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Variational foundations and generalized unified theory of RVE-based multiscale models

Pablo J. Blanco · Pablo J. Sánchez · Eduardo A. de Souza Neto · Raúl A. Feijóo

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Abstract A unified variational theory is proposed for a general class of multiscale models based on the concept of Representative Volume Element (RVE). The entire theory lies on three fundamental principles: (i) *kinematical admissibility*, whereby the macro- and micro-scale kinematics are defined and linked in a physically meanigful way; (ii) *duality*, through which the natures of the force- and stress-like quantities are uniquely identified as the duals (power-conjugates) of the adopted kinematical variables; and (iii) the *Principle of Multiscale Virtual Power*, a generalization of the well-known Hill-Mandel Principle of Macrohomogeneity, from which equilibrium equations and homogenization relations for the force- and stress-like quantities are unequivocally obtained by straightforward variational arguments. The proposed theory provides a clear, logically-structured framework within which existing formulations can be rationally justified and new, more general multiscale models can be rigorously derived in well-defined steps. Its generality allows the treatment of problems involving phenomena as diverse as dynamics, higher order strain effects, material failure with kinematical discontinuities, fluid mechanics and coupled multi-physics. This is illustrated in a number of examples where a range models is systematically derived by following the same steps. Due to the variational basis of the theory, the format in which derived models are presented is naturally well suited for discretization by finite element-based or related methods of numerical approximation. Numerical examples illustrate the use of resulting models, including a non-conventional failure-oriented model with discontinuous kinematics, in practical computations.

Keywords Multi-scale formulations · RVE · Duality · Constitutive theory · Hill-Mandel · Heterogeneous kinematics · Variational methods

P.J. Blanco · R.A. Feijóo
National Laboratory for Scientific Computing, LNCC/MCTI, Av. Getlio Vargas, 333, Petrópolis-RJ, 25651-075, Brazil
Tel.: +55-24-22336067
Fax: +55-24-22336071
E-mail: feij@lncc.br

P.J. Blanco · R.A. Feijóo
National Institute of Science and Technology in Medicine Assisted by Scientific Computing, INCT-MACC, Petrópolis, Brazil

P.J. Sánchez
CIMEC-UNL-CONICET, Güemes 3450, 3000 Santa Fe, Argentina

P.J. Sánchez
GIMNI-UTN-FRSF, Lavaise 610, 3000 Santa Fe, Argentina

E.A. de Souza Neto
Zienkiewicz Centre for Computational Engineering, Swansea University, Swansea SA2 8PP, United Kingdom

1 Introduction

1.1 RVE-based multiscale methods. A brief review

Multiscale theories, i.e. theories that link the macroscopic behaviour of continua to phenomena occurring at smaller spatial scales, date back at least to the mid-twentieth century. Fundamental early contributions are found in the seminal series of papers by Kirkwood and co-workers [52,54,55,56], where continuum governing equations are derived from statistical molecular mechanics arguments in the context of transport phenomena. In solid mechanics, significant theoretical developments in the estimation of macroscopic properties of heterogeneous materials began with the pioneering work of Hashin and Shtrikman [41], Hill [42,43,44,45], Budiansky [17], Mandel [72] and Gurson [40], among others. A further stream of significant developments

in this direction took place beginning in the mid- to late 1970's, based on the asymptotic analysis of partial differential equations with periodic coefficients in the modelling of periodic media. Fundamental contributions in this context are the books by Bensoussan *et al.* [10] and Sanchez-Palencia [105]. Common across the range of different approaches is the fact that macroscopic continuum quantities (often referred to as homogenized quantities) are invariably linked to their micro-scale counterpart fields by means of some kind of averaging process.

Over the last two decades or so, a surge in the use of multiscale theories has been seen especially within the context of computational mechanics. Attention has been focused particularly on theories that rely on the concept of *Representative Volume Element (RVE)* where stresses and strains at the macro-scale are obtained as volume averages of their micro-scale counterparts over the RVE. The RVE itself is usually modelled as a continuum, but may also be described in terms of discrete interactions. The use of RVE-based theories in situations of practical interest relies almost exclusively on techniques of computational homogenization, based on finite element methods [30,57,64,77,78,79,80,81,82, 93,115,121]. In solid mechanics, reported applications encompass at present the modelling of a wide range of phenomena, including plasticity, thermomechanical coupling, size effects, material failure and dynamics, among others.

In plasticity, for example, the recent review by McDowell [76] presents a comprehensive account of the use of multiscale theories not only in the continuum setting, but also at the molecular and atomistic scales. The literature in this area provides clear evidence of the ability of the multiscale approach to overcome several challenges in the modeling of the plastic response resulting from complex phenomena such as dislocation dynamics, crystal plasticity and phase transformation under complex strain histories. However, many fundamental problems, related both to the understanding and modeling of micro-scale mechanisms and to the development of suitable multiscale theories, remain open, even in this relatively classical field of research (see [76] and references therein).

Multiscale formulations have proved useful also in deriving higher order constitutive models [58,59,65,66, 114]. These formulations are suitable for modeling material behavior when the scales are not sufficiently separated and size-dependent behaviour becomes relevant. An appealing aspect of RVE-based strategies in this case is that they are capable of endowing the macro-scale with higher order constitutive models that are retrieved from conventional micro-scale descriptions with first-order kinematics. The associated length-scale here arises as a natural consequence of the kinematical transfer between scales, which includes a contribution of the second-order macro-scale gradient to the first order micro-scale deformation gradient field. This approach was shown to be an interesting alternative to phenomenological models in addressing problems such as strain localization, as a length-scale parameter does not need to be artificially introduced.

