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Effective properties of optimized composites

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***Abstract*—Homogenization and shape optimization of fibers in a composite structure has been solved by many authors mostly by means of FEM. In this paper a new procedure for homogenization of composites is proposed, based on the idea of Hashin bounds, leading to combination BEM-FEM approach, which seems to be promising right to applications to composites.**

***Keywords*—Composites, effective properties, combination FEM-BEM, homogenization, optimization**

I. Introduction

Conventionally, the optimal shape design problem consists of minimization of an appropriate cost functional with certain constraints, such as equilibrium and compatibility conditions and design requirements. One of a reasonable and practical form of the cost functional respects the minimization of the strain energy of the body subject to a specific load.

The formulation is naturally connected with finite element method, which starts with energy formulation. On the other hand combination of finite and boundary elements seems to be more suitable for such problems.

Advantages of the boundary element method in solving shape optimization are obvious from formulations presented in paper [1]. The way on how to formulate the localization and concentration factors in terms of the boundary integrals the idea of the Hashin-Shtrikman variational principles, [2] is used and developed in this paper.

Since we are concentrated on optimization of composite structures using homogenization, the theory for periodic media given by Suquet, [3] is fully utilized in this paper. The trick presented in [4] is also used in the optimization problem.

II. Homogenization

The unit cell is considered, as described in Fig. 1. This unit cell is cut out of the composite and periodic boundary conditions are applied, according to [3].

The elasticity system (equilibrium equations, kinematical conditions and Hooke's law) is defined in Ω as:

$$\operatorname{div}\boldsymbol{\sigma}(\boldsymbol{y}) = 0, \boldsymbol{\sigma}(\boldsymbol{y}) = \boldsymbol{L}(\boldsymbol{y}) : \boldsymbol{\varepsilon}(\boldsymbol{y}), \boldsymbol{\varepsilon} = \frac{1}{2}(\nabla\boldsymbol{u} + \nabla^{\mathrm{T}}\boldsymbol{u}) \qquad (1)$$

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and periodic boundary conditions along the boundary of the unit cell $\partial\Omega$ are given, see [3]. Stress $\boldsymbol{\sigma}$, strain $\boldsymbol{\varepsilon}$ and displacement $\boldsymbol{u}$ are to be determined, $\nabla$is nabla operator.

The geometry and denotation is seen from Fig. 1. The shaded area is considered in the next computation, because of symmetry.

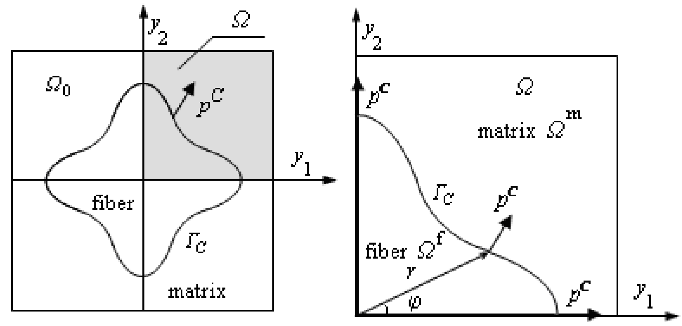

Fig. 1: Geometry and denotation of the unit cell

Localization consists of the solution of system of elasticity equations on the representative volume element (or unit cell) for concentration factors $\boldsymbol{A}^{\mathrm{f}}$ of fibers and $\boldsymbol{A}^{\mathrm{m}}$ for matrix:

$$\varepsilon^{\mathrm{f}}_{ij}(\boldsymbol{u}) = A^{\mathrm{f}}_{ijkl}E_{kl}, \boldsymbol{y}\in\Omega^{\mathrm{f}}\, \varepsilon^{\mathrm{m}}_{ij}(\boldsymbol{u}) = A^{\mathrm{m}}_{ijkl}E_{kl}, \boldsymbol{y}\in\Omega^{\mathrm{m}} \qquad (2)$$

The local strain tensor $\boldsymbol{\varepsilon}(\boldsymbol{u})$ is split into its average $\boldsymbol{E}$ and a fluctuating term $\boldsymbol{\varepsilon}^*(\boldsymbol{u})$ as:

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \boldsymbol{E} + \boldsymbol{\varepsilon}^*(\boldsymbol{u}), \quad \boldsymbol{\varepsilon}^*(\boldsymbol{u}) = \boldsymbol{\varepsilon}(\boldsymbol{u}^*), \quad <\boldsymbol{\varepsilon}(\boldsymbol{u}^*)>= 0 \qquad (3)$$

The fluctuating displacement $\boldsymbol{u}^*$ may be considered a *periodic field*, up to a rigid displacement that will be disregarded.

