Modeling of Composite Materials in SIMULIA Abaqus with the Help of Analytical Solutions of Generalized Eshelby Problem

Dmitriy B. Volkov-Bogorodsky, and Sergey A. Ryzhov

"TESIS" Co Ltd, Moscow, Russia

Abstract: In the work is presented new numerical-analytical approach for the static analysis of composite materials filled by inclusions with various geometrical form and mechanical properties essentially distinguish from the properties of the matrix. It is considered two basic cases of spherical and prolate spheroid inclusions, which can contain additional interface layers. For this problem it was developed analytical method for a two-scale analysis of composite construction (micro- and macro-level) under SIMULIA Abaqus. For the micro-level problem it has been developed a special class of high accuracy analytical elements constructed on the base of spherical and generalized spherical functions. These elements analytically describe the stress/strain structure near inclusions with interface layer and strongly accounting various conditions on the curvilinear interface boundary, including slip and loss contact conditions. On the base of these elements are estimated effective properties of composite material for the macro-level problem. These elements are included into SIMULIA Abaqus through the standard UMAT technique and allow high accuracy modeling of constructions of composite materials with detailed accounting of its internal microstructure.

Keywords: Dispersed Composites, Interface Layer, Strong Analytical Representations of stress/strain Structure, Special High Accuracy User Elements.

1. Introduction

Static and dynamic analysis of constructions on the base of composites materials requires detailed representation of the internal microstructure of the material in the FEM model for acceptable quality of the numerical results of finite-element modeling. In present time composites materials have very complex internal structure not only due to geometrical complexity of inclusions on micro-level, but also due to transition of geometrical sizes to nano-level (nanofullerens, nanotubes etc), where arising new physical effects (scale effects) leading to the large changes in the behavior of composites materials. Attempt of taking into account all these phenomena by the traditional approach based on the big amount of simple FEM elements and on h-convergence is soon restricted by the computational resources of computer systems even for the modern parallel systems.

The most advancement in the modeling of composite materials is connected with multi-scale modeling and homogenization theory (Bakhvalov, Panasenko, 1989). Success of this scientific method is in the separation of global (macro-level) and local (micro-level) physical processes in composites and in the mathematically rigorous description of local behavior near inclusions formalized in the homogenization theory as the series problems on the cell with inclusions.

Investigations of molecular structures in the nanocomposites filled by nanoinclusions has explained some scale effects by the presence of the interface layer near inclusion's boundary, which has fractal structure and large volume amount in common correlation of fractions in composite material. This property of nanostructures emphasizes the significance of mathematical description of interface layer in the finite element modeling of composite materials.

In this paper is presented analytical approach for building special type finite elements intended for accurate analysis of composite materials filled by spherical inclusions with spherical interface layer and by prolate spheroid inclusions. These elements analytically describe the local stress/strain behavior of the material near inclusions with interface layer and take rigorous into account (by analytical form of presentation) special behavior of solution due to various contact conditions on the curvilinear interface boundary.

This numerical analytical approach combines ideas of the finite element theory with ideas of the homogenization theory and is based on the advanced theory of special functions and special type representation of elements for micro-level problem called as analytical elements considered the structure of nonhomogeneities in the material. These elements are constructed on the base of generalized Eshelby problem for one inclusion in the infinite matrix with polynomial behaviour of solution at the infinity, and make up certain class of elements with complex computational organization. They make use in various fields of computational analysis: strength analysis of inhomogeneous media, thermoelasticity, acoustics, filtration, electrodynamics etc.

Realization of these elements in SIMULIA Abaqus is fulfilled by the standard UMAT technique required algorithmic realization in FORTRAN with procedures of calculation effective properties homogenized material and micro-stress distribution near inclusions. It is convenient that this realization is based on the ordinary finite element mesh and can be easy fulfilled in the frameworks of the usual steps of preparing finite element model in Abaqus/CAE.

The advances in analytical construction of user elements are connected with advances in algorithmic representation of special solutions of generalized Eshelby problem for one inclusion with interface layer based on the advanced theory of special functions (Volkov-Bogorodsky, 2008). Also this analytical approach can be applied to the building finite elements with singularities for analyses of geometrical singularities cased stress concentration in material.

The final goal of this investigation is to develop computational tools for optimization of constructions of composite materials based on the high accurate modeling of physical process on micro-level, where is working ideas of high level p-approximation. It can present common view on the approach as h-approximation on the macro-level and p-approximation on the micro-level. One should sign that such type computational organization is closed to the computational organization of today parallel systems and can be effective realized on the CPU+GPU systems.

