Estimation of effective elastic moduli of random structure composites by the method of fundamental solutions

Valeriy A. Buryachenko*

Micromechanics and Composites LLC, 2520 Hingham Lane, Dayton, OH 45459, USA

Abstract

One considers linearly elastic composite media, which consist of a homogeneous matrix containing a statistically homogeneous random set of aligned homogeneous heterogeneities of non canonical shape. Effective elastic moduli as well as the first statistical moments of stresses in the phases are estimated through the averaged boundary integrals over the inclusion boundaries. The modified popular micromechanical models are based on the numerical solution for one inhomogeneity inside the infinite matrix loaded by remote homogeneous effective field. This solution is obtained by a meshfree method based on fundamental solutions basis functions for a transmission problem in linear elasticity. The problem here addressed, consists in computing the displacement and traction fields of an elastic object, which has piecewise constant Lamé coefficients, from a given displacement (or stress) field on the infinity. The main properties of the method are analyzed and illustrated with several numerical simulations in 2D domains.

Keywords: Boundary integral equations, Method of fundamental solutions, Mechanics of deformable solids, Homogenization, determination of effective properties

1. 1. Introduction

The prediction of the behavior of composite materials in terms of the mechanical properties of constituents and their microstructure is a central problem of micromechanics, which is evidently reduced to the estimation of stress fields in the constituents. Appropriate, but by no means exhaustive, references for the estimation of effective elastic moduli of statistically homogeneous media are provided by the reviews [1-8]. It appears today that variants of the effective medium method [9, 10] and the mean field method [11, 12] are the most popular

*Corresponding author

Email address: buryach@aol.com (Valeriy A. Buryachenko)

and widely used methods. Recently a new method has become known, namely the multiparticle effective field method (MEFM) was put forward and developed (see for references Buryachenko [6]). The MEFM is based on the theory of functions of random variables and Green's functions. Within this method one constructs a hierarchy of statistical moment equations for conditional averages of the stresses in the inclusions. The hierarchy is then cut by introducing the notion of an effective field. This way the interaction of different inclusions is taken into account. The popular schemes of micromechanical analysis are based on numerical solutions for estimation of stress (or strain) distribution tensor for single (at least) inclusion inside infinite matrix subjected to so-called effective field.

Obtaining analytical solutions is not feasible in general even for a finite number of interacting particles, so various numerical methods have been developed, mostly based on the finite element analysis (FEA) and boundary integral equation (BIE) technique. A distinct advantage of the BIE compared to the FEA is that the BIEs require meshing only the boundary surface of computational domain as opposed to the entire 3-D domain for FEA. In the BIE singular forces distributed, e.g., on the surface of particles, depend on the external field, thus yielding an integral equation for the singularity strengths. The most popular formulation is the direct one where the variables of interest are the surface displacement and traction fields that leads to a set of ill-conditioned linear systems on discretization. The indirect formulation (e.g. the completed double layer boundary element method, see [13, 14]) results in a set of integral equations of the second kind, and therefore is numerically well-behaved. Although this formulation is more complicated than the direct method, however, it leads to an unconditionally convergent iterative scheme.

Despite the FEM's and BEM's popularity, there are many problems (e.g. meshing surface in 3D, computing of singular integrals) where it is desirable to improve the efficiency of traditional methods. In the alternative (proposed by Trefftz), the trial functions must satisfy the governing equation exactly and the error in the satisfaction of the boundary conditions is minimised. As a consequence, it is interesting to develop some alternative so-called meshless methods (see [15] for an overview and historical background on the subject) of the local boundary integral equation, boundary knot method, boundary collocation method, non-dimensional dynamic influence functions method, and the method of fundamental solutions (MFS) belonging to a boundary method for solving boundary value problems, which can be recognized as a discrete type of the indirect boundary element method with a concentrated source instead of distribution (see for references [16-19]). In this study, we will bring the MFS systematically for a single inclusion inside the infinite homogeneous matrix subjected to homogeneous loading. The MFS belonging to the BIE technique has a very attractive option since it is truly meshless, simple to program, and is able to take into account a sharp changes in geometry. The MFS and related methods over the last years have found extensive application in computing solutions to a broad range of problems [20, 21].

In the MFS the solution is approximated by a finite linear combination

55 of fundamental solutions (FS, assumed to be explicitly defined) with respect
 to source points which are positioned outside the solution domain. The un-
 known coefficients in the mentioned linear approximation can be determined by
 matching the boundary conditions in a variety of ways, the simplest (and most
 popular) being by collocation on a set of physical boundary points. In contrast
 60 to domain discretization methods such as the finite element (FEM), the MFS
 is a boundary method which means that only the boundary of the solution do-
 main needs to be considered. Moreover, the MFS is a boundary-type meshless
 method which does not need a boundary element mesh, either for purposes of
 interpolation of the trial and test functions of the solution variables, or for the
 65 integration, and only a set of source points is required for the discretization of
 the problem being analyzed. However, unlike the BEM, no potentially trouble-
 some integration is required in the MFS due to the placement of source points
 outside the solution domain when the singular integrals are avoided. At last
 MFS is adaptive in the sense that it can take into account sharp changes in
 70 the solution and in the geometry of the domain and can easily handle complex
 boundary conditions. Despite the mentioned advantages, a few disadvantages
 are that the positioning of the source points are preassigned and also the result-
 ing system of algebraic equations is ill-conditioned that leads to oscillation of
 the convergence curve of the numerical solution when a large number of source
 75 points are used. Optimization of source points allocation substantially reduces
 computational time while some regularization methods, such as the damped sin-
 gular value decomposition, the truncated singular value decomposition or the
 Tikhonov [22] regularization, can be used to mitigate the ill-conditioned effect
 (see [23]). The next step is checking the approximation in other (not collocation)
 80 points at the physical boundary (or interface) surface. The strain and
 stress field variables outside the boundary can be obtained directly when the
 derivatives are analytically calculated from the MFS expansion representation
 over the source points with the coefficients found by matching the boundary
 condition at the given collocation points at the physical surface.

85 Thus, the stress distributions inside a single inclusions inside infinite matrix
 are assumed to be found. This solution then can be incorporated into the one
 or another general framework of analytical micromechanics for self-consistent
 estimations of so-called effective field (see for details Buryachenko [6]). However,
 all mentioned methods are based on the effective field hypothesis (EFH, even
 90 if the term “*effective field hypothesis*” was not indicated) according to which
 each inclusion is located inside a homogeneous so-called effective field (see for
 references [6]). Effective field hypothesis is apparently the most fundamental,
 most prospective, and most exploited concept of micromechanics. This concept
 has directed a development of micromechanics over the last sixty years and made
 95 a contribution to their progress incompatible with any another concept. The
 idea of effective field was added by the hypothesis of “*ellipsoidal symmetry*” for
 the distribution of inclusions attributed to Willis [24]. However, Buryachenko
 [25, 26] has proved that the EFH is a central one and other concepts play a
 satellite role providing the conditions for application of the EFH.

100 The paper is organized as follow. In Section 2 we present the basic field

equations of linear elasticity, notations, statistical description of the composite microstructure as well as representation of the effective properties through the surface integrals over the inclusion boundaries. In Section 3, one presents the method of fundamental solution (MFS) adapted to the solution for one homogeneous noncanonical inclusion inside the infinite homogeneous matrix. The known micromechanical method of the effective field (MEF, see for references [6]) and Mori-Tanaka method (MTM, [11, 12]) are presented in Section 4 with the stress concentration factors and effective compliances expressed through the boundary integral of statistical averages over the boundary inclusions. In Section 5 we estimate the numerical errors of both the different versions of the MFS and the different choices of the source sets. The numerical evaluation of the effective Young modulus are shown for a statistically homogeneous composites reinforced by aligned identical homogeneous heterogeneities of noncanonical shape.

2. Preliminaries

Let a full space R^d with a space dimensionality d ($d = 2$ and $d = 3$ for 2- D and 3- D problems, respectively) contains a homogeneous matrix $v^{(0)}$ and, in general, a statistically inhomogeneous set $X = (v_i)$ of heterogeneities v_i with indicator functions V_i and bounded by the closed smooth surfaces $\Gamma_i := \partial v_i$ ($i = 1, 2, \dots$) defined by the relations $\Gamma_i(\mathbf{x}) = 0$ ($\mathbf{x} \in \Gamma_i$), $\Gamma_i(\mathbf{x}) > 0$ ($\mathbf{x} \in v_i$), and $\Gamma_i(\mathbf{x}) < 0$ ($\mathbf{x} \notin v_i$). It is assumed that the heterogeneities can be grouped into components (phases) $v^{(q)}$ ($q = 1, 2, \dots, N$) with identical mechanical and geometrical properties (such as the shape, size, orientation, and microstructure of heterogeneities).

