Computational Analytical Micromechanics (CAM). Background, Opportunities, and Prospects

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The sketch of micromechanics of random structures can be subdivided on computational micromechanics (CM) and analytical micromechanics (AM). CM contains both the analytical and numerical solutions for deterministic fields of heterogeneities in the infinite homogeneous matrix. CM reflects the explosive character of the progress in modern nano- and micromechanics caused by the development of improved materials processing, image analyses and computer-simulation methods. AM presents, first of all, a set of both the hypotheses and tools for interactions of these hypotheses with the numerical results of the CM. However, explosive character of the progress in the CM (especially in front of nanotechnology challenges) has led to the conflict with successively increasing gap between the high level of presented possibilities of the CM and poor consumer's opportunities of AM rigidly restricted by its background proposed by Mossotti (1850) and others (see for references [15]).

The most popular methods of AM are based just on a few basic concepts. The effective field hypothesis (EFH, also called the **H1a** hypothesis, p. 253 in [1]) is apparently the most fundamental, most prospective, and most exploited concept of micromechanics (see [1] where other references can be found). The idea of this concept dates back to Mossotti (1850) who pioneered the introduction of the effective field concept as a local homogeneous field acting on the inclusions and differing from the applied macroscopic one. Among a few hypotheses used by Mossotti (1850), one of the most important ones was the quasi-crystalline approximation (closing hypothesis **H2a**, p. 264 in [1], see also its multiparticle generalization, hypothesis **H2b**, p. 255 in [1]) proposed 100 years later by Lax (1952) in a modern concise form. The idea of the effective field and quasi-crystalline approximation was added by the hypothesis **H3** of "ellipsoidal symmetry" (p. 265 in [1]) for the distribution of inclusions just for providing the applicability of EFH. As a tool for concrete applications of the concepts mentioned, Eshelby (1957) solution was used although the Eshelby's theorem has a fundamental conceptual sense rather than only an analytical solution of some particular problem for the ellipsoidal homogeneous inclusion. The concept of the EFH (even if this term is not mentioned) in combination with subsequent assumptions totally dominates (and creates the fundamental limitations) in all four groups of AM in physics and mechanics of heterogeneous media: model methods, perturbation methods, self-consistent methods [e.g., Mori-Tanaka method (MTM), and the Method of Effective Field, MEF], and variational ones (see for refs. [1]).

However, one shows that the EFH is a central one and other concepts play a satellite role providing the conditions for application of the EFH. Moreover, one shows that all mentioned hypotheses are not really necessary and can be relaxed. The first attack on a citadel called EFH was produced by creation in [3]-[5] the exact general integral equation

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \langle \boldsymbol{\varepsilon} \rangle(\mathbf{x}) + \int [\mathbf{U}(\mathbf{x}-\mathbf{y})\boldsymbol{\tau}(\mathbf{y}) - \langle \mathbf{U}(\mathbf{x}-\mathbf{y})\tau(\mathbf{y})\rangle(\mathbf{y})] d\mathbf{y}. \tag{1}$$

where $\boldsymbol{\tau}(\mathbf{x}) \equiv \mathbf{L}_1(\mathbf{x})\boldsymbol{\varepsilon}(\mathbf{x})$ (see [1, 4] for complete notations). Equation (1) was obtained without any auxiliary assumptions such as, e.g., the version of the EFH $\langle \mathbf{U}(\mathbf{x}-\mathbf{y})\tau(\mathbf{y})\rangle(\mathbf{y}) = \mathbf{U}(\mathbf{x}-\mathbf{y})\langle \tau(\mathbf{y})\rangle(\mathbf{y})$ (hypothesis **H1b**, p. 253 in [1]) implicitly exploited in the known centering methods and reducing Eq. (1) for statistically homogeneous media subjected to the homogeneous boundary conditions to the known one

$$\boldsymbol{\varepsilon}(\mathbf{x}) = \langle \boldsymbol{\varepsilon} \rangle + \int \mathbf{U}(\mathbf{x}-\mathbf{y})[\boldsymbol{\tau}(\mathbf{y}) - \langle \tau \rangle] d\mathbf{y}, \tag{2}$$

which goes back to Lord Reyleigh (1892). One demonstrates (see [4] and [5]) that Eq. (2), erroneously recognized as an exact one after the proofs by Shermergor (1977) and by O'Brien (1979), is correct only after the additional asymptotic assumption **H1b**. The mentioned conflict between CM and AM is presently overcome in a conceptual sense very effectively by the new general integral Eq. (1) and their generalizations [15,16] forming a new background of micromechanicsthat that allows one to completely abandon the hypotheses **H1** and **H3** while the hypothesis **H2** can be used for multiparticle generality.

