B \subset [W^{1,2}(Y)]^3$. These functions are linear on every tetrahedron and in every element. They are chosen to be non zero only in the set of tetrahedrons which have a common apex. If we take a certain apex, then the basis function in this apex will have only one non zero element. This element is equal to one.

The setting of the matrix of system of linear equations and of vector of right sides

To set the matrix we use the method of transformation to a basic element. This method is based on the choice of a basic element and the following transformation of other elements in that way.

Let us define the basic tetrahedron V_0 with apexes $R_1 = [1, 0, 0]$, $R_2 = [0, 1, 0]$, $R_3 = [0, 0, 0]$ and $R_4 = [0, 0, 1]$. Now we take any tetrahedron V_p with apexes

$P_i[x_i, y_i, z_i]$, $i = 1, 2, 3, 4$. Let us define the matrix of transformation

$$T = \begin{pmatrix} \bar{x}_2 & \bar{x}_3 & \bar{x}_4 \\ \bar{y}_2 & \bar{y}_3 & \bar{y}_4 \\ \bar{z}_2 & \bar{z}_3 & \bar{z}_4 \end{pmatrix},$$

where

$$\begin{aligned} \bar{x}_i &= x_i - x_1, \\ \bar{y}_i &= y_i - y_1, \\ \bar{z}_i &= z_i - z_1 \end{aligned}$$

for $i = 2, 3, 4$. Those are distances of apexes of a given tetrahedron from its the first apex. We denote J the determinan of matrix T , this means $J = \det T$. Now we want to transform the computing on element V_p to element V_0 and old variables x, y, z (we denote them s_i for $i = 1, 2, 3$ for the following considerations) to transform to a new σ_i for $i = 1, 2, 3$. Linear functions f on the tetrahedron V_p are given by values in apexes $f(P_i)$. By the linear transformation we transform function f to f_0 on the tetrahedron V_0 where are given by values $f(R_i)$. This transformation can be rewritten in the form

$$f_0 = b^T \cdot \omega,$$

where $\omega = (\sigma_1, \sigma_2, \sigma_3, 1)^T$, $b = (b_1, b_2, b_3, b_4)^T$. It must also hold on element V_p , so

$$\underbrace{\begin{pmatrix} \sigma_1 & \sigma_2 & \sigma_3 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix}}_S \cdot \underbrace{\begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}}_{b^T} = \underbrace{\begin{pmatrix} f(P_1) \\ f(P_2) \\ f(P_3) \\ f(P_4) \end{pmatrix}}_{\hat{f}}.$$

Then

$$f_0 = b^T \cdot \omega = (S^{-1} \cdot \hat{f})^T \cdot \omega.$$

Now we perform the transformation

$$\int_{V_p} a_{ijgh} \frac{\partial \varphi_g^m}{\partial y_h} \frac{\partial \varphi_i^n}{\partial y_j} dx dy dz = a_{ijgh} \cdot |J| \cdot (\hat{\varphi}_g^m)^T \cdot (S^{-1})^T \cdot \int_{V_0} \frac{\partial \omega}{\partial \sigma_k} \frac{\partial \omega^T}{\partial \sigma_l} \cdot \frac{\partial \sigma_k}{\partial s_h} \frac{\partial \sigma_l}{\partial s_j} d\sigma \cdot S^{-1} \hat{\varphi}_i^n,$$

where $\hat{\varphi}_i^n = (\varphi_i^n(P_1), \varphi_i^n(P_2), \varphi_i^n(P_3), \varphi_i^n(P_4))$. Let us denote $\frac{\partial \sigma_i}{\partial s_i} = T_{ij}^{-1}$ and there holds $\frac{\partial \omega}{\partial \sigma_k} = (0, \dots, 0, 1, 0, \dots, 0)$ with 1 at the k -th place. The integral in previous relation can be written as

$$\begin{aligned} & \int_{V_0} \frac{\partial \omega}{\partial \sigma_k} \frac{\partial \omega^T}{\partial \sigma_l} \cdot \frac{\partial \sigma_k}{\partial s_h} \frac{\partial \sigma_l}{\partial s_j} d\sigma = \int_{V_0} \frac{\partial \omega}{\partial \sigma_k} \frac{\partial \omega^T}{\partial \sigma_l} \cdot T_{kh}^{-1} \cdot T_{lj}^{-1} d\sigma = \\ & = \int_{V_0} \begin{pmatrix} T_{1h}^{-1} T_{1j}^{-1} & T_{1h}^{-1} T_{2j}^{-1} & T_{1h}^{-1} T_{3j}^{-1} \\ T_{2h}^{-1} T_{1j}^{-1} & T_{2h}^{-1} T_{2j}^{-1} & T_{2h}^{-1} T_{3j}^{-1} \\ T_{3h}^{-1} T_{1j}^{-1} & T_{3h}^{-1} T_{2j}^{-1} & T_{3h}^{-1} T_{3j}^{-1} \\ 0 & 0 & 0 \end{pmatrix} d\sigma = \int_{V_0} B_{hj} d\sigma = \frac{1}{6} B_{hj}. \end{aligned}$$

If we denote

$$K_{hj} = \frac{|J|}{6} (S^{-1})^T B_{hj} S^{-1}$$

and

$$\hat{\varphi}^m = \left((\hat{\varphi}_1^m)^T, (\hat{\varphi}_2^m)^T, (\hat{\varphi}_3^m)^T \right)^T,$$

then we will be able to write

$$(A)_{m,n} = (\hat{\varphi}^m)^T \cdot \underbrace{\begin{pmatrix} a_{1j1h}K_{hj} & a_{1j2h}K_{hj} & a_{1j3h}K_{hj} \\ a_{2j1h}K_{hj} & a_{2j2h}K_{hj} & a_{2j3h}K_{hj} \\ a_{3j1h}K_{hj} & a_{3j2h}K_{hj} & a_{3j3h}K_{hj} \end{pmatrix}}_K \cdot \hat{\varphi}^n = (\hat{\varphi}^m)^T \cdot K \cdot \hat{\varphi}^n \quad (3.33)$$

