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SEURAT SYSTEM. SYNTHESIS OF COMPOSITE MATERIALS

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Most of the materials we are faced with are in fact, due to their structure highly heterogeneous. In contemporary thus developed materials are treated as composites or mixtures. The paper presents the kind of computer program, SEURAT System. The program SEURAT has been built at the Center of Computer Methods of Civil Engineering Department of Warsaw University of Technology. The aim of the SEURAT System is to predict the effective properties of composite from properties, and the geometrical arrangement of constituents.

1. Introduction

Investigation of the existing materials and designing new ones can be made with the aid of computer synthesis of material programm. This makes it possible to conduct such experiments which cannot be performed by usual methods – e.g. with the use of testing machines and real samples. Here an key part is played by technique of a computer image analysis which enables the structure of medium to be encoded into the computer memory (cf Gajl and Żmijewski (1989)).

Our intuition suggests that overall properties we observe depend upon:

- properties of components
- structure, viz. distribution or layout of the components

- mechanism of synergic interaction.

Basic concepts of the SEURAT System were presented by Gajewski et al. (1991), Izdebski and Żmijewski (1991), Łukasik and Żmijewski (1991a,b), Węglarz and Żmijewski (1991). For the time SEURAT System is composed of several main blocks (Fig.1) described in this paper.

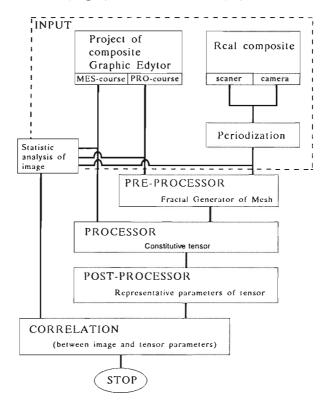


Fig. 1. The SEURAT System scheme

2. INPUT block

In this block the image of composite material is utilized as a basis for further analysis. The image can be obtain from a camera (Fig.2), a scanner (for real composites) or with the help of Graphic Editor of Composite Sample Picture in the case of project of a new structure (Fig.3).

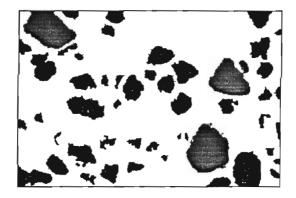


Fig. 2. The real composite structure

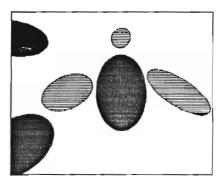


Fig. 3. The project of the composite structure

The Graphic Editor of Composite Sample Picture developes and modifies the idea which was presented by Węglarz and Żmijewski (1991). The algorithm of random numbers generation due to described probability arrangements have been taken after Rajski and Tyszer (1986), Zieliński (1979). The statistic analysis procedures are the results of studies carried out by Krzykowski (1991) and Niedokos (1990). The Monte Carlo method, which is used in this paper, is precisely displayed in the well known monograph by Zieliński (1972).

The Graphic Editor of Composite Sample Picture can work in two courses:

- "MES" that allows a direct creation of data for FEM programs
- "PRO" that allows the creation of the picture of sample of designed material of composite and, if needed, preparation of data for the FEM mesh generating programs.

The picture of sample of material is written down in a parametrical form in the disc file. It gives us the possibility of a quick reproduction and modification of pictures of composite that originated from sample, and facilitates making the statistic analysis of parameters that describe the picture. As the result information about the structure of the object is obtained.

Because most of composite structures have in fact probabilistic character, the Graphic Editor can produce images of project of structure in the probabilistic process.

3. Shape reconstruction

The aim of reconstruction process is, in this case, to calculate screecoordinates of polygon nodes with the same (or approximate) shape parameters as the analysed figure.

The considerations are limited to analyzing the shape of plan, monochromatic figures. It is assumed, that parameters describing the shape figure are their geometrical characteristics (3.1), calculated in relation to the selected coordinate system

$$S_{ij} = \int_{A} x^{i} y^{j} dA$$
 $i, j = 0, 1, ...$ (3.1)

where: x^i, y^j - coordinates, A - domain of a figure.

Having at one's disposal the complete set of S_{ij} we could reproduce an approximate shape of figure. This process we called the shape reconstruction.