In the field of thermoelasticity, the use of thermomechanically coupled multiscale formulations has led to the development of more refined constitutive descriptions. Early work exploring RVE-based theories in this case embraced the standard scales separation assumption, which is typical of the asymptotic analysis approach to the problem [10,25,33,106]. For example, in [91,92,107,118] the problem is addressed under the hypothesis of scales separation, requiring the use of a uniform temperature field in the micro-scale mechanical problem. This is consistent with a standard thermodynamics setting at the macro-scale. Alternatively, in [15], a thermomechanical multiscale formulation is proposed to account for temperature fluctuations in the micro-scale mechanical problem. This approach is based on purely variational arguments to define the kinematic transfer between scales and to naturally derive homogenization rules for the flux quantities (stress and heat flux in this case). The formulation proposed in [15] is in line with [31,51,83,84] in the sense that the continuum model at the macro-scale features a higher order thermal behavior, with the stress depending on the temperature gradient. This is consistent with an extended thermodynamics framework at the macro-scale.

Another interesting area where multiscale theories have a clear potential to promote significant advances in modeling, is failure mechanics. Macro-scale failure, i.e. loss of load carrying capacity leading to eventual fracturing of the material, is the result of a number of complex interacting micro-scale mechanisms whose nature depends crucially on the specific material in question. One of the main challenges here is the formulation of objective models, i.e. models for which the energy dissipated by the failure mechanisms is well-defined – unaffected by RVE size and convergent with mesh refinement. Classical, standard RVE-based formulations are inherently non-objective in this sense as the inherent size-effect associated with strain localization [6] at the micro-scale translates into a lack of objectivity of the macro-scale response with respect to RVE size [37]. To circumvent this problem several strategies have been developed. For instance, in [9,8,109] a specific stress homogenization procedure has been proposed which excludes strain localization zones from the

stress averaging domain. In addition, a dependence of numerical parameters (such as finite element size) on RVE domain size has been introduced. In [19,20] a second-order framework has been adapted to model material failure, with classical boundary conditions partially modified to account for strain localization, but without a strict direct relation between the macro-scale strain and the localized strain. Verhoosel *et al.* [125] proposed a method for deriving a homogenized macro-scale cohesive model from micro-structures with possible nucleation of micro-cohesive cracks and adhesive micro-interfaces. In [87] this approach was extended to include RVEs with a gradient-enhanced regularized damage material model (see also [85,86,88]).

1.2 Current trends and perspectives

It is clear from the above that the range of applications of RVE-based formulations is very wide. It should be added here that, at present, the interest in such approaches is growing at a faster pace than ever. This is confirmed by the shear number of papers published on the subject over the last few years as well as on the number of conferences and conference sessions organized on the topic. One of the main driving forces behind the advancement of multiscale techniques is the pressing need for more accurate computational tools for prediction of material response in situations where the macro-scale effects of complex micro-scale mechanisms cannot be easily captured by the conventional phenomenological modelling approach. In this context, computational RVE-based methods can be used either in the simulation of macroscopic structures by a coupled multiscale approach (often referred to as FE^2) or as a basis for the development of new phenomenological models, or calibration of material parameters of existing models, by means of so-called *numerical material testing* [32, 38,94,113,119,120,129]. An interesting application in this context is the development of constitutive laws for micromorphic materials [27,28,31,50,51]. In this field, the lack of practicality lies in the development of experiments to aid the identification of constitutive laws. Multiscale formulations can be employed to create the link between high-order continua at macro-scale and first-order continua at micro-scale.

Another key reason for the growing interest in RVE-based multiscale methods is the need to better understand how micro-scale mechanisms affect macro-scale behavior [122,126]. This understanding, together with the ability to numerically predict their impact on macro-scale behaviour, is crucial to optimize the use of existing materials as well as to assist the design of new materials in a rational, scientifically-based manner.

The design of new materials, in particular, is an area of research where significant resources have been injected in recent years. The wider availability of equipment at relatively low cost, allied to recent advances in sophisticated manufacturing processes, such as additive layer manufacturing, are creating great expectations for the development of materials with bespoke mecanical, thermal, optical, chemical and electromagnetic properties. This includes the promising development of new alloys, composites in general, bio-inspired and bio-compatible materials. Of particular interest are the so-called *metamaterials* – materials with useful exotic behavior [26]. Auxetic materials – materials with negative Poisson's ratio [62,63,128] – are a typical example. But exotic, counterintuitive behavior, can be associated with thermodynamical, electromagnetic [13, 12,11] and other mechanical properties [18,29,67,68, 70,130]. The unusual behavior displayed by such materials is a consequence of their micro-structural arrangement. Del Vescovo and Giorgio [23] provide an interesting overview covering a range of exotic materials and the tools currently available to model them. The ability to design micro-scale architectures that produce a specific material behaviour is of utmost importance in this context [39,75,108]. RVE-based computational multiscale methods aiming, for instance, the optimization of certain material properties [3,53,124] have shown to offer a solid tool to assist the material design process.

In summary, the track record of RVE-based computational multiscale methodologies in dealing with complex phenomena, allied to the current trends in the development and design of new materials, makes it reasonable to expect that the demand for more general, refined and accurate computational multiscale methods will only increase in the years to come.

1.3 Critical appraisal of the state-of-the-art

Despite the widespread use of RVE-based multiscale theories, a general unified framework for the development and treatment of theories of this class appears to be lacking at present. In fact, the RVE-based approach to classical multiscale solid mechanics – with both macro- and micro-scales described in terms of conventional kinematics – is very well understood and lies on the solid theoretical grounds set in the works of Hill [45] and Mandel [72]. However, any attempts to extend this approach beyond the classical scenario is likely to face challenges. This is due mainly to the fact that the classical theory (and existing extensions) evolved without a clear distinction being highlighted between fundamental assumptions and their consequences. Hence, it is not straightforward in general to ascertain precisely

what changes will be required to the classical theory if, for instance, dissimilar physical regimes are to be linked across the scales or, in the case of the purely mechanical theory, more complex loading systems become relevant or more sofisticated kinematical descriptions are adopted to model phenomena such as strain localization, fracturing or higher order strain effects.