Under the above described circumstances Hill's energy condition holds valid, as proved, e.g., by Suquet, [3]:

$$<\sigma_{ij}(\boldsymbol{y})\varepsilon_{ij}(\boldsymbol{y})>= S_{ij}E_{ij} \qquad (4)$$

Using (2), (3) and (4) the components of the overall stresses S_{ij} are written in relation to the overall strains E_{ij} as:

$$\begin{aligned} S_{ij} &=< \sigma_{ij}(\boldsymbol{y})>= L^*_{ijkl}E_{kl} =< L_{ijkl}(\boldsymbol{y})\varepsilon_{kl}(\boldsymbol{y})>= \\ &= (< L^{\mathrm{f}}_{ijkl}A^{\mathrm{f}}_{kl\alpha\beta}(\boldsymbol{y})>_{\mathrm{f}} + < L^{\mathrm{m}}_{ijkl}A^{\mathrm{m}}_{kl\alpha\beta}(\boldsymbol{y})>_{\mathrm{m}})E_{\alpha\beta} \end{aligned} \qquad (5)$$

where $<.>_{\mathrm{f}}$ stands for the average on fiber and $<.>_{\mathrm{m}}$ is the average on matrix, . This averaging process is made in such a way that the integrals are taken over fiber and matrix, respectively, and meas $\Omega = 1$ and $\boldsymbol{L}^*$ is the homogenized stiffness.

III. Localization

In the first step, the unit cell obeys static equilibrium equations and linear homogeneous Hooke's law (homogeneous and isotropic medium):

$$\sigma^0_{ij} = L^0_{ijkl}\varepsilon^0_{kl}, \text{ in } \Omega, \qquad (6)$$

and the boundary conditions at the concrete state. L^0_{ijkl} are components of not yet determined material stiffness matrix (stiffness tensor). These components will be stated later. Such a medium is called comparative one.

The solution of (6) is easy, as the comparative medium is homogeneous and isotropic:

$$u_i^0 = E_{ij} y_j, \varepsilon_{ij}^0 = E_{ij} \text{ in } \Omega, \text{ and boundary conditions on } \partial\Omega \quad (7)$$

In the second step a geometrically identical unit cell is considered. Also the loading and boundary conditions on $\partial\Omega$ remain valid. Define

$$\begin{aligned} \bar{u}_i &= u_i - u_i^0 = u_i - E_{ij} y_j, \quad \bar{\varepsilon}_{ij} = \varepsilon_{ij} - \varepsilon_{ij}^0 = \varepsilon_{ij} - E_{ij}, \\ \bar{\sigma}_{ij} &= \sigma_{ij} - \sigma_{ij}^0 = \sigma_{ij} - L_{ijkl}^0 E_{kl} \quad \text{in } \Omega \end{aligned} \quad (7)$$

Our next aim is to determine primed quantities, components of displacement vector $\bar{u}_i$ and components of strain and stress tensors $\bar{\varepsilon}_{ij}$ and $\bar{\sigma}_{ij}$. In order to do so, system (1) has to be formulated for the primed set. We start with Hooke's law, which is valid for heterogeneous medium:

$$\sigma_{ij}(\boldsymbol{y}) = L_{ijkl}(\boldsymbol{y})\varepsilon_{kl}(\boldsymbol{y}) = L_{ijkl}^0 \varepsilon_{kl}(\boldsymbol{y}) + \tau_{ij}(\boldsymbol{y}) \quad \text{in } \Omega \quad (8)$$

where τ_{ij} are components of polarization tensor and the direct relation between stresses and strains becomes homogeneous and isotropic, so that integral formulation of elastic problem may be formulated.