The characteristics of the polygon could be calculated as the sums of characteristics of the component triangles

$$S_{ij} = \sum_{k=1}^{n} S_{ij}^{\Delta k} \qquad S_{ij}^{\Delta k} = \int_{\Delta k} x^{j} y^{i} d\Delta k \qquad (3.2)$$

The integrals which appear in the right hand side of Eq (3.2) are calculated from the exact formulae (3.3) which can be adopted after transformation into barycentric coordinate system $(L_0L_1L_2)$

$$\int_{\Delta k} x^{j} y^{i} d\Delta k = \sum_{\Delta k} C(i, j) x_{0}^{a} x_{1}^{b} x_{2}^{c} y_{0}^{d} y_{1}^{e} y_{2}^{f} \int_{\Delta k} L_{0}^{\alpha} L_{1}^{\beta} L_{2}^{\gamma} d\Delta k$$
 (3.3)

where

$$C(i,j) \in C$$
 $\alpha = a + d$
 $a + b + c = j$ $\beta = b + e$
 $d + e + f = i$ $\gamma = c + f$

One of possible approaches to the question of shape reconstruction is the optimization of some function of vertex coefficients of reconstructed polygon. From the variety of optimization methods the Hook-Jeeves (IIJ) method has been selected. The analyzed function (3.4) is a sum of the squared errors of characteristics determined at subsequent steps of iteration and that is why further on it is called the error function

$$\Psi = \sum_{k=1}^{N} (J_{ij}^{k} - S_{ij}^{k})^{2}$$
(3.4)

where as before S_{ij} are the characteristics of reconstructed blank and J_{ij} are the current characteristics of a polygon during successive iteration.

The process of reconstruction consist in evaluating such coordinates of vertex for which the error function attains minimum (for the case under consideration the minimum is known $\Psi_{\min} = 0$). Note that the number of adopted characteristics is now arbitrary i.e. is independent of the number of vertices. However if too few characteristics are included the correct solutions is not warranted.

The formula (3.4) presents the simplest version which can be used in the problem. One of the possible modifications is normalization of the error function constituents

$$\Psi' = \sum_{k=1}^{N} \left(\frac{J_{ij}^{k} - S_{ij}^{k}}{(S_{00})^{p}} \right)^{2}$$
 (3.5)

where: $p = \frac{i+j+2}{2}$.

The normalization factor need not to be the area of the figure but it could be any other positive characteristic or their combination. Normalized error functions have an additional advantage. Their values are much smaller then these of non-normalized functions. This is especially important when the reconstructed shape is strongly irregular.

The algorithm described above produces acceptable and trustworthy results for rather compact and convex figures.

Some results are presented in Fig.4.

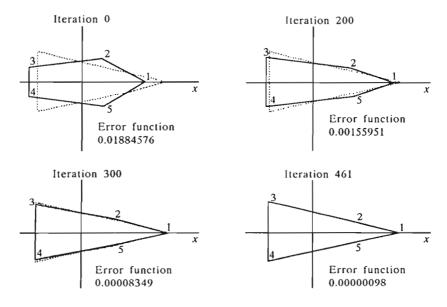


Fig. 4. Reconstruction of a triangle from a pentagon

4. PRE-PROCESSOR block

At this stage of the prediction of the effective properties of composite two steps are made. Periodization, if necessary, according to the requirements of the special FEM processor and discretization of the periodic cell of composite structure (Fig.5).

In the SEURAT system two possibilities of periodization exist. First of them can be used only for design of composite (the PRO course in the Graphic Editor), and second allows to periodize both the design and the real composite structure.

In the finite element method discretization always plays an essential role. The discretization in the SEURAT system can be performed in two ways. For the real composite structures the Fractal Generator (cf Lukasik and Żmijewski (1991a)) (based on Lindenmayer's grammar, Prusinkiewicz (1989)) of meshes was build. The formalism of Lindenmayer's grammar allows us to code the way in which the mesh generator should act. The refining aspect of the procedure is essential.

A very simple primary mesh can be locally enriched (for example subdivited) according to the complexity of the discretized object. The results were shown by Lukasik and Żinijewski (1991a) and (1993). Later on a similar con-



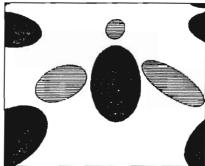


Fig. 5. Periodic structures

cept has been developed by Bova and Carey (1992). Some result of the fractal generator activity for a composite structure are presented in Fig.7.

In the case of project of composite two kinds of discretization can be used: the FEM course in the Graphic Editor (Fig.6) or the Fractal Generator program.

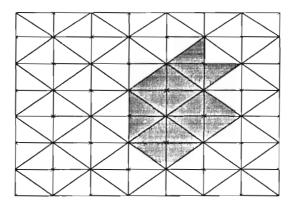


Fig. 6. The mesh for composite cell obtained by the Graphic Editor

As a final result in both methods we obtain standard lists of nodes and elements that constitute the basic data for computational programmes of the composite material model.