In the treatment of higher order strain effects, for example, the homogenization formulae for stress-like quantities is derived from a modified Hill-Mandel principle in [58,59]. More recently, in [71], a similar approach was adopted with kinematical conditions based on orthogonality restrictions proposed to construct a consistent kinematical transfer between scales. The resulting boundary conditions in the latter work are slightly different from those of the former, raising questions about the validity range and limitations of each formulation, and about what ultimately drives the kinematical transfer between the two scales. As they stand, it is not easy to compare these two theories and find a definite answer to these questions.

A rather blurred scenario emerges in the multiscale modeling of material failure – possibly one of the most challenging applications of RVE-based theories. An interesting point to observe here is that failure kinematics differs considerably from the classical case due to the inherent discontinuities that characterize the phenomenon. Hence, an appropriate extension of classical principles of kinematical transfer across scales requires very careful consideration and may not be easily established correctly on the basis of physical intuition alone. Note that this is a determining factor in the definition of RVE boundary conditions. Like the kinematical transfer (or the RVE boundary conditions), the homogenization formulae for the stress-like quantities are also generally postulated [8,9,109], without an underlying fundamental principle. More recently, in [104,123] a failure-oriented multiscale theory has been proposed where, rather than postulated, the RVE boundary conditions are derived from a robust kinematical principle and homogenization formulae for stress-like quantities (including the traction vector associated with the macro-scale displacement jump) are, in turn, derived from solid variational arguments based on a suitably extended Hill-Mandel Principle. This model extends the classical theory by accommodating a non-uniform insertion of macro-scale strain into the micro-scale under a strain localization regime in a way that the magnitude of the kinematical quantities involved are preserved in the micro-macro transition. This was shown to offer a possible solution to open problems, such as the construction of objective formulations, even when the process evolves from initially continuous media to domains featuring strong macro-scale discontinuities caused by micro-scale strain localization. At a closer look, this theory reveals an emerging pattern containing all the necessary ingredients that allow the problem to be dealt with using a minimum set of fundamental assumptions. This structure will be explored and generalized in the present paper.

The study of multiscale dynamics is of particular relevance to the development of a range of materials (including metamaterials), as well as to the analysis of multiscale problems involving high impact loads. Curiously, this topic has so far received relatively little attention in the context of RVE-based formulations and it is only recently that contributions to this area began to appear in the literature [69,98]. Similarly to multiscale material failure theories, a robust theoretical framework for the treatment of RVE-based multiscale dynamics appears to be missing at present. This becomes clear when we observe some potential shortcommings in the (currently scarce) available literature. For example, in [98] a split of the micro-scale displacement fluctuation into a steady-sate and a dynamic contribution is proposed, with each component subjected to a different kinematical constraint. Interesting numerical results are reported in this contribution, but the variational consequences of such constraints to the corresponding equilibrium equations are not easy to ascertain within the framework the theory is presented. Neither is the range of validity of the adopted micro-macro kinematical transfer which, in principle, should preserve the magnitude of the displacements involved. A related problem is briefly discussed in [100] where body forces (which could also be seen as arising from micro-scale inertia effects) are added to the classical formulation and then the corresponding macro-scale force is shown to vanish as a consequence of variational considerations. The conclusions in this case are reached in a variationally consistent manner, but the lack of a clear principle of kinematical transfer beween scales appears to lead to an erroneous conclusion. Inconsistencies of this type are obviously quite understandable, given that such theories are just starting to spring. With the above comments we only wish to emphasize that the modeling of multi-scale dynamics can also benefit significantly if a framework is established, based on clear fundamental principles, whereby multiscale theories of this type can be more easily derived in a systematic manner, free from potential inconsistencies.

Fluid mechanics is an area where, to the authors' knowledge, RVE-based theories have not been reported so far in the modeling of multiscale phenomena. This is probably a consequence of the natural difficulties in identifying an RVE in fluid flow. Depending on the de-

scription, the RVE could be understood as a representative volume of flowing particles (Lagrangian description) or as a representative volume window through which particles flow (Eulerian description). To date, multiscale fluid mechanics has been approached mainly from two points of view: (i) the celebrated *two-scale convergence method*, based on asymptotic expansions [2]; and (ii) the *variational multiscale method* [47]. The first approach is largely associated with the development of multiscale formulations for flow through porous media (see [117]). In [1] a basis was set to analyze, using the two-scale convergence method, the limit of Navier-Stokes equations in the presence of obstacles in the micro-scale. A very recent contribution [46] addressed the problem of multiscale modeling in turbulence based on asymptotic expansions for the Navier-Stokes equations. The interesting result is that, by modeling the convection of additional quantities at macro-scale (proper convection of small-scale information), it is possible to achieve a closed-form representation of the Reynolds stress for arbitrary geometries. The *variational multiscale method*, has also been successfully employed to model turbulence [7,48,49]. This approach proposes a direct link between the role of the micro-scale (called *subgrid* scale) and the discretization of the equations at the macro-scale. Despite their success, a limiting factor of both the two-scale convergence and the variational multiscale method is that they assume the problem to be governed by the same phenomenology at both scales. Distinct physical models at macro- and micro-scale, such as, for example, a macro-scale high-order formulation linked to a first-order micro-scale formulation – an approach that has been successfully employed in solid mechanics [58] – cannot in principle be treated by such methods. In this sense, an RVE-based framework could provide a interesting alternative, with a rather general setting, particularly for problems in which complete scale separation cannot be assumed.

1.4 Contribution of the present work

In response to the issues highlighted above – the current lack of a general framework and the pressing need for development of more sophisticated multiscale models – the present paper proposes a unified variational theory for a very broad class of RVE-based multiscale models. Our main purpose is to create a sufficiently general framework within which new multiscale models, incorporating more general mechanical settings and capable of accounting for more complex micro-scale phenomena, can be developed in clear, systematic steps. The proposed theory should be capable of handling multi-physics problems, material failure due to micro-scale strain localization or fracturing, dynamical effects and fluid mechanics, among other phenomena, and we shall limit ourselves to the use of a single temporal scale common to both spatial scales.