Since the material stiffness tensor appears to be non-homogeneous and anisotropic, idea used in [2], will be adapted here. From (8) it follows immediately

$$\tau_{ij} = [L_{ijkl}]\varepsilon_{kl}, \qquad [L_{ijkl}] = L_{ijkl} - L_{ijkl}^0 \quad (9)$$

which can be considered a definition of polarization tensor. Moreover, a transformation to the primed system will not disturb the direct relation stresses – strains, as after substituting (9) to (7_3) gives:

$$\begin{aligned} \bar{\sigma}_{ij} &= \sigma_{ij} - \sigma_{ij}^0 = L_{ijkl}^0 \varepsilon_{kl} + \tau_{ij} - \sigma_{ij}^0 = \\ &= L_{ijkl}^0 \varepsilon_{kl} + \tau_{ij} - L_{ijkl}^0 E_{kl} = L_{ijkl}^0 \bar{\varepsilon}_{kl} + \tau_{ij} \end{aligned} \quad (10)$$

Since both σ_{ij} and σ_{ij}^0 are statically admissible, it holds (the following equations must be defined in the sense of distributions):

$$\frac{\partial(L_{ijkl}^0 \bar{\varepsilon}_{kl} + \tau_{ij})}{\partial y_j} = 0 \text{ in } \Omega, \ \bar{s}_i = s_i - s_i^0, s_i = u_i, \text{or } p_i \ \ \partial\Omega \quad (11)$$

Owing to constant distribution of L_{ijkl}^0 in Ω, the equivalent integral formulation can be written as:

$$\begin{aligned} \bar{u}_m(\boldsymbol{\xi}) &= \int_{\partial\Omega} p_{mi}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{u}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) - \int_{\partial\Omega} u_{mi}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{p}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) + \\ &+ \left([L_{ijkl}^{\mathrm{f}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{f}}} + [L_{ijkl}^{\mathrm{m}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{m}}} \right) \varepsilon_{mij}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{\varepsilon}_k(\boldsymbol{y})\,\mathrm{d}\Omega \\ &\qquad \boldsymbol{\xi} \in \Omega \end{aligned} \quad (12)$$

$$\begin{aligned} c_{mn}(\boldsymbol{\xi})\bar{u}_n(\boldsymbol{\xi}) &= \\ &= \int_{\partial\Omega} p_{mi}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{u}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) - \int_{\partial\Omega} u_{mi}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{p}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) + \\ &+ \left([L_{ijkl}^{\mathrm{f}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{f}}} + [L_{ijkl}^{\mathrm{m}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{m}}} \right) \sigma_{mij}^*(\boldsymbol{y},\boldsymbol{\xi})\bar{\varepsilon}_k(\boldsymbol{y})\,\mathrm{d}\Omega \\ &\qquad \boldsymbol{\xi} \in \partial\Omega \end{aligned} \quad (13)$$

where c_{mn} are components of a tensor depending on position $\boldsymbol{\xi} \in \partial\Omega$ and the quantities with asterisks are given kernels.

Differentiating (12) by ξ_n and putting $\boldsymbol{\xi} \in \partial\Omega$ provides

$$\begin{aligned} \bar{\varepsilon}_{mn}(\boldsymbol{\xi}) &= \int_{\partial\Omega} P_{mi}^*(\boldsymbol{y},\xi)\bar{u}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) - \int_{\partial\Omega} U_{mi}^*(\boldsymbol{y},\xi)\bar{p}_i(\boldsymbol{y})\,\mathrm{d}\gamma(\boldsymbol{y}) + \\ &+ \left(\left([L_{ijkl}^{\mathrm{f}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{f}}} + [L_{ijkl}^{\mathrm{m}} - L_{ijkl}^0] \int_{\Omega^{\mathrm{m}}} \right)\right) \Sigma_{mij}^*(\boldsymbol{y},\xi)\bar{\varepsilon}_k(\boldsymbol{y})\,\mathrm{d}\Omega + \\ &+ \text{convected term} \end{aligned} \quad (14)$$

First, let $L_{ijkl}^0 \equiv L_{ijkl}^{\mathrm{f}}$. Eliminating unknown boundary values from (13) obtain the relation

$$\varepsilon_{mn}^{\mathrm{m}}(\bar{\boldsymbol{u}}(\boldsymbol{y})) = \chi_{mnkl}^{\mathrm{m}}(\boldsymbol{y}))E_{kl}, \ \varepsilon_{mn}^{\mathrm{f}}(\bar{\boldsymbol{u}}(\boldsymbol{y})) = \chi_{mnkl}^{\mathrm{f}}(\boldsymbol{y}))E_{kl} \quad (15)$$

if $L_{ijkl}^0 \equiv L_{ijkl}^{\mathrm{m}}$. This process leads us to a fourth-order "concentration factor tensor" $\boldsymbol{A}$ defined as

$$\varepsilon_{mn}^p(\boldsymbol{u}(\boldsymbol{y})) = [\boldsymbol{I}_{\boldsymbol{mnkl}} + \chi_{mnkl}^{\boldsymbol{p}}(\boldsymbol{y})]E_{kl} = A_{mnkl}^p E_{kl} \quad (16)$$

