

ПСЕВДОМАСШТАБНОЕ И МАСШТАБНОЕ ОПИСАНИЕ И ПЕРЕНОС ПО МАСШТАБАМ СВОЙСТВ НЕОРГАНИЧЕСКИХ И ОРГАНИЧЕСКИХ ПОЛИМЕРОВ И ПОЛИМЕРНЫХ КОМПОЗИТОВ

В.С. Травкин¹, Н.Н. Болотина^{1,2}

¹Hierarchical Scaled Physics and Technologies (HSPT), Los Angeles, CA, USA

E-mail: travkin@travkin-hspt.com

²University of Applied Sciences, Rheinbach, Germany

Заключение совета рецензентов: 01.04.10 Заключение совета экспертов: 11.04.10 Принято к публикации: 24.04.10

Мы начинаем с краткого очерка, в котором представлены некоторые определения из физики нескольких масштабов и некоторый полученный объем результатов, используемых в современной физике. Далее мы напоминаем об истории связи между структурой и свойствами материалов так, как они были сформулированы в 80-х и 90-х годах, включая и постепенное угасание этой кампании, и затем мы обсуждаем подходы, предлагаемые в настоящее время. Получение искомым специфических свойств сложных материалов, биоматериалов и искусственных биологических тканей вряд ли возможно без компонентов на полимерной основе. Для этого и необходимо изучение многомасштабных явлений в этих материалах и их композитах. Мы оцениваем новые технологии «многомасштабности», которые якобы соединяют свойства различных масштабов в полимерах и композитах, материалах на полимерной основе. Критический обзор будет главным образом посвящен попыткам «многомасштабности», псевдомасштабности, квазимасштабности, произвольной масштабности в физических методах и технологиях, в основном в механике сплошных сред и материаловедении, и в областях, связанных с моделированием полимеров, биополимеров и материалов на полимерной основе и их композитов. Претензии такого рода было бы лучше назвать методами множественного разрешения одного масштаба. В то же время мы сравниваем и описываем в деталях истинные полимасштабные механизмы, вытекающие из использования гетерогенных аналогов теоремы Гаусса-Остроградского (GOT) и дальнейшего использования этих теорем (WSAM) для тех же целей, для которых используется однородная теорема Гаусса-Остроградского в физике. В обзоре специальное внимание уделяется некоторым проблемам многомасштабных материалов, композитов с разномасштабными, гетерогенными, нелокальными и нелинейными свойствами.

Ключевые слова: полимеры, биополимеры, органические полимеры, полимерные композиты, гетерогенный, многомасштабный, полимасштабный, моделирование, многомасштабное моделирование, физическая модель, теорема Гаусса-Остроградского, теории осреднения, перенос по масштабам.

PSEUDO-SCALED AND SCALED DESCRIPTION AND SCALEPORTATION OF INORGANIC AND ORGANIC POLYMER AND POLYMER COMPOSITES PROPERTIES

V.S. Travkin¹, N.N. Bolotina^{1,2}

¹Hierarchical Scaled Physics and Technologies (HSPT), Los Angeles, CA, USA

E-mail: travkin@travkin-hspt.com

²University of Applied Sciences, Rheinbach, Germany

Referred: 01.04.10 Expertise: 11.04.10 Accepted: 24.04.10

We start with a short outline in which some definitions of a few scales physics and a developed volume of results used in the contemporary physics will be introduced. We continue with the reminding of the history of structure-properties relation as it was formulated in the 80s-90s including the calm fading of that campaign, and then we go on with the currently proposed approaches. The specific attributes of complex materials, biomedica and tissue engineering are hardly to be achieved without polymer-based constituents. That is of interest in promoting the understanding of multiscale studies. We consider the new techniques of “multiscaling” that allegedly connect different scale properties of polymers and polymer-based composites, materials. The critical review will be dealing mostly with the attempts to “multiscale”, pseudo-scale, quasi-scale, ad-hoc scaling approaches and techniques in physics, mostly in continuum mechanics and materials science and related to polymer and polymer-based materials and composite modeling fields. The claims of this kind would be better to name as the multi-resolution ones. At the same time, we compare and describe in some detail the true multiscale mechanisms stemmed from the heterogeneous analogs of Gauss-Ostrogradsky theorem (GOT) and further use of these theorems (WSAM) for the same purposes in which the homogeneous GOT is used. The interests will be focused on the problems of scaled materials, composites with multiscale, heterogeneous, nonlocal and nonlinear character.

Keywords: polymer; biopolymer; organic polymers; polymer composite; heterogeneous; multiscale; polyscale; modeling; multiscale modeling; physical model; Gauss-Ostrogradsky theorem; averaging theories; scaleportation.

Introduction

1. *Some definitions of scale dependent physics and hierarchical modeling of scaled phenomena and processes tied to continuum physics and modeling of polymers, polymer composites, and biopolymers as scaled media*

In spite of the fact that great progress was achieved regarding the power and speed of scientific computations, still many issues, tasks will remain unsolved in the near future.

It is also the point in discussion whether relying on computer power will solve “all” our problems with scale, interscale dependent issues. Of course, not, it is a too mechanistic human approach to structure and function dependence up to our needs hoping to resolve it with our tools at hand.

By present time, there have been developed numerous mostly experimental (including and numerical experiments) tools, methods for communication of physical properties usually established and applicable at one or another description scale to the other (mostly Upper) scale description methodologies.

This way of doing scale-to-scale [StS] communication has been in need for many decades. Mostly these attempts have been failing throughout this time span. We will talk on the reasons for failure.

Nevertheless, in the latest 8-10 years a huge number of attempts have started again claiming the direct connection, communication of thermal, electrical, mechanical characteristics at different scale description physics.

We start with a short outline in which some definitions of a few scales physics and a developed volume of results used in the contemporary physics will be introduced.

We continue with the reminding of the history of structure-properties relation-formulation in the 80s-90s including the calm fading of that campaign, then the nowadays proposed approaches.

The specific attributes of complex materials, biomedica and tissue engineering are hardly to be achieved without polymer-based constituents. That is of interest in promoting the understanding of multiscale studies.

We consider the new techniques of “multiscaling” that allegedly connect properties of polymers and polymer-based composites, materials. The critical review will be dealing mostly with the attempts to “multiscale”, pseudo-scale, quasi-scale, ad-hoc scaling approaches and techniques in physics, mostly in continuum mechanics and materials science and related to polymer and polymer-based materials and composite modeling fields. The claims of this kind would be better to name as multi-resolution ones.

The scaled exact governing equations and solutions for classical homogeneous and nonlocal heterogeneous Bottom-Up physical problems in different physical

disciplines, fields, which are under stable development path through more than 40 last years, will be used to analyze the current trends in multiscaling. A few ideas regarding the composites modeling, simulation with the purposes of Scaleportation (Scaleportation was introduced some years ago as a definition for the means and procedures of the direct and strict “transformation” of data at one scale to the data of the neighboring Upper or Lower Scale) would be introduced for the scale ranges from $(10^{-10}-10^{-6})$ m and up to $(10^{-3}-10^{-2})$ m.

These ~4 orders of decimal magnitude are at the most of physical theories to provide for the approximate or even ad-hoc adjusting mechanisms for the two-scale Bottom-Up mathematical algorithms. They will be re-entered with the examination of the strict Bottom-Up ⇕ Top-Down scale communications.

We should be concerned about the drawbacks within the techniques themselves along with the proper, correct communication of the different scale fields. Having this in mind, we shall try to maintain a balance between the methods employed at this time while demonstrating what arrays of possibilities can be explored in the future studies. In all other nature prescribed cases the physical matters are of scaled or multiscale character by existence.

There is no substance of physical content in our known universe that is not a *heterogeneous* one. The question is at what scale down the matter is still homogeneous? That answer we don't know yet. And mind the scale: an Upper or Lower one, then we will have the Heterogeneous matter anyway.

There is no action or process that we can name a *local* one, unless we want to declare that. Obviously, many actions or processes can be separated from their less important, at the moment or case, surroundings or/and forces. But that is always more or less an artificial choice. That says the connections of the scale inherited fields are of great significance/importance.

The strictest definition for the different scale related fields communication – transformation we suggested in 2004 as the Scaleportation. Scaleportation is the means and procedures of the direct and strict “transformation” of data at one scale to the data of the neighbouring Upper or Lower Scale. These interscale communications, scale transformations of data are mostly not by formulae, but using the scaled governing equations for the phenomena.

When more than 2 neighbouring scales of physical fields are involved, we have introduced the definition of Scaleleaping (or Leapscaling).

For example, we never think that the temperature of $1 \text{ mm}^3 = 10^{-9} \text{ m}^3$ and then of the same volume part of $10^{-9} (10^{-9}) \text{ m}^3 = 10^{-18} \text{ m}^3 = 1 \text{ } \mu\text{m}^3$ or then of the $10^{-9} \text{ } \mu\text{m}^3 = 10^{-27} \text{ m}^3 = 1 \text{ nm}^3$ volume part are different, even if that 1 mm^3 is at the thermodynamic equilibrium. But they are different. Depending on the type of boundaries and particular phenomena of the subscales for scales n_{ss} that means of this inequality $10^{-15} [m, Sc] \geq n_{ss} [m, Sc]$, which is usually out of the picture.

Well, here we need to confirm that, yes, all interatomic forces can be explained by electromagnetic forces. That means the attractive interactions named as van der Waals forces (dipole-dipole and London) and hydrogen bonding, as well as Coulomb long range collective forces, in principle can be evaluated (and will be probably in the near future) via the field generating scaled (two scales [Sc]) governing equations that are much more depicting and are of much more accurate description. Thus, it is much more difficult in simulation than the use of any kind of potentials.