2.1. Basic equations

Let a linear elastic body occupy an open bounded domain $w \subset R^d$ with a smooth boundary Γ and with an indicator function W and space dimensionality d ($d = 2$ and $d = 3$ for 2- D and 3- D problems, respectively). The domain w contains a homogeneous matrix $v^{(0)}$ and a statistically inhomogeneous set $X = (v_i, V_i, \mathbf{x}_i)$ of inclusions v_i with indicator functions V_i and centers $\mathbf{x}_i$. It is assumed that the inclusions can be grouped into component (phase) $v^{(1)}$ with identical mechanical and geometrical properties (such as the shape, size, orientation, and microstructure of inclusions). For the sake of definiteness, in the 2- D case we will consider a plane-strain problem. At first no restrictions are imposed on the elastic symmetry of the phases or on the geometry of the inclusions¹.

¹It is known that for 2- D problems the plane-strain state is only possible for material symmetry no lower than orthotropic (see e.g. [27]) that will be assumed hereafter in 2- D case.

The problem is governed by the local equations of elastostatics of composites

$$\nabla \boldsymbol{\sigma}(\mathbf{x}) = \mathbf{0}, \quad (1)$$

$$\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{L}(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x}), \text{ or } \boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{M}(\mathbf{x})\boldsymbol{\sigma}(\mathbf{x}), \quad (2)$$

$$\boldsymbol{\varepsilon}(\mathbf{x}) = [\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^\top]/2, \quad \nabla \times \boldsymbol{\varepsilon}(\mathbf{x}) \times \nabla = \mathbf{0}, \quad (3)$$

where $(\cdot)^\top$ denotes transposition, $\otimes$ and $\times$ are the tensor and vector products. $\mathbf{L}(\mathbf{x})$ and $\mathbf{M}(\mathbf{x}) \equiv \mathbf{L}(\mathbf{x})^{-1}$ are the known stiffness and compliance fourth-order tensors, and the common notation for contracted products has been employed.

In particular, for isotropic constituents the stiffness tensor $\mathbf{L}$ is given in terms of the local bulk modulus k and the shear modulus μ : $\mathbf{L} = (dk, 2\mu) \equiv dk\mathbf{N}_1 + 2\mu\mathbf{N}_2$, $\mathbf{N}_1 = \boldsymbol{\delta} \otimes \boldsymbol{\delta}/d$, $\mathbf{N}_2 = \mathbf{I} - \mathbf{N}_1$ ($d = 2$ or 3); $\boldsymbol{\delta}$ and $\mathbf{I}$ are the unit second-order and fourth-order tensors. For the fiber composites it is the plane-strain bulk modulus $k_{[2]}$ – instead of the 3-D bulk modulus $k_{[3]}$ – that plays the significant role: $k_{[2]} = k_{[3]} + \mu_{[3]}/3$, $\mu_{[2]} = \mu_{[3]}$. The tensors $\mathbf{g}$ ($\mathbf{g} = \mathbf{L}, \mathbf{M}$) of material properties are piecewise constant and decomposed as $\mathbf{g} \equiv \mathbf{g}^{(0)} + \mathbf{g}_1(\mathbf{x}) = \mathbf{g}^{(0)} + \mathbf{g}_1^{(1)}(\mathbf{x})$ where $\mathbf{g}^{(0)} = \text{const}$, $\mathbf{g}(\mathbf{x}) \equiv \mathbf{g}^{(0)}$ at $\mathbf{x} \in v^0$ and $\mathbf{g}_1^{(1)}(\mathbf{x}) \equiv \mathbf{g}_1^{(1)}$ is a homogeneous function of the $\mathbf{x} \in v^{(1)}$:

$$\mathbf{L}_1^{(1)}(\mathbf{x}) = \mathbf{L}_1^{(1)} \equiv \text{const. at } \mathbf{x} \in v^{(1)}. \quad (4)$$

The upper index (m) indicates the components and the lower index i indicates the individual inclusions; $v^{(0)} = w \setminus v$, $v \equiv v^{(1)}$, $V(\mathbf{x}) = V^{(1)} = \sum V_i(\mathbf{x})$, and $V^{(1)}(\mathbf{x})$ and $V_i(\mathbf{x})$ are the indicator functions of $v^{(1)}$ and v_i , respectively.

The introduction of jumps of material properties allows one to define the stress $\boldsymbol{\tau}$ and strain $\boldsymbol{\eta}$ polarization tensors by two equivalent ways ($\mathbf{x} \in R^d$)

$$\boldsymbol{\tau}(\mathbf{x}) = \mathbf{L}_1(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x}), \quad \boldsymbol{\eta}(\mathbf{x}) = \mathbf{M}_1(\mathbf{x})\boldsymbol{\sigma}(\mathbf{x}), \quad \boldsymbol{\tau} = -\mathcal{L}^{(0)}\boldsymbol{\eta}, \quad (5)$$

$$\boldsymbol{\tau}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x}) - \mathbf{L}^{(0)}\boldsymbol{\varepsilon}(\mathbf{x}), \quad \boldsymbol{\eta}(\mathbf{x}) = \boldsymbol{\varepsilon}(\mathbf{x}) - \mathbf{M}^{(0)}\boldsymbol{\sigma}(\mathbf{x}), \quad (6)$$

which are simply a notational convenience and vanish inside the matrix $\boldsymbol{\tau}(\mathbf{x}) \equiv \boldsymbol{\eta}(\mathbf{x}) \equiv \mathbf{0}$ ($\mathbf{x} \in v^{(0)}$). Hereafter $\mathbf{M}_1(\mathbf{y})$ is the jumps of $\mathbf{M}^{(k)}$ inside the component $v^{(k)}$ ($k = 0, \dots, N$) with respect to the $\mathbf{M}^{(0)}$, respectively. It is interesting, the popular polarization tensors (5) (see, e.g., Willis, [1]) are attributed to Hashin and Shtrikman [28] and Hill [29] who introduced, in fact, these notions in the equivalent form (6). For both local and nonlocal elasticity theory, Eqs. (5) and (6) are also equivalent; however, the form (6) is preferable for subsequent manipulation because Eq. (6) does not explicitly use the constitutive equation (2) for the heterogeneities $\mathbf{x} \in v$.

We assume that the phases are perfectly bonded, so that the displacements and the traction components are continuous across the interphase boundaries, i.e.

$$[[\mathbf{u}]] = \mathbf{0}, \quad [[\boldsymbol{\sigma}\mathbf{n}^{\text{int}}]] = \mathbf{0} \quad (7)$$

on the interface boundary Γ^{int} where $\mathbf{n}^{\text{int}}$ is the normal vector on Γ^{int} and $[[(\cdot)]]$ is the jump operator. The traction $\mathbf{t}(\mathbf{x}) = \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}(\mathbf{x})$ acting on any plane with

the normal $\mathbf{n}(\mathbf{x})$ through the point $\mathbf{x}$ can be represented in terms of displacements $\mathbf{t}(\mathbf{x}) = \hat{\mathbf{t}}(\mathbf{n}, \nabla)\mathbf{u}(\mathbf{x})$, where $\hat{t}_{ik}(\mathbf{n}, \nabla) = L_{ijkl}n_j(\mathbf{x})\partial/\partial x_l$ is the conormal derivative operator. The boundary conditions at the interface boundary will be considered together with the mixed boundary conditions on Γ with the unit outward normal $\mathbf{n}^\Gamma$

$$\mathbf{u}(\mathbf{x}) = \mathbf{u}^\Gamma(\mathbf{x}), \quad \mathbf{x} \in \Gamma_u, \quad \boldsymbol{\sigma}(\mathbf{x})\mathbf{n}^\Gamma(\mathbf{x}) = \mathbf{t}^\Gamma(\mathbf{x}), \quad \mathbf{x} \in \Gamma_t, \quad (8)$$

where Γ_u and Γ_t are prescribed displacement and traction boundaries such that $\Gamma_u \cup \Gamma_t = \Gamma$, $\Gamma_u \cap \Gamma_t = \emptyset$. $\mathbf{u}^\Gamma(\mathbf{x})$ and $\mathbf{t}^\Gamma(\mathbf{x})$ are, respectively, prescribed displacement on Γ_u and traction on Γ_t . Of special practical interest are the homogeneous boundary conditions

$$\mathbf{u}^\Gamma(\mathbf{x}) = \boldsymbol{\varepsilon}^\Gamma \mathbf{x}, \quad \boldsymbol{\varepsilon}^\Gamma \equiv \text{const.}, \quad \mathbf{x} \in \Gamma, \quad (9)$$

$$\mathbf{t}^\Gamma(\mathbf{x}) = \boldsymbol{\sigma}^\Gamma \mathbf{n}^\Gamma(\mathbf{x}), \quad \boldsymbol{\sigma}^\Gamma = \text{const.}, \quad \mathbf{x} \in \Gamma, \quad (10)$$

where $\boldsymbol{\varepsilon}^\Gamma$ and $\boldsymbol{\sigma}^\Gamma$ are the macroscopic strain and stress tensors, which are the given constant symmetric tensors.

