HYBRID, FINITE ELEMENT-ARTIFICIAL NEURAL NETWORK MODEL FOR COMPOSITE MATERIALS

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An application of Artificial Neural Networks for a definition of the effective constitutive law for a composite is described in the paper. First, a classical homogenisation procedure is directly interpreted with a use of this numerical tool. Next, a self-learning Finite Element code (FE with ANN inside) is used in the case when the effective constitutive law is deduced from a numerical experiment (substituting here a purely phenomenological approach). The new contribution to the classical self-learning procedure consists of its adaptation to a case of a non-monotonic loading (non one-to-one load-deformation curve). This new ability of the method is principally due to the incremental form of the constitutive equation and the respective scheme of the neural network structure. Also an organisation of a constitutive data-base containing learning patterns is suitably modified. It is shown by examples that the training process is very quick. The error of this method is smaller, comparing to other schemes of data acquisition.

Key words: Artificial Neural Networks, composite materials, self-learning FE method

1. Introduction

The paper is concerned with the presentation of some applications of Artificial Neural Networks (ANN) in the analysis of composites. Not only a formulation of the constitutive law for a composite but also its representation inside a finite element code is described in the paper. The methods presented here are intended only for composites with a very fine microstructure.

In the introductory part we explain why the representation of the constitutive law by ANN is useful, and we suggest what kind of problems can be reasonably treated with it.

The main problem in the analysis of composites is the estimation of the effective mechanical stiffness, effective thermal conductivity, effective thermal expansion, effective electrical resistance and so on. Effective – means here – significant when the structure is considered as a fictious, homogeneous body, disregarding details of its internal composition. These properties characterise global (or macro) behaviour, i.e. the behaviour observed at the macroscale. The perturbation of fields of variables of the problem due to the micro-heterogeneity is insignificant from this perspective. It is obvious that the global behaviour is determined at the microlevel, by geometry of components and their individual physical properties. Despite this, we want to carry out the estimation of global effects without pushing a finite element mesh down, into the geometry of the microstructure, while the global boundary value problem under global loading conditions is to be solved. Because of the scale separation between structural levels a mesh fine enough for the microlevel would result in a huge number of elements at the macro-structural level, thus, with a huge number of unknowns in the model. This can be avoided using theory of homogenisation. The theory of homogenisation (or rather a variety of theories) can be considered as a fundamental tool of a reasonable analysis of materials with a microstructure.

Alternatively, a set of experimental observations of the behaviour of a macro-sample of the heterogeneous material must be performed to define the effective properties of the composite. Recently this phenomenological approach has been frequently substituted with a so-called "numerical experiment" (Bandeira *et al.*, 2001; Wriggers and Lohnert, 2002). In the paper we use mainly such substitution as a source of constitutive data.

We note first that in the frame of the classical homogenisation theory some regularity of the microgeometry of the composition is assumed. It is necessary to simplify the description of a heterogeneous body. There are two principal idealisations of real structures. Asymptotic homogenisation of periodic media is applicable to the analysis of structures obtained by translation of an elementary cell (called the cell of periodicity) while in a self-consistent approach one assumes that the considered composite is made by multiple, irregular repetitions of a scaled pattern. The third possibility is a stochastic description, which is out of the scope of this paper.

In the case of periodic composites the mathematical formalism allows us to build a qualitative theory without any *a priori* restriction concerning the form of the resulting effective constitutive law (see, for example Sanchez-Palencia, 1980). However, in the practice of physically non-linear composites the nature of non-linearity must be taken into account at an early stage of the de-

velopment. For example, exponential non-linearity of components requires a theoretical formulation quite different than that for an elastic-plastic physical framework (Suquet, 1985). Because of this, many individual, particular theories have been built for particular classes of materials sometimes combined with particular geometries of the cell of periodicity.

Using asymptotic homogenisation, a solution to the problem of periodic media typically splits into two boundary value problems. The first one is formulated at the microlevel, for the repetitive microstructural domain. Its solution determines effective material characteristics and allows for the construction of stress distribution at the level of microstructure in the phase of "unsmearing". The second boundary value problem (the global one) is stated for the homogeneous, fictious body. The constitutive description of this material is obtained at the first stage. The principal difficulties result from the fact that in the non-linear material or geometrical frame the superposition of micro- and macro-behaviours is not allowed. Moreover, the coupling between these two levels is explained by the fact that the solution to the micro BV problem depends on the micro-geometry which changes during the global solution, which, in turn, depends on the results of the micro BV problem through the values of constitutive parameters in the global constitutive law. In the case of a complicated physical and geometrical composition the mentioned problems are rather difficult to overcome. This situation is even more difficult from the point of view of a designer who needs a method that works well for many geometric and physical arrangements suitable for various schemes of the structure that should be considered in the design process. This analysis is simpler if can be done without revision of the mathematical formulation at each stage of design and at each level of the structure.

Wriggers and others (Wriggers and Lohnert, 2002; Bandeira *et al.*, 2001) have made an important step toward such a solution. The proposed method consists of some numerical experiments using FE method at the meso- or microlevel. The proposed approach is consistent with fundamental findings of the homogenisation theory: as in the theory of homogenisation the global behaviour is deduced from a small sample of a composite material but now the method is fully numerical. It assumes the application of pre-existing numerical procedures in the modelling of contact, friction and other effects at the microlevel (inter-particular mechanics is considered for granular assemblies for example). Another important direction in the numerical homogenisation is represented by Kouznetzova, Brekelmans and co-workers (see Kouznetzova *et al.*, 2001). Also in this approach an expected form of the resulting, effective constitutive law should be imposed *a priori*.

A self-consistent approach can be considered as the most suitable theoretical frame resulting with a closed-form expression giving the effective material characteristics as a function of the volume fraction of the forcing material dispersed in the matrix. This approach, (see Zaoui, 1997; Kroner, 1978; Boutin, 2000; Hashin, 1968) is less sensitive on the morphology of the sample of the composite. Boutin, Zaoui and many other authors have developed expressions for different effective properties in the case of three separate levels of porosity: micro, meso and macro (Boutin *et al.*, 1998; Zaoui, 1997). Unfortunately, also this method assumes some qualitative *a priori* decisions concerning the global constitutive law. Finally, it seems to be very difficult to take into account all possible non-linear, unilateral microfeatures defining "generic heterogeneity" for this method. Also the geometry of the scalable cell should be very simple in this approach (concentric ellipsoids).