We would follow so far in this review the conventional classical set of Maxwell-Heaviside-Lorentz-Lorentz's (MHLL) EM homogeneous governing equations. We will not discuss here their validity and meaning. Nevertheless, it would be appropriate to mention the vague (at least) semi-empirical base for the derivation of these fundamental equations as well as the regauging of the sought Maxwell EM equations by Lorenz. And that brought in even more unanswered contradictions.

There is a need for future development of the more strict set of fundamental governing electrodynamics equations for the homogeneous matter first.

2. An example of polymer with the scale phenomena and the need for scaled physical and mathematical models

It is not a surprise that the complicated polymeric materials after more than 70 years of study still don't have a strong enough theory to explain and predict elastic properties and gain some inputs for manufacturing. One of the brightest examples of that is rubber. A presentation of rubber polymer as an array of elastic interpenetrating (or simpler) networks of elastic strains (polymeric chains) has not yet brought a good quantitative explanation and simulation depiction.

The whole conceptual approach traditionally used in rubber elasticity is leaning toward one distinguished piece (element) of medium – polymer molecule with analytical tools applied toward it. Then, the various techniques developed in particle physics for the point-like objects have been applied in the field, for example, see [1] among other numerous models.

We can mention the two major drawbacks of these 70+ year-old rubber structure polymer network viewpoints and analysis.

1) One is that at the level of a separate, single polymeric molecule the models have been constructed as for the kinetic array of springs (phantom model). Thus, the Hamiltonian is used as a source of energy retained dependency.

2) The second negative issue is that in the ways, models to go from an array of springs (which by itself is a pretty simplistic model) to the continuum presentation workers are also using particle physics concepts and solutions – unrealistic ones, where averaging is simplified (static, homogeneous).

In this path of modeling there will be hardly found a way to construct a solid scaled theory for the rubber. The final goal of that theory would be to develop scaleportation procedures, models for the continuum rubber material from at least one of 3D polymeric molecule scale to the one of continuum medium scale.

Hierarchical scaled volume averaging theory (HSVAT) introductory concepts and theorems for continuum mechanics general

Because this field – the Continuum Mechanics is forming the base for many sub-disciplines, particularly in Solid State mechanics, we ought to discuss on a few major developments as the examples of wrongdoing, of false science, that has been strangling Continuum Mechanics for more than 40 years.

To understand why the Homogeneous GO (divergence) theorem based studies are among hundreds of inappropriate others, we can mention just a few [2-34] prominent, influential, probably, studies of such kind. These insufficient, mildly saying, or incorrect reports for the Heterogeneous media problems in Continuum Mechanics we have to study laboriously with attention to detail.

We further need a few basic statements from the hierarchical description of heterogeneous media (HSVAT). The basic idea of hierarchical medium description is that the physical phenomena, mathematical presentation of those phenomena, and their models can be very different and in most of situations are different, even if the phenomena themselves are similar or looking as identical, but the scales are different and the lower scale features should be transported to the upper level of description in such a mode that the useful information would be added to the characteristics on the upper level.

The volume average value of one phase in a two phase composite medium $\langle s_1(\bar{x}) \rangle$ in the REV and its fluctuations in various directions are defined [35-43]

$$s_1(\bar{x}) = \langle s_1(\bar{x}) \rangle + \hat{s}_1(\bar{x}), \quad \langle s_1 \rangle = \frac{\Delta\Omega_1}{\Delta\Omega}$$

Five types of two-phase medium averaging over the REV (Fig. 1) function f are defined by the following averaging operators arranged in the order of seniority [38, 44, 45].

$$\langle f \rangle = \langle f \rangle_1 + \langle f \rangle_2 = \langle s_1 \rangle \tilde{f}_1 + (1 - \langle s_1 \rangle) \tilde{f}_2,$$

where the phase averages are given by

$$\langle f \rangle_1 = \langle s_1 \rangle \frac{1}{\Delta\Omega_1} \int_{\Delta\Omega_1} f(t, \bar{x}) d\omega = \langle s_1 \rangle \tilde{f}_1;$$

$$\langle f \rangle_2 = \langle s_2 \rangle \frac{1}{\Delta\Omega_2} \int_{\Delta\Omega_2} f(t, \bar{x}) d\omega = \langle s_2 \rangle \tilde{f}_2,$$

and the internal phase averaged functions are given by

$$\{f\}_1 = \tilde{f}_1 = \frac{1}{\Delta\Omega_1} \int_{\Delta\Omega_1} f(t, \bar{x}) d\omega;$$

$$\{f\}_2 = \tilde{f}_2 = \frac{1}{\Delta\Omega_2} \int_{\Delta\Omega_2} f(t, \bar{x}) d\omega,$$

where \tilde{f}_1 is an average over the space of phase one $\Delta\Omega_1$ in the REV, \tilde{f}_2 is an average over the second phase volume $\Delta\Omega_2 = \Delta\Omega - \Delta\Omega_1$, and $\langle f \rangle$ is an average over the whole REV. There are also important averaging theorems for the averaging of the spatial ∇ operator – heterogeneous analogs of Gauss-Ostrogradsky theorem. Those are plenty already since 70-80s [36, 39, 40, 42-49]. The first several of them needed to average the field equations are the WSAM theorem (after Whitaker-

Slattery-Anderson-Marle) and the one is for intraphase ∇ averaging. The differentiation theorem for the intraphase averaged function reads

$$\{\nabla f\}_1 = \nabla \tilde{f} + \frac{1}{\Delta\Omega_1} \int_{\partial S_w} \hat{f} \vec{d}s_1;$$

$$\hat{f} = f - \tilde{f}, \quad f \nabla \Delta\Omega_1,$$

where ∂S_w is the inner surface in the REV, $\vec{d}s_1$ is the second-phase, inward-directed differential area in the REV ($\vec{d}s_1 = \vec{n}_1 dS$). The WSAM theorem sets the averaged operator ∇ in accordance with

$$\langle \nabla f \rangle_1 = \nabla \langle f \rangle_1 + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} f \vec{d}s_{12}.$$

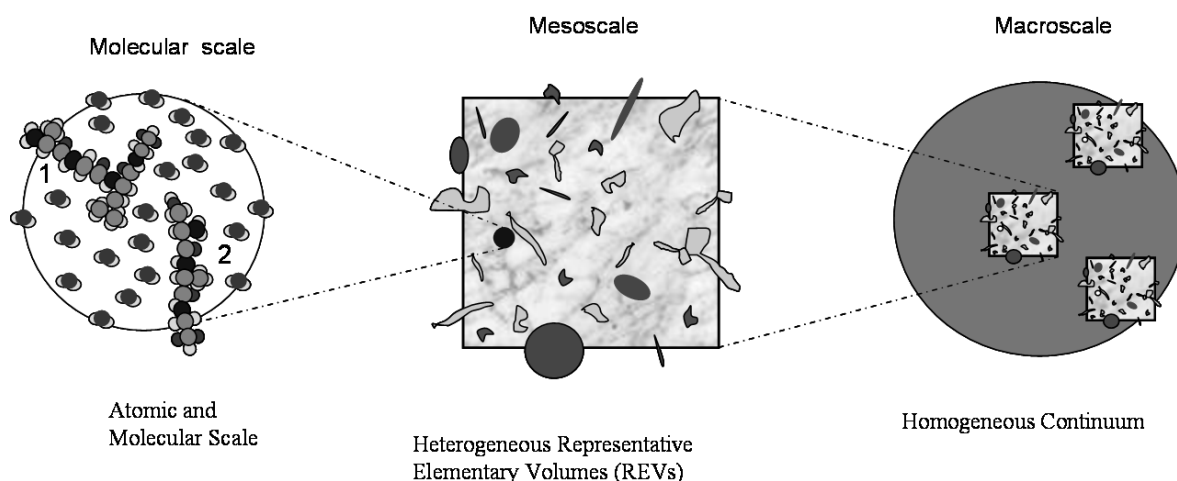


Рис. 1. Упрощенная схема «снизу вверх» (телескопического) последовательного ряда Представительных Элементарных Объемов (ПЭО) в 3 масштабах от молекулярного до масштаба сплошной среды: 1 – полипептид – аланин-глицин-валин-глицин; 2 – серин-аланин-глицин в водном растворе

Fig. 1. Simplified draft of Bottom-Up consecutive series of Representative Elementary Volumes (REV) at three scales from molecular to continuum ones: 1st polypeptide – alanine-glycine-valine-glycine; 2nd – serine-alanine-glycine in the solvent of water

Meanwhile, the foundation for the averaging made, for example, by Nemat-Nasser and Hori [26] (and many others) is based on the conventional homogeneous Gauss-Ostrogradsky theorem (see pp.59-60 in [26]), and not on its heterogeneous analogs as the WSAM theorem.

The following averaging theorem has been found for the **rot** operator

$$\langle \nabla \times \mathbf{f} \rangle_1 = \nabla \times \langle \mathbf{f} \rangle_1 + \frac{1}{\Delta\Omega} \int_{\partial S_{12}} \vec{d}s_{12} \times \mathbf{f},$$

and as a consequence, the theorem for the intraphase average of $(\nabla \times \mathbf{f})$ is found to be

$$\{\nabla \times \mathbf{f}\}_1 = \nabla \times \{\mathbf{f}\}_1 + \frac{1}{\Delta\Omega_1} \int_{\partial S_{12}} \vec{d}s_{12} \times \mathbf{f}.$$

More details on the non-local VAT procedures and governing equations for the different physical problems modeled in the homogeneous media by linear mathematical physics equations can be found in many publications [35-36, 43, 50-52]. Meanwhile, features depicting closure, nonlinear theory, polyphysics applications, polyscale developments, exact solutions, etc. can be found only in the works as [38, 44-49] and other studies.

It might help with the understanding of our approach to the more strict mathematically and physically description of many materials science, polymer science, and biological subjects, because those are mostly of Heterogeneous, Scaled, and Hierarchical character, made by nature itself.