2.2. Statistical description of random structure composites

It is assumed that the representative macrodomain w contains a statistically large number of realizations α of inclusions $v_i \in v^{(1)}$ ($i = 1, 2, \dots$) of the constituent $v^{(1)}$ (providing validity of the standard probability theory technique). A random parameter α belongs to a sample space $\mathcal{A}$, over which a probability density $p(\alpha)$ is defined (see, e.g., Willis [1]). For any given α , any random function $\mathbf{g}(\mathbf{x}, \alpha)$ (e.g., $\mathbf{g} = V, \boldsymbol{\sigma}, \boldsymbol{\varepsilon}$) is defined explicitly as one particular member, with label α , of an ensemble realization. Then, the mean, statistical or ensemble average is defined by the angle brackets enclosing the quantity $\mathbf{g}$

$$\langle \mathbf{g} \rangle(\mathbf{x}) = \int_{\mathcal{A}} \mathbf{g}(\mathbf{x}, \alpha) p(\alpha) d\alpha. \quad (11)$$

No confusion will arise below in notation of the random quantity $\mathbf{g}(\mathbf{x}, \alpha)$ if the label α is dropped for compactness of expressions unless such indication is necessary. One treats two material length scales (see, e.g., Torquato [4]): the macroscopic scale L , characterizing the extent of w , and the microscopic scale a , related with the heterogeneities v_i . Moreover, one supposes that applied field varies on a characteristic length scale Λ . The limit of our interests for both the material scales and field one is presented in an asymptotic sense

$$L \gg \Lambda \geq a, \quad (12)$$

as the scale of microstructure a relative to the macroscale L tends to zero. All the random quantities under discussion are described by statistically homogeneous random fields. For the alternative description of the random structure of a composite material let us introduce a conditional probability density $\varphi(v_i, \mathbf{x}_i | v_1, \mathbf{x}_1)$, which is a probability density to find the i -th heterogeneity with the center $\mathbf{x}_i$

in the domain v_i with fixed heterogeneity v_1 with the centers $\mathbf{x}_1$. The notation $\varphi(v_i, \mathbf{x}_i; v_1, \mathbf{x}_1)$ denotes the case $\mathbf{x}_i \neq \mathbf{x}_1$.

To prevent overlapping of different inclusions $\varphi(v_i, \mathbf{x}_i; v_m, \mathbf{x}_m) = 0$ for values of $\mathbf{x}_i$ lying inside the “excluded volumes” $\cup v_{mi}^0$, where $v_{mi}^0 \supset v_m$ with indicator function V_{mi}^0 is the “excluded volumes” of $\mathbf{x}_i$ with respect to v_m (it is usually assumed that $v_{mi}^0 \equiv v_m^0$), and $\varphi(v_i, \mathbf{x}_i; v_m, \mathbf{x}_m) \rightarrow \varphi(v_i, \mathbf{x}_i)$ as $|\mathbf{x}_i - \mathbf{x}_m| \rightarrow \infty$ (since no long-range order is assumed). $\varphi(v_i, \mathbf{x})$ is a number density, $n(\mathbf{x}) = n$ of component $v \ni v_i$ at the point $\mathbf{x}$ and $c^{(1)}$ is the concentration, i.e. volume fraction, of the component $v_i \in v$: $c^{(1)} = \langle V \rangle = \bar{v}_i n$, $\bar{v}_i = \text{mes } v_i$ ($i = 1, 2, \dots$), $c^{(0)}(\mathbf{x}) = 1 - \langle V \rangle$. Hereafter, if the pair distribution function $g(\mathbf{x}_i - \mathbf{x}_m) \equiv \varphi(v_i, \mathbf{x}_i; v_m, \mathbf{x}_m)/n^{(k)}$ depends on $\mathbf{x}_m - \mathbf{x}_i$ only through $|\mathbf{x}_m - \mathbf{x}_i|$ it is called the radial distribution function (RDF, see for references and details Buryachenko *et al.* [30]). The notations $\langle (\cdot) \rangle(\mathbf{x})$ and $\langle (\cdot) | v_1, \mathbf{x}_1 \rangle(\mathbf{x})$ will be used for the average and for the conditional average taken for the ensemble of a statistically homogeneous field $X = (v_i)$ at the point $\mathbf{x}$, on the condition that there are inclusions at the points $\mathbf{x}_1$. The notation $\langle (\cdot) \rangle_i(\mathbf{x})$ at $\mathbf{x} \in v_i$ means the statistical average over an ensemble realization of surrounding inclusions at the fixed v_i whereas $\langle (\cdot) \rangle_{(i)}$ indicates the volume average over an inclusion v_i in a single realization and $\langle (\cdot) \rangle_i \equiv \langle \langle (\cdot) \rangle_{(i)} \rangle$.

2.3. Effective properties

For statistically homogeneous media and homogeneous boundary conditions, the effective stiffness $\mathbf{L}^*$ and effective compliance $\mathbf{M}$ governed by the expectation of Eqs. (2)

$$\langle \boldsymbol{\sigma} \rangle = \mathbf{L}^* \langle \boldsymbol{\varepsilon} \rangle, \quad \langle \boldsymbol{\varepsilon} \rangle = \mathbf{M}^* \langle \boldsymbol{\sigma} \rangle \quad (13)$$

are defined by general relations

$$\mathbf{L}^* = \langle \mathbf{L} \mathbf{A}^* \rangle, \quad \mathbf{M}^* = \langle \mathbf{M} \mathbf{B}^* \rangle, \quad (14)$$

where $\mathbf{A}^*(\mathbf{x})$ and $\mathbf{B}^*(\mathbf{x})$ are the local strain and stress concentrator factors, respectively, obtained under pure mechanical loading $\boldsymbol{\varepsilon}(\mathbf{x}) = \mathbf{A}^*(\mathbf{x}) \boldsymbol{\varepsilon}^\Gamma$ (9) and $\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}^*(\mathbf{x}) \boldsymbol{\sigma}^\Gamma$ (10), respectively. By the use of the decomposition of the material tensor $\mathbf{g}$ ($\mathbf{g} = \mathbf{L}, \mathbf{M}$) Eqs. (14) can be rewritten in an equivalent form

$$\mathbf{L}^* = \mathbf{L}^{(0)} + \langle \mathbf{L}_1 \mathbf{A}^* V \rangle, \quad \mathbf{M}^* = \mathbf{M}^{(0)} + \langle \mathbf{M}_1 \mathbf{B}^* V \rangle. \quad (15)$$

The effective properties evaluations (15) are based on the estimations of the averages of polarisation tensors $\boldsymbol{\tau}$ (5₁) and $\boldsymbol{\eta}$ (5₂) averaged over the inclusion volume v . However, the representations $\boldsymbol{\tau}$ (6₁) and $\boldsymbol{\eta}$ (6₂) allows one to use only surface averages of these tensors. Namely, the volume averages of the strains and stresses inside inclusions can be expressed through the averages over the inclusion boundaries by the use of the Gauss’s theorem

$$\langle \boldsymbol{\varepsilon} V \rangle = \frac{1}{2\bar{v}} \int_{\Gamma} [\mathbf{u}(\mathbf{s}) \otimes \mathbf{n}(\mathbf{s}) + \mathbf{n}(\mathbf{s}) \otimes \mathbf{u}(\mathbf{s})] d\mathbf{s}, \quad (16)$$

$$\langle \boldsymbol{\sigma} V \rangle = \frac{1}{2\bar{v}} \int_{\Gamma} [\mathbf{t}(\mathbf{s}) \otimes \mathbf{s} + \mathbf{s} \otimes \mathbf{t}(\mathbf{s})] d\mathbf{s}, \quad (17)$$

where in Eq. (17) one used the equality $\nabla(\mathbf{s} \otimes \boldsymbol{\sigma}) = \boldsymbol{\sigma}$. Then the effective properties (15) can be expressed through the boundary integrals

$$\begin{aligned} \mathbf{L}^* &= \mathbf{L}^{(0)} + \mathbf{S}^{\epsilon*}, \\ \mathbf{S}^{\epsilon*} \langle \boldsymbol{\epsilon} \rangle &:= \frac{1}{2\bar{v}} \int_{\Gamma} \left\{ \mathbf{t}(\mathbf{s}) \otimes \mathbf{s} + \mathbf{s} \otimes \mathbf{t}(\mathbf{s}) - 2\mathbf{L}^{(0)}[\mathbf{u}(\mathbf{s}) \otimes \mathbf{n}(\mathbf{s})] \right\} d\mathbf{s}, \end{aligned} \quad (18)$$

$$\begin{aligned} \mathbf{M}^* &= \mathbf{M}^{(0)} + \mathbf{S}^{\sigma*}, \\ \mathbf{S}^{\sigma*} \langle \boldsymbol{\sigma} \rangle &:= \frac{1}{2\bar{v}} \int_{\Gamma} \left\{ \mathbf{u}(\mathbf{s}) \otimes \mathbf{n}(\mathbf{s}) + \mathbf{n}(\mathbf{s}) \otimes \mathbf{u}(\mathbf{s}) - 2\mathbf{M}^{(0)}[\mathbf{s} \otimes \mathbf{t}(\mathbf{s})] \right\} d\mathbf{s}, \end{aligned} \quad (19)$$

for the boundary conditions (9) and (10), respectively. The representation (18) for a particular case of the isotropic matrix is reduced to the corresponding equations proposed in [31, 32].