where the superscript $p \equiv \mathrm{f}$ holds for $y \in \Omega^{\mathrm{f}}$ and $p \equiv \mathrm{m}$ for $y \in \Omega^{\mathrm{m}}$. Since it obviously holds

$$< A_{mnkl}^{\mathrm{f}} >_{\mathrm{f}} + < A_{mnkl}^{\mathrm{m}} >_{\mathrm{m}} = I_{mnkl} \quad (17)$$

one does not need to compute both concentration factors. It is sufficient to draw concentration, say, on fiber, when dealing with concrete composites (the fiber ratio is very small), or on matrix, if the matrix volume ratio is large and the material behavior of stresses on matrix is almost uniformly distributed.

IV. Optimization

A natural question for engineers dealing with composites could be: determine such shape of fibers that the bearing capacity of the entire composite structure increases and attains its maximum. This is a problem of optimal shape of structures and can be formulated for composites as follows: Let the uniform strain field E_{kl} be applied to the domain Ω (in our case, a periodic distribution of fibers is considered). This produces concentration factors A_{mnkl}^{f} and A_{mnkl}^{m}, obeying (16,17). Let $\Pi(\boldsymbol{A}^{\mathrm{f}}, \boldsymbol{A}^{\mathrm{m}}, \Omega)$ be a real functional of A_{mnkl}^{f}, A_{mnkl}^{m} and Ω. The problem of optimal shape consists of finding such a domain Ω^{f} from a class O of admissible domains, which minimizes Π. This may symbolically be written as

$$\text{Minimum}\ \{\ \Pi(\boldsymbol{A}^{\mathrm{f}}, \boldsymbol{A}^{\mathrm{m}}, \Omega^{\mathrm{f}})\ ;\ B(\boldsymbol{u}, \Omega^{\mathrm{f}}) = \boldsymbol{0}\} \tag{18}$$

where B is an operator which for each Ω^{f} from O uniquely determines the displacement field $\boldsymbol{u}$ (in our case, this is the system of equations (1)).

The (19) problem may be formulated in terms of minimum Lagranigian. In order to ensure the correctness of this formulation, additional constraints have to be applied. In our case, the constant volume of fibers is assumed. Hence, the admissible set is defined as

$$O = \{\Omega^{\mathrm{f}}\ ; \text{meas}\ \Omega = C, \ \ \text{the fiber fully lays in the unit cell}\}$$

where C is the fiber area ratio.

It remains to state the shape parameters $\boldsymbol{p}$ identifying the change of the boundary of fiber. A natural choice is a movement of the boundary Γ_C. The Lagrangian involving the side condition using the Lagrangian multiplier is written as:

$$\begin{aligned}\Pi(\boldsymbol{u}, \Omega^{\mathrm{f}}) &= \frac{1}{2}\int_{\Omega} \sigma_{ij}(\boldsymbol{y})\varepsilon_{\boldsymbol{ij}}(\boldsymbol{y})\, \mathrm{d}\Omega + \lambda\Big(\int_{\Omega^f} \mathrm{d}\Omega^{\mathrm{f}} - C\Big) = \\ &= \frac{1}{2} S_{ij} E_{ij} + \lambda\Big(\int_{\Omega^f} \mathrm{d}\Omega^{\mathrm{f}} - C\Big)\end{aligned} \tag{19}$$

owing to Hill's energy condition (4). Coefficient λ is the Lagrangian multiplier. Substituting (5) to (20) gives:

$$\begin{aligned}\Pi(\boldsymbol{u}, \Omega^{\mathrm{f}}) = \frac{1}{2}[L^{\mathrm{f}}_{ijkl} < A(\boldsymbol{p})^{\mathrm{f}}_{kl\alpha\beta}(\boldsymbol{y}) >_{\mathrm{f}} + L^{\mathrm{m}}_{ijkl} < A(\boldsymbol{p})^{\mathrm{m}}_{kl\alpha\beta}(\boldsymbol{y}) >_{\mathrm{m}}] \times \\ \times E_{ij} E_{\alpha\beta} + \lambda\Big(\int_{\Omega^f} \mathrm{d}\Omega^{\mathrm{f}} - C\Big)\end{aligned} \tag{20}$$

and only the concentration factors are dependant of the vector $\boldsymbol{p}$.

