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Multiscale Modeling in the Mechanics of Materials: Cohesion, Interfacial Interactions, Inclusions and Defects

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Abstract. The models of media with multiscale effects are constructed based on the variational formalism. The internal interactions are determined by kinematic constraints of general character. These models take into account the superficial effects and internal interactions similar to interatomic forces of coupling. The models of media with a continuous field of defects of various types are considered. Descriptions of the media with defects, cohesion field models as a special case of the Cosserat models are considered. This paper is devoted to the consideration of disperse composite materials reinforced by nanoparticles. For numerical simulation, the new efficient block analytical-numerical method is developed oriented to the general case of solving problems in complex-shaped 2D and 3D domains. As an example of numerical investigation of the interfacial interactions in heterogeneous media, the medium with inclusions is considered.

1 Kinematic variational modeling of the medium

A variant of the variational formalism is developed. The variant proposed allows us to obtain constitutive equations, the system of equilibrium equations and boundary conditions [1]-[4]. A functional is constructed by taking into account kinematic constraints. The basic idea is that the general character of kinematic constraints determines the internal interactions. An algorithm proposed for the formulation of the model includes the following stages:

- Studying kinematic models, we can state kinematic constraints in media.
- Using the variational principle of possible displacements, we can determine the variation of the work done by internal forces on the kinematic constraints. As a result, the tensor of the Lagrange multipliers describes a spectrum of interactions that corresponds to the internal kinematic constraints.
- Integrating by part, we obtain a linear variational form and a set of arguments.
- Assume that only the reversible processes are considered. Then, the linear variational form is integrable and the potential energy can be formulated. For a linear elastic medium, the quadric form for the density of potential

energy can be obtained. The potential energy is formulated taking into account the tensor's dimensions of the arguments.

- Taking into account the expression of potential energy, we can arrive at the constitutive equations.
- The constitutive equations allow us to obtain particular expressions for the potential energy, which defines the mathematical statement of the model as a whole.

It is worth emphasizing that the proposed variational method needs fixed sets of arguments in the volume and in the superficial parts of potential energy. These sets of arguments are dictated by the introduced kinematic constraints. The correct mathematical statement is realized as a result of the proposed algorithm. By comparison, the set of arguments for the Sedov variational formalism is determined only for the volumetric part of the potential energy; consequently, some additional physical assumptions should be introduced to define the set of arguments for the superficial part of the potential energy.

2 Kinematic models

Let us represent a nonsymmetric distortion tensor referred associated with the Cartesian coordinates as follows:

$$\frac{\partial R_i}{\partial x_j} = \gamma_{ij} + \frac{1}{3}\theta\delta_{ij} - \omega_k \mathcal{E}_{ijk} . \tag{1}$$

Here, R_i are the components of the displacement vector, γ_{ij} and θ are the components of the deviator of the deformation tensor and the deviator of the spherical tensor, ω_k are the components of the rotation vector, $\mathcal{E}_{ijk}$ is the Levi–Civita tensor, δ_{ij} is the Kronecker delta, and $\omega_k = -\frac{1}{2}\mathcal{E}_{ijk}\frac{\partial R_i}{\partial x_j}$.

The conditions of the existence of the quadratures (the conditions of the existence of corresponding line (contour) integral) for the generalized Cauchy relationships (1) can be written in the following from:

$$\frac{\partial}{\partial x_m}\left(\gamma_{in} + \frac{1}{3}\theta\delta_{in} - \omega_k \mathcal{E}_{ink}\right)\mathcal{E}_{nmj} = 0 . \tag{2}$$

These relationships (2) are known as the Papkovich equations. Similarly, the well-known Saint-Venant equations can be obtained as the necessary and sufficient conditions of continuity for the rotation vector ω_k. The Cauchy relationships (1), the Papkovich equations (2), and the Saint-Venant equations may be treated as kinematic constraints [2]-[4]. All these relationships are used in the algorithm of the model proposed. The quasi-classical model of a medium with a nonsymmetric stress tensor can be formulated by using the nonsymmetric Cauchy relationships (1). Considering the Papkovich equations (2) and the Saint-Venant equations as kinematic constraints, we can obtain a Cosserat model for a medium with nonfree rotations, that is, rotations that depend on other generalized coordinates. In particular, the