3. Method of Fundamental Solutions (MFS)

3.1. The scheme of the Method of Fundamental Solutions (MFS)

Estimation of the effective properties (18) and (19) through the boundary integrals over the inclusion surfaces Γ_i is performed by substitutions of the corresponding integrals for a single representative inclusion v_i into one or another micromechanical model (some of them will be considered in Section 4). Although an estimation of the boundary integrals for a single particle v_i can be performed by the different BEMs, we consider the Method of Fundamental Solutions (MFS) which is a straightforward method that allows to approach the solution of Eqs. (1)–(3) for the known fundamental solutions. The solution is treated as a series of the fundamental solutions with singularities located outside the computational domain of the problem under consideration. The unknown coefficients of the series of the fundamental solutions are regarded as the strengths or the densities of the corresponding fundamental solutions. Namely, let the domains v_i and $\hat{v}_i^{(1)}$ be open subsets in R^d separated by the smooth boundary Γ_i (see, e.g., [33]). We say that $\hat{v}_i^{(1)}$ with the smooth pseudo-boundary $\hat{\Gamma}_i^{(1)} := \partial\hat{v}_i^{(1)}$ embraces v_i if $(v_i \cup \Gamma_i) \subset \hat{v}_i^{(1)}$. In a similar manner, one can define a pseudo-boundary $\hat{\Gamma}_i^{(0)} := \partial\hat{v}_i^{(0)}$ of an open subset $\hat{v}_i^{(0)}$ embracing the open domain $R^d \setminus (v_i \cup \Gamma_i)$. So, the grey regions in Figs. 1 and 2 are the inclusion v_i with the boundary $\Gamma_i = \partial v_i$. The pseudo-boundaries $\hat{\Gamma}_i^{(0)}$ are constructed from $\Gamma_i = \partial v_i$ by a homothety transformation (26) (Fig. 1a) and by a normal direction choice for the source points (27) (Fig. 1b), respectively, which will be considered later.

One introduces the infinite body Green's function $\mathbf{G}^{(k)}$ of the Navier equation with homogeneous elastic modulus tensor $\mathbf{L}^{(k)}$, defined by

$$\nabla \left\{ \mathbf{L}^{(k)} [\nabla \otimes \mathbf{G}^{(k)}(\mathbf{x})] \right\} = -\boldsymbol{\delta} \delta(\mathbf{x}), \quad (20)$$

of order $O(\int |\mathbf{x}|^{1-d} d|\mathbf{x}|)$ as $|\mathbf{x}| \rightarrow \infty$ and vanishing at infinity ($|\mathbf{x}| \rightarrow \infty$) in 3-D. We will also use the tensors of the fundamental stresses, tractions, and

strains

$$\begin{aligned}\mathbf{D}^{(m)}(\mathbf{x} - \mathbf{s}) &= \mathbf{L}^{(m)} \nabla \mathbf{G}^{(m)}(\mathbf{x} - \mathbf{s}), \\ \mathbf{T}^{(m)}(\mathbf{x}, \mathbf{s}) &= -\mathbf{n}^\Gamma(\mathbf{x}) \mathbf{D}^{(m)}(\mathbf{x} - \mathbf{s}), \\ \mathcal{E}^{(m)}(\mathbf{x} - \mathbf{s}) &= \nabla \mathbf{G}^{(m)}(\mathbf{x} - \mathbf{s}).\end{aligned}\tag{21}$$

In particular, for isotropic medium we reproduce the compact representation of the mentioned Green functions valid for both 2-D and 3-D cases (see e.g. [4, 34]) in Appendix.

Fig. 1: The boundary $\Gamma_i = \partial v_i$ and the pseudo-boundaries $\hat{\Gamma}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$ constructed by Eqs. (26) (1a) and (27) (1b), which will be considered later.

We place m points of the admissible singularities (or sources) $\{\mathbf{y}_p^k\}_{p=1}^m$ corresponding to the external ($k = 0$) and internal ($k = 1$) problems on the prescribed pseudoboundary surfaces $\hat{\Gamma}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$, respectively. A slight modification of Alves and Silvestre [35] (see also [36]) results shows that it is possible to approach the boundary conditions for the displacement approximated by linear combinations of the corresponding fundamental solutions. Let the effective field $\bar{\mathbf{u}}(\mathbf{x})$ be prescribed in the collocation points $\{\mathbf{x}_j\}_{j=1}^m \in \Gamma_i$. Then the strength of FSs $\mathbf{f}_i^{(k)} = (\mathbf{f}_{ip|1}^{(k)}, \dots, \mathbf{f}_{ip|d}^{(k)})^\top$ ($p = 1, \dots, m$) hold a $dm \times dm$ linear system of equations ($j = 1, \dots, d$, $l = 1, \dots, m$)

$$\sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(1)} G_{jq}^{(1)}(\mathbf{r}_{lp}^1) = \sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(0)} G_{jq}^{(0)}(\mathbf{r}_{lp}^0) + \bar{u}_j(\mathbf{x}_l),\tag{22}$$

where $\mathbf{r}_{lp}^k = (\mathbf{x}_l - \mathbf{y}_p^k)$ and $|\mathbf{r}_{lp}^k|$ is the distance between the collocation point (the field point), $\mathbf{x}_l$, and the location of the FSs (the source point), $\mathbf{y}_p^k \in \hat{\Gamma}_i^{(k)}$ ($k = 0, 1$). In a similar manner, the traction boundary conditions (7₂) can be obtained directly by taking summation of the traction FSs with the same strength $\mathbf{f}_i^{(k)} = (\mathbf{f}_{ip|1}^{(k)}, \dots, \mathbf{f}_{ip|d}^{(k)})^\top$ (22) over the source points $\mathbf{y}_p^k \in \hat{\Gamma}_i^{(k)}$ outside

the boundary Γ_i ($j, q = 1, \dots, d$; $p = 1, \dots, m$; $k = 0, 1$):

$$\sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(1)} T_{jq}^{(1)}(\mathbf{r}_{lp}^1) = \sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(0)} T_{jq}^{(0)}(\mathbf{r}_{lp}^0) + \bar{t}_j(\mathbf{x}_l), \quad (23)$$

where $\bar{\mathbf{t}} = \bar{\boldsymbol{\sigma}} \mathbf{n}^{\Gamma_i}(\mathbf{x}_l)$. We assumed in the system (22) and (23) that the numbers of both the field points $\{\mathbf{x}_l\}_{l=1}^m$ and source ones $\{\mathbf{y}_p^k\}_{p=1}^m$ ($k = 0, 1$) coincide. In such a case the strength of the FSs, $\mathbf{f}_i$, are determined uniquely, provided that the corresponding coefficient matrix is nonsingular. If $\bar{\mathbf{u}}(\mathbf{x})$ is prescribed in more points $\mathbf{x}_1, \dots, \mathbf{x}_n \in \Gamma_i$, with $n > m$, the system (22) and (23) is overdetermined, and the strength can be chosen by the discrete least-squares method (see [33, 35]) which is not considered in more details in the current paper.

Once the strength of the FS, $\mathbf{f}_i^{(k)}$, are found by solving the system (22) and (23) at $\{\mathbf{x}_l\}_{l=1}^m \in \Gamma_i$, the displacement vector in both the inclusion v_i and matrix $R^d \setminus v_i$ is then calculated straightforwardly by using the left-right side and right-hand side, respectively, of Eq. (22) with values of replaced radius-vectors $\mathbf{x}_l \rightarrow \mathbf{x}_s$ corresponding to location of a point $\mathbf{x}_s$. All other field variables can be obtained directly by taking summation of the same strength $\mathbf{f}_i^{(k)}$ (22) and (23) of the corresponding FSs over the source points $\mathbf{y}_p^k \in \hat{\Gamma}_i^{(k)}$ ($k = 0, 1$) outside the boundary Γ_i , e.g. the displacement and stress induced by m FSs can be estimated by the equations ($j, l = 1, \dots, d$):

$$u_j(\mathbf{x}_s) = \sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(k)} G_{jq}^{(k)}(\mathbf{r}_{sp}^k) + \bar{u}_j(\mathbf{x}_s) \delta_{k0}, \quad (24)$$

$$\sigma_{jl}(\mathbf{x}_s) = \sum_{p=1}^m \sum_{q=1}^d f_{ipq}^{(k)} D_{jlq}^{(k)}(\mathbf{r}_{sp}^k) + \bar{\sigma}_{jl}(\mathbf{x}_s) \delta_{k0} \quad (25)$$

for $\mathbf{x}_s \in v_i$ ($k = 1$) and $\mathbf{x}_s \in (R^d \setminus v_i)$ ($k = 0$), respectively.

