Shape optimization of composites using the BEM

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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 the FEM. In this paper a new procedure for homogenization of composites is proposed. This is based on the BEM, which seems to be more efficient and more accurate in applications than the FEM solution. Special properties of the distribution of stresses (or concentration factors) on a unit cell are used. Averaging process including integration over the unit cell, particularly in the case of fiber reinforced concrete (when the fiber ratio is relatively small) follows the fact that the stresses "relax" on the matrix and their distribution converges to constant except for a zone being in the vicinity of the fiber–matrix interfacial surface. This is why boundary element method is more suitable than finite element method, particularly in problems concerning fiber reinforced concretes.

A comparison medium is employed and the jump in material properties is involved in integral form, Procházka, Šejnoha². Hence, no Eshelby forces have to be applied along the interface fiber–matrix, Suquet³. Then, inverse variational principles, Procházka² (including variation of the domain of fiber under subsidiary condition that the volume of the fiber is fixed), may be used and the mechanical behavior on the interface fiber–matrix is more viewable during the iteration process solving this strictly nonlinear problem).

From the point of view of numerical solution, two basic steps will be observed:

1 the homogenization (periodic medium),
2 the optimization strategy (inverse variational problems).

1 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. The formulation of the cost functional depends on the concrete intention of a designer. One of a reasonable and practical form of the cost functional respects the minimization of the strain energy of the body subjected to a specific load. Such a problem can easily be formulated in terms of inverse variational principles.

Inverse variational principles are naturally connected with finite element method, as shown by Tada, Seguchi & Soh. But, the FEM is less suitable for the problems involving the optimal shape of boundary because of the division (in any case compulsory when using the FEM) of the domain, while boundary element method (the BEM) seems to be more suitable for such problems. On the other hand, the direct connection of the BEM with the variational principles is not seen at first sight and desires a deeper study.

2 Homogenization of periodic structures

Localization and homogenization is concisely described in Suquet. Recall some basic consumptions which we use later in the integral formulation.

First, we denote quantities used in this text. Two different scales will naturally be introduced. The macroscopic scale, the homogeneous law in which is sought, will be described in coordinate system $x \equiv \{x_1, x_2, x_3\}$ and the microscopic scale – heterogeneous – is characterized in the system of coordinates $y \equiv \{y_1, y_2, y_3\}$. The medium is generally heterogeneous, but locally – in the microscopic scale – is assumed to be periodic, thus a representative volume element may be cut out from the structure and the periodicity conditions can be introduced on the boundary of this element. The idea is illustrated in Fig. 1, which is copied from Suquet. Author of this paper is convinced that this picture describes the philosophy of micro- and macro levels in an outstanding way.

Let us distinguish the quantities under study in dependence of the macroscopic or microscopic scale in the following manner: The displacements in the macroscopic level will be denoted as $U \equiv \{U_1, U_2, U_3\}$ while in the microscopic level as $u \equiv \{u_1, u_2, u_3\}$. Moreover, in macroscopic level, let us denote strains as $E \equiv E_{ij}, i, j = 1, 2, 3$ and stresses as $S \equiv S_{ij}, i, j = 1, 2, 3$. In the microscopic level let us denote strains as $\varepsilon \equiv \varepsilon_{ij}, i, j = 1, 2, 3$ and strains as $\sigma \equiv \sigma_{ij}, i, j = 1, 2, 3$. Also define the microscopic-macroscopic relation of the averaged stresses and strains by

$$S_{ij} = \frac{1}{\text{meas } \Omega} \int_{\Omega} \sigma_{ij} \, d\Omega(y) = <\sigma_{ij}>,$$

$$E_{ij} = \frac{1}{\text{meas } \Omega} \int_{\Omega} \varepsilon_{ij} \, d\Omega(y) = <\varepsilon_{ij}>,$$ (1)
where \(<.>\) stands for the average, \(\Omega\) is the representative volume element, and \(\text{meas } \Omega\) is its volume, \(\Omega = \Omega^f \cup \Omega^m\), where respectively \(\Omega^f\) describes the domains adjacent to fiber and \(\Omega^m\) adjacent to matrix.