Papkovich equations (2) give us the following variational equation:

$$\begin{aligned}\delta U = \iiint \Big\{ &\sigma_{ij}\delta\left[\gamma_{ij} + \frac{1}{3}\theta\delta_{ij} - \omega_k \mathcal{E}_{ijk} - \frac{\partial R_i}{\partial x_j}\right] \\ &- m_{ij}\delta\left[\frac{\partial}{\partial x_m}\left(\gamma_{in} + \frac{1}{3}\theta\delta_{in} - \frac{\partial\omega_k}{\partial x_m}\mathcal{E}_{ink}\right)\mathcal{E}_{nmj}\right]\Big\}\, dV .\end{aligned} \tag{3}$$

Here, σ_{ij} and m_{ij} are the components of the stress tensor and the components of the Cosserat stress tensor, respectively. These equations may be used as a base for the mathematical description of the generalized Cosserat model with restricted rotations.

Let us assume that the linear form (3) is integrable. Then, we can represent the potential energy as follows:

$$\begin{aligned}\delta U = &\iiint U_V\left(\frac{\partial\omega_i}{\partial x_j}, \gamma_{ij}, \frac{\partial\theta}{\partial x_n}, \omega_n, R_n, \theta\right) dV \\ &+ \oiint U_F\left(R_i, \frac{\partial R_i}{\partial x_q} n_q\right) dF .\end{aligned} \tag{4}$$

Here, n_j are the components of the normal vector of the boundary surface F of the elastic body under consideration.

Thus, for a linear elastic medium, we can obtain the quadric form for the density of the potential energy. The system of constitutive equations can be found with the aid of the Green relationships. The components of generalized static strain and stress state in the body and the superficial forces on the surface can be found by using the formulas:

$$\sigma_{ij} = \partial U_V \Big/ \partial\left(\frac{\partial R_i}{\partial x_j}\right), \quad m_{ij} = \partial U_V \Big/ \partial\left(\frac{\partial\omega_i}{\partial x_j}\right), \quad \mu_i = \partial U_V \Big/ \partial\left(\frac{\partial\theta}{\partial x_i}\right),$$

$$\sigma_i = \partial U_V / \partial R_i, \qquad f_{ij} = \partial U_F / \partial R_i, \qquad m_i = \partial U_F / \partial \dot{R}_i$$

where $\dot{R}_i = (\partial R_i / \partial x_q) \cdot n_q$.

It is worth emphasizing that the coefficients of quadratic terms of U_V in (4) are determined by the deformations γ_{ij}, ω_n, and θ. These coefficients define the system of conventional elastic properties of the medium and have dimensions of stresses. The constant coefficients of quadratic terms which are associated with the vectors R_n, ω_n, and $\frac{\partial\theta}{\partial x_n}$ and the tensor $\frac{\partial\omega_i}{\partial x_j}$ are of the remaining dimensions. The multiscale effects of other type can be determined with the aid of these constants. We further suppose that some of these constants allow us to describe the interactions corresponding to the internal cohesion.

On the other hand, U_F (4) can be represented as

$$\begin{aligned}U_F = \frac{1}{2}\big\{&(AR_iR_j + 2A_1R_i\dot{R}_j + A_2\dot{R}_i\dot{R}_j)n_in_j + BR_iR_j(\delta_{ij} - n_in_j) \\ &+ 2B_1R_i\dot{R}_j(\delta_{ij} - n_in_j) + B_2\dot{R}_i\dot{R}_j(\delta_{ij} - n_in_j)\big\} .\end{aligned} \tag{5}$$

The constants A, A_1 and A_2 in (5) determine the surface effects associated with the normal to the surface of the body, and the constants B, B_1, and B_2 in (5) determine the superficial effects in the tangential plane.