The work reported here builds on the authors' past experience in the axiomatization of the classical theory [97,110,111,112] and in the treatment of problems involving kinematical discontinuities at both micro- and macro-scales [104]. Within the proposed framework, named *method of multiscale virtual power*, the entire theory sits on the three fundamental axioms/principles of: (i) *kinematical admissibility*[1]; (ii) *mathematical duality*, and (iii) *multiscale virtual power*. The idea of *kinematical admissibility* establishes a link between the macro- and micro-scale kinematics by means of two operators named the *insertion operator* and the *kinematical homogenization operator*, respectively. These effectively define the kinematical transfer between the scales and must impose constraints on admissible kinematical fields so as to ensure that, in some sense, their magnitude is preserved in the micro-macro transition. In addition, these kinematical constraints automatically prescribe the functional sets within which the solution of the associated equilibrium problems is to be sought. The concept of *duality*, in turn, plays a fundamental role in the correct definition of the generalized external force-like and generalized internal stress-like (or flux) quantities compatible with a given model. That is, force- and stress-like quantities cannot be defined *a priori*, independently of the underlying kinematics. Rather, they are seen here as *consequences* of the adopted kinematics. Once the kinematics is defined by postulating a sound principle of kinematical admissibility for a particular problem at hand, the corresponding force- and stress-like quantities emerge unequivocally as a result of considerations based on their mathematical duality (power-conjugacy) with respect to the adopted kinematical variables. Finally, the *principle of multiscale virtual power* is a generalization of the classical Hill-Mandel Principle of Macro-homogeneity [45,72], here extended and stated in variational form in terms of the total virtual power at the micro- and macro-scales. As we shall see, once this principle is applied to a particular problem in question, *all* equations of the theory, including equilibrium and ho-

[1] Within the generalized setting of the present paper, the term *kinematics* (and corresponding *kinematical variables*, etc) should be understood, in a broader sense, as relating to the primal variables of a given formulation. That is, we refer to kinematical variables as those whose rates produce power with the corresponding fluxes (stress- or force-like variables). In mechanical problems – the main motivation of our work – it has obviously the conventional meaning of generalized displacements and strains and their rates. In thermal problems, it refers to temperature, temperature gradient, and so on.

mogenization relations for the relevant force- and stress-like variables are naturally *derived* in a straighforward manner by means of simple variational arguments. This is in contrast with the usual approach, where such relations are often *postulated* instead, and makes the causal relations between the fundamental assumptions and their consequences very clear. This, in our view, endows the proposed framework with a logical structure and a degree flexibility that, not only provides a rational justification for many existing models but, more importantly, significantly facilitates the rigorous development of a wide range of new, more refined, multiscale theories in systematic, well-defined steps.

A crucial consequence of this rational structure is that, in developing any particular model within the present framework, the *only* degree of arbitrariness one has lies in the definition of: (a) the kinematical variables adopted at macro- and micro-scales; and (b) how these kinematical variables are linked (subject to the condition that their magnitudes are preserved in the micro-macro kinematical transfer). Once these have been postulated – ideally, so as to capture the kinematics of the corresponding real physical phenomena in the best possible way – the remainder of the model equations will be unequivocally derived on the basis of *duality* and *multiscale virtual power*. Also crucial is the fact that, as a result of the *Principle of Multiscale Virtual Power* any derived RVE equilibrium equations are presented in a variational format that is naturally well-suited for discretization by finite element or related methods of numerical approximation. Through this, a clear separation and differentiation between the fundamental theoretical aspects of the formulation and its numerical approximation is well-established, something which is confusing in many scientific publications.

1.5 Article overview

In presenting the proposed theory we have opted to follow a format where all derivations are first presented in a very general setting. For this purpose, a rather abstract notation is adopted. The need for an abstract notation is justified by the fact that, as mentioned in the preceding text, our intention here is to show a very general framework, capable of dealing with a wide range of problem descriptions – including, among others, conventional solid mechanics formulations, higher order strain theories, generalized stresses and strains, structural elements, discrete formulations in general, potential problems, and so on. To avoid an excessive level of abstraction, as the building blocks of the theory are presented, the meaning of the adopted notations is made clearer by showing how they specialize in the case of the classical infinitesimal solid mechanics. Once the complete theory is set, a number of examples of specializations are presented. These include existing theories – casting them within this framework gives, in our view, an interesting insight – as well as the derivation of new models, including problems involving solid dynamics, distinct physical models across the scales, fluid mechanics and thermo-mechanics.

The paper is organized as follows. As the proposed theory relies heavily on the concept of *virtual power*, a brief historical account of the Method of Virtual Power (MVP) is presented in Section 2 together with a review of its use in the modelling of general (single-scale) physical systems. The main purpose here is to emphasize that the modelling by means of the MVP is a three-step procedure consisting of: (i) *definition of kinematics*; (ii) the use of *mathematical duality* to characterize the virtual power functionals and the corresponding flux (force- and stress-like) variables consistent with the theory in question; and (iii) a statement of the Principle of Virtual Power (PVP) for the problem in question. With an appropriate PVP at hand, the Euler-Lagrange form of the equilibrium equations for the system under consideration can be derived straightaway.

Our main contribution – the proposed general unified RVE-based multiscale theory – is presented in Section 3. The proposed theory is an extension of the PVP-based modeling approach of Section 2 to problems involving two spatial scales. This extension is devised, effectively, by generalizing the three-step procedure of the MVP to problems involving two scales. This extension is named the *Method of Multiscale Virtual Power (MMVP)*. It requires the definition of the kinematics at *each* of the two scales as well as of how the micro- and macro-scale kinematics are linked in a physically consistent manner. Another essential feature is the *Principle of Multiscale Virtual Power (PMVP)* – an extension of PVP – linking the virtual power of the macro-scale to that of the micro-scale. The PMVP proposed here generalizes the well-known Hill Mandel Principle, upon which the classical RVE-based multiscale theory lies.

In Section 4, the general model of Section 3 is specialized to the case where only the *internal* (macro- and micro-) virtual powers are accounted for in the MMVP. Most standard multiscale models available in the current literature fit within this class. In particular, multiscale descriptions of this class define macro-scale constitutive functionals relating the macro-scale flux (stress-like) variables to the history of the associated kinematical variables alone.

