Calculation of the effective properties of the prestressed nonlinear elastic heterogeneous materials under finite strains based on the solutions of the boundary value problems using finite element method

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Abstract. This paper describes the approach and algorithms for numerical estimation of the effective properties of the prestressed nonlinear elastic heterogeneous materials under finite strains. To numerically evaluate effective properties on a representative volume (or periodicity cell), a series of sequences of elasticity problems differing in the type of the applied boundary conditions is solved. In all the problems being solved, along with the specially applied boundary conditions, the model undergoes the same predetermined prestress. In addition, a separate problem is being solved, in which, besides the prestressed state, zero displacement of the model boundary are set. The results of solving each problem in the form of stress tensors are averaged over the volume. Numerical calculations were carried out using the Fidesys Composite software module of the Fidesys CAE system using the finite element method. The paper presents the solution to a number of problems to estimate the effective coefficients of the porous material prestressed by pore pressure. Dependence graphs of effective properties on porosity and on size of pore pressure are constructed.

1. Introduction
In the numerical strength modeling of heterogeneous materials (composite, porous), it is necessary to know their average (effective) mechanical properties. Therefore, the problem of averaging their mechanical properties arises. Given the known geometry of the heterogeneous material and the known properties of its constituents, it is necessary to calculate the effective (i.e. averaged) properties of the heterogeneous material [1-8]. There are various ways to solve such a problem: both analytical ones – with the help of formulas, and numerical ones – using modern computer facilities.

The paper considers an approach to the numerical estimation of the effective nonlinear elastic properties of heterogeneous materials under finite strains, based on the numerical solution of boundary
value problems on a representative volume or cell of the periodicity of the material. Calculations on a representative volume were carried out using the finite element method [4, 5] with the help of CAE Fidesys [6].

2. Method for calculating the effective properties of the prestressed material
A representative volume of a heterogeneous material is the minimum volume of the material, on which it is possible to carry out any experiments or measurements on the basis of which results can be drawn some conclusions on the material behavior in general. If the heterogeneous material has an irregular structure, its representative volume must contain a sufficiently large volume of each component to allow averaging the properties of the entire material. If the material has a periodic structure, then a periodicity cell is used instead of a representative volume.

2.1. Estimation of the effective nonlinear-elastic properties of the unstressed heterogeneous material
We shall first give a definition of effective elastic properties. We call an effective (averaged) material (in terms of elasticity) such a homogeneous material that will satisfy the following condition: if we consider the representative volume of the original heterogeneous material and fill exactly the same volume with this homogeneous material, then the average (averaged over the volume) stresses on these two volumes will be equal for the same displacements at the volume boundaries. The elastic properties of the effective material will be called effective elastic properties of the original heterogeneous material.

Using this definition, we describe the technique for estimating the effective nonlinear-elastic properties of the heterogeneous material under finite strains. For a representative volume \( V_0 \) in the form of a rectangular parallelepiped of size \( 2A \times 2B \times 2C \), which faces are parallel to the coordinate planes, a certain sequences of boundary value nonlinear elasticity problems are solved in the coordinates of the initial (unstrained) state [9] (for the equilibrium state):

\[
\nabla \cdot \sigma = 0 \quad \text{or} \quad \nabla \cdot \mathcal{R} = 0
\]  

(1)

with non-periodic boundary conditions in the form of a given displacement vector of each boundary point

\[
\left. u \right|_0 = r \cdot (\Psi' - I)
\]  

(2)

or with periodic boundary conditions in the form of links to displacements of opposite points of the boundary

\[
\begin{align*}
    u^1_1 - u^{-1}_1 &= -2A(\nu_{11} - \delta_{11}) \\
    u^2_2 - u^{-2}_2 &= -2B(\nu_{22} - \delta_{22}) \\
    u^3_3 - u^{-3}_3 &= -2C(\nu_{33} - \delta_{33})
\end{align*}
\]  

(3)

where \( \sigma \) is a true stress tensor, \( \mathcal{R} \) is the first Piola stress tensor, \( \nabla \) is a gradient operator, \( r \) is a radius vector, \( \Psi' \) is an effective deformation gradient, \( \nu_{ij} \) are its components, and \( u \) is the displacement vector of the point. For periodic boundary conditions:

1) pair (1; -1) – opposite nodes on faces of representative volume perpendicular to the \( X \) axis;
2) pair (2; -2) – opposite nodes on faces of representative volume perpendicular to the \( Y \) axis;
3) pair (3; -3) – opposite nodes on faces of representative volume perpendicular to the \( Z \) axis.