2. Generalized Eshelby problem

Introducing analytical special type element is based on the strong solution of the Eshelby problem (Eshelby, 1961; Christensen, 1979) for spherical and prolate spheroid inclusions. We consider more general problem in difference to Eshelby supposed more arbitrary geometrical form of spherical and prolate spheroid inclusion, also arbitrary polynomial behavior of displacements at the infinity and more general contact conditions on the interface boundary, included slip and loss contact cases. Our analytical technique based on Papkovich-Neuber representation of elastic displacements (Papkovich, 1939) and on using spherical and generalized spherical functions allowed us to solve generalized Eshelby problem in exact and convenient form suitable for effective numerical realization.

We consider following boundary value problem for the spherical inclusion with spherical interface layer (see Fig. 1a) and prolate spheroid inclusion (see Fig. 1b) embedded in the infinite matrix subjected to arbitrary polynomial stresses at the infinity:

$$\mu\,\nabla^2 \boldsymbol{U} + (\mu+\lambda)\,\nabla\,\mathrm{div}\boldsymbol{U} = 0, \quad \boldsymbol{U}(P) \to \boldsymbol{U}_0(P),\ \ P\to\infty, \quad P=(x,y,z)\,. \tag{1}$$

Material constants (Lame coefficients) are of arbitrary quantities and can possess null values for hole instead inclusion.

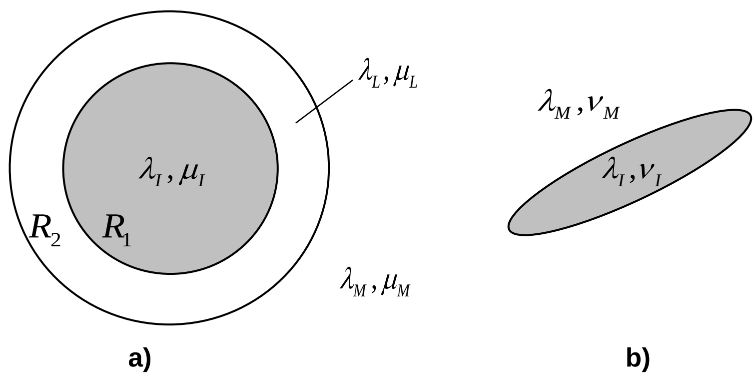

Figure 1. Two types inclusions of spherical a) and prolate spheroid b) form in the infinite matrix.

On the interface boundary can be various contact conditions corresponded to various behavior of the material near inclusion. In particular, it can be slip, shear friction, loss contact or classical ideal contact conditions on interface boundary:

$$\left[\boldsymbol{U}\right] = \left[\boldsymbol{p}(\boldsymbol{U})\right] = 0\,, \tag{2}$$

where $\boldsymbol{p}(\boldsymbol{U})$ indicates surface forces caused by displacements $\boldsymbol{U}$.

2.1 Analytical representation of displacements near inclusion

The analytical method for boundary values problem given by Equation 1 is based on the analytical representation of displacements by auxiliary potentials subjected to Laplace equation (Papkovich-Neuber representation, see Papkovich, 1939):

$$\boldsymbol{U}(P) = \frac{\boldsymbol{f}(P)}{\mu} + \frac{\nabla(\phi - \boldsymbol{r}\,\boldsymbol{f})}{4\mu(1-\nu)}\,, \quad \nabla^2 \boldsymbol{f}(P) = 0\,, \quad \nabla^2\phi(P) = 0\,, \quad \nu = \frac{\lambda}{2(\mu+\lambda)}\,. \tag{3}$$

For spherical and spheroid inclusions this representation are completed by special decompositions of auxiliary potentials on spherical and generalized spherical harmonic functions with the help of radial function $\chi_n^m(r)$ or $\chi_n^m(\alpha)$ for spheroid inclusion (α is a parameter of spheroid coordinate system, defined by the ratio of minor and major semi-axis of spheroid, see Fig. 2).