2.1 Kinematic model for the Cosserat pseudocontinuum (the fields of defects)

To describe the models of media with a continuous field of defects, we will consider the conditions of nonintegrability of the Cauchy relationships (1) instead the Papkovich equations (2):

$$\frac{\partial}{\partial x_m}\left(\gamma_{in}+\frac{1}{3}\,\theta\delta_{in}-\omega_k\mathcal{E}_{ink}\right)\mathcal{E}_{nmj}=\Xi_{ij}\,. \tag{6}$$

The tensor Ξ_{ij} is such that $\frac{\partial\Xi_{ij}}{\partial x_j}=0$. This tensor determines the field of incompatibility for displacements. A vector of jumps in displacements can be found by using the tensor (6). In other words, we can say that the virtual Burgers vector is represented by Ξ_{ij}. Furthermore, when this vector is written as the flux of the tensor Ξ_{ij} through any surface, this flux gives the virtual Burgers vector of dislocation. That is why the tensor Ξ_{ij} is called the dislocation density tensor.

Using the relationships (6) as kinematic constraints, we can construct the Cosserat pseudocontinuum with free deformations and rotations, that is, with deformations and rotations considered as independent generalized coordinates. In this case, the mathematical statement of the problem is based on the following variational equation:

$$\begin{aligned}\delta U=\iiint\Big\{&\sigma_{ij}\delta\left(\gamma^0_{ij}+\frac{1}{3}\,\theta^0\delta_{ij}-\omega^0_k\mathcal{E}_{ijk}-\frac{\partial R^0_i}{\partial x_j}\right)\\&+\,m_{ij}\delta\left[\Xi_{ij}-\frac{\partial}{\partial x_m}\left(\gamma^{\Xi}_{in}+\frac{1}{3}\,\theta^{\Xi}\delta_{in}-\omega^{\Xi}_k\mathcal{E}_{ink}\right)\mathcal{E}_{nmj}\right]\Big\}\,dV\,.\end{aligned} \tag{7}$$

Here, γ^{Ξ}_{ij}, ω^{Ξ}_k, and θ^{Ξ} are defined by the right-hand part of the tensor equation (6) and can be considered as particular solutions of this tensor equation.

Taking into account the definition of the Cosserat continuum, we will define γ^0_{ij}, θ^0, and ω^0_n as nonfree deformations and γ^{Ξ}_{ij}, θ^{Ξ}, and ω^{Ξ}_n as free deformations.

Similarly, the Cosserat models based on the conditions of nonintegrability for the Papkovich equations was obtained, the disclination density tensor was defied, and the mathematical statement of the problem for the generalized Cosserat pseudocontinuum was formulated in [5].

This process may be continued and the conditions of nonintegrability for the Saint-Venant relationships with respect to the gradient of the volume deformation θ may be obtained [4]. As a result, a new type of defects is modeled. This type of defects is additional to the dislocations and disclinations.

These defects are determined by jumps in $\partial\theta/\partial x_n$ and are described with the aid of the density tensor. Thus, the procedure of modeling proposed gives us the natural classification of models for continuums with defects [5].

3 The model of the cohesion field

One particular case of the Cosserat pseudocontinuum (7) gives us the variant of the cohesion field model [4], [5]:

$$\iiint \left\{ L_{ij} \left[-\frac{l_0^2}{\mu} L_{jk}(\dots) + \delta_{jk}(\dots) \right] R_k + X_i \right\} \delta R_i \, dV + \oiint \left[-\widehat{M}_i \delta \frac{\partial R_i}{\partial x_q} n_q + \widehat{Y}_i \delta R_i \right] dF = 0 \,. \tag{8}$$

Here,

$$L_{ij}(\dots) = (2\mu + \lambda) \frac{\partial^2(\dots)}{\partial x_i \partial x_j} + (\mu + \chi) \left(\delta_{ij} \Delta(\dots) - \frac{\partial^2(\dots)}{\partial x_i \partial x_j} \right)$$

$$\widehat{M}_i = \frac{2(\mu+\chi)^2}{\mu} l_0^2 [n_m n_j \mathcal{E}_{ijn} + (1 - 2\nu_*) n_n n_j \mathcal{E}_{ijm}] \frac{\partial \omega_n}{\partial x_m} - \frac{2(\mu+\lambda)^2}{\mu} l_0^2 \frac{\partial \theta}{\partial x_k} n_k n_i$$