To look through, browse our previous analytical reports in other areas where the Heterogeneous, multi-

phase, scaled media and phenomena are in the core of subject matter, and that should help in the estimation -

<http://www.travkin-hspt.com/fundament/03.htm> Why is it Different from Homogeneous and other Theories and Methods of Heterogeneous Media Mechanics/(other Sciences) Description?

<http://www.travkin-hspt.com/fundament/04.htm> Are there any other Methods and Theories available?

Solid state and particle physics methods used to apply for polymers and polymer composites properties determination

The word “nematic” finds an original prototype in the Greek word “νημα” (thread) that might be explained via the “director” (vector) orientation or the thread of the polymer blocks in a polymer medium. Meanwhile, unfortunately it does almost no input with regards to polymeric molecular scale $\sim(10^{-8}-10^{-5})$ m structure, morphology of molecule itself for the function, properties of the Upper continuum scale of polymeric medium. That structure of nematic as well as of cholesteric or smectic (for example) phases of liquid crystal polymers, meanwhile can be very helpful while assessing or modeling their properties via the hierarchical tools of HSP-VAT. In the Lower (smaller) scale ranges, we can find a lot of general meaning texts on physical, chemical and solid state emphasizing methods used for meso- and nanoscale description of polymers and polymer composites, materials.

We are interested here mostly in the works that define and treat these tasks as the “multiscale” which are usually only of two scale models. Here is the work [53] with a tremendous workload given that is done in an attempt to connect the famous from the middle of XX century particle physics, statistical mechanics theories to a pure continuum mechanics, complicated, heterogeneous polyscaled cellular dynamics task. That is not unusual when physicists use the tools they have been taught at universities to any other than statistical mechanics, particle physics theme. From the abstract: “...We introduce a model for describing the dynamics of large numbers of interacting cells. ...We present here a detailed description of the model, and use successive mean-field approximations to connect it to more coarse-grained approaches, such as discrete cell-based algorithms and coupled partial differential equations.” In p. 612 we can read: “In this paper we introduce a framework for modeling multicellular systems... This framework uses “subcellular elements” (defined below) as the fundamental dynamical variables, along with overdamped Langevin dynamics [19, 27] for temporal development of the system.”

This is the many-body approach with the point objects and also this is finite mathematics, discrete mathematics schematics for the Continuum Mechanics subject. The dynamics statistical mechanics governing equation takes the form (the equation number here and

all of the equations numbered below are from their original publications)

$$\dot{y}_{\alpha_i} = \eta_{\alpha_i} - \nabla_{\alpha_i} \sum_{\beta_j \neq \alpha_i} V_{intra} (|y_{\alpha_i} - y_{\beta_j}|) - \nabla_{\alpha_i} \sum_{j \neq i} \sum_{\beta_j} V_{inter} (|y_{\alpha_i} - y_{\beta_j}|). \quad (1)$$

The gradient terms on the right-hand side of this equation represent, respectively, the intra- and intercellular interactions between the elements with the phenomenological potentials V_{intra} and V_{inter} . As usual in this modeling, everything is included into these “free” terms.

One can read: “Finally, after three levels of coarse-graining, we have arrived at a partial differential equation for the cell density, as given in equations (10) and (11).”

The following can be said regarding this multi-coarse-graining statistical mechanics approach:

1) These tools of “statistical mechanics, many-body physics” – they don't work well for many-body field and for particle physics as a whole, and they are obsolete and partly are incorrect because of the fundamental assumptions put in the derivation of the governing equations (using definitions of point-like particles, homogeneous GO theorem, and incorrect averaging procedures – coarse graining).

2) All the fields and forces in this study are artificial; all of them have appeared as a result of imaginary interactions without a field of interaction.

3) What is the intracellular interaction potential V_{intra} ? Morse potential? What is the extracellular interaction potential V_{inter} ? What are their connections to the continuum fields of extracellular space or other cells environment?

4) The governing equations obtained in this study – equations (5)–(11), especially (5), (10) are of pure speculative nature based on the procedures developed in many-body and statistical mechanics for the point-like indistinguishable particles arrays.

We can not get equations (5), (10) with the heterogeneous GOT which are the WSAM theorems application, period.

5) Well, but the GO theorem can not be used for a particulate medium Upper scale (averaging), or coarse graining as it is used in statistical mechanics. What to do with this problem? All those adjustable functions as V_{intra} , V_{inter} , noise term η_{α_i} , and their numerous parameters are just pure speculative adjusting functions and constants, baring nothing or very little of the real physics related to the collective interactions of fields, phases, biochemical characteristics of a cell, extracellular environment, etc.

6) That construction of order parameters and coarse grain procedures are simplifying (not simplistic) tools and are designed for well adjusting to some averaged experimental results. Being within the concept of the one scale for the entire scaled problem is not helpful to solve

the many-body task, even the understanding and correct statement is impossible. Also, the most known techniques in traditional statistical mechanics (SM) many-body problem are approximate by nature.

7) Most of physicists who do the “SM for biology work” are familiar with these discussions on the validity of point particles – no volume, no features apart of those we would like to assign to them. Unfortunately, workers-physicists prefer to work with biological matters – those are polyscaled, in the same way as particle physicists work with volumeless particles.

Among selected publications some are in the same polyphase, polyscale biopolymeric media areas.

In the paper [54] the talk is about the difficult and in some points even not having proper developed continuum mechanics theories in relation to, let us take, two-phase and actually two-scale biomedias which consist of macromolecule (one) as a polymeric nonlinear elastic homogeneous medium with electrical (and might be electrodynamic) constant characteristics, and a solvent with constant phase electrical characteristics (electrical permittivity) and “The dielectric constant ϵ and the modified Debye-Hückel parameter κ are piecewise constants in domains Ω_{mf} , Ω_{mr} , Ω_s . In particular, $\kappa = 0$ in Ω_{mf} and Ω_{mr} because it models the free mobile ions which appear only in the solvent region Ω_s .”

There is only one polymeric elastic molecule in Ω_{mf} and one rigid molecule Ω_{mr} , meanwhile, it is supposed to be a lot of both kinds. One can learn from the abstract: “In this paper we propose a nonlinear elasticity model of macromolecular conformational change (deformation) induced by electrostatic forces generated by an implicit solvation model...” “The Poisson-Boltzmann equation for the electrostatic potential is analyzed in a domain varying with the elastic deformation of molecules, ... We derive the estimates of electrostatic forces ... and establish the existence of an equilibrium configuration using a fixed-point argument, under the assumption that the change in the ionic strength and charges due to the additional molecules causing the deformation are sufficiently small.”

In fact, the problem in this paper is not solved – there are given the estimations for numerous separate situations for electrostatic potential without coupled elastic deformation of macromolecule; then the general result of the “Existence of Solutions to the Coupled System” is given. That's it. Actually, the mathematical statement is given as de-coupled because the body forces in elasticity statement are depending on the potential function solution, but potential is given in the equation for the already occurred macromolecule elastic deformation? That's the current state of the art.

In p. 136 one can read important statement: “This article takes an important step in this direction by describing and analyzing the first mathematical model for the interaction between the nonlinear elastic deformation and the electrostatic potential field of macromolecules.” Because there is no established model

for coupling of physics of electrostatic fields (in both macromolecules and a solvent) and elasticity in a system with electrical field dependent deformation of polymer, the authors have developed the intricate method with the “supposed” change of Poisson-Boltzmann equation to “return” it to the form (which is not supposed to exist, because the taken form of the Poisson-Boltzmann equation is valid for only “while the Poisson-Boltzmann equation (2) holds true for real deformed configurations”).

That means the authors do not know the electrodynamics governing equations for the two-phase system with macromolecules and solvent interdependent (interacting) in their dynamics. The Poisson-Boltzmann equation (PBE)

$$-\nabla \cdot (\epsilon \nabla \phi) + \kappa^2 \sinh(\phi) = \sum_i^{N_f + N_r} q_i \delta(x_i)$$

is the equation in which there is happening a mixing of the two scales (at least) phenomena:

a) of the atomic scale;

and

b) of the continuum media scale – which is not even specified; these two scales are combined with the introduction of the Dirac's function and the Debye-Hückel parameter κ . And this was a conventional thing to do – in the first half of the XX century (1923 actually).

Because of the not quite correct physical and mathematical initial statement – in solvent the physics of electrostatics is of the Debye's time (hundred years old), the PBE essentially is incorrect; in macromolecules the physics of electrostatics is incorrect also – there are thousands and thousands of those charged atoms within the macromolecules; plus – the boundary conditions at the interfaces between the solvent and macromolecules are complex, heterogeneous mostly, the problem's present statement is hardly worth solving. Anyway, the attempt was made.

At present time, nobody knows exactly – How to develop Continuum Mechanics constitutive relations accounting for the coupling forces of elasticity within the macromolecules and of electrodynamics of the two-phase solution dynamical system? The authors have appeared to develop some substitutive model going via the assessment of the electrostatic energy of the system with the necessity to approximate the Lower scale (atomic and sub-atomic) singularities in the body force density that is modeled by a Gaussian function; and with the application of the infinitesimal displacement h of the molecular surface in its out normal direction.

Authors recognize that “...is the determination of the elasticity properties of macromolecules within the continuum framework, which requires new theoretical models and quantitative comparisons between the continuum modeling and the classical molecular dynamical simulation and/or experimental measurements.”

In conclusion to this study:

1) This is just another situation to confirm that the protein, macromolecules conformation problem is not going to be resolved by taking chances in developing the one more one-scale coefficient dependent theory. Because the correct way is to recognize that the Lower scale – atomic-molecular scale physical phenomena in polymeric solution have a major impact onto the conformation and consequently on the continuum elasticity and electrostatics of macromolecules. Therefore, the efficiently counted impacts are of the continuum mechanics scales – so the Bottom-Up / Top-Down Scaleportations need to be tackled. That will give the base for constitutive multiphysics macro-dependencies which appear naturally.