Localization consists of the solution of system of equilibrium equations on the representative volume element (or unit cell) for concentration factors \(A^f\) and \(A^m\):

\[
\epsilon_{ij}^f(u(y)) = A_{ijkl}^f(u(y)) E_{kl}, \quad y \in \Omega^f, \\
\epsilon_{ij}^m(u(y)) = A_{ijkl}^m(u(y)) E_{kl}, \quad y \in \Omega^m.
\] (2)

Denoting the boundary of the representative volume element (we rather use unit cell) by \(\partial \Omega\), the periodic boundary conditions will be employed on \(\partial \Omega\) (\(n = \{n_1, n_2, n_3\}\) is unit outward normal to \(\Gamma\) with respect to fiber \(\Omega^f\), see Fig. 2):

- stress: \(p_i = \sigma_{ij}n_j\) are opposite on the opposite sides, \(n_j\) is the \(j\)-th component of the unit outward normal,
- strains: the local strain \(\epsilon(u)\) is split into its average and a fluctuating term \(\tilde{\epsilon}\) as:

\[
\epsilon(u) = E + \epsilon(\tilde{u}) = E + \tilde{\epsilon}, \quad <\epsilon(\tilde{u})> = 0.
\] (3)

The fluctuating displacement \(\tilde{u}\) may be considered as a periodic field, up to a rigid displacement that will be disregarded.
Eq. (3) obeys the Hill’s energy condition, as proved, e. g., by Suquet:

\[ < \sigma_{ij} \varepsilon_{ij} > = S_{ij} E_{ij} \quad (4) \]

Using (2) we write:

\[ S_{ij} = < \sigma_{ij}(y) > = < L_{ijkl}(y) \varepsilon_{kl}(u(y)) > = \]

\[ = \left( < L_{ijkl}^f(y) A_{k\alpha\beta}^f(y) >_f + < L_{ijkl}^m(y) A_{k\alpha\beta}^m(y) >_m \right) E_{\alpha\beta} \quad (5) \]

where \(< \cdot >_f\) stand for average on fiber and \(< \cdot >_m\) is the average on matrix. This averaging process is made in such a way that the integrals are taken over fiber and matrix, respectively, but the denominator remains meas \( \Omega \), see (1).

By definition, the homogenized stiffness matrix \( L^* \) is written as:

\[ S_{ij} = L^*_{ijkl} E_{kl} \quad (6) \]

Comparing (5) and (6) the overall stiffness matrix follows as

\[ L^*_{ijkl} = L_{ijkl}^f < A_{k\alpha\beta}^f(y) >_f + L_{ijkl}^m < A_{k\alpha\beta}^m(y) >_m \quad (7) \]

It is worth noting that the homogenized stiffness matrix is symmetric with similar properties as that of the classical stiffness matrix.

3 Localization using the BEM

Without lack of generality, let us consider a symmetric unit cell, Fig. 2. The overall strain \( E_{ij} \) is given independently of location in \( \Omega \). The loading of this unit cell will be given by unit impulses of \( E_{ij} \), i.e. we successively select \( E_{i_0j_0} = E_{j_0i_0} = 1; E_{ij} = 0 \) for either \( i_0 \neq i \) or \( j_0 \neq j \).
The procedure is split into two steps. Assume the above described surface displacements to be prescribed along the entire boundary $\partial \Omega$ and there are no body forces. In the first step, the cell obeys static equilibrium equations and linear homogeneous Hooke’s law:

$$\sigma_{ij}^0 = L_{ijkl}^0 E_{kl} \text{ in } \Omega, \quad u_i^0 = E_{ij} y_j \text{ on } \partial \Omega(y),$$  \hspace{1cm} (7)

where $L_{ijkl}^0$ is the stiffness matrix (stiffness tensor) of a comparison medium. The meaning of $L^0$ will be stated later.

The solution of (7) is easy:

$$u_i^0 = E_{ij} y_j, \quad \varepsilon_{ij} = E_{ij} \text{ in } \Omega, \quad p_i^0 = \sigma_{ij}^0 n_j \text{ on } \partial \Omega.$$  

where $n = \{n_1, n_2\}$ is the unit outward normal to $\partial \Omega$.