A fundamental deficiency of Eq. (2) is a dependence of the renormalizing term $\mathbf{U}(\mathbf{x}-\mathbf{y})\langle\boldsymbol{\tau}\rangle(\mathbf{y})$ [obtained in the framework of the asymptotic approximation of the hypothesis **H1b**] only on the statistical average $\langle\boldsymbol{\tau}\rangle(\mathbf{y})$ while the renormalizing term $\langle\mathbf{U}(\mathbf{x}-\mathbf{y})\boldsymbol{\tau}\rangle(\mathbf{y})$ in Eq. (1) explicitly depends on on details distribution $\langle\boldsymbol{\tau}|v_i,\mathbf{x}_i\rangle(\mathbf{y})$ $(\mathbf{y}\in v_i)$. What seems to be only a formal trick is in reality a new background of micromechanics defining a new field of micromechanics called computational analytical micromechanics (CAM). CAM makes it possible to abandon basic concepts of AM **H1a**, **H1b**, **H3** (either completely [5] or partially [6]) in the framework of hypotheses either **H2a** [5] or **H2b** [7-9] at the solutions of truncated hierarchies of averaged Eq. (1) by the use of any available numerical method (VIE [5], BEM, FEM [6, 13], hybrid FEM-BEM, multipole expansion method, complex potential method, and other, see for refs. [1]). So, the final classical representations of the effective properties obtained by both the MEF and MTM (see for details [1]) depend only on the average strain concentrator factor $\mathbf{A}_i$, with $\langle\boldsymbol{\varepsilon}\rangle_i=\mathbf{A}_i\langle\overline{\boldsymbol{\varepsilon}}\rangle_i$, while the effective properties estimated by the new approach (1) implicitly depend on the inhomogeneous tensor $\mathbf{A}_i(\mathbf{x})$. The detected dependence allows us to abandon the hypothesis **H1b** whose accuracy is questionable for inclusions of noncanonical shape. We obtained a fundamental conclusion that effective moduli in general depend not only on the strain distribution inside the considered heterogeneity (describing by the tensor $\mathbf{A}_i(\mathbf{x})$, $\mathbf{x}\in v_i$) but also on the strains in the vicinity of heterogeneity i.e. extension of $\mathbf{A}_i(\mathbf{x})$, $\mathbf{x}\notin v_i$ is necessary. Then the size of the excluded volume as well as the binary correlation function will impact on the effective field even in the framework of hypothesis **H2a**.

It is expected to get a larger difference (which can reach infinity with the change of the sign of predicted local stresses) between the results obtaining the use of either Eqs. (1) and (2) for composites reinforced by heterogeneities demonstrating greater inhomogeneity of stress distributions inside heterogeneities. This inhomogeneity can be produced by the different contributors: *a*) peculiarities of heterogeneities manifested even in the framework of the hypothesis **H1a**, *b*) multiparticle interaction of heterogeneities (even homogeneous ellipsoidal ones), *c*) special feature of both the microstructure and applied loading. The next problems were solved (partialy, of course, see for refs. [1]) in the framework of the EFH and can be recast in the framework of the CAM with detection of significant improvement of predicted accuracy by the use of Eq. (1) instead of Eq. (2):

a). Composites with nonellipsoidal [6, 10, 11, 13], coated, continuously inhomogeneous [5] heterogeneities with either nonideal interface (including sliding, debonding, cohesive phenomena, as well as surface stress and surface tension ones [14]), nonlocal constitutive law (p. 581 in [1]), or wave propagation phenomena [15] (including metamaterials).

b) Inhomogeneity of statistical moments of stresses for homogeneous ellipsoidal heterogeneities detected for binary interacting heterogeneities [7].

c) Any nonlocal problem (inhomogeneous remote loading, functionally graded materials, clustered materials, bounded media, nanocomposides, nonlocal constitutive law [8, 9, 15] either inside or outside the heterogeneities).

d) Variational methods currently postulated homogeneity of polarization tensors inside the heterogeneities (this assumption is even more restrictive then EFH) can be renewed by using (1) instead of (2). e) Multi-physics coupled problems (e.g., electromagnetic, piezoelectric) [15, 16].

f) Wave motion phenomena in composites (including metamaterials) with electromagnetic, optic, and mechanical responses [15, 16].

g) Infiltration in porous media [20].

i) Peridynamic composites [17-19] [especially in the light that the definition of effective properties of peridynamic composites is unknown and any counterpart of GIE (neither (1) nor (2)) was recently absent].

j) Micromechanics of contact of randomly rough surfaces.

The solutions of mentioned problems obtained in the framework of the EFH were used as the basic elements in analyses of wide classes of dynamic, nonlinear, and coupled problems (see for refs. [1]). The generalisation of these schemes can be also performed in the framework of the CAM.

The researches can now forget about the restrictions of AM (such as, e.g., Eshelby tensor and the hypothesis **H1** and **H3**) and use the numerical solutions for one and a few (perhaps) heterogeneities obtained by any available method of CM (e.g., FEM, BEM, hybrid FEM-BEM, multipole expansion method, complex potential method, and other). The use of the hypothesis **H2** (and their generalizations, see [1]) is a technical problem rather than fundamental one. In a few years, it is expected the renewal of a lot of results (with discovery of fundamentally new effects) in the mentioned directions at a higher level of generality without the classical assumptions. New background of micromechanics proposed is just a second one (the first one was proposed by Mossotti, 1850). CAM offers the opportunities for a fundamental jump in multiscale research of composites and nanocomposites. However, these opportunities can be realized only in the case of joint efforts of both computational micromechanic's society and the analytical one, and the societies of material science and physics.

Acknowledgments

The author acknowledges the support of the US Office of Naval Research.

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