Our method of solving the problem of the effective constitutive law for a material with a microstructure is entirely numerical. It is based on the assumptions that the Cauchy stress (or its increment) in the fictitious, homogenised body is an unknown, non-linear function of mean strains, strain increment, physical parameters defining the microphysics of composition, and the geometry of the representative volume. The history of loading-unloading can affect all this data. We assume a form of this function representing it by an Artificial Neural Network with hidden layers. At the input of this network we have all independent variables, mentioned in the above sentence. At the output we obtain a state of stress in the point of the body at the macrolevel. Since the components of the strain tensor are present among the input variables, the Artificial Neural Network acts as a numerical representation of the effective constitutive law. It is well known that the ANN can be considered as a universal approximation of a function, functional or operator (a formal proof of this statement can be found in Chen and Chen (1995)). Because of this, this representation does not constrain the generality of the global, effective constitutive law we are looking for. To define the ANN we must determine all weights of the links between neurones belonging to various layers of the network. The coefficients in this very rich and flexible representation are defined during an iterative process of "training". The source of knowledge for the learning can be a real or numerical experiment. If a numerical experiment is considered, an auxiliary FE modelling process is similar to that proposed by Wriggers and Lohnert (2002) with the exception that in our case the form of the constitutive equation is defined by the ANN thus, it does not restrict the possible effective behaviour. In this case, like in the periodic homogenisation, we discover rather than impose the global constitutive law, but now – also

for a possibly non-linear effective behaviour. The FE analysis of a sample of the composite is a source of "examples" for the training process. These examples form a knowledge base containing the constitutive data. The considered sample of the composite that defines the microstructure consists of only one repetitive cell or a representative volume. In examples presented in this paper the representative volume will be replaced, for simplicity, by an array of cells. The equivalence between the composite structure and its homogeneous counterpart is defined in the paper in an original manner, consistent with the proposed numerical procedure (different from that, described in the frame of the theory of homogenisation).

The use of the ANN in the role of the constitutive operator is not new. Classical application of Artificial Neural Networks for constitutive modelling of concrete was originally proposed by Ghaboussi *et al.* (1991). An improved technique of ANN approximation for a problem of mechanical behaviour of drained and undrained sand is presented in Ghaboussi and Sidarta (1998). In the latest surveys Waszczyszyn (1997, 1998), Yagawa and Okuda (1996) the role of neural computing in the constitutive modelling is clearly pointed out. A similar approach is employed in Garcia *et al.* (2000), Gawin *et al.* (2001), Kortesis and Panagiotopoulos (1993), Mucha (1997), Penumadu and Zhao (1999) and many other papers.

The essence of the ANN technique is to construct an application that attributes a given set of output vectors to a given set of input vectors. When applied to the constitutive description, the physical nature of these input-output data is clearly determined by measured quantities: strains-stresses or displacements-forces. The neural "black box" operator, replacing the existing symbolic description, cannot be directly used in the symbolic development of the formulae and is useless for a closed-form solution. It can be very efficient as an element of a FE code, as it is shown in Gawin *et al.* (2001), Mucha (1997). A hybrid FE-ANN code is described also in Shin and Pande (2000, 2001). The authors show that the insertion of the constitutive law presented in the form of a neural operator leads to some qualitative improvements in the application of FE in engineering practice. Namely, the ANN representation can be modified to reduce the error of a FE numerical experiment with respect to the real experiment. Our representation of the constitutive law with the ANN is slightly different. It is incremental while in Shin and Pande (2000, 2001) the $\varepsilon - \sigma$ functions are directly approximated.

Obviously, there is no need to use the presented method in the case of a simple micro-geometry of the composite and when the behaviour of components is linear. In this case the classical description of the effective behaviour

is much better. The ANN representation can be useful in a case, when the physical or geometrical non-linearity dominates the micro-description and the FE analysis at the level of the representative volume (or a direct experiment) is the only possible tool for its effective analysis.

The paper contains academic examples illustrating the assumed strategy of the modelling. We refer the interested reader to our previous papers (Lefik and Schrefler, 2002a,b) in which some aspects of practical applications of the presented method to the analysis of mechanical behaviour of a superconducting cable is shown.

2. The effective constitutive law for acomposite and its representation by an Artificial Neural Network with hidden layers

2.1. Effective properties of the composite

For usual analysis of a two scale composite we define two sets of coordinates: local $\boldsymbol{y}$ related to the single, repetitive cell of periodicity Y and the global $\boldsymbol{x}$ for the entire body Ω (composed of a finite number of the cells, Fig. 1).
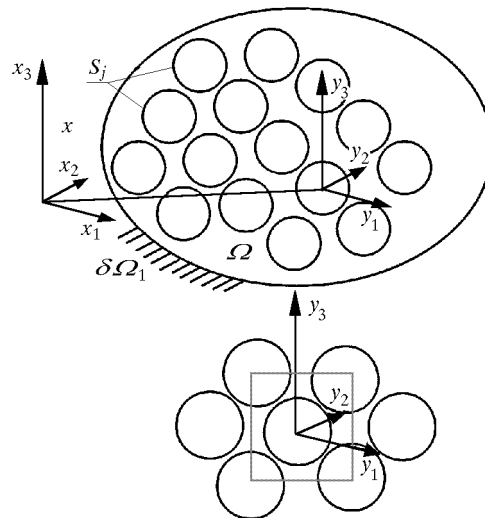

Fig. 1. The cell of periodicity and two systems of coordinates

The dimensionless characteristic length ε of the cell Y is treated as a small parameter tending to zero (the "length" of the cell Y related to the "length" of Ω). Let the displacement field $\boldsymbol{u}^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y})$ be an ε-depending solution to the problem

$$\text{find } u_i^{\varepsilon} \in V \text{ and } \sigma_{ij}^{\varepsilon} \in L^2 \text{ such that:} \tag{2.1}$$

$$\forall v_i(\boldsymbol{x}) \in V \qquad \int_{\Omega} \sigma_{kl}^{\varepsilon}(\boldsymbol{u}) v_{k,l} \, d\Omega = \int_{S_f} F_i v_i \, dS_f$$

where the stress tensor σ is computed via $(2.2)_1$ and remains inside the admissible set P $(2.2)_2$ defined by any usual yield criterion (an associated flow rule completes the constitutive description)

$$\sigma_{ij}^{\varepsilon}(\boldsymbol{u}^{\varepsilon})(\boldsymbol{x}, \boldsymbol{y}) = a_{ijkl}(\boldsymbol{y}) e_{kl}(\boldsymbol{u}^{\varepsilon}(\boldsymbol{x}, \boldsymbol{y})) \qquad \sigma_{ij}^{\varepsilon} \in P(\boldsymbol{y}) \tag{2.2}$$

V is the usual space of kinematically admissible displacements, $\boldsymbol{e}(\boldsymbol{v})$ is the linearized strain tensor computed at $\boldsymbol{v}$, $\boldsymbol{F}$ denotes a vector of external load. Components of the fourth order elasticity tensor $\mathbf{a}$ are piece-wise constant functions of $\boldsymbol{y}$ with discontinuities along regular surfaces, and satisfy the classical conditions of symmetry, ellipticity and positivity.