Section 5 presents an abstract derivation of tangent operators for the general framework developed in Sec-

tion 3. Such operators are fundamental in the computational implementation of the associated theories. For instance, in the case of non linear multiscale problems discretized by finite element methods, they provide the tangential stiffness matrices required by Newton-type iterative schemes for solution of the associated equilibrium problems.

In Section 6 several specializations of the general theory of Section 3 are presented, involving solid mechanics, fluid dynamics and thermomechanical problems. These illustrate the suitability of the proposed multiscale framework to model a wide range of physical phenomena. In addition, they show that the theory provides a rigorous justification to some otherwise intuitive postulates and can highlight inconsistencies present in some existing RVE-based models.

Computational application of the theory is illustrated in Section 7 where two finite element-based numerical examples are presented – one describing the use of a finite plasticity-based phase change model for polycrystals and another one describing material failure. In particular, the latter example illustrates how the present theory can be used with confidence in situations where the usual, unstructured approach to multiscale problems has failed to provide a consistent and clearly justified formulation.

The paper ends in Section 8, where some concluding remarks are made.

2 Method of virtual power

This section presents a method of primal (kinematical) variational modeling of a general physical system (of single scale) based on the Principle of Virtual Power. Our main aim is to review all essential definitions, mathematical operators, functional spaces and principles required to formulate models of physical systems by means of the PVP. The concepts reviewed here will be generalized in Section 3, where we propose a multiscale extension of the virtual power-based framework. We remark that a rather general, abstract notation will be adopted throughout the text. To avoid an excessive level of abstraction in the presentation, as the concepts and the corresponding abstract notation are introduced, their specialization to the well-established case of classical infinitesimal continuum solid mechanics is also presented. We begin below with a brief historical review of the Method of Virtual Power and then move on to the actual presentation of the PVP-based framework for general physical systems.

2.1 Brief historical review

With origins dating back to ancient Greece, the Principle of Virtual Power appears to have been formalized only in the eighteenth century in the work of d'Alembert [22]. In more modern times, the *method of virtual power* (or, equivalently, *method of virtual work*) has been acknowledged as a systematic, rational and intuitive approach to formulate models of continua [35,74]. It can be argued that the concept of virtual velocity or virtual power itself is a very intuitive one to most people. For example, to estimate the weight of a suitcase, one usually tries to lift it up instinctively and assess the "work" required to do so. That is, we intuitively estimate a force (the weight of the suitcase) by means the "work" or "power" expended when it is subjected to a kinematical action (lifting motion in this case). In this sense, the concept of work- or power-duality between forces and displacement or velocities appears to be somewhat ingrained in human mind.

On one hand, the application of this method to continuum physics modeling is more mathematically elaborate than the more classical approach deriving from vectorial rational mechanics – an approach largely followed in the undergraduate teaching of mechanics at present. On the other hand, the method of virtual power has an extremely appealing aspect in that it provides, in a most natural, axiomatic way, all the fundamental ingredients required in the formulation of a given problem, such as natural boundary conditions, jump conditions and the variational form of the equilibrium equations, regardless of the constitutive behavior of the underlying continuum. These advantages become more pronounced as the physical system under study increases in complexity and this, in our view, significantly outweighs the seemingly greater mathematical demands of the method. For example, the method completely avoids any ambiguities that could otherwise be present in the definition of force- and stress-like quantities compatible with a given physical system. In fact, the nature of force- and stress-like quantities associated with a system is not a fundamental assumption of the method but, rather, a derived concept resulting from mathematical duality. That is, *forces* are representations of the so-called *external virtual power functional* and *stresses* are representations of the so-called *internal virtual power functional* – they are fully characterized by the virtual power (or work they exert) and emerge unequivocally as a result of this duality once the kinematics of the system in question has been defined.

We remark that, in the context of the present paper, the terms *force* and *stress* should be understood in a *generalized* sense. This lack of potential ambigu-

ity in the derivation of force- and stress-like variables is particularly welcome in the development of new, more complex continuum models. In addition, it should be noted that the PVP naturally leads to governing equations stated in a variational format that is particularly well-suited for discretization by means of finite element (in the case of continuum models) or related methods of numerical approximation.

Some interesting fundamental developments based on the method of virtual power are particularly worth of mention. The method was used, for example, in [36] in the derivation of high order models of continua, making the role of kinematics in the modeling of force- and stress-like quantities very clear. These dual quantities were introduced exclusively through the characterization of *virtual power functionals* in the context of an extended kinematics of higher order. In the same spirit, the method of virtual power was employed in [74] to derive governing equations for electromagnetic high order continua. The axiomatic framework adopted in this case had the same goal: the modeling of forces by means of the mathematical duality between the functional spaces of forces and velocities. Similarly, in [21] the method of virtual power was used to deal with the presence of singular interfaces in continuum media. More recently, the same approach had its applicability extended to the field of thermomechanics [99] and thermodynamics [101]. These are further examples of the success and enormous potential of the method in dealing with the modeling of a wide range of physical phenomena.