Let us suppose that $A^{\mathrm{f}}_{kl\alpha\beta}$ is very precisely determined by the procedure described in section III. Hence, using (5), (17) and (18), (21) will be simplified as:

$$\begin{aligned}\Pi(\boldsymbol{u}, \Omega^{\mathrm{f}}) = \frac{1}{2}[(L^{\mathrm{f}}_{ijkl} - L^{\mathrm{m}}_{ijkl}) < A^{\mathrm{f}}_{kl\alpha\beta}(\boldsymbol{p})(\boldsymbol{y}) >_{\mathrm{f}} + L^{\mathrm{m}}_{ij\alpha\beta}] \times \\ \times E_{ij} E_{\alpha\beta} + \lambda\Big(\int_{\Omega^f} \mathrm{d}\Omega - C\Big)\end{aligned} \tag{21}$$

Our aim will now be to formulate the domain Ω^{f} by means of its corresponding boundary. This can be done in many ways. For example, suppose that the shape of the fiber under study is a polygon. One can choose some fixed point P (pole - in our case this is the origin of the coordinate system) and connect it with each vertex of this polygonal boundary. In this way we obtain N triangles T_k, $k = 1,...,N$, where $N + 1$ is the number of vertices. Since $\int_{\Omega^f} \mathrm{d}\Omega = \text{meas}\ \Omega^{\mathrm{f}}$, meas Ω^{f} is:

$$\text{meas}\ \Omega^{\mathrm{f}} = \sum_{k=1}^{N} \text{meas}\ T_k \tag{22}$$

where meas Ω^{f} or meas T_k stands for the measure of Ω^{f} or algebraic measure of T_k , respectively.

The situation is described in Fig. 2. In order to determine the area of the domain, it is easy to calculate the area of one arbitrary triangle T_k .

One rule has to be obeyed: the first vertex is the pole, the second vertex and the third have to hold the order of nodal points on the boundary of the domain, in our case the order of points is anticlockwise. Hence, the triangles denoted in Fig. 2 by thick line are added and that denoted by thin line are subtracted.

The stationary requirement leads to differentiation of the functional by the shape (design) parameters p_s

$$\begin{aligned}\frac{\partial \Pi(\boldsymbol{u}, \Omega)}{\partial p_s} = \frac{1}{2}[L^{\mathrm{f}}_{ijkl} < \frac{\partial A^{\mathrm{f}}_{kl\alpha\beta}(\boldsymbol{p})}{\partial p_s} >_{\mathrm{f}} + \\ + L^{\mathrm{m}}_{ijkl} < \frac{\partial A^{\mathrm{m}}_{kl\alpha\beta}(\boldsymbol{p})}{\partial p_s} >_{\mathrm{m}}] E_{ij} E_{\alpha\beta} + \lambda \frac{\partial}{\partial p_s} \int_{\Omega^{\mathrm{f}}} \mathrm{d}\Omega = 0\end{aligned} \tag{23}$$

which can be rewritten as:

$$E_s + \lambda = 0, \quad s = 1, 2, \ldots, n \tag{24}$$

where

$$\lambda = -\frac{\frac{1}{2}[L^{\mathrm{f}}_{ijkl} < \frac{\partial A^{\mathrm{f}}_{kl\alpha\beta}(\boldsymbol{p})}{\partial p_s} >_{\mathrm{f}} + L^{\mathrm{m}}_{ijkl} < \frac{\partial A^{\mathrm{m}}_{kl\alpha\beta}(\boldsymbol{p})}{\partial p_s} >_{\mathrm{m}}] E_{ij} E_{\alpha\beta}}{\frac{\partial}{\partial p_s} \int_{\Omega^{\mathrm{f}}} \mathrm{d}\Omega}$$

for each s =1,…,n

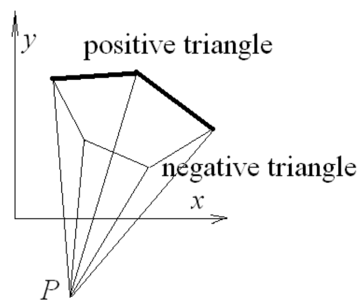

Fig. 2: Calculation of the area of domain Ω^{f}

If p_s, s = 1,...,n is claimed as the distances of the origin from the current boundary of the fiber, E_s corresponds to the strain energy density at the point of the interfacial boundary, in our case at the nodal point ξ_s . The equation (24) requires E_s to have the same value for any s. In other words, if the strain energy density were the same at any point on the "moving" part of the boundary, the optimal shape of the trial body would be reached. For this reason, the body of the structure should increase its area (in 3D its volume) at the nodal point ξ_s of the boundary, if E_s is larger than the true value of -λ , while it should decrease its value when E_s is smaller than the correct $-\lambda$. As, most probably, we will not know the real value $-\lambda$ in advance; we estimate it from the average of the current values at the nodal points.