Let $\boldsymbol{u}^0$, $\boldsymbol{\sigma}^0$ be the solution to the "homogenised" problem, i.e. problem (2.1) in which the variable material coefficients $\mathbf{a}(\boldsymbol{y})$ are replaced with some unknown constant values $\mathbf{a}^h$. We suppose that the periodicity of material characteristics imposes an analogous periodical perturbation on the quantities describing the mechanical behaviour of the body. Hence, for the displacements we have

$$\boldsymbol{u}^{\varepsilon}(\boldsymbol{x}) \equiv \boldsymbol{u}^0(\boldsymbol{x}) + \varepsilon \boldsymbol{u}^1(\boldsymbol{x}, \boldsymbol{y}) \tag{2.3}$$

$\boldsymbol{u}^1$ Y-periodic.

The same can be obtained for strains and the stress tensor via a simple total differential formula with respect to $\boldsymbol{x}$

$$\boldsymbol{e}^{\varepsilon}(\boldsymbol{x}) = \boldsymbol{e}^0(\boldsymbol{x}, \boldsymbol{y}) + \varepsilon \boldsymbol{e}^1(\boldsymbol{x}, \boldsymbol{y}) + ... + 0(\varepsilon^2)$$

$$\boldsymbol{\sigma}^{\varepsilon}(\boldsymbol{x}) = \boldsymbol{\sigma}^0(\boldsymbol{x}, \boldsymbol{y}) + \varepsilon \boldsymbol{\sigma}^1(\boldsymbol{x}, \boldsymbol{y}) + ... + 0(\varepsilon^2) \tag{2.4}$$

Thanks to (2.4), problem (2.1) splits into a sequence of problems of the order ε^0, ε^1 and ε^2.

The problem of the order ε^0 leads to equation (2.5) in which the perturbation of the displacement is computed according to (2.6) (this last expression

is not an assumption, it follows from the detailed analysis of the problem, see for example Sanchez-Palencia (1980) and references given there)

find $\chi_i^{pq} \in V_Y$ such that:

$$\forall v_i \in V_Y \qquad \int\limits_Y a_{ijkl}(\boldsymbol{y})(\delta_{ip}\delta_{jq} + \chi_{i,j(\boldsymbol{y})}^{pq}(\boldsymbol{y})v_{k,l(\boldsymbol{y})}(\boldsymbol{y})\,d\Omega = 0$$

(2.5)

$$u_i^1(\boldsymbol{x}, \boldsymbol{y}) = e_{pq(\boldsymbol{x})}(\boldsymbol{u}^0(\boldsymbol{x}))\chi_i^{pq}(\boldsymbol{y}) + C_i(\boldsymbol{x})$$

(2.6)

We call $\chi^{pq}(\boldsymbol{y})$ the homogenisation functions for displacements.

For $\mathbf{a}^h$ uniquely defined via the classical homogenisation procedure $\boldsymbol{u}^\varepsilon$ converges weakly to $\boldsymbol{u}^0$ as ε tends to zero. In this case, the tensor $\mathbf{a}^h$ defines an effective constitutive relationship between $\boldsymbol{e}(\boldsymbol{u}^0)$ and $\boldsymbol{\sigma}^0$ (a new admissible set in the stress space P^h makes a part of this effective constitutive description)

$$a_{ijpq}^h = |Y|^{-1} \int\limits_Y a_{ijkl}(\boldsymbol{y})(\delta_{kp}\delta_{lq} + \chi_{k,l(\boldsymbol{y})}^{pq})\,dY$$

(2.7)

$$\sigma_{ij}^0(\boldsymbol{x}) = a_{ijkl}^h e_{kl}(\boldsymbol{u}^0)$$

(2.8)

The heterogeneous structure can now be studied as a homogeneous one with effective material coefficients given by (2.7). The global displacements, strains and average stresses can be computed at that moment.

In this paper, instead of looking for $\mathbf{a}^h$ and P^h we are going to use a numerical representation of the effective constitutive law by a suitably trained ANN N. The input-output vector of N contains components of the strains $\boldsymbol{e}(\boldsymbol{u}^0)$ and stress tensor $\boldsymbol{\sigma}^0$ (in the vector-like notation)

$$\boldsymbol{\sigma}^0 = N@\boldsymbol{e}(\boldsymbol{u}^0) \qquad \sigma_i = \sum_q w_{qi}^{(2)} f_{(q)}(e_p w_{p(q)}^{(1)} + \theta_{(q)}^{(1)}) + \theta_i^{(2)}$$

(2.9)

Symbol @ denotes a result of an action of an operator at the specified operand. In this case it is the value of the neural operator at the input vector. Repetition of the subscript indicates summation over all its range (unless it is enclosed by paranthesis). Superscripts denote the number of a layer of neurones.

The parameters $\boldsymbol{w}$, θ and f in $(2.9)_2$ will be interpreted as weights, biases and transfer functions of the Artificial Neural Network defined and discussed in the next section. The finite element code with N included as a material description subroutine can be used to solve numerically problem (2.10) for $\boldsymbol{u}^0$

find $u_i^0 \in V$ and $\sigma_{ij}^0 \in L^2$ such that:

$$\forall v_i(\boldsymbol{x}) \in V \qquad \int\limits_{\Omega h} \sigma_{kl}^0(\boldsymbol{u})v_{k,l}\,d\Omega = \int\limits_{S_f} F_i v_i\,dS_f \qquad \boldsymbol{\sigma}^0 = N^h@\boldsymbol{e}(\boldsymbol{u}^0)$$

(2.10)

The correct, effective constitutive law in (2.10), represented by the ANN called N^h assures the following requirement

$$\forall \boldsymbol{F} \quad \|\boldsymbol{u}^\varepsilon - \boldsymbol{u}^0\|_{L^2(\Omega)} \leqslant \tau \qquad \qquad \tau \leqslant \varepsilon \|\boldsymbol{u}^1\|_{L^2(Y)} \quad \text{as} \quad \varepsilon \to 0 \qquad (2.11)$$

Estimation $(2.11)_2$ follows from a direct application of Cauchy's inequality. Expression (2.11) defines a correspondence between the heterogeneous the homogeneous (homogenised) fictitious body in a manner suitable for our purpose. In the numerical practice, comparison (2.11) of the effective solution with the exact one will be checked only in a few strategic points. Condition (2.11) formulated for any $\boldsymbol{F}$ is verifiable in practice only for a finite number of prescribed loads. Searching for the N^h, we employ an iterative procedure called the "training of Artificial Neural Network" proposed in all textbooks devoted to ANNs, as for example Hertz *et al.* (1991), Osowski (1996), Tadeusiewicz (1993) and shortly described in the next section.