For a representative volume (or periodicity cell), 21 sequences of boundary value elasticity problems are solved. Various problem sequences differ in the type of applied boundary conditions (i.e., in the type of the effective strain tensor on a representative volume). Different tasks within the
same sequence are distinguished by the strain value for the same type (each sequence contains 3-4 problems or more, if necessary). Strains of the following types are applied:

1) tension/compression (along each of the coordinate axes);
2) shears (in each of the coordinate planes);
3) biaxial tensile strain
4) superposition of tension strain and shear;
5) superposition of shears.

As a result of the solution of each boundary value elasticity problem, the distribution of the true stresses tensor $\sigma$ on a representative volume (or periodicity cell) is calculated. It is averaged over the strained volume by the formula

$$\sigma^e = \frac{1}{V} \int \sigma dV$$ (4)

Thus, we get an effective (average) stress tensor $\sigma^e$.

The effective Green stress tensor $E^e$ is calculated from the known effective strain affinor given in (2) according to the formula:

$$E^e = \frac{1}{2} (\Psi^e \cdot \Psi^e - I)$$ (5)

Whereas, the effective second Piola-Kirchhoff stress tensor $\Sigma^e$ is calculated from the effective deformation gradient and the effective stress tensor computed in (4):

$$\Sigma^e = (\det \Psi^e)(\Psi^e)^{-1} \cdot \sigma^e \cdot (\Psi^e)^{-1}$$ (6)

Thus, for each problem of each sequence, an effective Green stress tensor $E^e$ is actually given; and the effective second Piola-Kirchhoff stress tensor $\Sigma^e$ is calculated. Since various problems in the same sequence differ only in the magnitude of the strain, and the type of strain is preserved, the dependence of the effective Piola-Kirchhoff tensor on the characteristic value of the strain magnitude $q$ is constructed for each sequence:

$$\Sigma^e_{ij} = a_{ij}^0 q + a_{ij}^1 q^2$$ (7)

The coefficients $a_{ij}^0$ and $a_{ij}^1$ for each of the 21 dependences are calculated using the least square method. Further on the basis of these dependences, the effective nonlinear-elastic properties of the material are estimated in the form of a quadratic dependence of the Piola-Kirchhoff stress tensor $\Sigma^e$ on the Green stress tensor $E^e$:

$$\Sigma^e_{ij} = C_{ijkl}^0 E^e_{kl} + C_{ijklm}^1 E^e_{kl} E^e_{mn}$$ (8)

Therefore, estimation of effective elastic properties in nonlinear form is a calculation of coefficients $C_{ijkl}^0$ and $C_{ijklm}^1$ from (8).
2.2. Taking account of prestress in the estimation of the effective nonlinear elastic properties

The main point of the above-described methodology for estimating the effective elastic properties of the heterogeneous material is as follows: an unstressed representative volume or periodicity cell (i.e., a volume or a cell average strains and stresses in which are initially equal zero) undergoes certain mechanical actions that cause some average strains, which result in some average stresses in the model. The relationship between the resulting average stresses and strains makes it possible to estimate the effective elastic properties of the material.

There is also the case when it is necessary to numerically estimate the effective properties of the heterogeneous material subjected to prestress, for example, a porous material stressed by pore pressure. If the problem is solved in linear statement, such prestress will not affect the effective elastic properties of the material in accordance with the principle of superposition. Therefore, we describe the approach to the estimation of the effective elastic properties of the prestressed heterogeneous material under finite strains, taking into account geometric and physical nonlinearity.

Differences from the technique described in the previous paragraph, are the following. For a representative volume (or periodicity cell), 21 sequences of boundary value nonlinear elasticity problems are similarly solved. However, in addition to non-periodic boundary conditions (2) or periodic ones (3), in each problem of each sequence, boundary conditions or stresses corresponding to the prestress, to which the material is subjected are also set. Furthermore, a separate problem is solved in addition to the 21 problem sequences for a representative volume (cell periodicity) of the heterogeneous material. In this separate problem, boundary conditions and stresses corresponding to the prestress of the material are also given, and boundary conditions (2) or (3) are written. In these boundary conditions the effective deformation gradient $\mathbf{Y}_e$ is the identity tensor, $\mathbf{S}_0$ the Green stress tensor is equal zero – thus, the average strains in the model are equal to zero. However, due to prestressing in a representative volume, nonzero average stresses are obtained. The true stress tensor for this particular problem is calculated by integrating over the volume using formula (4). Let us denote it $\mathbf{s}_0$. From the known $\mathbf{s}_0$ by the formula (6) for the described separate problem, the average second Piola-Kirchhoff stress tensor is calculated. Let us denote it $\mathbf{S}_0$.