$$\widehat{Y}_i = Y_i - \left[2\mu\gamma_{ij} + \left(\frac{2\mu}{3} + \lambda \right) \theta \delta_{ij} - 2\chi\omega_k \mathcal{E}_{ijk} + \frac{2(\mu+\chi)^2}{\mu} l_0^2 \Delta\omega_n \mathcal{E}_{ijn} - \frac{2(\mu+\lambda)^2}{\mu} l_0^2 \Delta\theta\delta_{ij} \right] n_j + (\delta_{qj} - n_q n_j) \times \frac{\partial}{\partial x_q} \left[-\frac{2(\mu+\chi)^2}{\mu} l_0^2 \left[\frac{\partial \omega_k}{\partial x_p} + (1 - 2\nu_*) \frac{\partial \omega_p}{\partial x_k} \right] n_p \mathcal{E}_{ijk} + \frac{2(\mu+\lambda)^2}{\mu} l_0^2 \frac{\partial \theta}{\partial x_k} n_k \delta_{ij} \right],$$

where Δ is the Laplace operator, R_i is the vector of total displacement, μ and λ are the Lame coefficients, ν_* is a dimensionless constant of the model, and l_0^2 is a dimensional constant of the Cosserat pseudocontinuum.

Let us introduce the classical displacement vector associated with the operator of the classical theory of elasticity L_{ij} and the cohesion displacement vector associated with non-classical scale effects:

$$R_i = U_i - u_i, \qquad U_i = \left[-\frac{l_0^2}{\mu} L_{ij}(\dots) + \delta_{ij}(\dots) \right] R_j \tag{9}$$

$$u_i = -\frac{l_0^2}{\mu} L_{ij}(R_j) \,.$$

Here, U_i is the classical displacement vector and u_i is the cohesion displacement vector.

Then, we can restate the mathematical statement of the problem (8). The variational equation (8) implies the following differential equilibrium equations and boundary conditions for the model under consideration:

$$
\begin{aligned}
&L_{ij}(U_j) + X_i = 0, \qquad L_{ij}(u_j) - \frac{\mu}{l_0^2} u_i + X_i = 0, \\
&\delta L = \oiint \{ \widehat{M}_i \delta \dot{U}_i + \widehat{Y}_i \delta U_i - \widehat{M}_i \delta \dot{u}_i - \widehat{Y}_i \delta u_i \} \, dF = 0 \, .
\end{aligned}
\tag{10}
$$

4 Numerical simulation of media with inclusions by the block analytical-numerical method

The simulation of physical processes in non-classical media with inclusions can be effectively performed by the method based on analytical representations of the solution (so-called block analytical-numerical method [6]-[8]). The general scheme of the method consists in covering the initial region by a set of simple sub-regions called blocks. A solution in every block is approximated by a series in terms of special functions (called multipoles), which best reproduce the analytical properties of the solution and strongly satisfy the problem's operator equations. Comparing with finite element and boundary element methods, the method proposed has the advantage that it gives us the possibility to employ more complicated functions, which can describe analytical properties of the solution near to boundary singularities of the domain (for instance, reentrant corners with small or zero rounding radii [6]). Besides the representation of the solution in analytical form, this method facilitates procedures of calculation and optimization of effective and local characteristics of the heterogeneous media with inclusions.

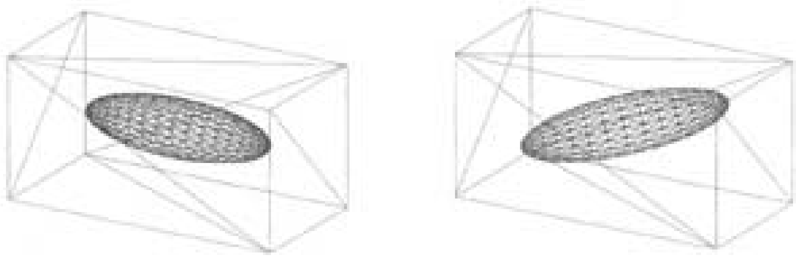

Fig. 1. Various types of inclusions

For various types of inclusions (see Fig. 1), the first step is to construct a block structure covered the initial region. The following method for the construction can be proposed.