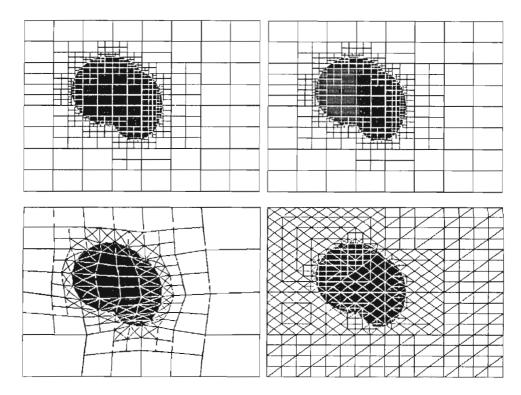


Fig. 7. The meshes for composite cell obtained by the Fractal Generator

5. PROCESSOR block

The typical way applied to approximation of the physical characteristic of composites is replacing them by the model of homogeneous body. The algorithm of homogenization of material uses the microlocal parameter method (cf Lewiński (1987)), bases of which were created by Woźniak (1986). The method uses modern tools of non-standard analysis. In spite of (or perhaps rather due to) application of such a subtle tool the numerical implementation results in a relatively simple and, what is more important, quite general FEM-like algorithm. According to this method the description of the model may simultaneously include variables of different range. Effective equations of the model consist only of the standard values. The starting point is a model with periodic structure. The effective constitutive tensor is obtained by the following simple formula

$$\mathbf{A}^{\text{eff}} = \mathbf{A} - \mathbf{B}^{\mathsf{T}} \mathbf{D}^{-1} \mathbf{B} \tag{5.1}$$

where

A - approximate average constitutive matrix of material

B - stress matrix

D - stiffness matrix.

The shape function should fulfill the following conditions

$$W(y) = \left\{ h_{\alpha} : h_{\alpha} \in \left(H_{\text{loc}}^{1}(\mathbb{R}^{N}) \right)^{N}, h_{\alpha} \text{ is } Y - \text{periodic} < \nabla h_{\alpha} > = 0 \right\}$$

$$(5.2)$$

where

$$<\nabla h_{\alpha}> = \frac{1}{|Y|} \sum_{e \in Z_{\alpha}} \int_{Y_{\bullet}} \nabla h_{\alpha} \ dY$$

and Z_{α} - set of elements which contain the node P_{α} .

The Y-periodicity conditions are satisfied provided that the discretization of specimen (Y) edge is symmetric (edge nodes have their duplicates on the opposite edges) with simultaneous identification of the appropriate degrees of freedom on opposite sides. The "oscillation" condition $\langle \nabla h_{\alpha} \rangle = 0$ is satisfied by assuming barycentric shape functions for example. This reduces the problem to the description of the specimen with the help of a typical FEM stiffness matrix.

In the implemented algorithm the space of shape function is modified by the supplementary matrix \bar{C}_e (originated from a nonlinear component of the shape function) introduced to the stiffnes matrix K_e of an element, this fact reads

$$\mathbf{C}_e = \xi \bar{\mathbf{C}}_e + \mathbf{K}_e \qquad \qquad \xi \in R \tag{5.3}$$

The above solution has been adopted because there is a possibility that the results can be obtained for "infinitesimally" small perturbation of the space " $\langle \nabla h_{\alpha} \rangle = 0$ ", limited by the factors independent of the applied method (kind of the linear set of equations solver, type of computer etc.)

On adopting the space " $\langle \nabla h_{\alpha} \rangle = 0$ " evaluation of effective modules for the fibrous composite was performed with the assumption that fibers and matrix are both linearly elastic. This is compared with the composite discussed by Więckowski (1986). Repeatable cell of composite is shown in Fig.8.

The effective constitutive tensor has also been determined using the analytical formulae under the assumption of plane strain state.

Więckowski shows results obtained with the help of both stress (eightnode, rectangular Bogner-Fox-Schmit elements) and displacement (four-node rectangular elements) finite elements method. Results of those computations are shown in Fig.9. In the presented algorithm calculations which discretize the whole cell with 72 or 336 three-node triangles have been.