However, to the authors' knowledge, the concepts of virtual power and duality have not been fully explored yet in the formulation of RVE-based multiscale theories. Given the current interest in RVE-based approaches and the demand for more complex models, it seems to us that it is high time now for the PVP to be explored in this context. However, before we proceed to do so, we shall review below the use of this concept to general physical systems in a conventional (single scale) setting. These ideas will form the basis for the multiscale extension of the PVP proposed in Section 3

2.2 Kinematics

The main kinematical concepts required to formulate models of physical systems in the context of the method of virtual power are reviewed here. For simplicity, we shall focus the presentation on continuum models. We remark, however, that the same concepts can be easily adapted for use in the modeling of discrete systems. Let $\mathcal{B}$ be a body occupying a domain Ω with sufficiently smooth boundary Γ and let $\mathbf{x} \in \Omega$ denote any point in this domain. The set of *generalized displacements* that characterize the kinematics of the physical model describing $\mathcal{B}$, belongs to a functional space $\mathcal{U}$. Elements $u \in \mathcal{U}$ are n-tuples of tensor fields, regular enough to yield mathematically well-posed formulations. Components of the n-tuple of an element $u \in \mathcal{U}$ are denoted u^i, $i = 1, \ldots, n$, so that $u = (u^1, \ldots, u^n)$. Each component u^i can be a zeroth-, first-, second-order (and so on) tensor field. Each component u^i is described through r^i scalar fields. Thus, the total number of scalar descriptors for an element u is $R = \sum_{i=1}^{n} r^i$. Each u^i has a domain of definition $\Omega^{\mathcal{U}_i} := \mathrm{Dom}(\mathcal{U}_i)$, $i = 1, \ldots, n$, i.e.

$$\begin{aligned} u^i : \Omega^{\mathcal{U}_i} &\to \mathcal{U}_i \\ \mathbf{x} &\mapsto u^i(\mathbf{x}), \end{aligned} \tag{1}$$

with $\Omega^{\mathcal{U}_i} \subseteq \Omega$. Each domain $\Omega^{\mathcal{U}_i}$ can be a set of points, surfaces or volumes. In compact form, we write

$$\begin{aligned} u : \Omega^{\mathcal{U}} &\to \mathcal{U} \\ \mathbf{x} &\mapsto u(\mathbf{x}), \end{aligned} \tag{2}$$

where $\Omega^{\mathcal{U}} := \mathrm{Dom}(\mathcal{U}) = (\mathrm{Dom}(\mathcal{U}_1), \ldots, \mathrm{Dom}(\mathcal{U}_n))$, or $\Omega^{\mathcal{U}} = (\Omega^{\mathcal{U}_1}, \ldots, \Omega^{\mathcal{U}_n})$.

Classical solid mechanics *In this case, the domain Ω is a region of the Euclidean space, the generalized displacement contains one single field – the conventional displacement vector field of the solid, $u = \mathbf{u}$ (a tensor field of order 1), and $\mathcal{U}$ is an appropriate Sobolev space of functions defined in Ω. Usually, it is considered that such space is $\mathcal{U} = \mathbf{H}^1(\Omega)$ of vector functions is with square integrable gradient in Ω. Hereafter we take put all the examples and functional spaces in this standard setting. Here we have $\Omega^{\mathcal{U}} = \Omega$. A more elaborate case arises when multi-physics interactions are considered. In electro-mechanically coupled problems the generalized kinematics is characterized as $u = (\mathbf{u}, \phi)$, comprising the displacement vector field $\mathbf{u}$ of the solid – a tensor field of order 1 – and by the electrostatic (scalar) potential field ϕ – a tensor field of order 0 (see [24]). For a general class of micromorphic fluids, the generalized displacement $u = (\mathbf{v}, \boldsymbol{\nu})$ contains the velocity vector field $\mathbf{v}$, a tensor field of order 1, and the rate of deformation tensor field $\boldsymbol{\nu}$, a tensor field of order 2 (see [27, 28]). Further examples will be given in Section 6.* ■

Next, we define the set $\mathrm{Kin}_u \subset \mathcal{U}$ of *kinematically admissible generalized displacements*. Elements $u \in \mathrm{Kin}_u$ satisfy some kinematical constraint (for example, prescribed boundary conditions or possible distributed constraints). A schematic diagram of the functional sets and relevant operators is shown in Figure 1. It is within Kin_u that we shall look for the solution of the equilibrium problem (to be defined later) associated with the physical system under consideration. For simplicity

we assume Kin_u to be a linear manifold (translation of a subspace). As a consequence, it is possible to characterize the subspace Var_u of *kinematically admissible generalized virtual displacements* or *velocities* as

$$\mathrm{Var}_u = \{\hat{v} \in \mathcal{U},\, \hat{v} = v_1 - v_2,\, v_1, v_2 \in \mathrm{Kin}_u\}. \tag{3}$$

Classical solid mechanics *For a body occupying a region Ω, with boundary Γ subject to the kinematical constraint $\mathbf{u} = \mathbf{u}^*$ on $\Gamma_u \subseteq \Gamma$, for a given $\mathbf{u}^*$, we have* $\mathrm{Kin}_u = \{\mathbf{u} \in \mathbf{H}^1(\Omega),\, \mathbf{u}|_{\Gamma_u} = \mathbf{u}^*\}$, *and* $\mathrm{Var}_u = \{\mathbf{u} \in \mathbf{H}^1(\Omega),\, \mathbf{u}|_{\Gamma_u} = \mathbf{0}\}$. ■

Another kinematical concept fundamental to the statement of the PVP is that of *generalized virtual strain action*. Generalized virtual strain rate fields belong to the *space of generalized strain actions*, denoted $\mathcal{E}$. In general, any field $D \in \mathcal{E}$ is an m-tuple of tensor fields. That is, $D = (D^1, \ldots, D^m)$, where each component D^i can be a scalar, a first-order, a second-order tensor field, and so on. Each component D^i, $i = 1, \ldots, m$, is described by s^i scalar fields, so that the total number of scalar descriptors of D is $S = \sum_{i=1}^{m} s^i$. Each components D^i has a domain of definition $\Omega^{\mathcal{E}_i} := \mathrm{Dom}(\mathcal{E}_i)$, i.e.

$$\begin{aligned} D^i : \Omega^{\mathcal{E}_i} &\to \mathcal{E}_i \\ \mathbf{x} &\mapsto D^i(\mathbf{x}). \end{aligned} \tag{4}$$

Each $\Omega^{\mathcal{E}_i} \subseteq \Omega$ can be a set of points, surfaces or volumes. In compact notation, we have

$$\begin{aligned} D : \Omega^{\mathcal{E}} &\to \mathcal{E} \\ \mathbf{x} &\mapsto D(\mathbf{x}), \end{aligned} \tag{5}$$

and $\Omega^{\mathcal{E}} := \mathrm{Dom}(\mathcal{E}) = (\mathrm{Dom}(\mathcal{E}_1), \ldots, \mathrm{Dom}(\mathcal{E}_m))$, that is $\Omega^{\mathcal{E}} = (\Omega^{\mathcal{E}_1}, \ldots, \Omega^{\mathcal{E}_m})$.