For algorithmic efficiency we use the following complex value submissions of harmonic polynomial (spherical functions) ϕ_n^m, on the base of which we have been constructed additional generalized spherical functions ϕ_n^{*m} and $\hat{\phi}_n^{*m}$ for spherical and spheroid coordinate system:

$$\phi_n^m(P) = \sum_{p=0}^{\left[\frac{n-m}{2}\right]} \frac{(-1)^p w^{m+p} \bar{w}^p}{4^p\, p!\,(m+1)_p} \left(\frac{d}{d\,z}\right)^{(2p)} \left(z^{n-m}\right), \;\; n \ge m, \quad w = x + i\,y\,, \quad \bar{w} = x - i\,y\,, \tag{4}$$

$$\phi_n^{*m}(P) = r^{-2n-1}\,\phi_n^m(P)\,, \qquad r = \sqrt{x^2 + y^2 + z^2}\,, \tag{5}$$

$$\hat{\phi}_n^{*m}(P) = \chi_n^m(\alpha)\,\phi_n^m(P)\,, \qquad \chi_n^m(\alpha) = \frac{Q_n^m(\mathrm{ch}\,\alpha)}{P_n^m(\mathrm{ch}\,\alpha)}\,. \tag{6}$$

Here P_n^m and Q_n^m are Legendre functions of the first and second kind (Bateman, Erdelyi, 1953). We can effective calculate and differentiate spherical and generalized spherical functions due to Equations 4-6.

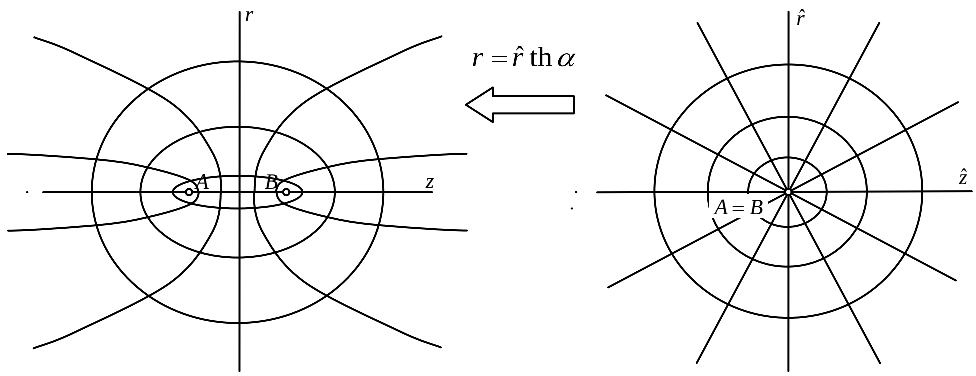

Figure 2. Spheroid coordinate system.

2.2 Definition auxiliary potentials for various interface boundary conditions

Exact solution of generalized Eshelby problem in the form of finite sum of generalized spherical functions is conditioned by the form of auxiliary potentials in Equation 3, which is different for various phases of regarded domain (Fig.1a). All potentials are defined by five harmonic vector polynomial $\boldsymbol{f}_0^{(I)}$, $\boldsymbol{f}_0^{(L)}$, $\boldsymbol{f}_0^{*(L)}$, $\boldsymbol{f}_0^{(M)}$ and $\boldsymbol{f}_0^{*(M)}$ with degree n consistent to degree of infinity function $\boldsymbol{U}_0(P)$. In all phases potential ϕ_0 is equal to zero.

In inclusion G_I potential $\boldsymbol{f}$ (see Equation 3) has form:

$$\boldsymbol{f}(P) = \boldsymbol{f}_0^{(I)} + C_0\, r^{2n+5}\, \nabla \operatorname{div} \boldsymbol{f}_L^*, \quad \boldsymbol{f}_L^* = r^{-2n-1} \boldsymbol{f}_0^{*(L)}, \quad P \in G_I, \tag{7}$$

where C_0 is still a free unknown constant. In the interface layer G_L potential $\boldsymbol{f}$ has the next form with three unknown constants:

$$\boldsymbol{f}(P) = \boldsymbol{f}_0^{(L)} + A_1\, \boldsymbol{f}_L^* + \left(B_1 + C_1\, r^{2n+5}\right) \nabla \operatorname{div} \boldsymbol{f}_L^*, \quad P \in G_L. \tag{8}$$

And in the infinite matrix G_M potential $\boldsymbol{f}$ has the form:

$$\boldsymbol{f}(P) = \boldsymbol{f}_0^{(M)} + \boldsymbol{f}_L^* + \boldsymbol{f}_M^* + B_2\, \nabla \operatorname{div} \boldsymbol{f}_M^*, \quad \boldsymbol{f}_M^* = r^{-2n-1} \boldsymbol{f}_0^{*(M)}, \quad P \in G_M. \tag{9}$$