In the second step a geometrically identical cell is considered. Define

$$\bar{u}_i = u_i - u_i^0, \quad \bar{\varepsilon}_{ij} = \varepsilon_{ij} - \varepsilon_{ij}^0, \quad \bar{\sigma}_{ij} = \sigma_{ij} - \sigma_{ij}^0 \text{ in } \Omega,$$  \hspace{1cm} (8)

The displacements $\bar{u}$, strains $\bar{\varepsilon}$ and stresses $\bar{\sigma}$ to be stated. Generalized Hooke’s law becomes:

$$\sigma_{ij} = L_{ijkl} \varepsilon_{kl} \text{ in } \Omega,$$  \hspace{1cm} (9)

Define the symmetric stress polarization tensor $\tau$ as:

$$\sigma_{ij} = L_{ijkl}^0 \varepsilon_{kl} + \tau_{ij},$$  \hspace{1cm} (10)

or subtracting (10) and (7):

$$\bar{\sigma}_{ij} = L_{ijkl}^0 \bar{\varepsilon}_{kl} + \tau_{ij}.$$  \hspace{1cm} (11)

Moreover, eliminating $\sigma$ from (10) and (9) we get a possible definition of polarization tensor:

$$\tau_{ij} = [L_{ijkl}^0](\varepsilon_{kl} + E_{kl}),$$  \hspace{1cm} (12)

where

$$[L_{ijkl}^0] = L_{ijkl}^0 - L_{ijkl}.$$

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

$$\frac{\partial(L_{ijkl}^0 \bar{\varepsilon}_{kl} + \tau_{ij})}{\partial y_j} = 0 \text{ in } \Omega,$$  \hspace{1cm} (14)

$$\bar{u}_i = u_i - u_i^0, \bar{p}_i = p_i - p_i^0 \text{ on } \partial \Omega,$$  \hspace{1cm} (15)

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

$$c_{mn}(\xi)\bar{u}_n(\xi) = \int_{\partial \Omega} p_{mi}^*(y; \xi)\bar{u}_i(y) \, d\gamma(y) - \int_{\partial \Omega} u_{mi}^*(y; \xi)\bar{p}_i(y) \, d\gamma(y) +$$

$$+ \left( [L_{ijkl}^f - L_{ijkl}^0] \int_{\Omega_f} + [L_{ijkl}^m - L_{ijkl}^0] \int_{\Omega_m} \right) \{\varepsilon_{miyj}(y; \xi)\bar{\varepsilon}_{kl}(y) + E_{kl} \} \, d\Omega.$$  \hspace{1cm} (16)
where \( c_{mn} \) depends of the position \( \xi \in \partial \Omega \) and the quantities with asterisks are known kernels.

Differentiating the last equation provides

\[
\varepsilon_{mn}(\xi) = \int_{\partial \Omega} P_{mi}^* (y; \xi) \tilde{\mu}_i (y) \, d\gamma(y) - \int_{\partial \Omega} U_{mi}^* (y; \xi) \tilde{\nu}_i (y) \, d\gamma(y) + \\
+ \left( [L_{ijkl}^f - L_{ijkl}^0] \int_{\Omega^f} + [L_{ijkl}^m - L_{ijkl}^0] \int_{\Omega^m} \right) \times \\
\times \{ \Psi_{mij}(y; \xi)(\varepsilon_{kl}(y) + E_{kl}) \} \, d\Omega(y) + \text{convected term} \tag{17}
\]

First, let \( L_{ijkl}^0 = L_{ijkl}^f \). Eliminating unknown boundary values from (16) and (17) we obtain the relation

\[
\varepsilon_{ij}^m (\tilde{u}(y)) = \varepsilon_{ij}^m (y) E_{kl}, \tag{18}
\]

and if \( L_{ijkl}^0 = L_{ijkl}^m \) then

\[
\varepsilon_{ij}^f (\tilde{u}(y)) = \varepsilon_{ij}^f (y) E_{kl}. \tag{19}
\]

This process leads to a fourth-order "concentration factor tensor" \( A_{ijkl} \) defined as

\[
\varepsilon_{ij}^p (\tilde{u}(y)) = \varepsilon_{ij}^p (y) E_{kl}, \quad \varepsilon_{ij}^p (u(y)) = [I_{ijkl} + \varepsilon_{ij}^p (y)] E_{kl} = A_{ijkl}^p (y) E_{kl}, \tag{20}
\]

where the superscript \( p = f \) for \( y \in \Omega^f \) and \( p = m \) for \( y \in \Omega^m \) (cf. (2)), and (7) follows.