2) It was noted for many instances that – as soon as one can see or understand that several different forces, effects, etc. act in the same volume, one should be immediately concerned that this description means – the different carriers (phases) in the same volume (or sub-volumes – also the same) are functioning or acting on behalf of different physical phenomena. That also means – we can freely designate the different phases to be the carriers of their respected physical effects – firstly, and those effects should be the subject of the appropriate heterogeneous scaled dynamics and static governing equations (GE) – secondly.

Pure continuum mechanics modeling methods applied for the upper scale polymer and polymer composites properties assessment

Throughout a few last decades the researchers in heterogeneous Continuum Mechanics (CM) Solid State fields as – Elasticity Theory, Continuum Damage Mechanics (CDM), Viscoelasticity, Plasticity Theories, Micromechanics, Biomechanics are making their science as in an ivory tower. While in some fields, not so distant from the above mentioned disciplines, there is known a spectrum of new related theories, that is not the case for the Solid State Continuum Mechanics. Despite that they do the false science of Heterogeneous materials for decades, this does not bring them a thought about their wrongdoings.

This is the deed of a great number of just errors, misunderstandings. People doing theoretical, mathematical, and experimental (because their experiments are controlled by their theories) errors in their research, they use public money and they deliver the trash or misrepresentations. They teach incorrect courses to students and professionals as well.

The authors, in spite that their work is about the scaled heterogeneous media, are not seeking and not using the only correct, appropriate, created for these purposes tools because:

1) They don't know that other than Gauss - Ostrogradsky (some know it as a divergence) theorem (GOT)

exists for Heterogeneous media – the WSAM theorem and others. Meanwhile, a few of them do know.

2) They don't know, don't develop and don't want to know whether the Governing Equations of the Upper (in most situations) scale physical fields exist?

3) They don't know what are these HSP-VAT GEs?

4) What are the Upper scale GE⁽²⁾? And why they need to use these concepts and tools?

5) They don't solve the equations of the 2-nd (Upper) scale. The equations they sometimes present as of the Upper averaged space are incorrect.

Despite a proper terminology and even figures, most of works on multiscaling in polymer composites are misleading. Workers use the conventional Homogeneous physical and mathematical instruments, in spite that polymers themselves are composite materials at molecular scale, adding the complications at the mixture scale. Thus, as one of numerous publications with the same Homogeneous treatment of Heterogeneous matter (hundreds of them), we can read in [30] that averaging of stress and strain components to get the “effective” ones must go with integrals

$$\langle \sigma_{ij} \rangle = \frac{1}{V} \int_V \sigma_{ij}(x_k) dV ; \tag{2}$$

$$\langle \varepsilon_{ij} \rangle = \frac{1}{V} \int_V \varepsilon_{ij}(x_k) dV . \tag{3}$$

When providing for these integrations in p. 12, the authors integrate over the simulated REV cell as – “The effective stress (Equation (2)) associated with this RVE realization (Fig. 2) is simply the average over all M elements (both matrix and platelet) contained in the RVE cell

$$\bar{\sigma}_{ij} = \frac{1}{A_{tot}} \sum_{m=1}^M A_m \sigma_{ij}^{(m)} , \tag{19}$$

where $\sigma_{ij}^{(m)}$ is the stress associated with m th element, and

$$A_{tot} = \sum_{m=1}^M A_m \tag{20}$$

is the total area of the RVE cell.”

Meanwhile, this is the wrong definition and calculations. According to scaled theory and modeling of the Upper scale nonlocal characteristic as this one, an ensemble average $\langle \sigma_{ij} \rangle$ or the volume average $\bar{\sigma}_{ij}$ are just averaged in some ordinary ways stress functions - but not the effective variables. Note also that the boundary conditions (BC) could not be set up as the true periodical – Fig. 2, because disjointed REV's have different BC than the snapped altogether.

The details and further analysis regarding these features of polyscale presentation of heterogeneous, scaled media we would like to concentrate on here.

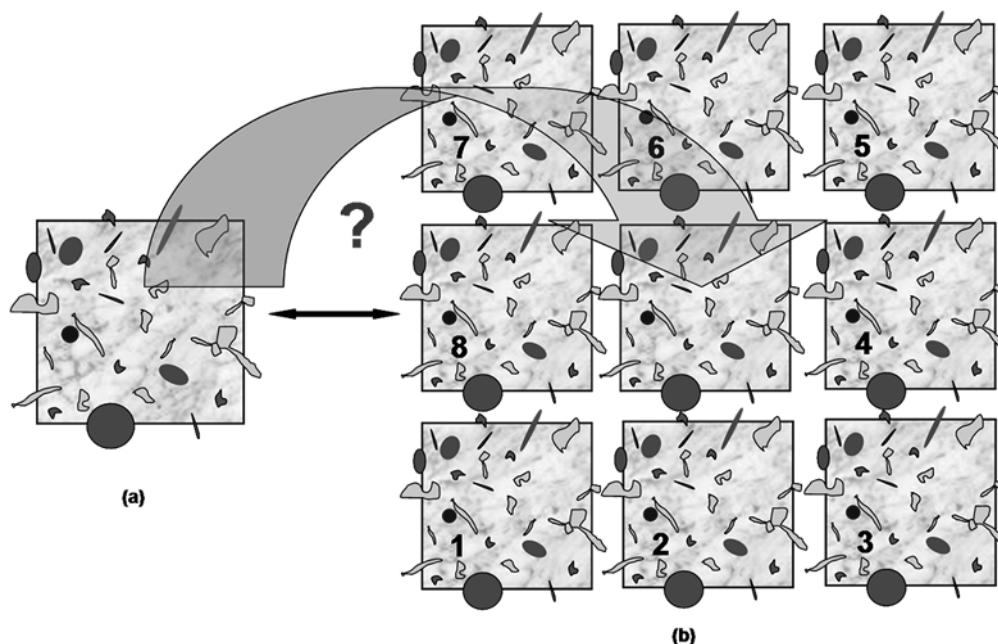


Рис. 2. Псевдоусреднение неперриодических ПЭО для 2D морфологии. (а) Один ПЭО, неперриодический. (b) Якобы правильная последовательность осреднений для масштабного псевдоиерархического вычисления (по сравнению со Spencer and Sweeney [30] Рис. 3)

Fig. 2. Pseudo-averaging with the non-periodical REV for the 2D morphology. (a) One REV, not periodical. (b) Assumed to be the proper arrangement of averaging for scaled pseudo-hierarchical simulation (comparing to Spencer and Sweeney [30] Fig. 3)

We need to start from several distant in time works, which left such a profound trace in education, science and engineering of composites afterwards that we have to scrape them off for good. The author of [4] discusses both an ensemble averaging as well as volume averaging techniques for the equations of mathematical physics. The author speaks on effective coefficients, also tells about the problem of the design of composite materials with the needed effective coefficients. The basic starting field's distribution equation (3) is

$$\frac{\partial}{\partial x_i} \left[\epsilon_{ij}(\bar{x}) \frac{\partial \phi'(\bar{x})}{\partial x_j} \right] = \rho(\bar{x}); \quad (3)$$

$$\epsilon_{ij} = \epsilon(\bar{x}) \delta_{ij}, \quad (4)$$

after averaging it has the form

$$\bar{\epsilon} \nabla^2 \{ \phi(\bar{x}) \} = - \frac{\partial}{\partial x_i} \left[\epsilon'(\bar{x}) \frac{\partial \phi'(\bar{x})}{\partial x_i} \right] + \rho(\bar{x}), \quad (31)$$

and we note that in this statistical averaging there are no techniques, recognition of the specifics for the left hand side operator's averaging. No difficulties with the GO theorem conditions fulfillment or about the WSAM theorem application if any at all?

Also, we have to note here that in this kind of problem analysis and evaluation, including a solution, there is no place for material's consideration – just statistics, no place for the phase (phases) description, no

place for interface description, and on the physics of interface elaboration. There are the statistics of morphology and morphology parameters that are not directly tied to the GE above. That is out of consideration because there are no tools and power for doing this in the statistical mechanics of one scale.

There was also no talking about the first (ground, Lower) scale (there is no scale consideration at all) physics and its mathematical representation. Taking an ensemble average of equations is not problem at all in statistical theory of heterogeneous materials.

1) The simple treatment of effective coefficients problem is given in the section V as for the equation

$$\epsilon^* \frac{\partial}{\partial x_i} \{ E_i(\bar{x}) \} = \rho(\bar{x}), \quad (60)$$

that needs to be compared to the original equation with the constant coefficient

$$\epsilon \frac{\partial}{\partial x_i} E_i(\bar{x}) = \rho(\bar{x}). \quad (52)$$

In this comparison, while actual substitution of one equation by another, there are so many issues mixed and out of description. Among them, the vital one is the issue of how to justify the connection of the initial equation to the effective coefficient equation? Another – is this equation with effective coefficient correct? What kind of fields (all of them) is used in these equations, etc.? Regarding a very important issue of the effective

coefficient bounds, we need to recognize that using the homogeneous concepts and theoretical constructions we inevitably develop the same kind of useless characteristics on bounds.

2) Thus, the substantial portion of section V is given to the detailed analysis of statistical theory using the three-point correlation function for the assessments of bounds for effective coefficients.

3) Section VI is devoted to the experiment which is meant to be in line with the assessment of some three-point correlation functions. All of this discussion on the issue of three-point correlation function is actually based on and brought to life by Miller's "cell model for real materials"? This model is quite simplistic and is far beyond the correct construction for averaging, averaged fields, and averaged equations.