It is similar representation of auxiliary potential in the case of the spheroid inclusion (Fig.1b). Substituting potential $\boldsymbol{f}$ to Papkovich-Neuber representation and then to the interface boundary conditions leads us to the system of boundary equations relative functions $\boldsymbol{f}_0^{(I)}$, $\boldsymbol{f}_0^{(L)}$, $\boldsymbol{f}_0^{*(L)}$, $\boldsymbol{f}_0^{(M)}$, $\boldsymbol{f}_0^{*(M)}$. These equations will contain differential operators (with constant coefficients) $\nabla \operatorname{div} \boldsymbol{f}_0$, $\boldsymbol{r} \operatorname{div} \boldsymbol{f}_0$ and $\nabla\left(\boldsymbol{r}\, \boldsymbol{f}_0\right)$, which not increase degree of harmonic polynomial $\boldsymbol{f}_0$, and also will contain operator $\boldsymbol{r}\left(\boldsymbol{r}\, \boldsymbol{f}_0\right)$, which increase degree of polynomial $\boldsymbol{f}_0$. The choice of unknown constants C_0, A_1, B_1, C_1 and B_2 is in requirement that coefficients on term $\boldsymbol{r}\left(\boldsymbol{r}\, \boldsymbol{f}_0\right)$ in boundary equations are equal to zero. Then we obtain system of four boundary equation, which is solving explicitly. So, we can explicitly express four function $\boldsymbol{f}_0^{(I)}$, $\boldsymbol{f}_0^{(L)}$, $\boldsymbol{f}_0^{*(L)}$, $\boldsymbol{f}_0^{*(M)}$ through function $\boldsymbol{f}_0^{(M)}$, so that boundary equations corresponding to the contact boundary conditions will be equal to zero. Hence, it will be satisfied contact conditions on interface boundary and asymptotic condition $\boldsymbol{U}(P) \to \boldsymbol{U}_0(P),\ P \to \infty$ at the infinity.

We expand all unknown functions on spherical harmonic ϕ_n^m (see Equation 4), and then solve boundary problem of re-expansion in terms of ϕ_n^m of differential operators $\nabla \operatorname{div} \boldsymbol{f}_0$, $\boldsymbol{r} \operatorname{div} \boldsymbol{f}_0$ and $\nabla\left(\boldsymbol{r}\, \boldsymbol{f}_0\right)$ on interface boundary. This problem is easy formulated in term of matrix equations about coefficients of four unknown functions. So, we obtain solution of generalized Eshelby problem with arbitrary polynomial asymptotic $\boldsymbol{U}_0$ at the infinity and with various contact conditions on interface boundaries.

2.3 Review of possible solutions by the analytical technique

Developing analytical approach can be applied not only to the static elasticity problem, but also to the another equations and to the dynamic processes, such as heat transfer equation, acoustic equation, Brinkman and Stokes filtration equations, Maxwell equations and so on. Dynamic equations (elasticity, Maxwell, acoustics or heat transfer, filtration) are considered as harmonic process with periodic time oscillation or Laplace integral transformed process, and then governing equations are represented by the Helmholtz equations. Modification of the analytical technique concerns Papkovich-Neuber representation and basic functions ϕ_n^m, ϕ_n^{*m} (Equations 3-5), which are now related with Helmholtz equation instead of the Laplace equation (Volkov-Bogorodsky, 2008). Analysis of the equations of the parabolic type (heat transfer and filtration) also leads to the Helmholtz equation and to the same analytical technique.

So, further generalization of the Eshelby problem to the another type of equations and to the dynamic problems allows us to build the necessary functions for construction such type high accuracy user elements for static and dynamic analysis of these equations on the micro-level.

3. Construction a form functions for the micro-level analysis

Solution of generalized Eshelby problem with various linear independent asymptotic $\boldsymbol{U}_0$ at the infinity generates complete and linear independent system of functions which is used for the effective micro-level analysis. In accordance with homogenization method (Bakhvalov, Panasenko, 1989; Christensen, 1979) this analysis gives possibility of estimation effective properties of the cell with one or several inclusions, and also possibility of high accuracy calculation of the stress/strain distribution in the cell near inclusions (see Figure 3). In the Abaqus/Standard there is various elements constructed on the base of tetrahedron and hexahedron with linear and quadratic approximation (C3D4 , C3D8 , C3D10 , C3D20). We have been constructed special form functions (Zienkiewicz, 1971) on the base of block least square method and generalized Eshelby problem for tetrahedron and hexahedron with linear and quadratic approximation, which is used for the micro-level analysis of the stress/strain distribution in the cell near inclusion. For the macro-level analysis is used standard Abaqus elements with effective properties of the cell (tetrahedron or hexahedron), calculated on the base of generalized Eshelby problem.