For a plane problem, in a domain with an elliptic inclusion (as an example, see Fig. 2), we use a rectangular grid and then additionally split those rectangular cells that are intersecting by the boundary of the inclusion. Then we

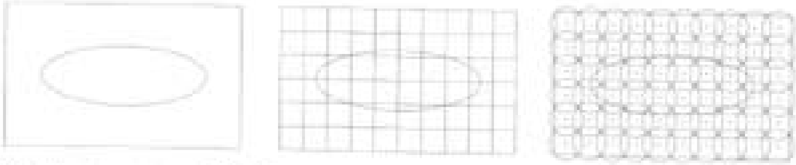

Fig. 2. Construction of block structure

circumscribe a circle about every cell and obtain circular blocks as it shown in Fig. 2.

Let us now consider the double plane problem ($R_1 = R$, $R_2 = R_3 = 0$) for the total displacement vector $R = U - u$ in the cell with constructed block structure. From the above discussion it appears that now the problem can be stated as follows:

$$\mathcal{L}_C\,\mathcal{L}\,R = 0, \quad \mathcal{L} = \mathcal{L}_C\big|_{C=0}, \quad \mathcal{L}_C = (2\mu + \lambda)\frac{\partial^2}{\partial x^2} + \mu\frac{\partial^2}{\partial y^2} - C,$$

$$R = \begin{cases} R_f & \text{in inclusion} \\ R_m & \text{in matrix} \end{cases}, \quad \mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{\nu E}{(1-2\nu)(1+\nu)};$$

these equations should be completed by the following conditions on the boundary of the inclusion and the cell:

$$[R] = \left[\frac{\partial R}{\partial n}\right] = 0, \quad [\hat{Y}] = 0, \quad [\widehat{M}] = 0,$$

$$R(\pm L, y) = \pm 1, \qquad \widehat{M} = 0, \quad 0 < y < H,$$

$$\frac{\partial R}{\partial n}(x, 0) = \frac{\partial R}{\partial n}(x, H) = 0, \qquad \hat{Y} = 0, \quad -L < x < L,$$

where E is the modulus of elasticity (Young's modulus), ν is Poisson's ratio, $C = 1/l_0^2$ is a dimensional constant of the Cosserat pseudocontinuum, $[R] = R_f - R_m$ is the jump at the inclusion, $\partial/\partial n$ is the derivative in the direction of the boundary normal vector with the components n_x and n_y, H is the height of the cell, and L is the half-width of the cell.

For a numerical example, let us assume the following values of parameters: $\nu_f = \nu_m = 0.3$, $E_f/E_m = 3$, and $C_m/\mu_m = C_f/\mu_f = 100$.

It may be proved that an approximate iterative algorithm for the solution of the problem (9) can be used. Here, to construct the approximate solution, we restrict ourselves to the first step in the iterative procedure, which has two stages.

First, the classical problem ($\mathcal{L}\, U = 0$) is solved for the following boundary conditions:

$$[U] = 0\,, \qquad \left[\mu\,\frac{\partial U}{\partial n} + (\mu + \lambda)\,\frac{\partial U}{\partial x}\,n_x\right] = 0\,, \tag{11a}$$

$$U(\pm L,\, y) = \pm 1, \qquad\qquad 0 < y < H\,, \tag{11b}$$

$$\frac{\partial U}{\partial n}(x,\,0) = \frac{\partial U}{\partial n}(x,\,H) = 0, \quad -L < x < L\,. \tag{11c}$$

Second, the displacement of the cohesion field u is found as a solution of the non-classical equation ($\mathcal{L}_C\, u = 0$) with the following boundary conditions at the contour of the inclusion and at the boundary of the cell:

$$[u] = \frac{[c^*]}{\langle c^* \rangle}\,\langle u \rangle\,, \qquad \left[\frac{\partial u}{\partial n} - \frac{\partial U}{\partial n}\right] = 0\,, \tag{12a}$$

$$u(\pm L,\, y) = 0, \qquad\qquad 0 < y < H\,, \tag{12b}$$

$$\frac{\partial u}{\partial n}(x,\,0) = \frac{\partial u}{\partial n}(x,\,H) = 0, \quad -L < x < L\,. \tag{12c}$$

Here,

$$\langle u \rangle = u_f + u_m, \qquad \langle c^* \rangle = c^*_f + c^*_m, \qquad c^*_{f,m} = C_{f,m}/E_{f,m}\,.$$

