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PREDICTION OF ESHELBY'S INCLUSION PROBLEM SOLUTION USING ARTIFICIAL NEURAL NETWORK

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Abstract: *In this contribution we present our new approach to obtain or better estimate mechanical fields (strain, stress and displacement) inside isotropic infinite body with ellipsoidal-like inclusions. The precise solution has been given by J. D. Eshelby (1957) to internal and external points of inclusion domains and form the basis of our work. When the Eshelby's solution is extended to take into account perturbations due to the presence of numerous adjacent inclusions (Novák et al., 2012; Oberrecht et al., 2013) the solution given for dozens of points is very time demanding. Utilizing Artificial Neural Network (ANN) trained by exact Eshelby's solutions to predict mechanical fields can be achieved considerable speedup at the cost of approximate solution. At this state we only focus on prediction of one component of a perturbation strain tensor for single ellipsoidal inclusion.*

Keywords: Micromechanics, Isotropic Ellipsoidal Inclusions, Eshelby's Solution, Artificial Neural Network.

1. Introduction

In these days, composite materials form an integral part of the world around us. Whether it's a well-known material or material being just developed, we want to know the most about their properties and their behaviour at the macro or micro level. In this paper, we focus on the micro level behaviour of composite non-dilute material consisting of isotropic ellipsoidal-like inclusions and isotropic infinite matrix. Our main interest is the evaluation of micromechanical fields (strain, stress and displacement) on this type of material.

2. Eshelby's Solution

The analytical solution for elastic fields caused by inclusions has been given by J. D. Eshelby (1957). In his work Eshelby shows that this problem can be decomposed into exactly two tasks of a known solution

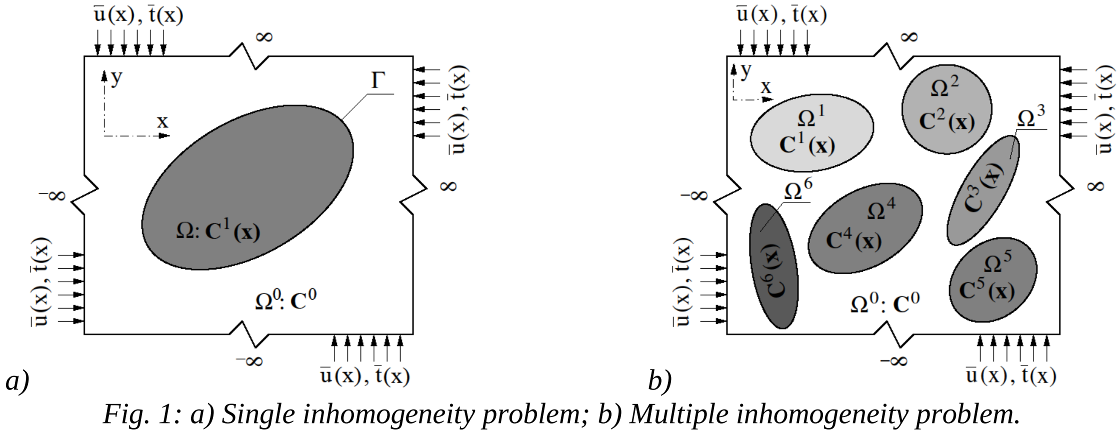

Fig. 1: a) Single inhomogeneity problem; b) Multiple inhomogeneity problem.

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and then assembled back by making use of the superposition principle. The solution of a single inhomogeneity problem, see Fig. 1a, is therefore given as the sum of homogeneous infinite body problem and homogeneous inclusion problem, so called perturbation part of mechanical fields (Eshelby, 1957; Mura, 1982). In case of multiple inhomogeneity (Fig. 1b), the solution of mechanical field within a body with N inclusions is obtained as the sum of N single inclusion tasks scaled by a multiplier associated with each inclusion so as to fulfil self-equilibrium as presented in paper by Novák (2008).

Using these solutions and computer programming the µMECH library (Novák et al., 2012; Oberrecht et al., 2013) was created for solving micromechanical fields in materials with single or multiple inclusions. But, despite the performance of computers, the solution for thousands of points (no matter if internal or external) is very time demanding. Therefore, we came up with the idea of speeding up the process with predicting approximate solutions by an Artificial Neural Network (ANN).

