Advances in Engineering Software 86 (2015) 80–84

Contents lists available at ScienceDirect

Advances in Engineering Software

journal homepage: www.elsevier.com/locate/advengsoft

Software for estimation of second order effective material properties of porous samples with geometrical and physical nonlinearity accounted for

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ARTICLE INFO

Article history:
Received 29 August 2014
Received in revised form 10 March 2015
Accepted 11 April 2015

Keywords:
Effective properties
Porous material
Finite strain
Physical nonlinearity
Finite-element method
Parallel computations

ABSTRACT

A method and an algorithm for numerical estimation of effective mechanical properties of porous materials are presented. The effective properties are sought in the form of the nonlinear relation between the second Piola–Kirchhoff stress tensor and the Green strain tensor for anisotropic materials with second-order nonlinearities accounted for. The effective characteristics of test models are computed by means of a CAE Fidesys program module based on the proposed algorithm. The effective material properties as functions of porosity are examined. The finite element mesh that contained more than a million of elements was used while performing stress analysis of a specimen. To reduce computing time, assembly and solution of the global equation system was done in parallel using CUDA technology. The computations were carried out on NVIDIA Tesla C2050 graphics processors. Our results show that accounting for nonlinear effects is essential for correct estimation of effective properties of porous materials.

1. Introduction

The problem of estimating the effective properties of porous materials [1] is important for the analysis of specimen properties during geological exploration of oil fields. Such material properties are used for computational modeling of physical processes in the course of field development and operation. At present the existing mathematical models do not allow to calculate the effective properties of porous materials with the accuracy suitable for industrial use. The effective material properties are usually determined experimentally, by testing of multiple specimens. Nevertheless, an efficient development of an oil field is impossible without complicated numerical modeling that requires significant computer power. It is necessary to perform multiple computer solutions for the determination of effective averaged properties of porous samples. Computational procedure for estimation of averaged properties of porous materials is suitable for effective parallelization using large number of computational nodes, such as in cluster-type systems. The use of hybrid supercomputers (MPI, CUDA, Open MP-based) allows enormous increase of the speed of modeling effective prototype properties thus decreasing time and cost of laboratory tests.

2. Problem statement

Let us consider the representative volume, filled with porous material. We assume that an effective (averaged) material should satisfy to the following condition: average volume stresses in real and effective materials are equal under the same displacements of faces that bound the representative volume [2–4].

Here we describe a method for creating effective constitutive relationships for the porous material with the use of definition given above. We solve certain sequences of boundary value problems of nonlinear elasticity for the representative volume V_0 in its initial state (before deformation) [6–8]:

$$\nabla \cdot \sigma = 0 \tag{1}$$

with boundary conditions

$$u|_{\Gamma_0} = R \cdot (F^{e^*} - I) \tag{2}$$

It is shown [9] that the superposition of a rigid motion on the deformation of a porous body does not change the effective constitutive equations.

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http://dx.doi.org/10.1016/j.advengsoft.2015.04.007
0965-9978/

The mechanical properties of a matrix material are described by Hooke's law or by constitutive relations of Murnaghan [5]:

$$\overset{0}{\Sigma} = \lambda(E:I)I + 2GE + 3C_3(E:I)^2 I + C_4(E^2:I)I + 2C_4(E:I)E + 3C_5E^2 \tag{3}$$

Here σ is the true total state stress tensor (Cauchy stress tensor); $\overset{0}{\Sigma}$ is the second Piola–Kirchhoff stress tensor; E is the Green strain tensor; I is the second-order identity tensor; F is the corresponding affinor (deformation gradient) [6], $F = \frac{dr}{dR}$; R is the radius vector of a particle in the initial state, r is the radius vector of a particle in the current state; $r - R = u, u$ is the displacement vector from the initial state to the current state; λ and G are the first-order elastic constants; C_3, C_4, and C_5 are the second-order elastic constants. The index e corresponds to the effective material. The colon in equations is the sign of double tensor contraction.

Each problem sequence corresponds to certain appearance of the Green strain tensor E^e of the effective material (and to certain deformation gradient F in boundary conditions). Also, different problems of one sequence differ by strain magnitude.

We find stress tensor σ by solving each problem of each sequence. Using σ it is possible to calculate stress tensor σ^e of effective material according to the following formula:

$$\sigma^e = \frac{1}{V}\int_V \sigma\, dV = \frac{1}{V}\int_\Gamma N\cdot\sigma r\, d\Gamma \tag{4}$$

where N is an external normal to boundary Γ and r is the radius vector.