While in the stochastic approach so nicely described in the works like in [4], one would note that this kind of approach has some features that we can name as unacceptable, for example, such as:

st1) There is no volume of statistical averaging, but either all the 3D Cartesian (or in another geometry) coordinates or the volume (body) of the problem. This assumption instantly brings the question on correctness of the boundary conditions all together with the principal issue of what kind of averaging theorem is being applied – the homogeneous GO theorem, or the heterogeneous WSAM kind of theorems (there are many of them).

st2) Further, the statistical averaging comes with the necessity to consider "an infinite statistical hierarchy of equations" ([4] p. 222). While we can read in p. 223 – "There is, however, no way in general to find a finite set without some approximation." That means – no dreams about the exact two scale, or even only an Upper scale rigorous solution of heterogeneous problem! That is a disappointing conclusion. Meanwhile, with HSP-VAT tools we are able to solve either scale – an Upper or Lower, or both scale problems.

st3) To solve the problem for the averaged fields in statistical averaging techniques [3, 4] suggested, the only way is by using the integro-differential equation of Dyson that is even hard to configure in the final form. Which anyway is incorrect due to the accepted derivation procedures.

This is an old but still representative result of a simplified approach, incorrect by the method.

The work [6] is a useless large laborious study with a good topic and still it is useless. Let us follow authors' arguments. One can read in page 161 the shocking disclosure of their preemptive ignorance regarding the control volume (REV) selection, features and existing other than GO theorems: "Physically irrelevant mathematical questions of continuity may arise from possible real physical discontinuities across s " which is the interface surface (boundary between the phases) "in the event that the unit cell faces ∂r_0 (bounding the unit cells r_0 externally) coincide partly or wholly with the phase boundaries s . Such unnecessary mathematical

complications can be avoided by reverting to the **artifice** adopted in I of imagining the unit cell faces to be drawn in such a way as to lie entirely within the continuous phase. This choice of "curvilinear unit cell: insures complete continuity of all functions across the cell faces ∂r_0 despite possible discontinuities across the phase boundaries s ..."

Then the author writes that this mathematical artifice is not of any meaningful value – which is a straightly wrong statement, that we are addressing below in the text.

This particular mathematical artifice is the one which allowed authors to draw their further incorrect studies. Reading more on we find that: "Indeed, ultimately we shall do away entirely with the concept of unit cells and revert wholly to a scheme based upon the introduction of spatially periodic functions satisfying boundary conditions only on the phase boundaries s (see §6). In such a scheme the unit cell boundaries play no role whatsoever." No more comment.

As the consequence of this derivation, finally the authors found the numerous irrelevant formulae. For example, on the dispersivity dyadic for a Darcy flow in porous media (5.4), (5.15) in pp. 170-171.

As of the most frivolous we can find the next one on the layered media effective overall conductivity coefficients – (8.45)-(8.47) – "Equations (8.45) – (8.47) apply for any one-dimensional spatially periodic conductivity field $D(z)$, continuous or discontinuous."? We might conclude on this work that the time of this paper was 1980-82 that is many years after publications in the 60s and 70s on the basics of the HSVAT, then these authors would regard on themselves that their work was useless and incorrect.

In the book [11] (we may say almost a classical good book for any but heterogeneous topics) the two last chapters – the 8th and 9th are devoted to the matter of suspension moving in liquid while considering mainly the very dilute and the more dense slow flow regimes. The whole content of these two chapters are to make assessments of dynamics of not a separate particle movement, but rather to describe and to find out the parameters of the "clouds" of particles – actually averaged characteristics of the Upper scale physics.

At the same time, there are no concepts or features (mind that was only the 60s and beginning of the 70s) describing the second (Upper) scale field's properties that are in fact sought in the studies described and formulated in these two chapters. These are averaged characteristics of bulk effects of the second dispersive phase as, for example, nonlocal pressure drop ΔP_s in liquid, differential volume element $d\tau$ (as REV), permeability coefficient K , filtration velocity U , effective viscosity of suspension μ , etc. etc. This one scale handling of problems does not allow obtaining correct analysis and mathematical formulae. For example, in chapter 9 we can find the definition of effective viscosity of suspension in expressions (9.1.1), (9.1.2) that are

incorrect as soon as the boundaries should not be considered as homogeneous surfaces, etc. etc.

Commonly, these two chapters in [11] book give a nice, broad analysis of single scale attempts to solve these broadly stated Two-scale heterogeneous problems – the flow of suspensions, and the flow in porous media. The chapters can be referred as for studying of **what cannot be done** with the one scale mathematical physics statement while the two scales are natural for the problems in this field.

There were a lot of citations (references) in the 80s and 90s to the publications authored and co-authored by Z.Hashin, for example, see [12-15]. In these studies dated back to the beginning of the 60s, there was already proclaimed the theory which was supposed to explain almost everything in continuum mechanics of composites (Heterogeneous Media) – elasticity, heat transport, electromagnetic fields basics, strength, etc.

The whole course of development in these studies is based on artificially (we explain why we use this word) simplified concepts and mathematics of bulk averaging through the Volume – Surface GO theorem, and the Virtual Work Theorem.

Using the assigned one phase boundary REV see, for example Fig. 2.1.2 in 1972 report for NASA by Hashin [14] – which explains why most of the formulae in this report, for example, like (5.3.5), (5.3.21) that are the key formulae among others, are illustrations of erroneous mathematics.

In the abstract of the study [17], one can find a valuable idea of comparison of two very often used methods: “The average-field theory and the homogenization theory are briefly reviewed and compared. These theories are often used to determine the effective moduli of heterogeneous materials from their microscopic structure in such a manner that boundary-value problems for the macroscopic response can be formulated. While these two theories are based on different modeling concepts, it is shown that they can yield essentially the same effective moduli and boundary-value problems.”

These authors' writing deserves to be commented here for the clarity of arguments regarding the important statements they provided to readers, for example, in the page 667 where one can read that: “Average-field theory. This theory is based on the fact that the effective mechanical properties measured in experiments are relations between the volume average of the strain and stress of microscopically heterogeneous samples. Hence, macrofields are defined as the volume averages of the corresponding microfields, and the effective properties are determined as relations between the averaged microfields.”

This definition is incorrect and incomplete. We would not be surprised that using this definition the authors came to their conclusions.

What is incorrect regarding this Average-field theory statement: a) “effective mechanical properties

measured in experiments are relations between the volume average of the strain and stress of microscopically heterogeneous samples,” – these properties are the result of experimental set-up made for Homogeneous medium, and as such bearing the features of GO homogeneous medium theorem based experimental set-up. Not a Heterogeneous Medium Experiment (HtME) on Elasticity properties. This is the experiment (HtME) where the dependency of stress on a displacement field as of an averaged field is usually established, thus this dependency would consist also within the HtME provided with the surficial integrals for the displacement fields over the interfaces within the measured volume, within the REV or one of possible REV's taken as for this certain experiment. So, this should not be the Homogeneous experiment, if we are determined to deal with our Heterogeneous medium. Well, in this case we have to obtain the Heterogeneous dependence between the average displacements and average stress in the whole Heterogeneous medium, in the separate phase(s) of the medium.

b) The Upper scale elasticity model fields are determined via not only the Lower scale microelasticity fields, but also, and that is the major constitutive part of Upper scale physics, by the Upper scale Ht Governing equations solution for the problem's domain Heterogeneous medium. Otherwise, if the Upper scale GE would be accepted as of Homogeneous medium, then the Upper scale Effective Coefficients (EC) and Boundary Conditions (BC) would not be the conventional Homogeneous medium EC and BC.

c) In many, most probably, situations the Upper scale statement conditions are of the prevailing importance for the Heterogeneous problem (elasticity in this case) and as such the Upper scale mathematical statement must be stated rigorously, as strict as the theory allows. That means – the Lower and the Upper scale GEs must be constructed directly mathematically tied, as they are in physical nature of the problem, usually. That means also – that the Top-Down as well as Bottom-Up sequences should be used for the mathematical formulation of the Two Scale Problem.

Also, the Upper scale GEs formulated as the conventional homogeneous statement are incorrect if taken separately from the correct Lower and Upper scale Heterogeneous GEs as in this paper, for example.

In the fundamental book by Nemat-Nasser and Hori [26] there are given the parts related to averaging procedures, theorems, etc. all applied towards the Elasticity theory for Heterogeneous materials. But the basics for averaging are made of conventional Gauss-Ostrogradsky theorem, not heterogeneous theorems as the WSAM theorem, for example, in pp. 59-60.

The excerpt in the page 471 shows explicitly that the authors are bearing in mind the averaging procedures in the book as for the one scale methodology. We read – “The second important difference between the concept of an RVE and the periodic model is that, through the

application of a Fourier series representation, the periodic (elasticity) model can be solved essentially exactly in many important cases, whereas in the case of a RVE, only estimates based on specialized models (e.g., the dilute distribution, the self-consistent, and the differential models) are possible.”

Which is stated as such because the authors do not believe in the existence of the second scale physics and mathematics, although, this statement is also incorrect, as soon as there are the Upper scale problems solved for many instances. The most clear, simple, and straightforward examples of them can be seen in our texts. That has been shown for many problems, by the means of the Two scale solutions, especially with the exact Two scale solutions of those few common textbooks known and taught in the universities' problems, see in –

<http://www.travkin-hspt.com/fluid/03.htm> Classical Problems in Fluid Mechanics;

<http://www.travkin-hspt.com/thermph/02.htm> Classical Problems in Thermal Physics;

<http://www.travkin-hspt.com/eldyn/glob1.htm> Globular Morphology Two Scale Electrostatic Exact Solutions.

This new kind of Mathematical Physics can successfully tackle and solve the old problems either.

Also, obtained after 2002 the analytical solutions of the following two scale classical problems that have not been solved for many decades by other methods (given in textbooks the Lower Homogeneous scale “solutions” are wrongly attributed to the Upper Heterogeneous scale averaged fields):

<http://www.travkin-hspt.com/eldyn/WhatToDo2.htm> When the 2x2 is not going to be 4 - What to do?;

<http://www.travkin-hspt.com/eldyn/photocrs1.htm> Two Scale EM Wave Propagation in Superlattices - 1D Photonic Crystals;

<http://www.travkin-hspt.com/acoustics/supercross.htm> Two Scale Solution for Acoustic Wave Propagation Through the Multilayer Two-Phase Medium.