A specific feature of the MFS is some freedom in choosing the source points with respect to the accuracy of the numerical solution. Young *et al.* [37] estimated an excellent accuracy of the MFS for the positions of the source points $\mathbf{y}$ in computational domain through the field points $\mathbf{x}_l$ ($l = 1, \dots, m$) by a homothety transformation:

$$\mathbf{y}_l = \mathbf{x}_i + b(\mathbf{x}_l - \mathbf{x}_i), \quad (26)$$

where $\mathbf{x}_i$ is a homothetic center coinciding with the particle center. Once the parameters $0 < b < 1$ and $1 < b$ for $k = 1$ and $k = 0$, respectively, are chosen, the distribution of the source points is determined. The pseudo-boundaries $\hat{\Gamma}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$ in Fig. 1a are obtained from the boundary $\hat{\Gamma}_i$ of the grey inclusion v_i by the homothety transformation (26).

However, for the thin inclusions with the thickness $2h$ (e.g. for the tri-axial ellipsoid with distinct semi-axis lengths $a_1 > a_2 \gg a_3$, $h = a_3$) the distances $D(\mathbf{y}_l, \Gamma_i)$ (defining the matrix coefficients $G_{jq}^{(k)}(\mathbf{r}_{lp}^1)$ (22) and $T_{jq}^{(k)}(\mathbf{r}_{lp}^1)$ (23) are

essentially differ one from another points $\mathbf{x}_i$. Here $D(\mathbf{y}_l, \Gamma_i)$ denotes the Euclidean distance between $\mathbf{y}_l$ and the boundary of v_i , or in other words, the radius of the largest inscribed disk with center $\mathbf{y}_l$. Because of this, for the thin inclusions the following allocations of the source points ($k = 0, 1$)

$$\mathbf{y}_l^k = \mathbf{x}_l + (2k - 1)d_k \mathbf{n}^{\Gamma_i}(\mathbf{x}_l) \quad (27)$$

with $d = D(\mathbf{y}_l, \Gamma_i) = 10 - 30\%h$ is preferable.

The algorithm of the normal direction choice for the source points (27) proposed by Alves and Antunes [38] was accomplished by so called global choice for the coefficient d_k ($k = 0, 1$) recently presented in [39]. A simplest choice of a constant d_k is a non-optimal one that works in most cases. In such a case, the pseudo-boundaries $\hat{\Gamma}^{(1)}$ and $\hat{\Gamma}^{(0)}$ can be presented as the boundaries of Minkowski addition and subtraction

$$\hat{v}^{(1)} = v_i \oplus (\mathbf{0}, d_0), \quad \hat{v}^{(0)} = v_i \ominus b(\mathbf{0}, d_1) \quad (28)$$

, respectively, of the domain v_i , where $b(\mathbf{0}, d_k)$ stands the ball of radius d centered at the origin $\mathbf{0}$. As an example, a grey cross-section of a spherocylinder (or a capsule) with the aspect ratio $\alpha = R/h$ is presented in Fig. 1b. The pseudo-boundaries $\hat{\Gamma}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$ in Fig. 1b are obtained from the boundary $\hat{\Gamma}_i$ of the grey inclusion v_i by the normal direction choice for the source points (27) with $d_1 = h/2$ and $d_0 = h/2$, respectively. In so doing, the aspect ratios of the domains with the pseudo-boundaries $\hat{\Gamma}_i^{(1)}$ and $\hat{\Gamma}_i^{(0)}$ are $(2\alpha + 1)/3$ and $(2\alpha - 1)$ while the aspect ratios of the corresponding domains obtained by the homothety transform (27) do not change and equal α .

Alves [39] (see also [38]) analysed optimisation of more general stresslet allocation techniques for convex and concave regions. However, more detail consideration of optimization of FS's allocation substantially reducing computational time for the elastic problem solution is beyond the scope of the current study.

3.2. The matrix representation of the MFS

Construction and solution of the linear algebraic system (22) is straightforward (see, e.g., [37, 40]). However, we consider it in more details for the 2D domain v_i . The singularities $Y_p^0 = (y_{p|1}^0, y_{p|2}^0)$ and $Y_p^1 = (y_{p|1}^1, y_{p|2}^1)$ ($p = 1, \dots, P$) are fixed on the boundaries $\hat{\Gamma}_i^{(0)}$ of $\hat{v}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$ of $\hat{v}_i^{(1)}$, respectively. A set of P collocation points $X_p = (x_{p|1}, x_{p|2})$ ($p = 1, \dots, P$) is chosen on Γ_i . Then the system (22) can be presented in the matrix form

$$\mathbf{A}\mathbf{f} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{1,2} & \dots & \mathbf{A}_{1,P} \\ \mathbf{A}_{2,1} & \mathbf{A}_{2,2} & \dots & \mathbf{A}_{2,P} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}_{P,1} & \mathbf{A}_{P,2} & \dots & \mathbf{A}_{P,P} \end{pmatrix} \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \vdots \\ \mathbf{f}_P \end{pmatrix} = \begin{pmatrix} \mathbf{g}_1 \\ \mathbf{g}_2 \\ \vdots \\ \mathbf{g}_P \end{pmatrix} = \mathbf{g} \quad (29)$$

where the $4P \times 4P$ matrix $\mathbf{A}$ with the submatrices

$$\mathbf{A}_{\alpha,\beta} = \begin{pmatrix} \mathbf{A}_{\alpha,\beta}^{1,1} & \mathbf{A}_{\alpha,\beta}^{1,2} \\ \mathbf{A}_{\alpha,\beta}^{2,1} & \mathbf{A}_{\alpha,\beta}^{2,2} \end{pmatrix} \quad (30)$$

are defined through the submatrices

$$\mathbf{A}_{\alpha,\beta}^{1,\delta+1} = (-1)^{\delta+1} \mathbf{G}^{(\delta)}(|X_\alpha - Y_\beta^\delta|) \in R^{2 \times 2}, \quad (31)$$

$$\mathbf{A}_{\alpha,\beta}^{2,\delta+1} = (-1)^{\delta+1} \mathbf{T}^{(\delta)}(|X_\alpha - Y_\beta^\delta|) \in R^{2 \times 2}, \quad (32)$$

and

$$\begin{aligned} \mathbf{f}_p &= (\mathbf{f}_p^{(0)}, \mathbf{f}_p^{(1)})^\top = (f_{p|1}^{(0)}, f_{p|2}^{(0)}, f_{p|1}^{(1)}, f_{p|2}^{(1)})^\top \in R^4, \\ \mathbf{g}_p &= (\mathbf{g}_p^{(0)}, \mathbf{g}_p^{(1)})^\top = (g_{p|1}^{(0)}, g_{p|2}^{(0)}, g_{p|1}^{(1)}, g_{p|2}^{(1)})^\top \in R^4, \end{aligned} \quad (33)$$

where $f_{p|j}^{(\delta)} = f_{p|j}^{(\delta)}(Y_p^\delta)$, $g_{p|j}^{(\delta)} = \bar{u}_{p|j} \delta_{0\delta} + \bar{t}_{p|j} \delta_{1\delta}$, and $j = 1, 2$; $p, \alpha, \beta = 1, \dots, P$; $\delta = 0, 1$. It is observed for $d = 2, 3$ that accurate numerical results could be obtained when the source points for the pseudoboundary $\hat{\Gamma}_i^{(0)}$ of the submerged stresslets are located off the boundary at about 70 – 90% (26) of the distance from the center (see for details Young *et al.* [37]).

It should be mentioned that for two limiting cases of the rigid inclusions and pores, one can consider one pseudo-boundary $\hat{\Gamma}_i^{(0)}$ instead of two pseudo-boundaries $\hat{\Gamma}_i^{(0)}$ and $\hat{\Gamma}_i^{(1)}$. Namely, the matrix Eq. (28) is formally kept without changes. However, now the matrix $\mathbf{A}$ has a dimension $2P \times 2P$ and for the rigid inclusions the submatrices

$$\mathbf{A}_{\alpha,\beta} = \mathbf{A}_{\alpha,\beta}^{1,1} \quad (34)$$

are defined by the displacement fundamental tensor

$$\mathbf{A}_{\alpha,\beta}^{1,1} = -\mathbf{G}^{(0)}(|X_\alpha - Y_\beta^0|) \in R^{2 \times 2}, \quad (35)$$

and

$$\mathbf{f}_p = (f_{p|1}^{(0)}, f_{p|2}^{(0)})^\top \in R^2, \quad \mathbf{g}_p = (g_{p|1}, g_{p|2})^\top \in R^2, \quad (36)$$

where $f_{p|j}^{(0)} = f_{p|j}^{(0)}(Y_p^0)$, $g_{p|j} = \bar{u}_{p|j}$, and $j = 1, 2$; $p, \alpha, \beta = 1, \dots, P$. In the case of replacement of rigid inclusions by the porous, the equations (34)–(36) should be also replaced by the following equations

$$\mathbf{A}_{\alpha,\beta} = \mathbf{A}_{\alpha,\beta}^{2,1} \quad (37)$$

$$\mathbf{A}_{\alpha,\beta}^{2,1} = -\mathbf{T}^{(0)}(|X_\alpha - Y_\beta^0|) \in R^{2 \times 2}, \quad (38)$$

$$\mathbf{f}_p = (f_{p|1}^{(0)}, f_{p|2}^{(0)})^\top \in R^2, \quad \mathbf{g}_p = (g_{p|1}, g_{p|2})^\top \in R^2, \quad (39)$$

respectively, where $f_{p|j}^{(0)} = f_{p|j}^{(0)}(Y_p^0)$, $g_{p|j} = \bar{t}_{p|j}$, and $j = 1, 2$; $p, \alpha, \beta = 1, \dots, P$.