3. Artificial Neural Network for constitutive description and a hybrid ANN-FE code

An inspiration for the application of Artificial Neural Networks (ANNs) to different branches of engineering sciences comes from the analysis of transmission and transformation of signals in human or animal neural systems. The importance of the method significantly increased during last years. Nowadays, the ANNs are successfully used in the computer-aided management, modelling of different physical dynamic processes depending on many fuzzy variables. In this application, the ANN will be included into the classical Finite Element procedure as a constitutive subroutine, as it is described in this section.

3.1. Artificial neural network with hidden layer for incremental representation of the constitutive law

The ANN can be considered as a universal, non-linear operator that transforms a set of suitably interpreted discrete values into another set of numerical data. Considering the structure of this operator, the ANN appears as a collection of some simple processing units (called neurones or nodes) that are mutually connected by links with adjustable strengths (see Fig. 1). This logical system, with nodes organized in layers, transforms the input signal presented at its "input" nodes into the output signal produced at the "output layer".

The sequence of signals presented at the input and that expected to be obtained at the output layer, are called the input and target patterns, respectively. The activity of the network consists of transformation of each input pattern into the output signal, and is defined by expression (3.1). After each cycle (forward transmission of the input signal and back propagation of the output error), the weights of connection are modified to reduce the error between the network response and the given output pattern

$$o_i = f\Big(f\big(w_{qr}^{(2)} f(i_p w_{pq}^{(1)}) + b_r^{(1)}\big) w_{ri}^{(3)} + b_i^{(2)}\Big) \qquad \sigma_i = o_i \qquad (3.1)$$

In this representation, f is a given sigmoid function of one variable x, Eq. (3.2), while $\boldsymbol{w}$ and $\boldsymbol{b}$ are weights and biases being constant during transmission of the signal

$$f_i(x) = \frac{p_i[1 - \exp(-\lambda_i x)]}{1 + \exp(-\lambda_i x)} \qquad (3.2)$$

All independent variables are in $\boldsymbol{i}$. It can be proved that this form approximates all continuous functions of several variables. A graph related to this formula is commonly known as a neural-like network. In Fig. 2 a special form of such a network, useful for our purpose, is illustrated.

In Fig. 2 we show a canonical scheme of the Artificial Neural Network for incremental approximation of the constitutive law.
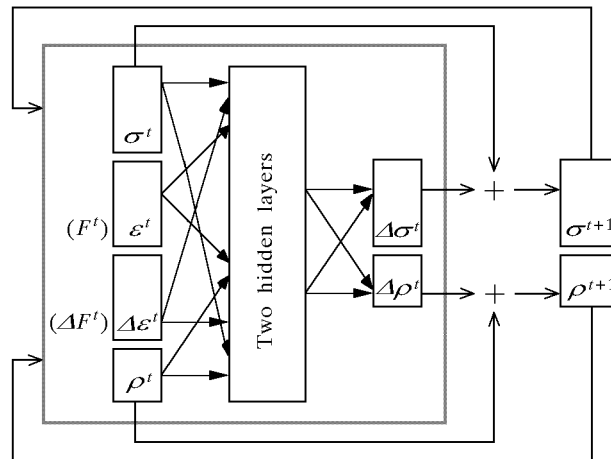

Fig. 2. A scheme of the ANN that is used throughout the paper. The light arrows show spontaneous activity of the net along a given path in the space of deformations. ρ is an internal parameter that allows for many suitable interpretations, depending on the field of application

For such a operational scheme there exist some well developed methods for finding the coefficients: weights and biases.

One can observe that the form of (2.9) for the approximation of the effective constitutive law is identical with expression (3.1), suitably truncated.

3.2. An incremental form of the constitutive equation

In our former papers (Lefik, 1997, 2001; Lefik and Schrefler, 2002, 2003), we showed that the incremental form of the constitutive equation is more suitable for approximation by an Artificial Neural Network. We shortly repeat here the arguments that support this idea.

We consider only a special form of the incremental constitutive law, namely (3.3)

$$\dot{\boldsymbol{\sigma}} = \boldsymbol{g}(\boldsymbol{\sigma}, F, \dot{F}, \rho) \tag{3.3}$$

In this representation F denotes the gradient of deformation, $\boldsymbol{g}$ is a function. It is well known that $\boldsymbol{g}$ in the representation (3.3) can be chosen to fulfill all conditions defining the admissible subspace P in the space of stresses. In this way, the solution $\boldsymbol{\sigma}$ to differential equation (3.3) can be statically admissible. This formulation, on one hand involves only unknown function $\boldsymbol{g}$ that can be well approximated by the ANN, on the other hand does not introduce any "geometric" object in the stress space like a yield surface or other potential usually defined in the case of non associated plastic flow. These are fundamental arguments supporting this representation when an ANN approximation is used. The third important argument is following. The approximation of the incremental form is simpler since the ANN learns only local and short segments of the stress-strain graph. In the hidden layers some neurons specialize in switching between different "current states of stress". Thus, the network can be small and learns quickly. This is shown by examples by Lefik and Schrefler (2003). Some graphs taken from that paper are presented in Fig. 3. In this Figure we see an approximation of the experimental graph of the mechanical histeresis of a superconducting cable, described by Nijuhuis et al. (1998). The graph in this Fig. 3a shows an autonomous activity of the trained ANN along the given "path", as it is expressed by equation (3.4), below. The approximation is realistic and the ANN – very small. Such a result is impossible to obtain by a non-incremental network. In that case a typical result is shown in Fig. 3b.

The incremental approximation of the constitutive law by the ANN can be defined as follows.
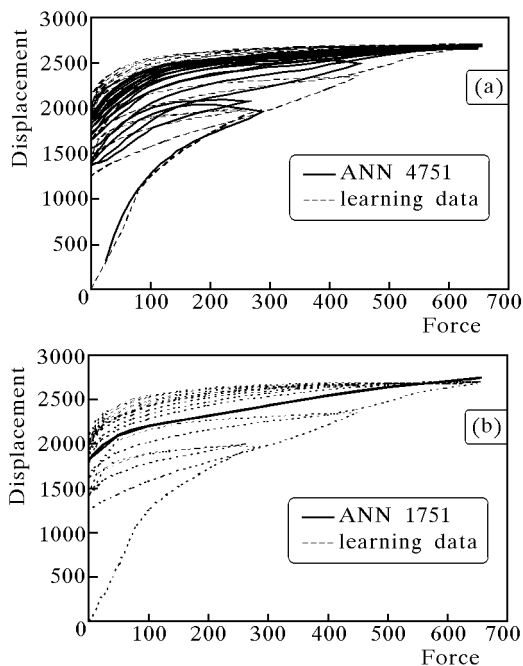
Fig. 3. Experimental graph (dashed line) taken from Nijuhuis *et al.* (1998),
approximated by the incremental and non-incremental ANN (solid line).
Autonomous generation of the graph by the networks for the points never shown in
the training, according to Lefik and Schrefler (2002b): (a) incremental approach,
(b) non-incremental one