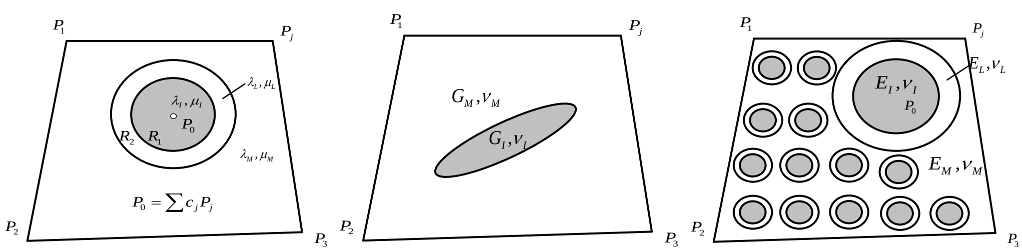

Figure 3. User element with spherical inclusion and interface layer.

3.1 Introducing analytical element in Abaqus/Standard

Implementation of the analytical elements in Abaqus/Standard is carried out through the standard UMAT technique (see "Abaqus User Subroutines Reference Manual", 2011). It is supposed realization of the all algorithms of the generalized Eshelby problem as FORTRAN 90 code, which is compiled by Abaqus before submitting of the finite element model for calculation. Now the library of user elements contains approximately 1200 lines of FORTRAN code and realizes algorithms of calculation effective properties of the cell with inclusions and stress/strain distribution in the cell on the micro-level near inclusions.

Description of the analytical elements in the input file of the FEM model associates with correspondent material with calculated effective properties, and assumes a common description of the element properties (parameters of inclusion and material) by the standard keys

```
*MATERIAL, name=U100_material
*USER MATERIAL, constants=…
```

which defines all needed parameters of group elements, associated with this material. The order of parameters for elements with spherical inclusions and interface layers is the next: E_I, ν_I, E_L, ν_L, E_M, ν_M (Young modulus and Poison ratio instead of Lame coefficients), c_0, c_1, where $c_1 = (R_1/R_2)^3$ is the relative volume fraction of inclusion inside the region occupied by the inclusion and interface layer, c_0 is common volume fraction of inclusions in material.

Using of the defined material is given by standard way:

```
*SOLID SECTION, ELSET=Matrix_strength, material= U100_material
```

So, introducing analytical elements in Abaqus/Standard numerical scheme comes to the preparing model with standard Abaqus elements $\mathrm{C3D4}$, $\mathrm{C3D8}$, $\mathrm{C3D10}$, $\mathrm{C3D20}$ and to the further substitution of some subset of elements to the elements with inclusions by standard UMAT keys:

```
*USER MATERIAL,…
*SOLID SECTION, elset=…
```

Then, it is executing macro-level numerical analysis in Abaqus/Standard with further correction internal stresses on the base of the solution of the generalized Eshelby problem. By this way it can be modeled complex dispersed composites structure with arbitrary distribution of inclusions (including random distributions).

4. Simple examples

As the demonstration we considered two simple problems of bulk and L-type domain loading with strengthening of the central zone by dispersed schungite particles with variation of the volume fraction and sizes of particles (Figures 4, 5). The length of the bulk is $1700\,mm$, the length of the strengthening zone is $500\,mm$ (Figure 4); the width of the leg in L-type domain (Figure 5) is $300\,mm$. Into the bulk section there is steel core of rectangular form surrounding by the soft matrix.

In the first case it is considered concentrated force in the central point of the bulk ($F_y = 100N$) and compressible matrix; strengthening zone was filling by particles without interface layer ($c_1 = 1$) with variation volume fraction c_0 from small to extreme values. In the second case (Figure 5) it is considered loading by uniform constant pressure $P = 10\,kPa$ with variation of the sizes of particles in micro- and nano-range into almost incompressible matrix. Under these conditions interface layer sharply increases and is observed scale effect of the improving mechanical characteristics (Vlasov, Volkov-Bogorodsky, Yanovskii, 2012). This case of strengthening is describing by the constant volume fraction $c_0 = 0.02$ and variation of the parameter c_1 from small to big amount. Mechanical characteristics of the matrix, interface layer and inclusions (of spherical form in our examples) are $E_I = 1.5\,GPa$, $\nu_I = 0.3$, $E_L = 987\,MPa$, $\nu_L = 0.3$, $E_M = 135\,MPa$, $\nu_M = 0.3, 0.4999$; for the first case $\nu_M = 0.3$, for the second $\nu_M = 0.4999$.