However, the MFS coefficient matrix $\mathbf{A}$ (29) (as well as (34) and (37)) of the system (22) and (23) is often severely ill-conditioned and the system of linear algebraic equations (22) and (23) cannot be solved by direct methods, such as,

e.g., the least-squares method, producing a highly unstable solution which increases dramatically as the number of boundary collocation points m increases. Several regularization procedures have been proposed to remedy the instability and accuracy loss in the solution of such ill-conditioned matrix equations (see, e.g., [41]). However, we only consider the Tikhonov regularization (TR) method, see e.g., Tikhonov and Arsenin [22], since it is simple, noniterative, and it provides an explicit solution. Namely, the TR procedure consists of seeking a solution which minimizes a criterion made up of the sum of two summands. The first one is a possibly weighted least square term while the second one is a quadratic penalty term on the solution, that is

$$\min\{\|\mathbf{A}\mathbf{f} - \mathbf{g}\|_2^2 + \lambda\|\mathbf{I}^{\text{dm}}\mathbf{f}\|_2^2\}, \quad (40)$$

where $\|(\cdot)\|_2$ denotes the Euclidean norm while for the zeroth order TR method, $\mathbf{I}^{\text{dm}} = \text{diag}(1, \dots, 1) \in R^{dm \times dm}$ is the identity matrix. Formally, the TR procedure provides an explicit solution $\mathbf{f}_\lambda$ of the regularized system of equations,

$$(\mathbf{A}^\top \mathbf{A} + \lambda \mathbf{I}^{\text{dm}})\mathbf{f} = \mathbf{A}^\top \mathbf{g}. \quad (41)$$

The regularization parameter $\lambda \geq 0$ often controls the relative weight of the penalty term in the criterion. For the parameter $\lambda = 0$, Eq. (41) degenerates to the solution of the least squares problem which is completely dominated by contributions from data errors and rounding errors. By adding the penalty term, we are able to reduce these contributions and maintain the penalty term to be of reasonable size. However, the optimal determination of a regularization parameter λ is essential for the effectiveness of the TR method applied to the ill-conditioned interpolation matrix equation. In the L-curve criterion, the optimal value λ is intuitively chosen at the “corner” of the L-curve defined as

$$L = \{\log \|\mathbf{A}\mathbf{f}_\lambda - \mathbf{g}\|_2, \log \|\mathbf{I}\mathbf{f}_\lambda\|_2, \lambda \geq 0\} \quad (42)$$

where the L-curve is a continuous curve when the regularization parameter λ is real in the TR method (see, e.g., [23, 41, 42]) That is the ill-conditioning of the MFS matrix $\mathbf{A}$ generally observed in the MFS does not lead to the resulting accuracy loss when both the TR method is used and the value of the spatial parameter b (26) is considered in the range $0.7 \leq b/a \leq 0.9$.

Substitution of the found solution $\mathbf{f}$ of the matrix Eq. (28) into Eqs. (23) and (24) allows one to present all field variables in an arbitrary point $\mathbf{x} \in R^d$ in a symbolic matrix notations ($k = 0, 1$)

$$\mathbf{u}(\mathbf{x}) - \bar{\mathbf{u}}(\mathbf{x})\delta_{0k} = \mathcal{G}^{(k)}\mathbf{A}^{-1}\mathbf{g}(\mathbf{x}), \quad (43)$$

$$\boldsymbol{\sigma}(\mathbf{x}) - \bar{\boldsymbol{\sigma}}(\mathbf{x})\delta_{0k} = \mathcal{D}^{(k)}\mathbf{A}^{-1}\mathbf{g}(\mathbf{x}), \quad (44)$$

$$\mathbf{t}(\mathbf{x}) - \bar{\mathbf{t}}(\mathbf{x})\delta_{0k} = \mathcal{T}^{(k)}\mathbf{A}^{-1}\mathbf{g}(\mathbf{x}), \quad (45)$$

which can be considered as a representation of the boundary inclusion perturbations defined at the pseudoboundaries either $\hat{\Gamma}_i^{(1)}$ or $\hat{\Gamma}_i^{(0)}$ at $k = 1$ or $k = 0$, respectively.

4. Effective elastic moduli of composite materials

4.1. Some classical hypotheses

The basic hypotheses of micromechanics are well known and presented in the form adopted to the use of the volume integral over the inclusion volume (see, e.g., [6]). We present in this Subsection the same hypotheses in the form which are most adopted for the subsequent application of the boundary integrals over the inclusion boundaries. Namely, we now apply so-called effective field hypothesis (EFH) which is the main approximate hypothesis of many micromechanical methods:

Hypothesis H1. *Each heterogeneity v_i is located in the field ($\vartheta = \varepsilon, \sigma$)*

$$\bar{\vartheta}_i(\mathbf{y}) \equiv \bar{\vartheta}(\mathbf{x}_i) \quad (\mathbf{y} \in v_i), \quad (46)$$

which is homogeneous over the heterogeneity v_i .

For the boundary variables ($\mathbf{s} \in \Gamma_i$), the hypothesis **H1** can be presented in the local coordinate systems connected with v_i

$$\bar{\mathbf{u}}_i(\mathbf{s}) \equiv \bar{\varepsilon}(\mathbf{x}_i)\mathbf{s} \quad \bar{\mathbf{t}}_i(\mathbf{s}) \equiv \bar{\sigma}(\mathbf{x}_i)\mathbf{n}^{\Gamma_i}(\mathbf{s}), \quad (47)$$

where $\mathbf{n}^{\Gamma_i}(\mathbf{s})$ is unit outward normal at $\mathbf{s} \in \Gamma_i$.

According to hypothesis **H1a** and in view of the linearity of the problem there exist constant fourth and second-rank tensors $\mathbf{B}_i(\mathbf{x})$, $\mathbf{R}_i(\mathbf{x})$, such that

$$\sigma(\mathbf{x}) = \mathbf{B}_i(\mathbf{x})\bar{\sigma}(\mathbf{x}_i), \quad \bar{v}_i\eta(\mathbf{x}) = \mathbf{R}_i(\mathbf{x})\bar{\sigma}(\mathbf{x}_i), \quad \mathbf{x} \in v_i, \quad (48)$$

where $v_i \subset v^{(1)}$ and $\mathbf{R}_i(\mathbf{x}) = \bar{v}_i\mathbf{M}_1^{(1)}(\mathbf{x})\mathbf{B}_i(\mathbf{x})$. According to Eshelby's [43] (see also [44]) theorem for the ellipsoidal inclusion v_i , there is the following relation between the averaged tensors (48) $\mathbf{R}_i = \bar{v}_i\mathbf{Q}_i^{-1}(\mathbf{I} - \mathbf{B}_i)$, where $\mathbf{g}_i \equiv \langle \mathbf{g}(\mathbf{x}) \rangle_{(i)}$ ($\mathbf{g}$ stands for $\mathbf{B}_i, \mathbf{R}_i$), where $\mathbf{Q}_i = \mathbf{L}^{(0)}(\mathbf{I} - \mathbf{S}_i)$ is represented through the Eshelby tensor $\mathbf{S}_i$. For example, for the homogeneous ellipsoidal domain v_i we obtain ($\mathbf{x} \in v_i$)

$$\mathbf{B}_i(\mathbf{x}) \equiv \mathbf{B}_i = \left(\mathbf{I} + \mathbf{Q}_i\mathbf{M}_1^{(i)} \right)^{-1}. \quad (49)$$

In the general case of coated inclusions v_i , the tensors $\mathbf{B}_i(\mathbf{x})$ can be found by the transformation method by Dvorak and Benveniste [45] (see for references and details [6]).

Different methods can be employed to truncate the hierarchies of corresponding integral equations (see for references, e.g., [6]). Probably the most popular closing assumption is "quasi-crystalline approximation" by Lax [46] which neglects direct interaction between each pair of heterogeneities although such an interaction takes place though the effective field generated by all surrounding inclusions.