The trained ANN is an operator that performs the the following operation

$$(\boldsymbol{\sigma}^t, \boldsymbol{F}^t, \rho^t, \Delta\boldsymbol{F}^t) \rightarrow (\boldsymbol{\sigma}^{t+1}, \boldsymbol{F}^{t+1}, \rho^{t+1}) \qquad \Delta\boldsymbol{F}^t = \dot{\boldsymbol{F}}^t \Delta t \qquad (3.4)$$

3.3. Insertion of the ANN into a Finite Element code

We show next that representations (2.9), (3.1) work well inside a finite element code. Let us suppose that the basic equation for the standard; displacement-based finite element method can be written in the form

$$\int\limits_V \mathbf{B}_N^\top : \boldsymbol{\tau} \, dV^0 = \int\limits_S \mathbf{N}_N^\top \boldsymbol{t} \, dS + \int\limits_V \mathbf{N}_N^\top \boldsymbol{f} \, dV$$

$$\boldsymbol{\varepsilon}(d\boldsymbol{u}) = \mathbf{B}_N d\boldsymbol{u} \tag{3.5}$$

where V is the volume of the body in the reference configuration, $\mathbf{B}_N$ is the matrix that operating on the vector of admissible variation of independent

variables to give the strain measure $\boldsymbol{\varepsilon}(d\boldsymbol{u})$ coupled with the material stress $\boldsymbol{\tau}$. In what follows in the paper, we will consider small transformations, thus an infinitesimal strain tensor. The index N means that $\mathbf{B}$ is constructed on the basis of the approximation of $\boldsymbol{u}$ by a set of interpolation functions $\mathbf{N}(\boldsymbol{x})$ on appropriate finite elements. On the right-hand side of (2.8) $\boldsymbol{t}$ is a stress vector given on the part S of the boundary, while $\boldsymbol{f}$ are body forces acting on the elementary volume dV.

Since the considered material behaviour is non-linear, the Newton algorithm will be applied to solve the system of equations (2.8). The Jacobian of the left-hand side of (2.8) can be written as follows

$$J = \int_V [d\boldsymbol{\tau} : \boldsymbol{\varepsilon}(d\boldsymbol{u}) + \boldsymbol{\tau} : d\boldsymbol{\varepsilon}(d\boldsymbol{u})] \, dV^0 \tag{3.6}$$

The first term in integral (2.9) can be computed using a usual constitutive assumption

$$d\boldsymbol{\tau} = \mathbf{D} : d\boldsymbol{\varepsilon} \tag{3.7}$$

where $D_{ij} = \partial\tau_i/\partial\varepsilon_j$.

We can rewrite the above equations, taking variation with respect to the independent variables of the problem $\boldsymbol{u}$ and obtaining (by definition) the stiffness matrix $\mathbf{K}$

$$K_{MN}^{main} = \int_{V^0} \mathbf{B}_M : \mathbf{D} : \mathbf{B}_N \, dV^0 \tag{3.8}$$

The second term in integral (3.6) represents the initial stress matrix.

Using the assumed representation of the constitutive law by the ANN, instead of (3.7) we obtain

$$d\boldsymbol{\tau} = N_{d,\sigma}@d\boldsymbol{\varepsilon} \tag{3.9}$$

The index d denotes that the network quality is best for some given value of the increment d, σ means that the stress increment is computed at the current value of $\boldsymbol{\tau} = \boldsymbol{\sigma}$. It is clear that we must replace the neural operator in (3.1) by the matrix $\mathbf{D}$ or simply, construct this matrix using the given representation of the constitutive law. This will be done by trial incrementation of $\boldsymbol{\varepsilon}$. Let us suppose that both tensors $d\boldsymbol{\tau}$ and $d\boldsymbol{\varepsilon}$ are represented by column vectors

$$\begin{aligned} d\boldsymbol{\sigma} &= [d\boldsymbol{\tau}_1, d\boldsymbol{\tau}_2, d\boldsymbol{\tau}_1] = [N_{d,\sigma}@d\boldsymbol{\varepsilon}_1, N_{d,\sigma}@d\boldsymbol{\varepsilon}_2, N_{d,\sigma}@d\boldsymbol{\varepsilon}_1] \\ [d\boldsymbol{\varepsilon}^t] &= [d\boldsymbol{\varepsilon}_1, d\boldsymbol{\varepsilon}_2, d\boldsymbol{\varepsilon}_3] \\ \mathbf{D} &= [d\boldsymbol{\sigma}][d\boldsymbol{\varepsilon}^t]^{-1} \end{aligned} \tag{3.10}$$

The matrix of trial vectors $d\varepsilon^t$ is always proportional to the strains in the last equilibrated point (σ, ε) during the Newton iteration process (preceding step). The trial vectors cannot be arbitrary because $N_{d,\sigma}@d\varepsilon \neq -N_{d,\sigma}@(-d\varepsilon)$, and in fact two different tangent stiffness matrices can be defined in any point: one for loading and the other for unloading. It is supposed then that the loading (unloading) is continued during current increment in the Newton iterations. Formulae $(3.10)_{1,2}$ are used here instead of computing the derivatives of the neural network with respect to input values.

The stress in the second term in integral (3.6) is computed using the neural network in the recall mode for a given constant step $d\varepsilon$, until the strain ε at the trial solution in the current step is reached. The ANN acts here in the autonomous activity mode as it is defined in Section 3. This process corresponds to classical integration of the incremental constitutive equation for updating σ. It always starts in the last equilibrated point, and the increment $d\varepsilon$ is proportional to the one defined for this step (loading or unloading).

4. Classical homogenisation procedure directly interpreted by the Artificial Neural Network

It can be shown that the vector of homogenisation functions, Eq. (2.5), appears as a perturbation field in the numerical experiment in which the cell of periodicity is loaded with a uniform displacement of points on the border. This imposes a given average strain state equal to the homogeneous one, computed from formula (2.9) in which $\boldsymbol{u}$ is to be applied on the border

$$u_i = e_{ij}^{ave} x_j \tag{4.1}$$

The corresponding stress can be obtained according to expression (4.2) with $\boldsymbol{t}$ used for the stress vector on the boundary of the cell

$$\sigma_{ij}^{ave} = \int\limits_{\partial Y} x_i \otimes t_j \; ds \tag{4.2}$$

Since Eq. (2.9) is a universal approximator, the introduced assumption does not restrict the possible effective behaviour. Like in the periodic homogenisation, we discover rather than impose the global constitutive law. All the constitutive information is in the data set furnished to the network.