Since it obviously holds

\[
< A_{ijkl}^f >_f + < A_{ijkl}^m >_m = 1 \tag{21}
\]

one needs not to compute both concentration factors. It is sufficient draw a concentration 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 nearly uniformly distributed.

4 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 \( E_{ij} \) be applied to the domain \( \Omega \) (in our case, a periodic distribution of fibers is considered). This produces concentration factors \( A_{ijkl}^f \) and \( A_{ijkl}^m \), obeying (21). Let \( \Pi(A^f, A^m, \Omega) \) be a real functional of \( A^f, A^m \) and \( \Omega \). The problem of optimal shape consists of finding such
domain $\Omega^j$ from a class $O$ of admissible domains, which minimizes $\Pi$. This may symbolically be written as

$$\min \{ \Pi(A^j, A^m, \Omega); A(u, \Omega) = 0, \text{ eq. (2) is fulfilled} \}, \quad (22)$$

where $A$ is an operator which for each $\Omega \in O$ uniquely determines the displacement field $u$.

Since there is no external loading in our solution for concentration factors, (the load is due to unit impulses of strain tensor or, equivalently, of prescribed displacements), one of a practical requirements of designers is an assumption of minimum strain energy of a structure subject to the above mentioned load distribution. Such a problem may be formulated in terms of inverse variational principles. In order to ensure the correctness of this formulation, additional constraint have to be applied. In our case, we assume the constant volume of fibers. Hence, the admissible set is defined as

$$O = \{ \Omega; \text{ meas } \Omega = C, \quad \text{Big} \left[ \frac{dg(x)}{dx} \right] \leq C_g \}, \quad (23)$$

where $C$ and $C_g$ are (reasonably) chosen constants and $g$ is a function describing the interfacial boundary $\Gamma$.

It remains to state the shape function $p$, or in a discretized form the internal - shape - parameters $\mathbf{p}$. A natural choice is a movement of $\Gamma$.

Because of the special nature of the loading, the energy functional can be written as:

$$\Pi(u, \Omega) = \frac{1}{2} S_{ij} E_{ij} + \lambda \left( \int_{\Omega^j} d\Omega - C \right) \rightarrow \text{stationary}, \quad i, j = 1, 2, 3, \quad (24)$$

owing to Hill’s energy condition (4). Coefficient $\lambda$ is lagrangian multiplier.

Substituting (7) to (24) we have:

$$\Pi(u, \Omega) = \frac{1}{2} [L_{ijkl}^f < A(p)_{kla\beta}(y) >_f + L_{ijkl}^m < A(p)_{kla\beta}(y) >_m] E_{\alpha\beta} E_{ij} + \lambda \left( \int_{\Omega^j} d\Omega - C \right), \quad (25)$$

and only the concentration factors are dependant of the function $p$.

Let us say that $A_{ijkl}^f$ is very precisely determined by the procedure described in section 3. Hence, using (21) and (7), eq. (25) will be simplified as:

$$\Pi(u, \Omega) = \frac{1}{2} [L_{ijkl}^m + (L_{ijkl}^f - L_{ijkl}^m) < A(p)_{kla\beta}(y) >_f] E_{\alpha\beta} E_{ij} + \lambda \left( \int_{\Omega^j} d\Omega - C \right), \quad (26)$$
Our aim will now be to formulate the domain $\Omega^f$ by means of its corresponding boundary. This can be done in many ways. For example, suppose the polygonal shape of the fiber under study. One can choose some fixed point $P$ (pole - in our case this is the origin) 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 $\int_{\Omega^f} d\Omega = \text{meas } \Omega^f$, the discretization of $\Omega^f$ may be written as

$$\text{meas } \Omega = \sum_{k=1}^{N} \text{meas } (T_k),$$

where $\text{meas } (T_k)$ stands for the measure of $T_k, k = 1, ..., N$.