Last equality in (4) has been received with the help of the divergence theorem and the following observation from tensor analysis:

$$\nabla\cdot(\sigma r) = (\nabla\cdot\sigma)r + \sigma(\nabla r)^* = (\nabla\cdot\sigma)r + \sigma\cdot I = \sigma \tag{5}$$

Knowing the deformation gradient (that was set by us) and true stress tensor, we can calculate Green strain tensor and second Piola–Kirchhoff stress of the effective material:

$$E^e = \frac{1}{2}(F^{e^*}\cdot F^e - I) \tag{6}$$

$$\overset{0}{\Sigma}{}^e = (\det F^e)(F^e)^{-1}\cdot\sigma^e\cdot(F^e)^{*-1} \tag{7}$$

We assume that the dependence of the Piola–Kirchhoff stress tensor components on a strain parameter q for each problem sequence (i.e. for each load type) can be described by a quadratic function:

$$\overset{0}{\Sigma}{}^e_{ij} = \alpha^0_{ij}q + \alpha^1_{ij}q^2 \tag{8}$$

Accordingly we will search for effective constitutive relations as a nonlinear dependence of the Piola–Kirchhoff stress tensor $\overset{0}{\Sigma}{}^e$ on the Green strain tensor E^e:

$$\overset{0}{\Sigma}{}^e_{ij} = C^0_{ijkl}E^e_{kl} + C^1_{ijklmn}E^e_{kl}E^e_{mn} \tag{9}$$

The second term in the right-hand side is introduced in order to take into account nonlinear effects in the effective constitutive equations.

The effective elastic moduli C^0_{ijkl} and C^1_{ijklmn} of the porous material depend on porosity.

It is worth noting that finding the effective constitutive relations of the porous material in the nonlinear case above requires solving 21 sequences of cases (equal to the number of independent elastic modules in (9)). Each sequence must contain no less than three problems (i.e. for each load type – no less than three load cases) in order to perform least squares method for determining coefficients in (8).

3. Solution method

In practice it is convenient to set the Green strain tensor and to employ it for computation of the deformation gradient using formula (6). Since the deformation gradient is a non-symmetric tensor of the second rank it cannot be uniquely determined from the symmetric Green strain tensor. That is why we set the deformation gradient as an upper triangular matrix. Then its six components are uniquely defined by six independent components of the Green strain tensor.

After calculation of the deformation gradient, we apply boundary conditions (2) to the model, solve the boundary value problem of nonlinear elasticity and find stresses σ.

The following sequences of problems are solved:

(1) $E_{11} = q$ – uniaxial tension or compression in the X direction;
(2) $E_{22} = q$ – uniaxial tension or compression in the Y direction;
(3) $E_{33} = q$ – uniaxial tension or compression in the Z direction;
(4) $E_{12} = E_{21} = q$ – shear in the XY plane;
(5) $E_{13} = E_{31} = q$ – shear in the XZ plane;
(6) $E_{23} = E_{32} = q$ – shear in the YZ plane;
(7) $E_{11} = E_{22} = q$ – biaxial tension or compression in the XY plane;
(8) $E^0_{11} = E^0_{33} = q$ – biaxial tension or compression in the XZ plane;
(9) $E^0_{11} = E^0_{22} = E^0_{33} = q$ – uniform tension or compression;
(10) $E_{11} = q, E_{12} = E_{21} = q$ – superposition of uniaxial tension or compression in the X direction and shear in the XY plane;
(11) $E_{22} = q, E_{12} = E_{21} = q$ – superposition of uniaxial tension or compression in the Y direction and shear in the XY plane;
(12) $E_{33} = q, E_{12} = E_{21} = q$ – superposition of uniaxial tension or compression in the Z direction and shear in the XY plane;
(13) $E_{11} = q, E_{13} = E_{31} = q$ – superposition of uniaxial tension or compression in the X direction and shear in the XZ plane;
(14) $E_{22} = q, E_{13} = E_{31} = q$ – superposition of uniaxial tension or compression in the Y direction and shear in the XZ plane;
(15) $E_{33} = q, E_{13} = E_{31} = q$ – superposition of uniaxial tension or compression in the Z direction and shear in the XZ plane;
(16) $E_{11} = q, E_{23} = E_{32} = q$ – superposition of uniaxial tension or compression in the X direction and shear in the YZ plane;
(17) $E_{22} = q, E_{23} = E_{32} = q$ – superposition of uniaxial tension or compression in the Y direction and shear in the YZ plane;
(18) $E_{33} = q, E_{23} = E_{32} = q$ – superposition of uniaxial tension or compression in the Z direction and shear in the YZ plane;
(19) $E_{12} = E_{21} = q, E_{13} = E_{31} = q$ – superposition of shears in the XY and XZ planes;
(20) $E_{12} = E_{21} = q, E_{23} = E_{32} = q$ – superposition of shears in the XY and YZ planes;
(21) $E_{13} = E_{31} = q, E_{23} = E_{32} = q$ – superposition of shears in the XZ and YZ planes;

here q is a strain parameter.

The effective stress tensor σ^e is calculated with the help of averaging (4). Using Eq. (7), the Piola–Kirchhoff stress tensor $\overset{0}{\Sigma}{}^e$ is determined.

Then the dependence of the Piola–Kirchhoff stress tensor on the strain parameter q is generated for each problem sequence. These dependences are approximated by expressions (8). Coefficients α^0_{ij} and α^1_{ij} are found using the least squares method.

The coefficients C^0_{ijkl} from (9) are determined through the coefficients α^0_{ij}, and coefficients C^1_{ijklmn} – through α^1_{ij} that are calculated