4.1.   Constitutive data-base for the training

A constitutive data-base contains pairs of input vectors and output vectors for the training of the network. The input and output is accorded with the structure of the ANN (Fig. 2) and is always of the form:

$$\{(\text{input vector}), (\text{output vector})\}$$

For the case of the incremental law, for the k-th pattern, we have

$$\{[\varepsilon_i, \boldsymbol{\sigma}(\varepsilon_i), \boldsymbol{\eta}_i, \Delta\varepsilon_i], \Delta\sigma_{\alpha\beta i}\}_k \tag{4.3}$$

Additionally, in the below shown example, we must satisfy the following condition imposed by isotropy of the approximated constitutive law (@ denotes the action of the neural network operator on the input data)

$$\forall i \ \text{ if } \ N@\left\{\begin{array}{c} \varepsilon_i \\ \boldsymbol{\sigma}_i \\ \eta \\ \Delta\varepsilon_i \end{array}\right\} = \{\Delta\boldsymbol{\sigma}_i\} \ \text{ then } \ \forall\boldsymbol{\Theta} \quad \boldsymbol{\Theta}^\top\boldsymbol{\Theta} = \mathbf{1} \ \text{ we have}$$

$$N@\left\{\begin{array}{c} \boldsymbol{\Theta}^\top\varepsilon_i\boldsymbol{\Theta} \\ \boldsymbol{\Theta}^\top\boldsymbol{\sigma}_i\boldsymbol{\Theta} \\ \eta \\ \boldsymbol{\Theta}^\top\Delta\varepsilon_i\boldsymbol{\Theta} \end{array}\right\} = \{\boldsymbol{\Theta}^\top\Delta\boldsymbol{\sigma}_i\boldsymbol{\Theta}\} \tag{4.4}$$

To satisfy condition (4.4), we must train the network with some supplementary data: the new subset of patterns is of the form

$$\left\{[\boldsymbol{\Theta}^\top\varepsilon_i\boldsymbol{\Theta}, \boldsymbol{\Theta}^\top\boldsymbol{\sigma}_i\boldsymbol{\Theta}, \boldsymbol{\eta}_i, \boldsymbol{\Theta}^\top\Delta\varepsilon_i\boldsymbol{\Theta}], \boldsymbol{\Theta}^\top\Delta\sigma_{\alpha\beta i}\boldsymbol{\Theta}\right\} \tag{4.5}$$

The subscript k refers to the pattern obtained from the ith experimental point by transformation via the kth rotation matrix $\boldsymbol{\Theta}$. The total number K of these additional terms in the matrix of patterns depends on the number of trial rotation needed to train the network up to a satisfactory level of tolerance. An artificial construction of the experimental data has been necessary to perform a 2D numerical experiment.

In this case, the source of constitutive data is a numerical experiment defined with expressions (4.1) and (4.2) executed on a single cell of periodicity of the composite. The results of FE computations for different (assumed and imposed over the cell) values of a small deformation tensor or tensor of deformation gradient must be completed by the manipulation prescribed by (4.4).

4.2. Example

As an example, we consider a hyperelastic composite, the repetitive cell of which consists of a neohookean material with a circular hole of the radius equal to the distance between the neighbouring, circular pore.

In Fig. 4 this situation is shown. In Fig. 5 some of deformed configurations are presented. The number of such numerical experiments was 1260, including incrementation. The full constitutive data base containing all rotated data was much bigger. As far as the increments with the negative sign were concerned it was about 15000 patterns. The training was organized by epochs that contained about 1250 patterns. After the first decisive reduction of the error of the training, most of the patterns used as the test data revealed very good coherence with the training results.
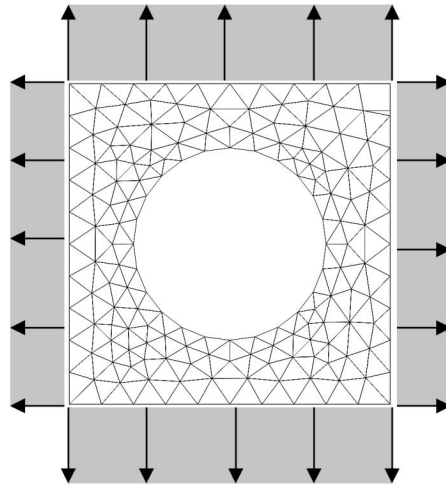

Fig. 4. A single cell of periodicity of the composite

5. The self-learning Finite Element code for deducing effective constitutive relationships from a numerical experiment

The self-learning finite element procedure is based on the standard FE code including the Newton-Raphson type iterative method. The neural constitutive model, Eq. (3.1), can be applied for the solution to general structural problems in the same manner as the conventional one. All details can be found
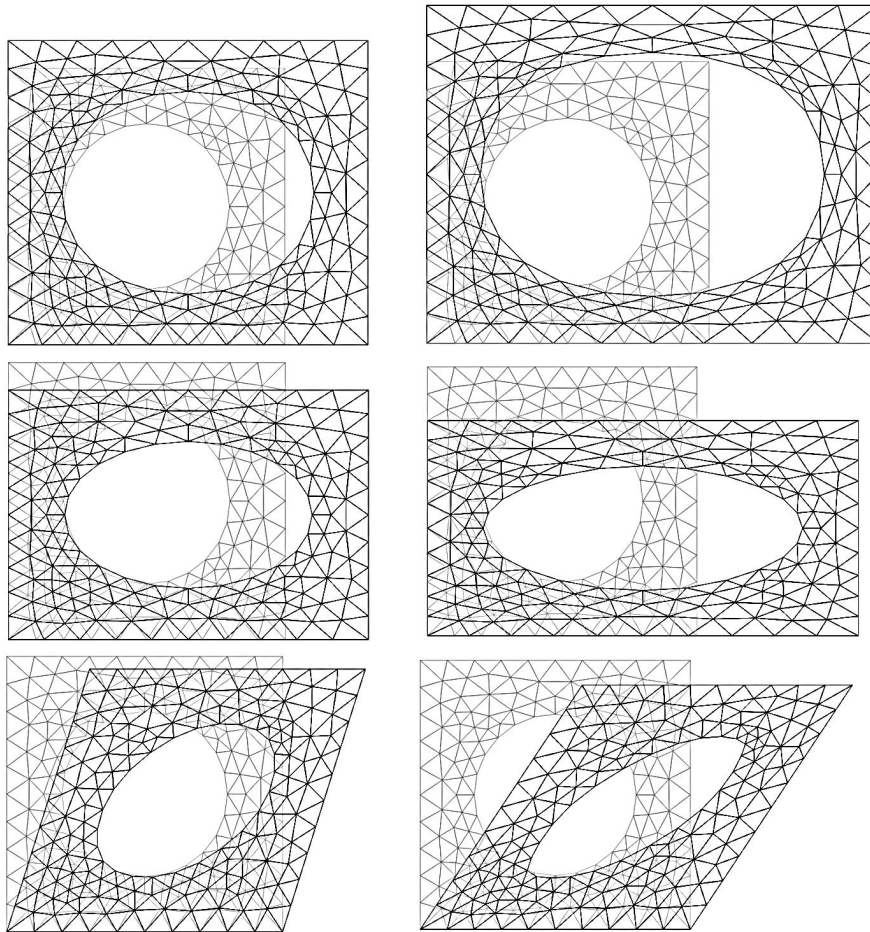
Fig. 5. Examples of trial deformations of the cell of periodicity – a source of the constitutive data