This process is described in Procházka.$^2$

5 Euler's equations

The stationary requirement leads to differentiation of the functional by the shape parameters $p_k$:

$$\frac{\partial \Pi(u, \Omega)}{\partial p_k} = \frac{1}{2} \left[ L^f_{ijkl} - L^m_{ijkl} \right] \left\{ \frac{\partial A(p)_{k\alpha\beta}(y)}{\partial p_k} \right\}_{I} >_{f} +$$

$$+ \frac{\partial A(p)_{k\alpha\beta}(y)}{\partial p_k} \right\}_{m} E_{\alpha\beta} E_{ij} + \lambda \frac{\partial}{\partial p_k} \int_{\Omega^f} d\Omega,$$

in the case of (25), and

$$\frac{\partial \Pi(u, \Omega)}{\partial p_k} = \frac{1}{2} \left[ (L^f_{ijkl} - L^m_{ijkl}) \right] \left\{ \frac{\partial A(p)_{k\alpha\beta}(y)}{\partial p_k} \right\}_{I} >_{f} E_{\alpha\beta} E_{ij} +$$

$$+ \lambda \frac{\partial}{\partial p_k} \int_{\Omega^f} d\Omega,$$

in the case of (26). Both latter formulas can be rewritten as

$$E_k + \lambda = 0, \quad k = 1, ..., N,$$

If we claim $p_k, k = 1, ..., N$ the distances from the current boundary of the fiber, $E_k$ corresponds to the strain energy density at the point of the interfacial boundary, in our case at the nodal point $k$. The equation (31) requires $E_k$ to have the same value for any $k$. 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 $k$ of the boundary, if $E_k$ is larger than the true value of $-\lambda$, whilst it should decrease its value when $E_k$ is smaller than the correct $-\lambda$. As, most probably, we will not know the real value of $-\lambda$ in advance, we estimate it from the average of the current values at the nodal points.
Since $E_k, k = 1, \ldots, N$, prove large differences in their values, the logarithmic scale was proposed by Tada, Seguchi & Soh\textsuperscript{4}. The computational procedure follows this idea.

The differentiation by $\lambda$ completes the system of Euler's equations:

$$\sum_{k=1}^{N} \text{meas}(T_k) = C.$$ \hspace{1cm} (32)

This numerical procedure is fully described in Procházka\textsuperscript{2}.

6 Example

Unit cells are considered with fiber volume ratio equal to 0.4 and 0.6. 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 $\Gamma$. As said in the previous section, the higher value of this energy, the larger movement of the nodal point of $\Gamma$ should aim at the optimum.

In both cases of volume ratios we used the following material properties of phases: Young's modulus of fiber $E^f = 210$ MPa, Poisson's ratio $\nu^f = 0.16$; on the matrix $E^m = 17$ MPa, and $\nu^m = 0.3$.

For fiber volume ratio 0.6 we started with radius $r = 0.714$ and "unit moves" of the parameters $p_i$ where given by the change of radius by 2.2 \%. This means that in the first step we successively applied radius 0.730 at each nodal point of the contact boundary. The homogenized matrix $L^*$ in the case $r = 0.714$ possessed the following values:

$$\begin{bmatrix}
182 & 62 & -0.05 \\
62 & 182 & 0.034 \\
-0.75 & -1.1 & 98
\end{bmatrix}$$

From the above matrix one can conclude that the responses on normal unit strains are computed with high accuracy while the results from shearing strains are less accurate.

In Fig. 3, the distribution of relative energies $E_k$ is depicted along the interfacial boundary and in Fig. 4 the optimal shape of the fiber is drawn. This results are in accordance with results gained from the FEM. The volume fiber ratio was in this case equal to 0.4.

![Figure 3. Relative energies](image)

![Figure 4. Optimal shape](image)
7 Conclusions

In this paper inverse variational principle together with boundary element method has been applied to the solution of optimal fiber shape design on a unit cell of periodic composite structure. The BEM procedure possesses many advantages in comparison with finite element method and is very prospective not only for applications to homogeneous media, but also for partly homogeneous materials, such as composites and soils. When searching for optimal shape design of fibers in composite structures, many formulations have been used in the past. They very often start with minimum strain energy function. This assumption is in inverse variational principles fulfilled implicitly. A natural requirement is the restriction to the constant volume or area in many methods of solution of optimal shape design of composites, say, when solving a periodic distribution of fibers.

The requirement of the constant volume or area seems to be restrictive, particularly when expecting application of inverse variational principles to larger range of problems. Actually, it is not so. The constant $C$ may change, too. Thus the formulation has to be extended in such a way that $C$ is involved into the problem as a new variable and may be variated (differentiated) in some reasonable way. It is necessary to point out that the extremum of the functional $\Pi$ is found as neither the minimum nor the maximum, but the functional should be minimum with respect to the displacements and maximum with respect to the lagrangian multiplier $\lambda$.

References


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