The matrix K has a size 12×12 . If at least one of functions φ^m, φ^n is equal to zero on the tetrahedron V_p , then the form (3.33) is equal to zero. If both functions φ^m, φ^n are non zero on V_p then vectors have 1 only on one place and elsewhere they are zero. If we denote a "non zero index" (the position of 1) of the vector $\hat{\varphi}^m - r_m$ and a "non zero index" of the vector $\hat{\varphi}^n - r_n$, we will get the relation for computing an elementary matrix $(A)_{m,n}$ on the basic element

$$(A)_{m,n} = \int_{V_p} a_{ijgh} \frac{\partial \varphi_g^m}{\partial y_h} \frac{\partial \varphi_i^n}{\partial y_j} dx dy dz = (K)_{r_m r_n}$$

The whole matrix A is set by the following process:

1. We prepare a zero matrix A , that means $A_{ij} = 0 \quad \forall i, j = 1, \dots, n$.
2. For every tetrahedron $V_p, p \in N$ from a mesh we set an auxiliary matrix K .
3. For every couple of functions φ^m, φ^n that are non zero on a given tetrahedron we find numbers r_m and r_n .
4. We set the corresponding elements to the resultant matrix A :

$$(A)_{r_m, r_n} = (A)_{r_m, r_n} + (K)_{r_m, r_n}.$$

The vector on the right hand side b^{kl} is set by an analogical process. The relation for the computing of b^{kl} on the element V_p is transformed to the basic element V_0 :

$$(b^{kl})_n = \int_{V_p} a_{ijkl} \frac{\partial \varphi_i^n}{\partial y_j} dx dy dz = \frac{|J|}{6} (\hat{\varphi}^n)^T \cdot v^{kl},$$

where

$$v^{kl} = (a_{1jkl}, a_{2jkl}, a_{3jkl}) \cdot (S^{-1})^T (T_{1j}^{-1}, T_{2j}^{-1}, T_{3j}^{-1}, 0)^T.$$

If the function φ^n is non zero on the tetrahedron V_p , then the vector $\hat{\varphi}^n$ has 1 only at one position and elsewhere is zero. This nonzero position is denoted by r . It holds

that $(\hat{\varphi}^n)_r = 1$. We add $\frac{|J|}{6} (v^{kl})_r$ to the n -th element of the resultant vector on the right hand side b^{kl} , that means

$$(b^{kl})_n = (b^{kl})_n + \frac{|J|}{6} (v^{kl})_r.$$

Further, we solve the system of linear equations $A\alpha^{kl} = b^{kl}$ by using a numerical method.

3.6 The computing of homogenized coefficients

The domain Y is composited from finite number of subdomains Y_i with Lipschitz boundaries. The material is considered Y -periodic. We assume that we already have computed coefficients α^{kl} by using the FEM. Now we choose the mesh of points, we make the corresponding space of basis functions B and we computed values of functions $\bar{\chi}^{kl}$ at points of the mesh. Last we approximate derivations of functions $\bar{\chi}^{kl}$ by using computed function values. The average of the biggest cube of the mesh is denoted h .

Functions $\bar{\chi}^{kl}$ are generally non continuous on cubes which are on the boundary of two different subdomains Y_m, Y_n . Therefore we can not approximate well their derivations from function values there. The set of all those elements is denoted M_1 . Its volume measure is of order h .

Further, we denote M_2 the set of all cubes which have at least one face is merged to Y , because functions $\bar{\chi}^{kl}$ are very different than functions χ^{kl} . The volume measure of M_2 is of order h too.

Functions $\bar{\chi}^{kl}$ have continuous second derivations on the set $Y \setminus (M_1 \cup M_2)$. Therefore we can approximate the first derivations $\bar{\chi}^{kl}$ by linear functions from the space B with the error of order h . Homogenized coefficients a_{ijkl}^H are computed by using the numerical integration

$$a_{ijkl}^H = \int_{Y \setminus (M_1 \cup M_2)} a_{ijgh} \left(\delta_{gk} \delta_{hl} - \frac{\partial \bar{\chi}^{kl}}{\partial y_h} \right) dV.$$

Because the integrated function is computed with error of order h and the volume measure of $(M_1 \cup M_2)$ is also of order h , computed homogenized coefficients a_{ijkl}^H convert to real values a_{ijkl}^0 with error of order h .

4 Conclusion

We described a mathematical model and by the means of it we can compute the field of stress and deformation inside of any material. We formulated the problem of linear elasticity for the anisotropic nonhomogeneous material. But the solution of this problem is difficult. Therefore, we described the method of homogenization that transforms a generally nonhomogeneous material to material that is piecewise homogeneous.

The structure of the material is described by Hook's coefficients of elasticity. By the method of homogenization we transform general coefficients to coefficients homogenized. Such recomputed coefficients can be set to the problem of elasticity. This problem can be solved by the FEM, by finding the minimum of the potential energy functional. This leads to the solving of the system of linear equations. Systems of linear equation, which arise from those problem, can be solved by the conjugate gradient method in the case of homogenization (the matrix has a small number of nonzero elements) or by the preconditioned conjugate gradient method in the case of an elasticity problem.