After solving a separate problem with zero average strain and prestress for the representative volume (or periodicity cell) and averaging of stresses, the dependencies of the difference between the effective Piola-Kirchhoff tensor $\mathbf{S}_e$ and the effective Piola-Kirchhoff tensor $\mathbf{S}_0$ for a separate problem with zero strains on the characteristic value of the strain magnitude are built for each of the 21 sequences. These dependences have the same form as (7):

$$\sum_{ij}^e - \sum_{ij}^0 = \alpha_{ij}^0 q + \alpha_{ij}^1 q^2$$

Next, on the basis of these dependences, the effective nonlinear-elastic properties of the material are estimated as a quadratic dependence of the difference of $\mathbf{S}_0$ and $\mathbf{S}_e$ on the Green stress tensor $\mathbf{E}^e$:

$$\sum_{ij}^e - \sum_{ij}^0 = C_{ijkl}^0 \mathbf{E}^{e(0)}_{kl} + C_{ijklm}^{(1)} \mathbf{E}^{e(1)}_{kl} \mathbf{E}^{e}_{mn}$$

The essence of the described approach is that prestress creates some strains and stresses (natural ones) in a representative volume (cell of periodicity), and, after prestressing, additional (artificial) average strains are applied to the model, causing additional (artificial) average stresses. The effective properties of the prestressed material represent the relationship between these additional stresses and strains.
3. Examples of calculations

The described method of numerical estimation of the effective nonlinear-elastic properties of prestressed heterogeneous materials is realized in the software module Fidesys Composite of the Fidesys CAE-system [10]. Boundary-value problems of nonlinear elasticity are solved using the program kernels of the CAE Fidesys by the finite element method [11, 12]. As an example, we give numerical solutions to the problem of estimating the effective elastic moduli of the first and second order for the porous material prestressed by pore pressure. The material is modeled by the Murnaghan model with the constants $\lambda = 1.09 \cdot 10^5$ MPa, $G = 0.818 \cdot 10^5$ MPa, $C_3 = -0.29 \cdot 10^5$ MPa, $C_4 = -2.4 \cdot 10^5$ MPa, $C_5 = -2.25 \cdot 10^5$ MPa. As a model for calculation, a periodicity cell in the form of a cube with a spherical pore in the center was taken (Fig. 1).

![Figure 1. Model for calculating the effective properties of the porous material in a section](image)

3.1. Dependence of effective properties of the porous material on porosity

A porous material stressed by pore pressure of $6 \cdot 10^3$ MPa was considered. The dependence of its effective elastic moduli of the first and second order on the porosity (the ratio of the pore volume to the total volume of the porous material) varied from zero to 10%. The graphs of such dependences are shown below.

![Figure 2. Dependence graph of the elastic modulus $C_{1122}$ on the material porosity](image)
Figure 3. Dependence graph of the elastic modulus $C_{11}$ on the material porosity

The elastic moduli of the first order with increasing porosity monotonically decrease (as shown in Figure 2 for the coefficient $C_{122}$). The elasticity moduli of the second order with increasing porosity monotonically decrease in modulus (they are negative). This is shown in Figure 3 for the coefficient $C_{11111}$. Dependences on the porosity of the effective nonlinear-elastic properties of porous materials without prestressing [4] have a similar nature.

It should be noted that if the porosity goes to zero, the coefficient $C_{122}$ tends to a constant $\lambda$ of the Murnaghan initial material, and the coefficient $C_{1212}$ – to a constant $G$. This corresponds to the theoretical relationship between the Murnaghan constants and elastic moduli of the first order $C_{ijkl}$ and may serve as a confirmation of the correctness of calculations.

3.2. Dependence of effective properties of the porous material on pore pressure

The porous material with the porosity 6.22% was considered. The dependence of its effective elastic moduli of the first and second orders on the pore pressure, varying from zero to $1.4 \cdot 10^4$ MPa, was investigated. The dependences graphs are given below.