in Shin and Pande (2000, 2001). The main advantage of this substitution is the possibility to modify the constitutive model simply by retraining the neural network. This feature results in a self-learning code, which evaluates the supplied ANN model and adjusts itself to a desirable response of the structure. This strategy permits the constitutive relationship to be built directly from experimental data or, alternatively, from the exact FE solution. In our case, it is solution of (2.1) for a structure composed of many repetitive cells of the given internal structure (may be very complicated). If the considered number of cells is large enough we are able to capture its effective (global) properties.

The procedure starts with calculation of the trial FE solution using any initial constitutive law (e.g. linear constitutive matrix). Pairs (e_I, σ_I) at each Gauss point on any considered load level are saved for future training of the ANN. The displacements at some strategic points of the structure are monitored δ_I and compared with the known data describing the behaviour of the composite material δ_D. Those vectors constitute, respectively, the output and the target of the whole procedure.

The current adjustment is measured by means of the normalized root-mean square error calculated as follows (instead of $(2.6)_1$)

$$Err = \frac{1}{\delta_D^{max} - \delta_D^{min}} \sqrt{\frac{1}{MN} \sum_{n=1}^{N} \sum_{m=1}^{M} (\delta_{II,n}^m)^2} < \tau \tag{5.1}$$

In (5.1), N is the number of load increments, M – number of monitored displacements, the vector $\delta_{II} = \delta_I - \delta_D$ represents the errors made by the ANN at the monitored points and δ_D^{max}, δ_D^{min} are the maximum and minimum values of $|\delta_D|$, respectively.

In the following, the displacement differences δ_{II} are treated as the load for the new solution. The obtained strain-stress pairs (e_{II}, σ_{II}) are used to correct the current guess (e_I, σ_I)

$$e^{train} = e_I \qquad\qquad \sigma^{train} = \sigma_I + \sigma_{II} \tag{5.2}$$

Such prepared training data (5.2) are used for retraining the neural network that forms the constitutive model. The new weights of the ANN are saved and the next step of the self-learning procedure starts with the corrected ANN constitutive model. If the value of E becomes lower than the tolerance level τ ? or the admissible number of self-learning steps is reached, the process is finished. According to Shin and Pande (2000, 2001), this procedure converges.

5.1. Example

We consider the same example as in Section 4.3. This time, however, a sample containing several cells is considered. The non-deformed cell of periodicity forms a square with a hole of diameter equal to half of the edge. For acquisition of the constitutive data we perform three different numerical FE experiments (because of (2.6)). All these experiments are qualitatively different than those proposed by Shin and Pande. We impose uniform displacements of borders of a portion of the composite. The nature of these kinematic loadings is easily seen in Fig. 8: two different tests of tension (free and constrained tension) and a shear test. The controlled quantities are now values of reactions in the boundary

nodes. A test like this was never proposed by the authors of the self-learning method since its original application was acquisition of the constitutive data from real and in situ observations. It is obvious that the point-wise reaction is not an observable quantity. In the context of the numerical experiment this strategy works quite well, even in the analysis of composite materials for which the stress jumps in the small scale of the body. In the approximation of the constitutive law an incremental constitutive description and the corresponding architecture of the ANN has been used (described by Lefik (2001)).
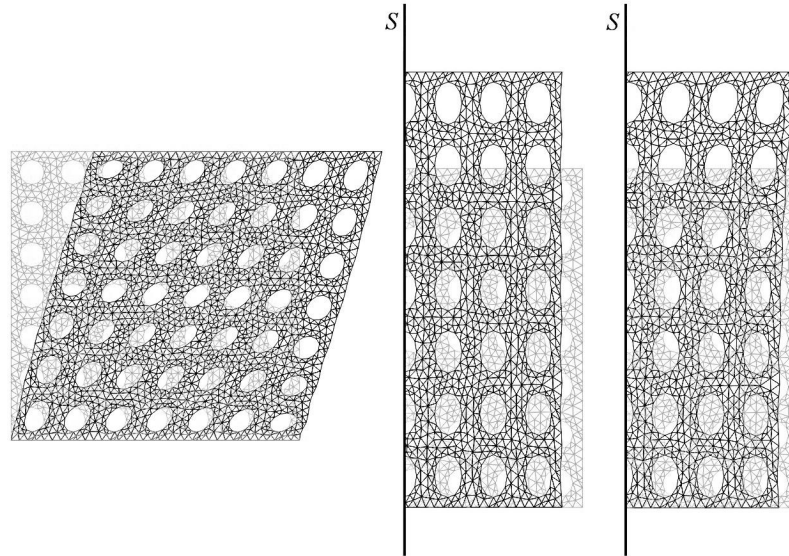

Fig. 6. Three numerical tests on a sample of the composite used simultaneously for the preparation of the data-base for ANN training