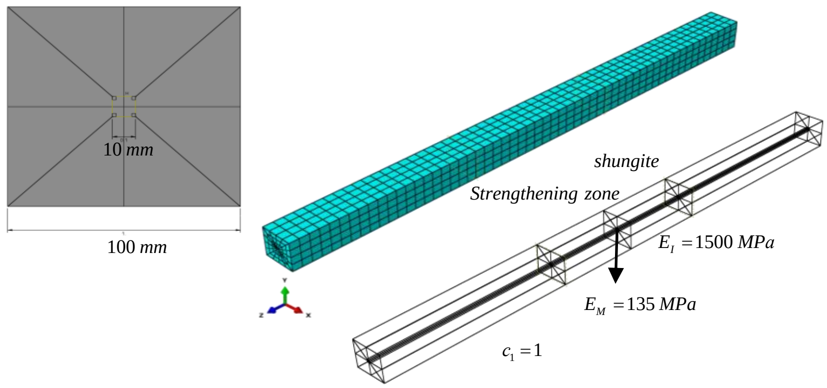

Figure 4. The test FEM model with spherical inclusion.

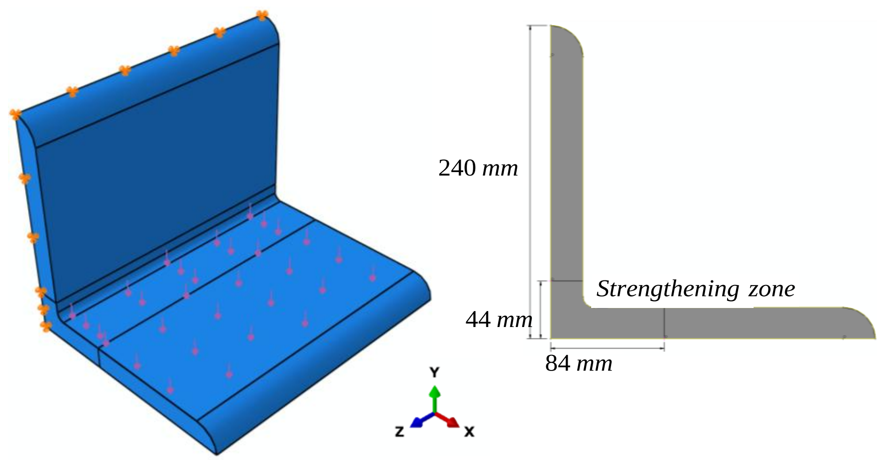

Figure 5. L-type test model with loading by the pressure.

On the Figure 6 is presented dependence of the effective characteristics of the strengthening zone on the volume fracture of shungite particles, calculated on the base of micro-level problem; it is classical three body Eshelby problem (Christensen, 1979). On the Figure 7 is shown profile and maximal bulk displacement for various volume fractures c_0 in the strengthening zone.

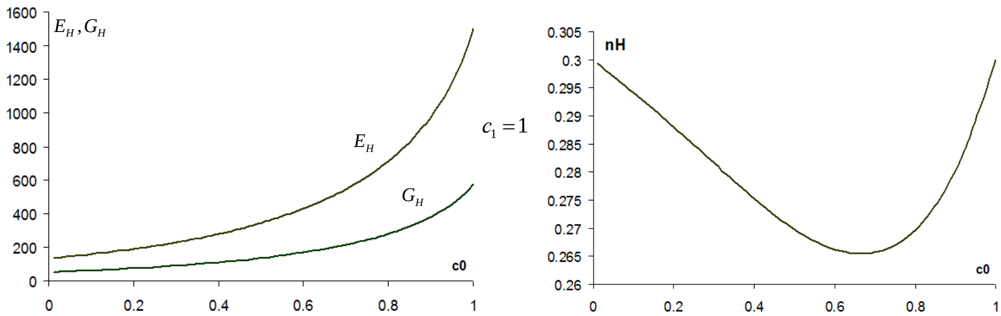

Figure 6. Effective properties of FEM model with spherical inclusion.