Since E_s, prove large differences in their values, logarithmic scale was proposed by Tada, Seguchi and Soh, [5]. The computational procedure follows this idea.

Differentiating by λ completes the system of Euler's equations:

$$\sum_{s=1}^{n} \text{meas } T_s = C \qquad (26)$$

Unit cell is considered with various fiber volume ratios. Since we compare energy densities at nodal points of the interfacial boundary, the relative energy density may be regarded as the comparative quantity influencing the movement of the boundary Γ_C. As said in the previous section, the higher value of this energy, the larger movement of the nodal point of Γ_C should aim at the optimum. The process of iterations will end if the Euclidean distance between current and previous energies be less then given admissible error.

In the following examples various combinations of stiffnesses of fiber and matrix is contemplated. Denote by $c_{\text{f}} = \text{meas }\Omega^{\text{f}}$ the area fraction of fiber and by $c_{\text{m}} = \text{meas }\Omega^{\text{m}}$ the area fraction of matrix. One phase possesses the material properties: Modulus of elasticity of fiber E^{f} = 210000 kN/ m^2 and that of matrix E^{m} = 180000 kN/ m^2, while Poisson's ratio of fiber ν^{f} =0.18 and ν^{m} = 0.3 is Poisson's ratio of matrix.

In the first numerical test it is: $c_{\text{f}} = 40\%$, $c_{\text{m}} = 60\%$, and the relative error is 3.8e-04 after twenty seven iterations using the step of iteration 0.1. The result is depicted in Fig. 3. In Fig. 4 the area ratios are as $c_{\text{f}} = 60\%$, $c_{\text{m}} = 40\%$ and the relative error is 3.3e-04 after thirty iterations using the step of iteration 0.1. The previous cases have not required respecting any restrictions on the length of beams.

In the last examples the same area fractions are accepted as in the first case (results in Fig. 5) and in the second case (Fig. 6), but the material properties are interchanged, the fiber is weaker than matrix. The approach have to involve the local iteration, as the beams are bounded by 0.05 from the external boundary $\partial\Omega$. The relative error is in the first case equal to 2.57e-03 after thirty five iterations using the step of iteration 0.1. The result is seen in Fig. 5. Fig. 6 shows the results from the same constellation as before (weak matrix, fiber and matrix area ratios interchanged, bounded beams requiring the local iteration). The error is 2.51e-2 after thirty six iterations.

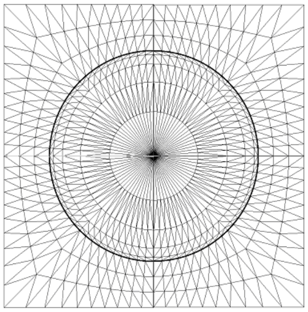

Fig. 3: First case

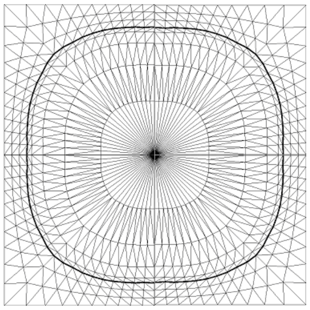

Fig. 4: Second case

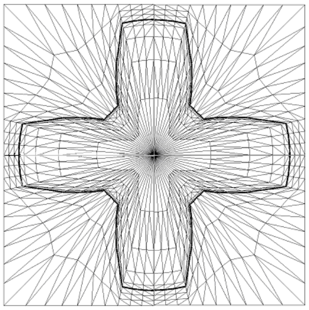

Fig. 5: First case

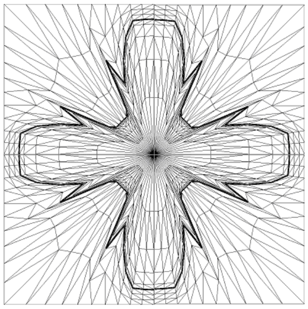

Fig. 6: Second case

The results show certain shapes of fibers which can be used in practice. The last case only shows possible direction on how to construct fiber, and while the previous cases are quite reasonable the last case is more or less scholar.

Acknowledgment

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