5.2. Discussion of the results

In Fig. 7 two testing finite element computations are shown. These computations have been executed for a loading never used in the training and with the FE code including the ANN inside. A relatively small ANN with 10 and 7 neurones in hidden layers have been trained with the constitutive data collected from each first Gauss point of the homogeneous problem (the black, rectangular mesh in Fig. 7). The performance of the trained ANN was checked with the loading scheme never used in the training. This scheme is shown in Fig. 7. The coarse, rectangular mesh (dark line) represents the displacements of the "effective", homogeneous body under action of the horizontal shearing
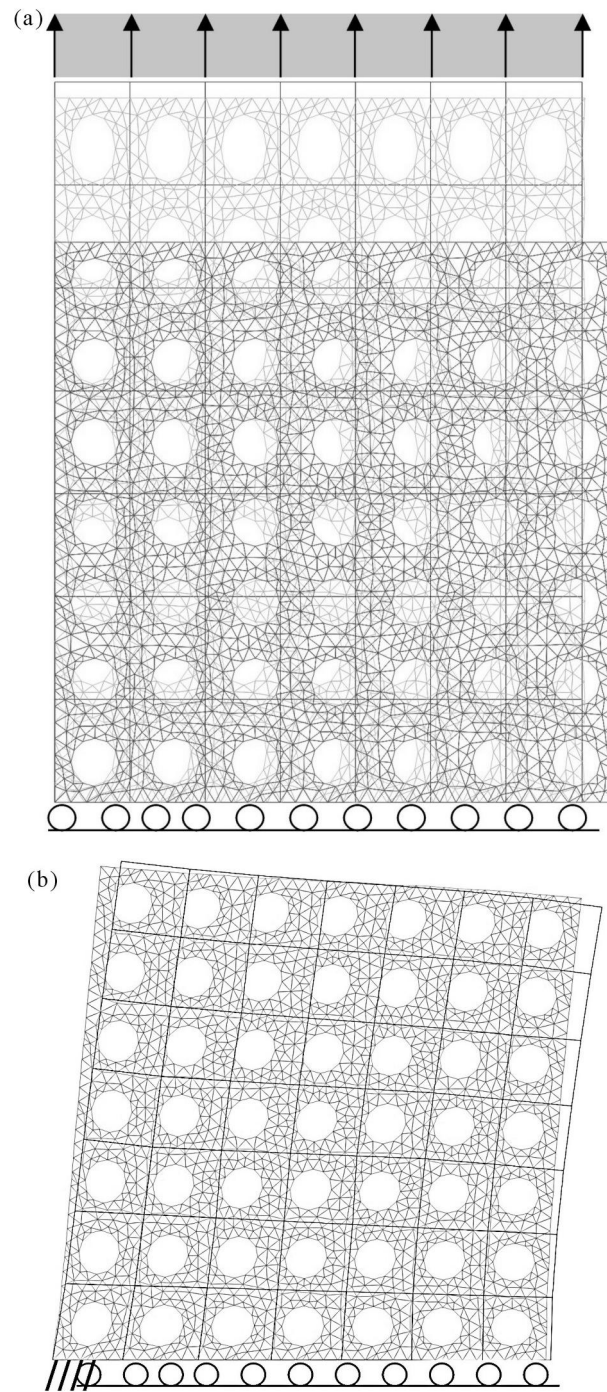
Fig. 7. Two numerical tests on a sample of the composite that have never been used
in the training. The coars mesh – results obtained for the effective model, the light
deformed mesh – "exact" solution

stress vector applied to the upper edge of the rectangular sample. This computation was carried out by FE-ANN code (the FE code published by Bonet and Wood (1997) was modified and used). The triangular mesh (light lines) represents the "true" deformed configuration. The coarse mesh is defined for the homogenised body. The qualitative accordance is good, the maximum error in displacements does not exceed 5%.

In Fig. 8, the difference of the return curve and the one obtained with the loading is used as the measure of the error. It is known that for hyperelastic composites these two curves should coincide. What is shown in Fig. 8 is obtained for the example trained within the direct approach. In Fig. 8b the curves coincide much better that in Fig. 8a. The self-learning method of data acquisition is more efficient. In this case the ANN is simply "tailored" for the Finite Element code in which will be included as a constitutive procedure.
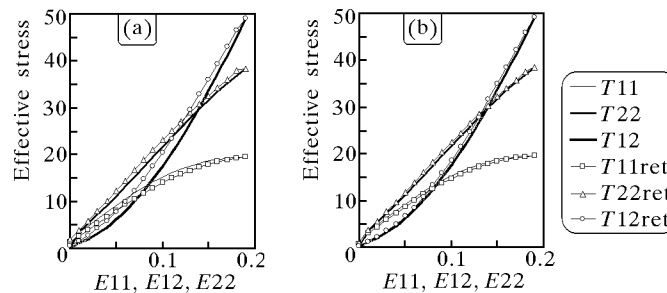

Fig. 8. Comparison of loading and unloading stress-strain curves used as the measure of the error of the ANN representation of the constitutive law inside the FE code

In the example, only three cases of load are reported. As far as the convergence to zero is concerned, see Bandeira *et al.* (2001), a relatively small trial portion of the composite is sufficient to predict the overall behaviour of the non-homogeneous material. In our example we consider only 20 cells of periodicity but even in this case we notice that the perturbation of the mean displacements is negligible.

6. Conclusions

We conclude that the effective constitutive law for a composite can by approximated by the Artificial Neural Network with hidden layers. This approximation does not constrain the form of unknown effective relationships.

The following condition must be fulfilled to assure successful approximation:

- The constitutive law must be formulated in the incremental form
- The ANN must be included as a subroutine in the Finite Element procedure.

Moreover:

- The self-learning procedure seems to be a very effective tool for the identification of the global behaviour of composites. The microstructure of the material (position of the monitored point on the cell of periodicity) does not influence the identification abilities of the program.
- The ANN representation of any constitutive law is a flexible tool for the representation of the effective (global) behaviour of materials with a complex internal microstructure.
- This representation is very suitable for analysis of composites since it is "automatic" in the sense that it does not require any *a priori* choice or adaptation of the existing constitutive theory for the description of the observed material behaviour.
- The convergence is surprisingly fast. Four steps are enough to obtain a qualitatively good model.
- A representation of the effective constitutive law can be very simple (a network of the architecture 3-6-3 is sufficient in the first example).
- The usefulness of the hybrid FE-ANN code has been confirmed since it opens up new possibilities in comparison with the standard FE codes in the sense that the constitutive models can be easily modified and its simplicity accelerates work of the program.

These conclusions have been supported by examples, not by a theoretical proof.

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Zastosowanie sztucznych sieci neuronowych w modelowaniu numerycznym kompozytów przy pomocy metody elementów skończonych

Streszczenie

W artykule opisano zastosowanie sztucznych sieci neuronowych do określenia efektywnego związku konstytutywnego dla kompozytów. To narzędzie numeryczne użyte zostało dwojako: do bezpośredniego zapisu wyników otrzymanych w ramach klasycznej metody homogenizacji oraz do wnioskowania o własnościach efektywnych na podstawie eksperymentu numerycznego (zastępującego eksperyment rzeczywisty) wykonanego na małej, lecz reprezentatywnej próbce kompozytu. W tym drugim przypadku zastosowano schemat „samouczącego się" programu metody elementów skończonych, w którym związek konstytutywny opisany jest siecią neuronową. Schemat ten zaadaptowano tak, że może być użyty w przypadku obciążeń niemonotonicznych oraz wtedy, gdy zależność: miara odkształcenia–miara naprężenia nie jest wzajemnie jednoznaczna. Te nowe możliwości uzyskane zostały dzięki przedstawieniu związku konstytutywnego w formie przyrostowej oraz opracowania odpowiedniej do tego budowy sieci neuronowej. Schemat „samouczącego się" programu MES charakteryzuje się tym, że proces formułowania nieznanego związku konstytutywnego jest szybki, a zgodność modelu numerycznego z eksperymentem większa niż dla innych metod.