3. Artificial Neural Network

Artificial Neural Networks (ANN) are computational models based on central nervous systems, especially on brain (Gurney, 2002; Haykin, 2009). These models are capable of machine learning and recognizing of patterns in given data. ANN consists of many simple processing nodes – so called neurons – interconnected into systems that can change their structure during the training (learning) phase. To each connection between two neurons is assigned an adaptive value representing synaptic weight of this connection. Based on given data and respective results used as an external information flowing through the system, these weights are balanced in a way that the output of ANN corresponds to the actual results.

There are numerous types of ANNs from single-directional systems to complicated multi-directional systems with many inputs and nested loops. One specific type of ANN is the feed-forward neural network. In this system, neurons are organized into layers where connections among neurons are placed only between adjacent layers, as shown in Fig. 2. There are no loops, cycles or feed-back connections.

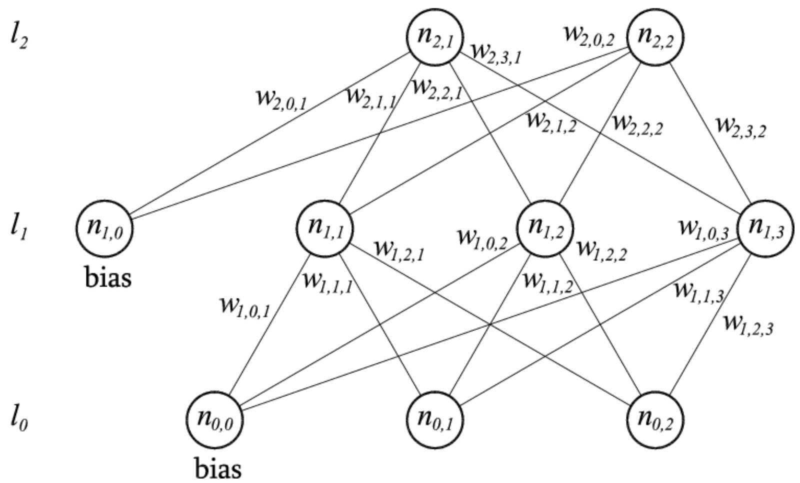


Fig. 2: Example of feed-forward Artificial Neural Network.

The most widely used example is the multi-layer perceptron (MLP) with the sigmoid transfer function and the gradient descent method of training – so called backpropagation learning algorithm. The power of MLPs lies in their ability to approximate nonlinear relations which corresponds to our problem, so when speaking about ANN in the following text, the MLP is considered.

4. Prediction of Eshelby's Solution

As described in section 2, the solution for materials with multiple inclusions is decomposed into separate solutions, each for every inclusion. Therefore, we assume here only single inclusion in the infinite isotropic body. But even so, the solution of mechanical fields depends on many input variables, such as load case, Young's modulus and Poisson's ratio of the inclusion and matrix, dimensions and rotations of the inclusion in space, coordinates of the inclusion centre and coordinates of a point where we want to evaluate mechanical fields.

4.1. ANN model and samples generation

For a sake of simplicity, we decided to start with the simplest model where the only variables are coordinates of a given point and all the inclusion and matrix parameters are fixed. In such a case, the coordinate system of the inclusion coincides with the coordinate system of the applied load case and we can limit the domain of point coordinates to only the first octant of the inclusion coordinate system. That is because the mechanical fields around inclusion are symmetrical to planes defined by semiaxes of inclusion. The centre of the inclusion matches the centre of a used coordinate system.

To generate uniformly distributed samples of point coordinates, we used software called SPERM 2.0 (Novák, 2011) based on method of Latin Hypercube Sampling (LHS). In total we generate *10 000* points with uniformly distributed coordinates *x*, *y* and *z* in range from *0.0* to *0.5*. Other material properties and used constants are listed in table 1. As the load case is always the remote unit strain, particular units are irrelevant thus it is only a question of scaling.

Tab. 1: Material properties and used constants.