Hypothesis H2, “quasi-crystalline” approximation. *It is supposed that the mean value of the effective field at a point $\mathbf{x} \in v_i$ does not depend on the stress field inside surrounding heterogeneities $v_j \neq v_i$ ($\mathbf{x} \in v_i$, $\mathbf{s} \in \Gamma_i$):*

$$\langle \bar{\boldsymbol{\vartheta}}_i(\mathbf{x}) |; v_j, \mathbf{x}_j \rangle = \langle \bar{\boldsymbol{\vartheta}}_i \rangle, \quad \langle \bar{\boldsymbol{\chi}}_i(\mathbf{s}) |; v_j, \mathbf{x}_j \rangle = \langle \bar{\boldsymbol{\chi}}_i \rangle. \quad (50)$$

To make further progress, the hypothesis of “ellipsoidal symmetry” for the distribution of inclusions attributed to Willis [24] is widely used:

Hypothesis H3, “ellipsoidal symmetry”. *The conditional probability density function $\varphi(v_j, \mathbf{x}_j |; v_i, \mathbf{x}_i)$ depends on $\mathbf{x}_j - \mathbf{x}_i$ only through the combination $\rho = |(\mathbf{a}_{ij}^0)^{-1}(\mathbf{x}_j - \mathbf{x}_i)|$:*

$$\varphi(v_j, \mathbf{x}_j |; v_i, \mathbf{x}_i) = h(\rho), \quad (51)$$

where the matrix $(\mathbf{a}_{ij}^0)^{-1}$ (which is symmetric in the indexes i and j , $\mathbf{a}_{ij}^0 = \mathbf{a}_{ji}^0$) defines the ellipsoid excluded volume $v_{ij}^0 = \{\mathbf{x} : |(\mathbf{a}_{ij}^0)^{-1}\mathbf{x}|^2 < 1\}$.

It is reasonable to assume that $(\mathbf{a}_{ij}^0)^{-1}$ identifies a matrix of affine transformation that transfers the ellipsoid v_{ij}^0 being the “excluded volume” (“correlation hole”) into a unit sphere.

4.2. Some popular methods

Hypotheses **H1–H3** allow one to obtain the explicit solution by the method of effective field (MEF, see for references and details [6]) for the stress distribution (the strain field can be considered in a similar manner) for identical aligned heterogeneities ($v_i = v_j = v_1$, $\mathbf{x} \in v_1$)

$$\langle \bar{\boldsymbol{\sigma}} \rangle_1(\mathbf{x}) = \mathbf{Y} \langle \boldsymbol{\sigma} \rangle, \quad (52)$$

$$\langle \boldsymbol{\sigma} \rangle_1(\mathbf{x}) = \mathbf{B}_i(\mathbf{x}) \mathbf{Y} \langle \boldsymbol{\sigma} \rangle, \quad (53)$$

$$\mathbf{M}^* = \mathbf{M}^{(0)} + n^{(1)} \mathbf{R}_i \mathbf{Y}, \quad (54)$$

$$\mathbf{Y}^{-1} = \mathbf{I} - n^{(1)} \mathbf{R}_i \mathbf{Q}_i^0, \quad (55)$$

where the matrix $\mathbf{Y}$ is determined by the action of the surrounding inclusions and for the sake of simplicity of the subsequent calculation it is usually assumed that the shape of “correlation hole” v_{ij}^0 does not depend on the inclusion v_j : $v_{ij}^0 = v_i^0$ and $\mathbf{Q}_{ij}^0 = \mathbf{Q}_i^0 \equiv \mathbf{Q}(v_i^0)$.

As pointed out by Benveniste [12], the essential assumption in the Mori-Tanaka [11] method (MTM) states that each inclusion v_i behaves as an isolated one in the infinite matrix and subject to some effective stress field $\bar{\boldsymbol{\sigma}}_i$ coinciding with the average stress in the matrix

$$\langle \bar{\boldsymbol{\sigma}}_i \rangle = \langle \boldsymbol{\sigma} \rangle^{(0)}. \quad (56)$$

Using Eq. (56) as the closing assumption and substituting the hypothesis **H2** leads to the next representation for both the statistical average local stresses

and effective compliance

$$\langle \boldsymbol{\sigma} \rangle_i(\mathbf{x}) = \mathbf{B}_i(\mathbf{x})[c^{(0)}\mathbf{I} + c^{(1)}\mathbf{B}_i]^{-1}\langle \boldsymbol{\sigma} \rangle, \quad (57)$$

$$\mathbf{M}^* = \mathbf{M}^{(0)} + c^{(1)}\mathbf{R}_i[c^{(0)}\mathbf{I} + c^{(1)}\mathbf{B}_i]^{-1}. \quad (58)$$

For the identical ellipsoidal inhomogeneous heterogeneities v_i homothetical to v_i^0 , equivalences of Eqs. (53), (54) and (57), (58), respectively, are demonstrated in, e.g., [6]). However, the representations (53), (54) and (57), (58), respectively, do not coincide even for the identical aligned isotropic fibers if v_i and v_i^0 are not homothetic (in particular, if v_i is not an ellipsoid, see [6]).

It should be mentioned that the effective compliances (54) and (58) are traditionally expressed through the averages of the tensors $\mathbf{B}_i(\mathbf{x})$ and $\mathbf{R}_i(\mathbf{x})$ over the inclusion volumes v_i . However, these tensors can be also estimated through the averages over the inclusion boundaries $\mathbf{s} \in \Gamma_i$ of the fields $\boldsymbol{\vartheta}(\mathbf{s})$ ($\boldsymbol{\vartheta} = \boldsymbol{\varepsilon}, \boldsymbol{\sigma}$) corresponding to the homogeneous loading $\bar{\boldsymbol{\sigma}} \equiv \text{const.}$ ($c \rightarrow 0$) of a single inclusion v_i :

$$\mathbf{B}_i\bar{\boldsymbol{\sigma}} = \frac{1}{2\bar{v}_i} \int_{\Gamma_i} [\mathbf{t}(\mathbf{s}) \otimes \mathbf{s} + \mathbf{s} \otimes \mathbf{t}(\mathbf{s})] d\mathbf{s}, \quad (59)$$

$$\mathbf{R}_i\bar{\boldsymbol{\sigma}} = \frac{1}{2} \int_{\Gamma_i} \{ \mathbf{u}(\mathbf{s}) \otimes \mathbf{n}(\mathbf{s}) + \mathbf{n}(\mathbf{s}) \otimes \mathbf{u}(\mathbf{s}) - 2\mathbf{M}^{(0)}[\mathbf{t}(\mathbf{s}) \otimes \mathbf{s}] \} d\mathbf{s}. \quad (60)$$

In such a case the effective compliances $\mathbf{M}^*$ (54) and (58) are estimated through the boundary integrals as in Eqs. (59) and (60). In so doing, the stress concentration tensor $\mathbf{B}_i(\mathbf{x})$ in Eqs. (53) and (57) is estimated by Eq. (45) at $k = 1$.

5. Numerical results

We consider the problem for one inclusion in the infinite homogeneous matrix with large elastic mismatch of the inclusion (the Young modulus $E^{(1)} = 100$ and Poisson ratio $\nu^{(1)} = 0.49$) and the matrix ($E^{(0)} = 1$, $\nu^{(0)} = 0.45$). In order to estimate the approximations introduced by discretizations implemented in the MFS in Section 4.2 and for the evaluation of the solution (29) we compare numerical results with a reference analytical solution for a single circle inclusion inside the infinite matrix in a plane strain problem. In the following experiments (Fig. 2), we considered uniformly spaced collocation points on Γ_i and the same number of source points on $\hat{\Gamma}_i^{(1)}$ and $\hat{\Gamma}_i^{(0)}$ when the source sets prescribed by Eqs. (26) and (27) coincide. We consider a uniform remote tension $\bar{\sigma}_{ij} = \delta_{i1}\delta_{j1}$ generating a homogeneous stress distribution inside circle inclusion $\boldsymbol{\sigma}(\mathbf{x}) = \mathbf{B}_i(\mathbf{x})\bar{\boldsymbol{\sigma}}$ ($\mathbf{B}_i(\mathbf{x}) \equiv \text{const.}$, $\mathbf{x} \in v_i$) which is analytically estimated by means of the Eshelby tensor. The value $B_{i|1111}(\mathbf{x}) \equiv 1.4587$ analytically evaluated is compared with their numerical values $B_{i|1111}(\mathbf{x})$ estimated by both the direct (least-squares) method of solution of Eq. (29) and the pseudo-inverse TR procedure (42) in the vicinity of the inclusion boundary $B_{i|1111}(\mathbf{s}) \equiv \lim B_{i|1111}(\mathbf{x})$ ($\mathbf{x} \rightarrow \mathbf{s}$, $\mathbf{x} \in v_i$, $\mathbf{s} \in \Gamma_i$) In Fig. 2 the curves 1 and

2 are estimated by the direct method and the TR procedure, respectively, for $P = 30$, $d = 0.6$ (27), and $\lambda = 10^{-5}$. The errors corresponding to the curves 1 and 2 equal 6.5% and 0.23%, respectively. Increasing of the number of source points $P = 60$ leads to increasing of accuracy of the TR procedure (42) (curve 4 with the error 0.00068%) and to osculation of the direct solution (29) (curve 3, the error 35%). Subsequent increasing of the number of source points $P = 200$ with $d = 0.1$ provide the error 0.000016% of the stress distribution $B_{i|1111}(\mathbf{s})$ ($\mathbf{s} \in \Gamma_i$) (42) while the approximative osculating solution (29) takes the negative values ($B_{i|1111}(\mathbf{s}) < 0$. at some $\mathbf{x} \in \Gamma_i$) and loses a physical meaning.