The spaces $\mathcal{U}$ and $\mathcal{E}$ are related by a linear operator, denoted $\mathcal{D}$,

$$\begin{aligned} \mathcal{D} : \mathcal{U} &\to \mathcal{E}, \\ u &\mapsto D = \mathcal{D}(u), \end{aligned} \tag{6}$$

that introduces the concept of *generalized strain actions* (and *generalized virtual strain rates*). This operator plays a fundamental role in the definition of duality.

Classical solid mechanics *In this case, $\mathcal{D}$ is the symmetric gradient operator, so that $\mathcal{D}(\mathbf{u}) = \nabla^S \mathbf{u}$, $n = 1$, $R = 3$, $m = 1$ and $S = 6$. The field $\nabla^S \mathbf{u}$ is defined over the entire body, so that $\Omega^{\mathcal{E}} = \Omega$, and belongs to the function space $\mathcal{E} = \mathsf{L}^2_{\mathrm{sym}}(\Omega) = \{\boldsymbol{\varepsilon} \in \mathsf{L}^2(\Omega),\, \boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}^T\}$ (recall we are in a standard mathematical setting). It is worth showing here more general examples in addition to the solid mechanics case. For eletro-mechanical coupled problems the generalized strain action is given by $\mathcal{D}((\mathbf{u}, \phi)) = (\nabla^S \mathbf{u}, \nabla\phi)$, where $\mathbf{u}$ and ϕ are the displacement (a vector) and the electrostatic potential (a scalar), respectively. Then, in this case,*

$$\mathcal{D} = \begin{pmatrix} \nabla^S & 0 \\ 0 & \nabla \end{pmatrix},$$

$n = 2$, $R = 4$, $m = 2$ and $S = 9$. For micromorphic fluids (see [36]), the generalized strain action is given by the triad $\mathcal{D}((\mathbf{v}, \boldsymbol{\nu})) = (\nabla\mathbf{v}, \nabla\mathbf{v} - \boldsymbol{\nu}, \nabla\boldsymbol{\nu})$, where $\mathbf{v}$ is the velocity (vector) and $\boldsymbol{\nu}$ the micro-velocity gradient (a second-order tensor). Then,

$$\mathcal{D} = \begin{pmatrix} \nabla & 0 \\ \nabla & -\mathbf{I} \\ 0 & \nabla \end{pmatrix},$$

$n = 2$, $R = 12$, $m = 3$ and $S = 45$. It should be noted that the meaning of ∇ depends on the configuration chosen to describe the problem. In micromorphic fluids, the adopted configuration is a spatial configuration. Hence, ∇ is the gradient relative to the spatial coordinates. ■

An element $D \in \mathcal{E}$ is said to be a *kinematically compatible generalized strain action* if there exists an element $u \in \mathcal{U}$ such that $D = \mathcal{D}(u)$. The domain of definition of kinematically compatible generalized strain actions is $\Omega^{\mathcal{E}}$ and can be expressed as $\Omega^{\mathcal{E}} = \mathrm{Dom}(\mathcal{D}(\mathcal{U}))$.

Remark 1 *Since $\mathcal{D}$ is linear, it has a well-defined (rectangular) matrix representation of the form*

$$\mathcal{D} = \begin{pmatrix} \mathcal{D}^{11} & \mathcal{D}^{12} & \ldots & \mathcal{D}^{1n} \\ \mathcal{D}^{21} & \mathcal{D}^{22} & \ldots & \mathcal{D}^{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}^{m1} & \mathcal{D}^{m2} & \ldots & \mathcal{D}^{mn} \end{pmatrix}. \tag{7}$$

With this representation, we have $\Omega^{\mathcal{E}_i} = \mathrm{Dom}(\mathcal{D}^{i1}(u^1)) = \ldots = \mathrm{Dom}(\mathcal{D}^{in}(u^n))$, $i = 1, \ldots, m$.

Another important subspace of $\mathcal{U}$ is the *kernel* of the operator $\mathcal{D}$, denoted $\mathsf{N}(\mathcal{D}) \subset \mathcal{U}$, defined as

$$\mathsf{N}(\mathcal{D}) = \{u \in \mathcal{U},\, \mathcal{D}(u) = 0\}. \tag{8}$$

That is, the subspace with null generalized strain action.

Classical solid mechanics *The kernel of the $\mathcal{D}$ – the symmetric gradient operator – is the space of all rigid infinitesimal displacements, i.e. displacements that admit the representation $\mathbf{u}(\mathbf{x}) = \mathbf{u}_o + \mathbf{W}(\mathbf{x} - \mathbf{x}_o)$, with $\mathbf{u}_o$ a uniform field, $\mathbf{W}$ a skew-symmetric second-order tensor and $\mathbf{x}_o$ a point.* ■

Also important is the image, $\mathcal{D}(\mathrm{Var}_u) \subset \mathcal{E}$, of Var_u under the operator $\mathcal{D}$. This is the space of *kinematically compatible generalized virtual strain actions*.