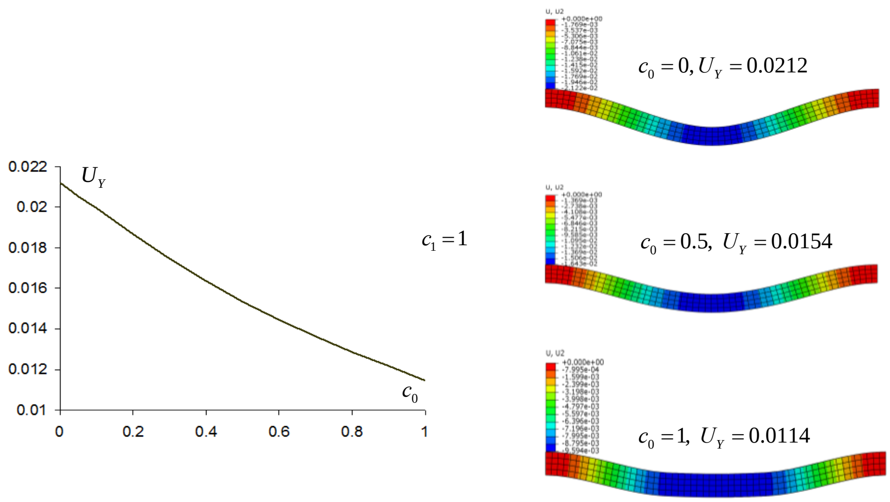

Figure 7. Bulk loading with strengthening zone.

On the Figure 8 is presented dependence on the size of interface layer of the effective characteristics of the strengthening zone, caused by sizes of shungite particles, also maximal displacement of loading leg. Effective characteristics were calculated in micro-level problem on the base of asymptotic homogenization theory (Bakhvalov, Panasenko, 1989). It should be noted that the results of asymptotic homogenization model on describing of the scale effect are in good agreement with experiment (see Vlasov, Volkov-Bogorodsky, Yanovskii, 2012).

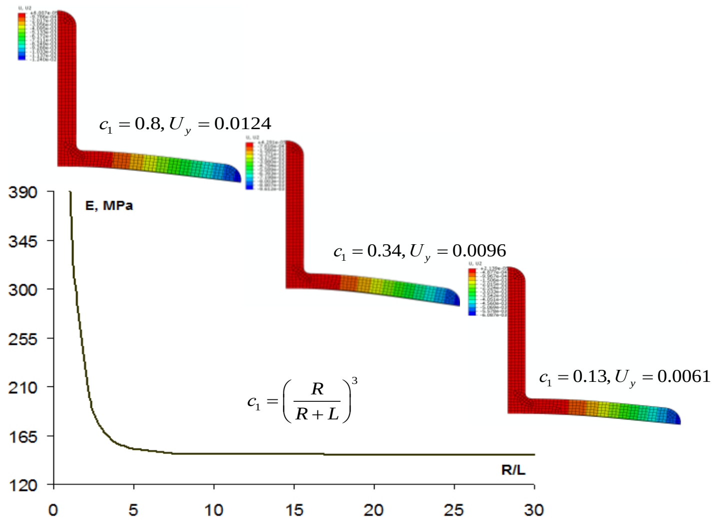

Figure 8. L-type domain loading with strengthening zone.

The micro-level problem gives us opportunity to estimate real stresses near inclusions on the base of the analytical solution of the asymptotic homogenization theory cell problem. On the Figure 9 is shown as example the distribution of the stress component σ_{zz} in the middle section $\{y=0\}$ near inclusion of the spheroid form with semi-axes ratio $\delta = 0.7$ under unit macro-strain $\varepsilon_{zz} = 1$. On the base of this micro-level distribution and calculated in Abaqus/Standard macro-level distribution we can estimate local stresses in whole model (Figure 10).