These solutions leave no chances for calculations or comparison with experiment of the Upper scale characteristics using the basis of Homogeneous GOT. This has no sense and is invalid for Heterogeneous problems.

The second failure after using the GO theorem for heterogeneous media as for homogeneous ones in continuum mechanics (in almost 100% of the books) is the acceptance and even sometimes “proofs” that the averaged product of fields is equal to the product of averaged fields:

$$\{\sigma : \epsilon\}_{V^o} \approx \{\sigma\}_{V^o} : \{\epsilon\}_{V^o} \approx \sigma^o : \epsilon^o .$$

We can read on this in p. 54 [26] – “Thus, averages taken over any RVE in B’ are essentially the same as

those taken over B when the RVE is suitably large. For statistically homogeneous B, it therefore follows that

$$\{\epsilon(\mathbf{y})\}_{V^o} = \bar{\epsilon}(\mathbf{y}) \approx \epsilon^o; \quad \{\sigma(\mathbf{y})\}_{V^o} = \bar{\sigma}(\mathbf{y}) \approx \sigma^o, \quad (2.6.4a,b)$$

where ϵ^o and σ^o are the prescribed uniform farfield strains and stresses.”

This is a false statement. This expression assumption allows authors to do unbelievable simplifications and stretching in many important issues.

For example, in pp. 54-57 [26] one can read the reasoning (“proofs”) that the operation of differentiation commutes with the operation of local averaging? That is incorrect by pure mathematics.

In the one of the numerous claims for multiscale modeling of physical phenomena [8] is used the asymptotic expansion of field variables with the following development of “multi-scale” Euler governing equations along. We will follow the main arguments and concepts referred to this paper in the effort (the next following many previous ones) to address the “Multi-scale” treatment issues raised in many CM papers.

In the Introduction to the paper there is given a nice review of the studies related to “multiscaling” in continuum mechanics. We can read in p. 1826: “Quasicontinuum method [12, 22, 23] has been proposed for problems requiring the simultaneous resolution of continuum and atomistic length scales in a unified manner. In this approach, the continuum part is furnished by finite element method where mesh adaptivity is employed to provide multi-scale analysis capabilities near lattice and other highly energetic regions, and proper weight distribution is introduced for handshaking regions. A bridging scale scheme has been proposed to separate basis functions of 2 scales in the handshaking region [26]...” etc.

The main objection to these and to the one in the reviewed paper [8] is that in these simulation techniques they can not describe properly the – “coupling,” “multiscaling,” “connection of scales,” “scale bridging,” etc., because they can not properly address and formalize the collective behavior, collective physical subjects phenomena at the neighboring physical scales as well as the surficial phenomena that all work simultaneously in Modeling Governing Equations.

That is because the authors use for GE developing the Homogeneous GO theorem. That's simple. These are really the Multi-Resolution methods sometimes using the different scales to solve the INCORRECT problem's statement.

Why it is incorrect – BECAUSE FOR THE MULTISCALE PROBLEM INSTEAD OF THE MULTISCALE PHYSICAL STATEMENT, FORMULATED AS THE MULTISCALE MATHEMATICAL STATEMENT, THE SINGLE SCALE PHYSICAL AND MATHEMATICAL PROBLEM USING THE MULTIREOLUTION STATEMENTS IS BEING USED AND “SOLVED”.

Having no different spaces - just a single space for any physical phenomena.

Where the DOT for every resolution statement IS THE POINT with no physical subject, physical meaning inside, just the value of the field at this dot. Where everything is being adjusted to the one scale experimental data (for any scale experiment) using the "coefficients", the magic property of adjusting coefficients. After all, these coefficients are also of the single scale Homogeneous matter. The authors write straight about that – the scale in y-coordinate is not a physical scale, it is the mathematical convenience, the mathematical habitat trick for the convenience of finding the solution. We are not looking into some physical sense while selecting this or numerous other kinds of coordinate resolution.

Summarizing the outlook for these excerpts in pp. 1827-1828, we can say that this kind of methodology, expressed in this work of 2004 and other works of the given authors group ([7], etc.), presents itself as the homogenization procedures [2] aimed to deal with the complicated heterogeneous media solid state mechanics problem. But this is not even a two-scale method. Not a "multi-scale" physics treatment as the authors want to position this work at. No interscale dependencies were properly set-up and determined in terms of Lower Scale Domain Upper Scale Point, etc. as can be expected from Fig. 1 (page 1827).

The large publication was recently issued by Ghoniem and Kioussis [9] on the noble nowadays topic "How to reach Multiscaling in Nanotech?" Because it was positioned as the one in between the Continuum Mechanics applications and the Nanotech fields related to Continuum Mechanics traditional writings, we need to address this one more "multiscaling" text. In page 2 one can read the good words of intention – "Multiscale interconnected approaches will need to be developed to interpret new and highly specialized nano-/micromechanical tests. One of the advantages of these approaches is that, at each stage, physically meaningful parameters are predicted and used in subsequent models, avoiding the use of empiricism and fitting parameters..." "...In this article, we review several components of mechanics that are collectively needed to design new nano and micro materials, and to understand their performance. We first discuss in Section 2 the main aspects of quantum mechanics based methods (ab initio)."

As usual in this kind of texts - there are a number of scientific techniques provided that had been developed during the last 60-40 years and nothing about – How we can transfer our models from one scale into other? That can not be done while using the mathematics of CM based on the homogeneous GO theorem. While without scaleportation (not of homogeneous statistical mechanics) all these publications are just a collection of old time homogeneous techniques swept together because the appropriate scientific language should be

used at present. For example, in p. 39 it is written that – "Understanding the collective behavior of defects is important because it provides a fundamental understanding of failure phenomena (e.g., fatigue and fracture)." "In an attempt to resolve these observations, two main approaches have been advanced to model the mechanical behavior in this meso length scale. The first is based on statistical mechanics methods [135-142]. In these developments, evolution equations for statistical averages (and possibly for higher moments)..."

"The second approach, commonly known as dislocation dynamics (DD), was initially motivated by the need to understand the origins of heterogeneous plasticity and pattern formation..." There are many studies referred to in this review, as just mentioned, and still all are based on the same homogeneous techniques that are not correct while applied to heterogeneous matter. In p.40: "Because of the high density of dislocations and the strong nature of their interactions, direct computer simulations of inhomogeneous plastic deformation and dislocation patterns is still unattainable."

That is incorrect, in the HSP-VAT this goal is quite attainable. Among a few more interesting for commenting techniques, one can find in this article the classical 1D layered medium problem, which is being tackled with the one scale methodology. This problem has been found in HSP-VAT completely solvable for both scales, which is not possible with the one scale statistical mechanics tools described in the reviewed paper.

We would cite more and more of the same mode one scale traditional Continuum Mechanics homogeneous studies of heterogeneous tasks and will not find any method to perform correct scaleportation of properties, or two scale portable solution.

Summary to these and generally to all homogeneous 1sc (one scale) method studies used for heterogeneous CM tasks

1) We can not avoid mentioning an important feature and the need for analytical solutions of heterogeneous problems - it is to give guidance and the cornerstone assessment and results for the future controlled comparison. It is vitally important to have correct analytical solutions for heterogeneous problems. In the problems for the two-scale local-nonlocal heterogeneous tasks there exist the solutions obtained only by the HSP-VAT.

2) Often the texts have the hidden facts and mathematical errors that consist of the mathematical treatment of the outer surface S_0 of the selected REV as it is intersected by the second phase elements, defects, cracks, voids, but the crack's surfaces S_q in real treatment are considered as if they are not intersected with the outer surface S_0 . This is an important hide or negligence. There was written a whole piece of analyses deliberating the mathematics to show why this intersection – Fig. 3,4,

is so important for the conventional homogeneous, one-scale physics, including electrodynamics and, of course, elasticity mechanics, presented in the “Heterogeneous Electrodynamics” section of the website – <http://www.travkin-hspt.com/eldyn/edeffectivecoeff.htm> Effective Coefficients in Electrodynamics.

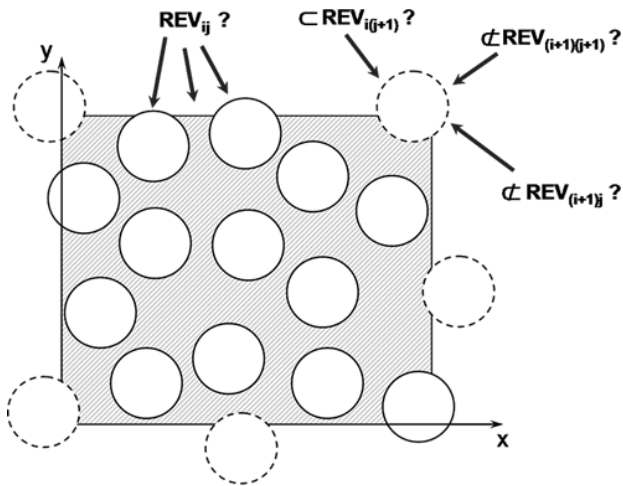


Рис. 3. Типичный рисунок двухфазного композита, подвергнутого ПЭО якобы свободной формы (следуя описанию в работах [22, 23])

Fig. 3. Typical drawing of the two-phase composite subjected to allegedly free form REV (following concepts in studies [22, 23])

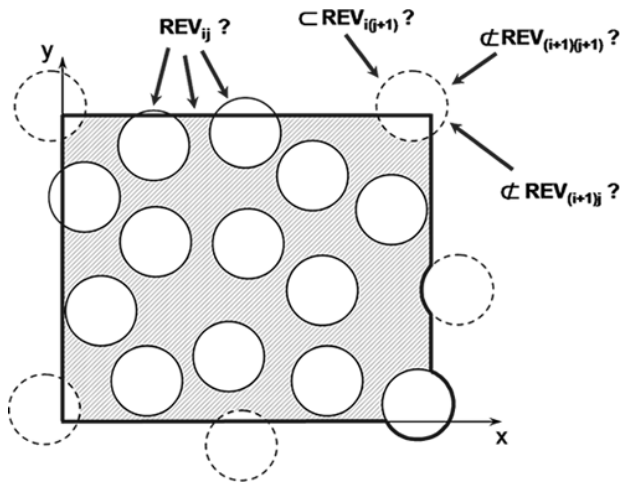


Рис. 4. Одна из предполагаемых форм ПЭО, которая может быть создана для двухфазного композита, учитывающая исчезновение из ПЭО нескольких пересекающих границу ПЭО волокон

Fig. 4. Guessed shape REV that might be drawn for a two-phase composite, accounting on eliminating from the REV a few boundary intersecting fibers

3) The lack of heterogeneous media scaled understanding brought out strange and erroneous statements used throughout the literature on Homogeneous Continuum Mechanics applied for heterogeneous problems, that the assignment of the

remote initial values for like “bulk” strain ϵ_{kl}^* and stress σ_{ij}^* (other field as temperature, potential, etc.) in the composite automatically determines the matrix effective, bulk characteristics $\langle \epsilon_{kl} \rangle, \langle \sigma_{ij} \rangle$.