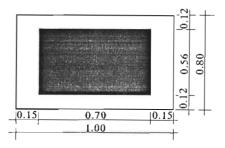


Fig. 8. The repeatable cell of fibrous composite

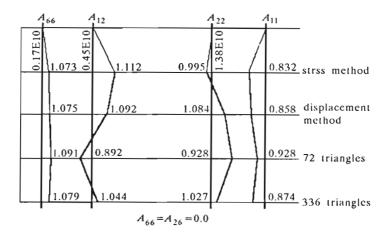


Fig. 9. Results for fibrous composite

6. POST-PROCESSOR block

Effective constitutive parameters obtained in the SEURAT System are the basis for next step of the process. They are employed for input data in the probabilistic analysis of composite properties. The choice of representative parameters for univocal description of properties of composite material is essential.

In our case, we decided to choose (for \mathbb{R}^2) the set of parameters

$$\lambda_1, \lambda_2, \lambda_3, \rho_1 l, \rho_2$$
 (6.1)

where

 λ_i - invariants of fourth order tensor ρ_i - invariants of second order tensor.

The constitutive fourth order tensor can be obtain with the help of formula

$$C^{ijkl} = \lambda_{1}(\rho_{1}v_{1}^{i}v_{1}^{j} + \bar{\rho}_{1}\bar{v}_{1}^{i}\bar{v}_{1}^{j})(\rho_{1}v_{1}^{k}v_{1}^{l} + \bar{\rho}_{1}\bar{v}_{1}^{k}\bar{v}_{1}^{l}) + + \lambda_{2}(\rho_{2}v_{2}^{i}v_{2}^{j} + \bar{\rho}_{2}\bar{v}_{2}^{i}\bar{v}_{2}^{j})(\rho_{2}v_{2}^{k}v_{2}^{l} + \bar{\rho}_{2}\bar{v}_{2}^{k}\bar{v}_{2}^{l}) + + \lambda_{3}(\rho_{3}v_{3}^{i}v_{3}^{j} + \bar{\rho}_{3}\bar{v}_{3}^{i}\bar{v}_{3}^{j})(\rho_{3}v_{3}^{k}v_{3}^{l} + \bar{\rho}_{3}\bar{v}_{3}^{k}\bar{v}_{3}^{l}) \qquad i, j, k, l, = 1, 2$$

$$(6.2)$$

For it the following equations must be satisfied (n = 1, 2, 3)

$$(\rho_n)^2 + (\bar{\rho}_n)^2 = 1$$

$$v_n^i v_n^i = 1 \qquad v_n^i \bar{v}_n^i = 0 \qquad \bar{v}_n^i \bar{v}_n^i = 1$$
(6.3)

and

$$\kappa_n^{ij}\kappa_n^{ij} = 1 \qquad \qquad \kappa_n^{ij}\bar{\kappa}_n^{ij} = 0 \qquad \qquad \bar{\kappa}_n^{ij}\bar{\kappa}_n^{ij} = 1 \tag{6.4}$$

where

$$\kappa_n^{ij} = v_n^i v_n^j \qquad \qquad \bar{\kappa}_n^{ij} = \bar{v}_n^i \bar{v}_n^j \tag{6.5}$$

The representative parameters utilized in the SEURAT System allow us to objectify the comparison of constitutive tensors on basis of five elements for \mathbb{R}^2 . Such an representation can be applied to the statistic analysis of the constitutive tensors and moreover it can be graphically interpreted (Fig.10).

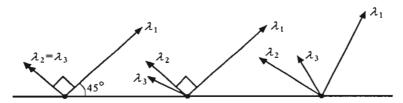


Fig. 10. Graphic representations for isotropic (a), ortotropic (b) and anizotropic (c) constitutive tensors

The knowledge of the parameters of this representation allows us to reconstruct the coefficients of the tensor in the arbitrary chosen coordinate system.

7. CORRELATION block

In fact, the analysis of composite properties is an analysis of coupled values (components of constitutive tensor). It requires the use of special kind of algorithms of probabilistic methods.

As a result a good correlation between the parameters of composite structure and the parameters of constitutive tensor is obtained.

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System SEURAT. Synteza materiałów kompozytowych

Streszczenie

W artykule przedstawiono opis Systemu SEURAT. System ten powstały w Ośrodku Metod Komputerowych Wydz. Inżynierii Lądowj PW jest programem komputerowym służącym do automatycznej analizy projektowanych i rzeczywistych kompozytów plaskich reprezentowanych przez ich obraz. W systemie można wyróżnić kilka "odrębnych" błoków dedykowanych specyficznym aspektom procesu badania struktur kompozytowych (edycja i analiza obrazu, rekonstrukcja ksztaltu, dyskretyzacja, określanie efektywnych wielkości itp.). Prace nad Projektem SEURAT trwają od II polowy lat osiemdziesiątych. W obecnej chwili system jest nadal rozwijany m.in. w kierunku zastosowania metod adaptacyjnych.

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