Fig. 2: Stress concentration factor $B_{i|1111}(\mathbf{s})$ vs a polar angle ϕ/π .

Now we compare the numerical solutions $B_{i|1111}(\mathbf{x})$ ($\mathbf{x} \in v_i$) obtained by the TR procedure (42) for two types of source sets generated by both the homothety transformation (26) and the normal direction choice (27) with $P = 375$, $b = 0.9$, $d = 0.1R_2$, $\lambda = 10^{-5}$. For demonstration of the difference between the mentioned numerical results, we analyse the elliptic inclusion

$$x_1^2/R_1^2 + x_2^2/R_2^2 = 1 \quad (61)$$

with distinct semiaxis lengths $\alpha := R_2/R_1 = 0.1, 0.2, 0.3$ corresponding to the analytical results $B_{i|1111}(\mathbf{x}) \equiv 5, 731, 3.402, 2.601$ ($\mathbf{x} \in v_i$, $\mathbf{x} = (x_1, 0)^T$), respectively. For $\alpha = 0.3$ both the source sets (26) and (27) provide the comparable accuracies (the errors 0.28% and, 0.016% respectively). However, at the flattening of the elliptical inclusion (with decreasing of α from 0.3 to 0.1) demonstrates an advantage of the algorithm (27) with respect to the homothety transformation (26). Indeed, the errors of the TP procedure (42) exploiting the source set (26) increases to 1.8% (Fig. 3, curve 1) and to 9.2% (curve 3) for $\alpha = 0.2$ and $\alpha = 0.1$, respectively, while the error of the same method (42) with the source set (27) leads to the errors 0.021% (curve 2) and 0.31%

(curve 4), respectively. The reason of so much dramatic decline of accuracy of the estimations corresponding to the source set (26) is explained by an essentially different variation of the distances $D(\mathbf{y}_l, \Gamma_i)$ of the source points from the boundary Γ_i . For the normal direction choice for the source points (27), this distance $d = D(\mathbf{y}_l, \Gamma_i) \equiv 0.1R_2$ is the constant for $\forall \mathbf{y}_l \in \hat{\Gamma}_i^{(k)}$ ($k = 0, 1$) while for homothety transformation (26), the distances $D(\mathbf{y}_l, \Gamma_i)$ equal $d_2 = 0.1R_2$ (as in Eq. (26)) and $d_1 = 0.1R_1 = 10d_2$ for $\mathbf{y}_l = (0, 0.9R_2)^\top$ and $\mathbf{y}_l = (0.9R_1, 0)^\top$, respectively. Thus, TR procedure (42) accompanied by the normal direction choice for the source points (27) provides an excellent accuracy of the solution of the elastic problem for a single inclusion $v_i \subset R^2$ in a wide range of both the elastic mismatch and the aspect ratio of the inclusion.

Fig. 3: Stress concentration factor $B_{i|1111}(x_1)$ vs a normalized coordinate x_1/R_1 .

With the non-essential restriction on space dimensionality d and on the shape of inhomogeneities we will consider 2- D plane strain problems for composites reinforced by aligned infinite fibers with noncircular cross-section schematically presented in the Fig. 4 and described by the curve

$$\begin{cases} (x - R + r)^2 + (y - R + r)^2 = r^2, & \text{for } \{|x| > R - r\} \cap \{|y| > R - r\}, \\ |x + y| + |x - y| = 2R, & \text{for } \{|x| < R - r\} \cup \{|y| < R - r\}, \end{cases} \quad (62)$$

which reduces to a circle and a square in the limiting cases $R = r = a$ and $r = 0$, respectively. Normalized effective Young moduli $E_{11}^*/E^{(0)}$ are presented in Fig. 5 as the functions of the volume concentration of inclusions at $r = 0.2, 0.4, 0.6, 1R$ (curves 1–4) estimated by the MEF. As can be seen, the estimations carried out for the different shape of inclusions defining by rs are essentially different at $c > 0.6$; $E_{11}^*(0.8)/E^{(0)}$ at $c = 0.8$ varies from 23.67 to 7.37 as r varies from 0.2 to 1.0. In so doing, the corresponding values $E_{11}^*(0.8)/E^{(0)}$

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estimated by the MT method at $c = 0.8$ varies from 8.46 (curve 5) to 7.37 (curve 4) as r varies from 0.2 to 1.0. The are known publications (see for references [6]) demonstrating equivalence of the MTM and MEF for composites with identical aligned homogeneous ellipsoidal heterogeneities v_i with the homothetic excluded volume v_i^0 . Because of this, the values $E_{11}^*(c)/E^{(0)}$ estimated by both the MTM and MEF for the circle inclusions $r = 1$ are expectedly coincide with each other (curve 4 in Fig. 5). However, the estimations of $E_{11}^*(c)/E^{(0)}$ (curve 5) carried out by the MTM for $r = 0.2$ are essentially different from the corresponding values evaluated by the MEF (curve 1). As can be seen, the MEF is basically sensitive with respect to the inclusion shape (defining by α) than the MTM.

Fig. 4: Schematic of a noncircular inclusion characterized by the shape parameter r/R

6. Conclusion

In the present paper, numerical results were obtained for composites with statistically homogeneous field of homogeneous aligned prolate identical heterogeneities of non canonical shape. At first, the solution for one inclusion inside infinite medium was obtained by the MFS adapted for analysis of infinite domains. In the MFS one considers representations of the solution as a linear combination of point source fundamental tensors centered at some points placed outside the boundary of interest. The vectorial coefficients of these linear combinations defining a coefficient matrix can be computed by imposing, on some boundary points (collocation points) at the interface, the boundary conditions of the transmission problem. Applications of the proposed techniques were illustrated through several numerical examples. Results obtained using the Tikhonov regularization techniques were compared to those obtained by the direct inversion of corresponding coefficient matrix for the different choices of

the source sets and to analytical values. Several numerical examples for smooth 2D domains and smooth boundary data were presented in order to show the accuracy and feasibility of the method. Possible extensions to the 3D problem require only a placement of both the collocation and source points at the interface Γ_i and the pseudo-boundaries $\hat{\Gamma}_i^{(0)}$, $\hat{\Gamma}_i^{(1)}$, respectively, are straightforward. The numerical evaluation of the effective Young modulus are shown for a statistically homogeneous composites reinforced by aligned identical homogeneous heterogeneities of noncanonical shape.

Fig. 5: Variation of the relative Young modulus $E_{11}^*/E^{(0)}$ as a function of the concentration of the inclusions c .

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Appendix. The representations of the fundamental solutions (20) and (21)

The tensors of the fundamental displacements, tractions, stresses, and strains (20), (21) have the following components ($d = 2, 3$)

$$G_{ij}(r) = Cr[(3 - 4\bar{\nu})\gamma(|\mathbf{x}|)\delta_{ij} + n_i n_j], \quad (\text{A.1})$$

$$T_{ij}(\mathbf{x}, \mathbf{s}) = -2\mu C[(1 - 2\bar{\nu})\delta_{ij} + dn_i n_j]n_k n_k^\Gamma(\mathbf{x}) + (1 - 2\bar{\nu})(n_i n_j^\Gamma(\mathbf{x}) - n_j n_i^\Gamma(\mathbf{x})), \quad (\text{A.2})$$

$$D_{ijk}(r) = -2\mu C[(1 - 2\bar{\nu})(\delta_{ik} n_j + \delta_{jk} n_i - \delta_{ij} n_k) + dn_i n_j n_k], \quad (\text{A.3})$$

$$\mathcal{E}_{ijk}(r) = -C[(3 - 4\bar{\nu})\delta_{ij} n_k - \delta_{ik} n_j - \delta_{jk} n_i + dn_i n_j n_k], \quad (\text{A.4})$$

respectively, where

$$\gamma(r) = \begin{cases} -\ln|\mathbf{x}| & \text{for } d = 2, \\ 1 & \text{for } d = 3, \end{cases} \quad \bar{\nu} = \begin{cases} \nu, & \text{for 3-D and plane strain,} \\ \frac{\nu}{1+\nu}, & \text{for plane stress problems.} \end{cases} \quad (\text{A.5})$$

Here $C = [4\omega_d\mu(1 - \bar{\nu})r^{d-1}]^{-1}$, ω_d is the surface area of the unit sphere in R^d , and the tensor $\mathbf{T}(\mathbf{x}, \mathbf{s})$ is defined at the surface $\mathbf{s} \in S$ with the unit outward normal $\mathbf{n}^\Gamma = (n_1^\Gamma, \dots, n_d^\Gamma)^\top$ at $\mathbf{s} \in S$, $r \equiv |\mathbf{x} - \mathbf{s}|$, $r_{,i} = r_i/r = n_i$.

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