Figure 4. Dependence graph of elasticity modulus $C_{1111}$ on pore pressure
The coefficient \( C_{0111} \) (Fig. 4) depends on pore pressure very weakly (when the pressure varies from zero to \( 1.4 \times 10^4 \) MPa, its change is not more than 1%), however, an interesting effect is observed: when the pore pressure increases to about \( 5 \times 10^3 \) MPa, \( C_{0111} \) it increases, and with a further increase in pressure it begins to fall monotonically. The coefficient \( C_{0122} \) (Figure 5) increases monotonically and linearly with increasing pore pressure within these limits by approximately 10%. The coefficient \( C_{1212} \) responsible for the material behavior under shear strains is practically independent of the pore pressure.

Negative elastic moduli of the second order \( C_{111111} \) (Fig. 6) and \( C_{111122} \) with increasing pore pressure grow in absolute value. Thus, if with increasing porosity (in the first problem) the coefficients \( C_{ijkl}^{(0)} \) and \( C_{ijklmn}^{(1)} \) decrease in magnitude (behaving identically), then in the second problem, with increasing pore pressure, they behave differently: elasticity moduli of the first order decrease in absolute value, while moduli of the second order increase in absolute value. It has the following physical significance: with increasing pore pressure, the non-linearly elastic porous material becomes less rigid, but nonlinearity is more pronounced in it (the more strain is, the stronger the stiffness decreases). The coefficient \( C_{121212} \) is very small, within 1% of the constants \( \lambda \) and \( G \) of the initial Murnaghan material.
4. Conclusion
The article describes an approach to the numerical estimation of the effective properties of the prestressed nonlinear elastic heterogeneous materials under finite strains. The approach is based on solving boundary-value problems of nonlinear elasticity for a representative volume (or cell of periodicity) of the material with subsequent averaging of the results over this volume. This algorithm is implemented in the software module Fidesys Composite of Fidesys CAE-system. Calculations were made for the porous material loaded by pore pressure.

Acknowledgments
The research for this article was performed in Lomonosov Moscow State University and was financially supported by Russian Ministry of Education and Science (project №14.610.21.0013, project ID RFMEFI61017X0013).

References
[1] Levin V A, Zingerman K M, Vershinin A V and Yakovlev M Ya 2015 Numerical analysis of effective mechanical properties of rubber-cord composites under finite strains Compos. Struct. 131 25–36.
[2] Vershinin A V, Levin V A, Zingerman K M, Sboychakov A M and Yakovlev M Ya 2015 Software for estimation of second order effective material properties of porous samples with geometrical and physical nonlinearity accounted for Adv. Eng. Softw. 86 80–84.
[3] Levin V A, Vdovichenko I I, Vershinin A V, Yakovlev M Ya and Zingerman K M 2016 Numerical estimation of effective mechanical properties for reinforced Plexiglas in the two-dimensional case Model. Simulat. Eng. Available online: http://www.hindawi.com/journals/mse/aip/9010576/
[4] Vdovichenko I I, Yakovlev M Ya, Vershinin A V and Levin V A 2016 Calculation of the effective thermal properties of the composites based on the finite element solutions of the boundary value problems IOP Conf. Ser.: Mater. Sci. and Eng. 158 (1) 012094 Available online: http://iopscience.iop.org/article/10.1088/1757-899X/158/1/012094/pdf
[5] Levin V A, Vdovichenko I I, Vershinin A V, Yakovlev M Y and Zingerman K M 2017 An approach to the computation of effective strength characteristics of porous materials Letters on Materials 7 (4) 452-454
[6] Konovalov D A and Yakovlev M Ya 2017 Numerical estimation of effective elastic properties of elastomer composites under finite strains using spectral element method with CAE Fidesys Chebyshevskiy sbornik 18 (3) 316-329
[7] Sevostianov I and Kachanov M 2014 On some controversial issues in effective field approaches to the problem of the overall elastic properties Mech. Mater. 69 (1) 93–105
[8] Fish J and Fan R 2008 Mathematical homogenization of nonperiodic heterogeneous media subjected to large deformation transient loading Int. J. Numer. Methods Eng. 76 (7) 1044–64
[9] Lurie A I 1990 Non-Linear Theory of Elasticity (North-Holland: Amsterdam, Netherlands) 617
[10] Fidesys LLC official website. Available online: http://cae-fidesys.com
[11] Zienkiewicz O C and Taylor R L 2000 The finite element method. Vol. 1. The basis. (Butterworth-Heinemann: Oxford, United Kingdom) 707
[12] Zienkiewicz O C and Taylor R L 2000 The finite element method. Vol. 2. Solid mechanics. (Butterworth-Heinemann: Oxford, United Kingdom) 479