That is strange because those properties are not equal. These characteristics are of different media and often even of different scales. Nevertheless, based on this erroneous assumption – the great number of studies are using the definition that the only functions they need to simulate are of the inclusions (or second) phase, because the matrix phase effective properties are known as assigned? This is wrong for heterogeneous scaled physics and math.

4) The great fundamental fault of all of this kind local-nonlocal, pseudo-Upper scale effective characteristics – “effective” stiffness tensor, “effective” strain ϵ_{kl}^* tensor, “effective” stress σ_{ij}^* tensor, and other “effective”-like properties is that the researchers while taking averaging (mean) functions just cut out them from the real heterogeneous physics and proper averaging mathematics.

For example, while tackling the strain tensor [20-24] the authors wrote the volumetric averages without any thought on the Hooke's law separately from the elasticity governing equations or the Upper scale in the respected two or more phases, dropping the part of boundary conditions – tractions at the interfaces, external boundary of the REV (they used the “invented” RVE notion), etc.

That kind of cheating or ignorance gives the possibility to write the wrong equality for the matrix averaged strain, for example, in [22] – eq. (60) (as well as the same kind of statement in every study of the mentioned co-authors)

$$\langle \epsilon_{ij} \rangle = \frac{1}{2V} \int_{\Sigma} (u_i^- n_j + u_j^- n_i) dS = E_{ij}, \quad (60)$$

and the assigned “bulk” macroscopic strain tensor E_{ij} , where u_i^- is the displacement vector in the matrix and Σ is the external REV surface, here going only through the matrix (Fig. 4, 5). Because generally

$$\langle \epsilon_{ij} \rangle \neq \frac{1}{2V} \int_{\Sigma} (u_i^- n_j + u_j^- n_i) dS \neq E_{ij}.$$

By doing this assignment the half-problem has become known and, at the same time – the problem of the Boundary Conditions (BC) at the Upper macroscopic scale has been created – Fig. 5. That is because the local strain tensor at the boundary from outside can not be easily assigned via using the homogeneous formulae for the BC for the nonlocal fields and for the “averaged” strain. In this way the authors assign the nonlocal Upper scale solution in the matrix (one of the phases) just at the beginning.

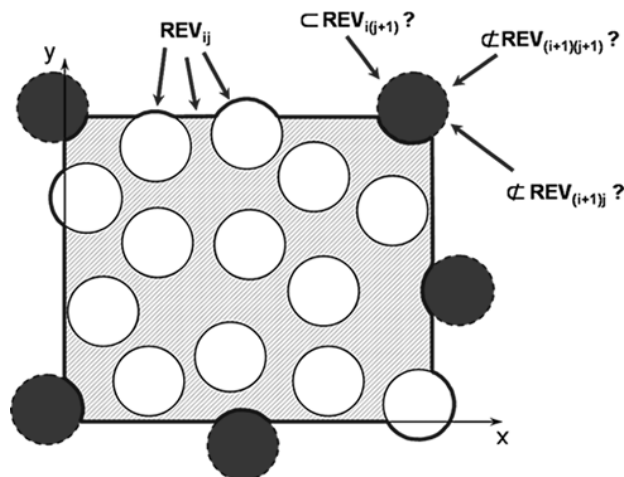


Рис. 5. Истинная форма ПЭО, используемая в работах [22, 23]. В ней намеренно присутствуют полностью или не присутствуют совсем пересекающиеся границей ПЭО волокна

Fig. 5. The true shape REV used in the works [22, 23]. There is no intersecting of the 2-nd fiber phase done on purpose

5) Meanwhile, the assignment of the Nonlocal macrostrain means not only the assignment of the one phase solution actually, but also the almost unsurpassed technical difficulties with the BCs and this Upper (nonlocal) scale problem – because the nonlocal boundary condition would demand the assignment also of the surficial integrals near the boundary within the heterogeneous medium already. Then, the assignment of both phases nonlocal HSP-VAT boundary conditions with surficial values means in its turn the solution of the both Upper Scale displacement – temperature, flow rate, electrical, and strain field problems in need.

6) This is the danger of ignorant usage of the Upper scale (macroscopic) variables to instantaneously (and not innocent) presenting the Lower scale (microscopic) wrong averaging operations for “finding” the “effective” strain? That is unacceptable.

7) In this way of doing “multiscale”, “macroscopic” – in reality the screwed homogeneous one-scale media elasticity theory, continuum damage mechanics, general continuum mechanics of heterogeneous, scaled media (HtSM) – the authors do not only perform incorrectly the Upper scale (macroscopic) assessments, simulation. And often even the Lower scale simulation goes wrong, because they assume that the different scales variables can be taken as equal. This we call the **Scaleblending**. The authors are loosing the substantial part of real science for Heterogeneous Scaled Media. This constitutes a great loss both for science and technologies and the financial loss for the wrong, unnecessary studies.

8) Also, doing the two-scale HSP-VAT problems as the one scale problems the authors are loosing the chance to address the most interesting phenomena in the physics of composite media – **the phenomena at the interfaces**, see Fig. 5. This is not achievable with the one scale local homogeneous mechanics.

9) Avoiding modeling and simulation formulated in terms of HSP-VAT for the Upper scale fields the authors have been deliberating on, acting in this mode to prevent themselves from the Upper scale problem's features:

9.1) They can not formulate, even know and investigate most of the Upper scale characteristics of interest: a) both scale surficial characteristics; b) both scale fluctuation characteristics, etc. Most of the authors have never even heard of those.

9.2) They can not study the morphology parameters of Ht Elasticity, Heat Transfer, Plasticity, Continuum Damage Mechanics, Fluid Mechanics, etc. Morphology parameters formulated and sought after as of the Upper scale – not those researchers usually count for, as – number of cracks, statistical characteristics of defects, interface morphology, etc. All these are of the Lower scale parameters first of all, not of the Upper one.

9.3) They can not study the properties of the interface – correctly determine the arisen characteristics, because the interface is the thing that connects and communicates both phases and has its own characteristics [55, 56]. Those would be studied later when researchers learn how to formulate the issues.

10) It can be said that the analyzed above issues are related to the problem of Scaleportation from Lower scale local field solutions to the Upper scale averaged nonlocal, but mostly sought after fields. These fields include also the effective properties of polymers, polymer composites, heterogeneous media. As we have depicted above the problem of scaleportation is itself not a trivial task of simulation with the Detailed Micro-Modeling – Direct Numerical Modeling (DMM-DNM) homogeneous physics mathematical statements.

11) It is interesting to mention, regarding the use of assigned averaged strain and stress, the other physical fields – whether the authors have thought about the verification of their solutions and have simulated the values of the effective characteristics as temperature, flow rates, strain and stress by averaging the Lower scale local fields? In this case they would find out the nonconservative fields. Which is unexplainable via the Homogeneous CM.

12) Not the last and definitely not the least remark is that the assignment of the averaged (Upper scale) gradient of the strain field (other physical fields of interest) is followed by the non-uniqueness of the solution for the Upper scale statement! Followed by the non-uniqueness of solutions for the Lower scale statements! Followed by the non-unique determination and simulation for the “effective” coefficients! Authors of the one scale solutions apparently do not realize this.

Acknowledgements

Dedicated to E.G. Travkina, mother of V.S.T., acknowledging her encouragement and spiritual strength.