In every block, we use a finite series (with sufficient number of multipoles) for the system of the following functions (see [8]):

$$\begin{aligned} \Phi^*_s(x,\, y) &= \Phi^*_s(\sqrt{2\mu + \lambda}\,\bar{x},\, \sqrt{\mu}\,\bar{y}) \\ &= \Gamma(s+1)(\sqrt{C}/2)^{-s}\, I_s(\sqrt{C}\,r)\, \exp(is\,\varphi)\,, \end{aligned}$$

where $\Gamma(s)$ is the Euler gamma-function, $I_s(r)$ is the modified Bessel function, $r = \sqrt{\bar{x}^2 + \bar{y}^2}$, and $\varphi = \arctan \bar{y}/\bar{x}$.

The local displacements $U^{(k)}$ and $u^{(k)}$ (in the block with the number k) are coupled to the displacements of adjacent blocks by a particular variant of the least square method for a multi-block system (see [8]); the conditions (11a)-(12c) are enforced by the same method. Some examples of the tension distribution are presented in Figs. 3 and 4. The parameters of the inclusion are taken as follows: the major axis of the ellipse $a = 1.4\,\varepsilon$, the minor axis of the ellipse $b = (0.5,\, 0.3)\,\varepsilon$, where $\varepsilon \;=\; (0.9,\, 0.7,\, 0.5)$ and the parameters of the cell are $L = 1$ and $H = 1.2$.

In Fig. 3, the tension patterns are depicted which belongs to the classical model. The first pattern corresponds to $2.4\,\mu_m$, the others correspond to the increment $0.2\,\mu_m$. The corresponding tension patterns associated with the cohesion fields are presented in Fig. 4.

As can be seen, the pattern of distribution differs essentially from the pattern corresponding to the classical model. This is due to the presence of

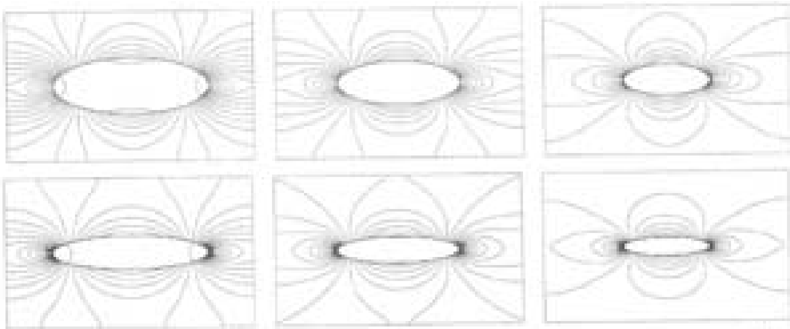

Fig. 3. Examples of the classical tension distributions $\sigma_x(U) = (2\mu + \lambda)\frac{\partial U}{\partial x}$

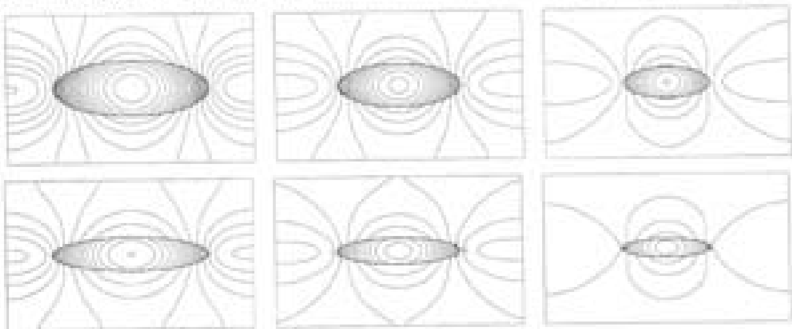

Fig. 4. Examples of tension distributions $\sigma_x(R)$ in the complete problem

the cohesion component u in the complete problem (9), (10). The change in the stress-strain state leads to the change in the balance of the potential energy between the inclusions and the matrix. As a result, the stiffness and strength parameters of a cell as a whole may vary. It seems plausible that an accurate estimation of these effects should be performed for the determination of the parameters of the models.

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