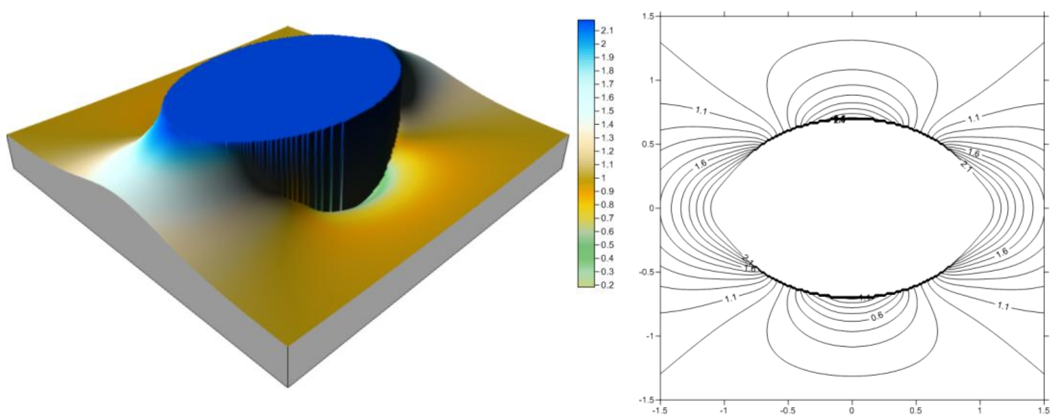

Figure 9. Local stresses in the cell near inclusion.

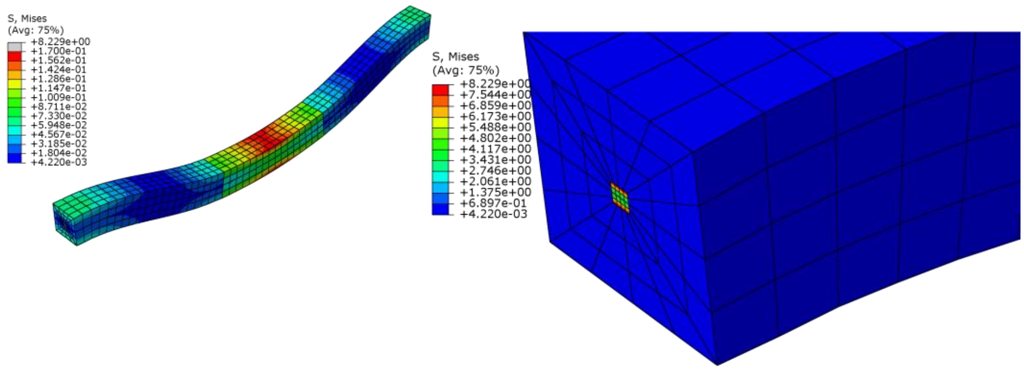

Figure 10. Local stresses estimation in whole model.

5. Summary

In this paper are presented numerical analytical approach combines ideas of the finite element theory with ideas of the homogenization theory and is based on the advanced theory of special functions and user elements are called as analytical elements considered the structure of inhomogeneities in the material. Realization in SIMULIA Abaqus of these elements is fulfilled by the standard UMAT technique required realization of algorithms in FORTRAN with calculation of effective mechanical characteristics of non-homogeneous media by asymptotic homogenization method. It is convenient that this realization is based on the ordinary finite element mesh and can be easy fulfilled in the frameworks of the usual steps of preparing finite element model in Abaqus/CAE.

These user elements make up certain class of elements with complex computational organization and makes use in various fields of computational analysis: strength analysis of inhomogeneous media, thermoelasticity, acoustics, filtration in porous media, electrodynamics etc.

6. References

1. Bakhvalov, N.S., and G.P. Panasenko, "Homogenization of processes in periodic media," Dordrecht, Boston, London: Kluwer, 1989.
2. Bateman, H., and Erdelyi, A., "Higher Transcendental Functions, Vol. 1" New York, Toronto, London: Mc Graw-Hill Book Company, 1953.
3. Christensen, R.M., "Mechanics of Composite Materials," John Wiley and Sons Inc, 1979.
4. Eshelby, J.D., "Progress in Solid Mechanics," (Edited by I.N. Sneddon and R. Hill), North Holland, Amsterdam, 1961, 89-140.
5. Papkovich, P.F., "Elasticity Theory," Moscow, Leningrad, 1939 (in Russia).
6. Volkov-Bogorodsky, D.B., "Application of Analytical Calculations on the Base of Block Method in Coupled Problems of Continuum Mechanics," Proceedings of Theoretical and

Practical Conference “Engineering Systems-2008”, Moscow, 7-11, April 2008. Moscow, 2008, 123-138 (in Russian).

7. Vlasov, A.N., Volkov-Bogorodsky, D.B., and Yanovskii, Yu.G. “Effect of Inclusion Size on the Mechanical Properties of Elastomeric Composites,” Doklady Physics, Mechanics, 2012, Vol. 57, No. 4, pp. 157-159.
8. Zienkiewicz, O.C., “The Finite Element Method in Engineering Science,” McGrow Hill, London, 1971.
9. Abaqus User Subroutines Reference Manual, Version 6.10-1, Dassault Systémes Simulia Corp., Providence, RI.