References

1. Mergell B., Everaers R. Tube Models for Rubber-Elastic Systems // *arXiv:cond-mat/0103584v4* [cond-mat.stat-mech], 2001.
2. Bakhvalov N.S., Panasenko G.P. Homogenization: Averaging Processes in Periodic Media. Mathematical Problems in the Mechanics of Composite Materials. Dordrecht: Kluwer Acad. Publishers, 1989.
3. Beran M.J. Statistical Continuum Theories. New York: Wiley-Interscience, 1968.
4. Beran M.J. Application of Statistical Theories for the Determination of Thermal, Electrical, and Magnetic Properties of Heterogeneous Materials // *Mechanics of Composite Materials*. 1974. № 2. P. 209-249.
5. Borisenko A.I., Tarapov I.E. Vector and Tensor Analysis with Applications. Englewood Cliffs: Prentice-Hall, Inc., 1968.
6. Brenner H., Adler P.M. Dispersion Resulting From Flow Through Spatially Periodic Porous Media. II. Surface and Intraparticle Transport // *Phil. Trans. R. Soc. Lond.* 1982. V. A307. P. 149-200.
7. Chen J.-S.; Mehraeen S. Multi-scale modelling of heterogeneous materials with fixed and evolving microstructures // *Modelling Simul. Mater. Sci. Eng.* 2005. V. 13. P. 95-121.
8. Chen J.-S.; Mehraeen S. Variationally Consistent Multi-Scale Modeling and Homogenization of Stressed Grain Growth // *Comput. Methods Appl. Mech. Engrg.* 2004. V. 193. P. 1825-1848.
9. Ghoniem N.M., Kioussis N. Hierarchical Models of Nanomechanics and Micromechanics // *Handbook of Theoretical and Computational Nanotechnology*. Rieth M., Schommers W., Eds. American Scientific Publisher. P. 1-97, 2005.
10. Golovchan V.T., Guz' A.N., Kokhanenko Yu.V., Kushch V.I. *Mechanics of Composites. Statics of Materials*, Volume 1. Kiev: Naukova Dumka, 1993. (in Russian).
11. Happel J., Brenner H. *Low Reynolds Number Hydrodynamics*. Alphen aan den Rijn: Sijthoff and Noordhoff, 1973.
12. Hashin Z. Elasticity of Random Media // *Trans. Soc. Rheol.* 1965a. № 9. P. 381-406.
13. Hashin Z. On Elastic Behaviour of Fiber Reinforced Materials of Arbitrary Transverse Phase Geometry // *J. Mech. Phys. Solids*. 1965b. № 13. P. 119-134.
14. Hashin Z. *Theory of Fiber Reinforced Materials* // NASA CR-1974 Report. Philadelphia: Univ. Pennsylvania. 1972.
15. Hashin Z. Analysis of Composite Materials – A Survey // *J. Appl. Mech.* 1983. № 50. P. 481-505.
16. Hill R. Elastic Properties of Reinforced Solids: Some Theoretical Principles // *J. Mech. Phys. Solids*. 1963. № 11. P. 357-372.
17. Hori M., Nemat-Nasser S. On Two Micromechanics Theories for Determining Micro-Macro Relations in Heterogeneous Solids // *Mech. Materials*. 1999. V. 31, Iss. 10. P. 667-682.
18. Kushch V.I. Conductivity of a periodic particle composite with transversely isotropic phases // *Proc. R. Soc. Lond.* 1997a. V. A453. P. 65-76.
19. Kushch V. I. Microstresses and effective elastic moduli of a solid reinforced by periodically distributed spheroidal particles // *Int. J. Solids and Structures*. 1997b. V. 34, Iss. 11. P. 1353-1366.
20. Kushch V.I., Sangani, A.S. Stress Intensity Factors and Effective Stiffness of a Solid Containing Aligned Penny-Shaped Cracks // *Int. Journal of Solids and Structures*. 2000a. V. 37. P. 6555-6570.
21. Kushch V.I., Sangani A.S. Conductivity of Composite Containing Uniformly Oriented Penny-Shaped Cracks or Perfectly Conducting Disks // *Proc. Roy. Soc. London*. 2000b. V. A456, P. 683-699.
22. Kushch V.I., Sevostianov I., Mishnaevsky L.Jr. Stress Concentration and Effective Stiffness of Aligned Fiber Reinforced Composite with Anisotropic Constituents // *Int. Journal of Solids and Structures*. 2008a. V. 45, № 18-19. P. 5103-5117.
23. Kushch V.I., Shmegeera S.V., Mishnaevsky L.Jr. Meso Cell Model of Fiber Reinforced Composite: Interface Stress Statistics and Debonding Paths // *Int. Journal of Solids and Structures*. 2008b. V. 45, № 9. P. 2758-2784.
24. Kushch V.I., Sevostianov I., Mishnaevsky L.Jr. Effect of Crack Orientation Statistics on Effective Stiffness of Mircocracked Solid // *Int. J Solids and Structures*. 2009. V. 46, № 6. P. 1574-1588.
25. Mura T. *Micromechanics of Defects in Solids*. New York: Martinus Nijhoff, 1987.
26. Nemat-Nasser S., Hori M. *Micromechanics: Overall Properties of Heterogeneous Materials*, 2nd Ed. Amsterdam: Elsevier Science B.V., 1999.
27. Nigmatulin R.I. *Dynamics of Multiphase Media*, Vol. 1, Revised and Augmented Ed. New York: Hemisphere Publish. Corp., 1991.
28. Nigmatulin R.I. *Dynamics of Multiphase Media*, Vol. 2, Revised and Augmented Ed. New York: Hemisphere Publish. Corp., 1991.
29. Papanicolaou G. *Wave Propagation in Complex Media*. New-York: Springer-Verlag, 1998.
30. Spencer P. E., Sweeney J. *Modelling of Polymer Clay Nanocomposites for a Multiscale Approach* // *arXiv Cornell University*, 2009.
31. Truesdell C. *A First Course in Rational Continuum Mechanics*. Baltimore: John Hopkins Univ., 1972.
32. Fish J.; Belsky V. Multi-grid Method for Periodic Heterogeneous Media, Part 1: Convergence Studies for One-Dimensional Case // *Comput. Methods Appl. Mech. Eng.* 1995. V. 126. P. 1-16.
33. Wagner G.J., Liu W.K. Coupling of Atomic and Continuum Simulations using a Bridging Scale Decomposition // *J. Comput. Phys.* 2003. V. 190. P. 249-274.

34. Weiler F.C. Fully Coupled Thermo-Poro-Elasto Governing Equations// Proc. Computational Mechanics of Porous Materials and Their Thermal Decomposition. ASME, AMD – Vol. 136. 1992. P. 1-28.
35. Gray W.G., Lee P.C.Y. On the Theorems for Local Volume Averaging of Multiphase Systems // Int. J. Multiphase Flow. 1977. V. 3. P. 333-340.
36. Gray W.G., Leijnse A., Kolar R.L., Blain C.A. Mathematical Tools for Changing Spatial Scales in the Analysis of Physical Systems. Boca Raton: CRC Press, 1993.
37. Marle C.M. Ecoulements Monophasiques en Milieu Poreux // Rev. Inst. Francais du Petrole. 1967. V. 22. P. 1471-1509.
38. Primak A.V., Shcherban A.N., Travkin V.S. Turbulent Transfer in Urban Agglomerations on the Basis of Experimental Statistical Models of Roughness Layer Morphological Properties // Transactions World Meteorological Organization Conference on Air Pollution Modeling and its Application. Geneva: WMO, Vol. 2. 1986. P. 259-266.
39. Quintard M., Whitaker S. One and Two-Equation Models for Transient Diffusion Processes in Two-Phase Systems // Advances in Heat Transfer, Vol. 23. New York: Academic Press. 1993. P. 369-465.
40. Slattery J.C. Momentum, Energy and Mass Transfer in Continua. Malabar: Krieger, 1980.
41. Whitaker S. Diffusion and dispersion in porous media // AIChE Journal. 1967. V. 13. P. 420-427.
42. Whitaker S. Simultaneous heat, mass and momentum transfer in porous media: a theory of drying // Advances in Heat Transfer, Vol. 13. New York: Academic Press. 1977. P. 119-203.
43. Whitaker S. The Method of Volume Averaging. Berlin, Heidelberg: Springer, 1998.
44. Travkin V.S., Catton I. Transport Phenomena in Heterogeneous Media Based on Volume Averaging Theory // Advances in Heat Transfer, Vol. 34. New York: Academic Press. 2001. P. 1-144.
45. Travkin V.S., Catton I. Porous Media Transport Descriptions – Non-Local, Linear and Nonlinear Against Effective Thermal/Fluid Properties // Advances in Colloid and Interface Science. 1998. V. 76-77. P. 389-443.
46. Travkin V.S., Catton I. Turbulent transport of momentum, heat and mass in a two level highly porous media // Heat Transfer 1994, Proc. Tenth Intern. Heat Transfer Conf., Vol. 5, Hewitt G.F., Ed. London: Chameleon Press. 1994. P. 399-404.
47. Travkin V.S., Catton I. A two temperature model for turbulent flow and heat transfer in a porous layer // J. Fluids Engineering. 1995. V. 117. P. 181-188.
48. Travkin V.S., Hu K., Rizzi M., Canino M., Catton I. Revising the Goals and Means for the Base-to-Air Cooling Stage for Semiconductor Heat Removal – Experiments and Their Results // Proc. 17th IEEE SEMI-THERM Symp. New York: IEEE Publishing. 2001. P. 85-94.
49. Travkin V. S., Catton I. Nonlinear effects in multiple regime transport of momentum in longitudinal capillary porous media morphology // Journal of Porous Media. 1999. V. 2, № 3. P. 277-294.
50. Crapiste G.H., Rotstein E., Whitaker S. A general closure scheme for the method of volume averaging // Chemical Engineering Science. 1986. V. 41. P. 227-235.
51. Gratton L., Travkin V.S., Catton I. The Influence of Morphology upon Two-Temperature Statements for Convective Transport in Porous Media // J. Enhanced Heat Transfer. 1996. V. 3, № 2. P. 129-145.
52. Luikov A.V. Heat- and Mass Transfer (Textbook). Moscow: Energiya, 1971. (in Russian).
53. Newman T.J. Modeling Multicellular Systems Using Subcellular Elements // Mathematical Biosciences and Engineering. 2005. V. 2, № 3. P. 611-622.
54. Zhou Y.C., Holst M., McCammon J.A. A Nonlinear Elasticity Model of Macromolecular Conformational Change Induced by Electrostatic Forces // J. Math. Analysis Applic. 2008. V. 340, Iss. 1. P. 135-164.
55. web-1: <http://www.travkin-hspt.com/elastic/whatsupf/whatsup.htm> What is in use in Continuum Mechanics of Heterogeneous Media as of Through ~1950–2005?
56. web-2: <http://www.travkin-hspt.com/elastic/ivorytower/ivorytower.htm> Who Are in the Continuum Mechanics Continuing to Dwell in an Ivory Tower? Who Tries to Re-Invent the Wheel? What Are the Damage and Financial Loss?