Properties and constants	***Infinite matrix***	***Inclusion***
Young modulus	*5*	*50*
Poisson's ratio	*0.25*	
Load case	*remote strain* ε_{xx} *= 1.0 in inclusion centroid*	
Semiaxes dimensions	*/*	$a_1 = 0.15; a_2 = 0.1; a_3 = 0.05$
Euler angles	*/*	$\alpha = \beta = \gamma = 0.0$

4.2. Model training

For the ANN training phase the reference results are needed. We used the above-mentioned µMECH library and for each point solve the perturbation fields. As another part of simplification we decide to predict only one element from the results, the perturbation strain ε_{xx}. From these results, we create a cumulative distribution function (CDF), as we want the results to be in uniform distribution.

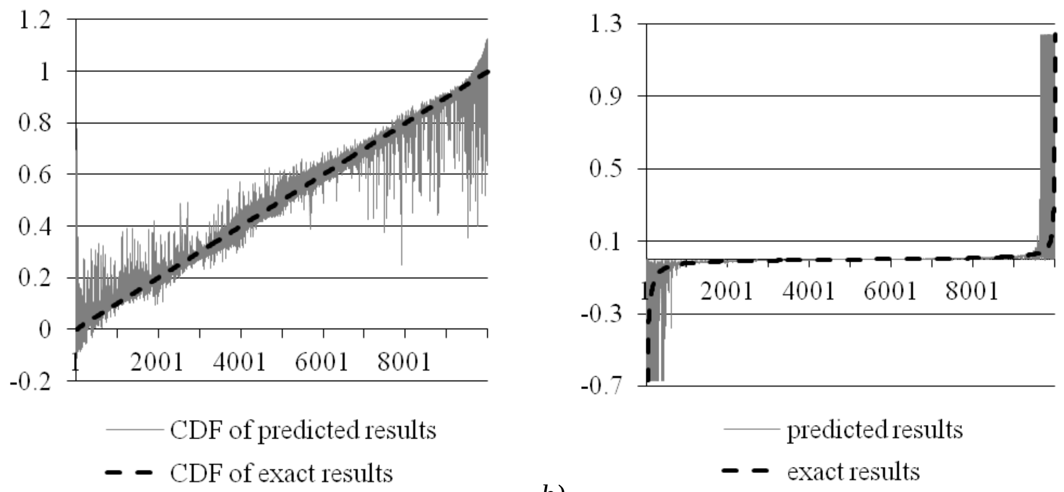
To create and train the ANN we used software called RegNeN 2012 (Regression by Neural Network) (Mareš and Kučerová, 2012) which is a software package for computing a regression for given data using artificial neural network. During the training phase the neural system itself is created. It is composed from three input neurons in the first layer, *n* neurons in the second so called hidden layer and one output neuron in the third layer. Numbers of neurons in hidden layer depend on the self validating process for which the software uses so called cross-validation method.

In this method the samples are divided into *m* parts from which *m-1* parts are used to calibrate the weights between neurons and the remaining part is used for validation. Then one neuron is added into hidden layer, the process of calibrating is repeated with different *m-1* parts and for validation is used the current remaining part. This is repeated *m-times* and finally the ANN with smallest error is saved.

4.3. Results verification

In practical use, this is the place when the desired prediction of results takes a turn. Material for which we want to know the mechanical fields must be distributed in the same data format as was used in the training phase. These simple inputs are forwarded to already trained ANN which in a split of a second return predicted results based on previously calibrated synaptic weights.

But because of the development of this method we are more interested in the accuracy of predicted results than the results itself. So we take all of the *10 000* input samples that we used for the ANN training and perform the prediction of results. Since we used the CDF values for ANN training, the predicted results were also in a scale from 0 to 1. The difference between exact and predicted data in CDF values is shown on Fig. 3a. Data on Fig. 3b are the same values only converted back using the inverse CDF.



a) *b)*

Fig. 3: Comparison of predicted results and exact results in: a) CDF values; b) Original values.

5. Brief Results

As can be seen from Fig. 3 the predicted results are distorted with an error which is most evident with the outlying data. In the case that the training data set will contain a sufficient representation of these outlying values the ANN should be able to better detect correlations for these values and predict better results. So we see a possible improvement in the use of a much larger set of training data.

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