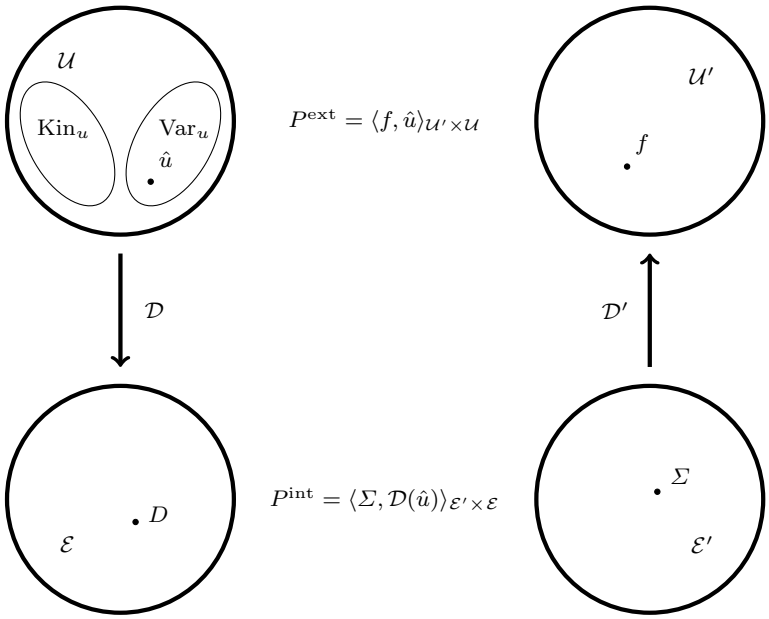

Fig. 1 Virtual Power Method for physical systems. Schematic diagram of basic functional sets and operators.

2.3 First hypothesis. Mathematical duality.

The **first hypothesis** of the MVP-based modeling approach is that the *generalized (external) forces* and *generalized (internal) stresses* admissible by a given physical system are duals of the kinematical variables chosen to describe that system. This allows the nature of admissible generalized stresses, denoted Σ, and forces, denoted f, to be determined solely as a consequence of duality arguments. That is, the nature of force- and stress-like variables cannot be postulated a priori. They are, rather, direct *consequences* of the adopted kinematics. With $\mathcal{E}'$ and $\mathcal{U}'$ denoting, respectively, the dual spaces of $\mathcal{E}$ and $\mathcal{U}$, the **first hypothesis** is stated as follows:

- The nature of the admissible generalized internal stresses $\Sigma \in \mathcal{E}'$ is characterized through a linear (and continuous) functional in $\mathcal{E}$, defined by the duality pairing denoted $\langle\!\langle \Sigma, D \rangle\!\rangle_{\mathcal{E}' \times \mathcal{E}}$.
- Similarly, the nature of the admissible generalized external forces $f \in \mathcal{U}'$ is characterized through a linear (and continuous) functional in $\mathcal{U}$, defined by the duality pairing denoted $\langle\!\langle f, u \rangle\!\rangle_{\mathcal{U}' \times \mathcal{U}}$.

These duality products must satisfy the well-known properties:

- $\langle\!\langle \Sigma, D \rangle\!\rangle_{\mathcal{E}' \times \mathcal{E}} = 0 \quad \forall D \in \mathcal{E} \Rightarrow \Sigma = 0,$
- $\langle\!\langle \Sigma, D \rangle\!\rangle_{\mathcal{E}' \times \mathcal{E}} = 0 \quad \forall \Sigma \in \mathcal{E}' \Rightarrow D = 0,$
- $\langle\!\langle f, u \rangle\!\rangle_{\mathcal{U}' \times \mathcal{U}} = 0 \quad \forall u \in \mathcal{U} \Rightarrow f = 0,$
- $\langle\!\langle f, u \rangle\!\rangle_{\mathcal{U}' \times \mathcal{U}} = 0 \quad \forall f \in \mathcal{U}' \Rightarrow u = 0.$

The first step in the characterization of the model of a real physical system is the definition of an appropriate duality pairing $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathcal{E}' \times \mathcal{E}}$. Obviously, the definition of this duality pairing will depend on the physical nature of the phenomena described by the model. And it will also play a fundamental role in the characterization of the duality pairing $\langle\!\langle \cdot, \cdot \rangle\!\rangle_{\mathcal{U}' \times \mathcal{U}}$. With the notation introduced in the previous section, for the duality pairing between generalized stresses and strain actions, we have

$$\langle \Sigma, \mathcal{D}(u) \rangle_{\mathcal{E}' \times \mathcal{E}} = \sum_{i=1}^{m} \langle \Sigma^i, (\mathcal{D}(u))^i \rangle_{\mathcal{E}'_i \times \mathcal{E}_i} \tag{9}$$

or, equivalently, by using (7),

$$\langle \Sigma, \mathcal{D}(u) \rangle_{\mathcal{E}' \times \mathcal{E}} = \sum_{i=1}^{m} \sum_{j=1}^{n} \langle \Sigma^i, \mathcal{D}^{ij}(u^j) \rangle_{\mathcal{E}'_i \times \mathcal{E}_i}, \tag{10}$$

where $\langle \cdot, \cdot \rangle_{\mathcal{E}'_i \times \mathcal{E}_i}$ denotes a generalized internal product over the domain of definition of component i. For example, if $\Omega^{\mathcal{E}_i}$ is a surface or a volume in Euclidean space, we could have

$$\langle \Sigma^i, (\mathcal{D}(u))^i \rangle_{\mathcal{E}'_i \times \mathcal{E}_i} = \int_{\Omega^{\mathcal{E}_i}} \Sigma^i \cdot (\mathcal{D}(u))^i d\Omega^{\mathcal{E}_i}, \tag{11}$$

whereas, if $\Omega^{\mathcal{E}_i}$ is a set of points, it could be

$$\langle \Sigma^i, (\mathcal{D}(u))^i \rangle_{\mathcal{E}'_i \times \mathcal{E}_i} = \sum_{i=1}^{N^{\mathcal{E}_i}} \Sigma^i \cdot (\mathcal{D}(u))^i, \tag{12}$$

with $N^{\mathcal{E}_i}$ denoting the cardinality of the set $\Omega^{\mathcal{E}_i}$. Once this pairing is defined one should be able to promptly identify the nature of Σ, as in the following example.

Classical solid mechanics *In this case, this duality pairing reads* $\langle \Sigma, \mathcal{D}(u)\rangle_{\mathcal{E}'\times\mathcal{E}} = \int_\Omega \boldsymbol{\sigma}\cdot\nabla^S\mathbf{u}\,d\Omega$. *The stress* $\boldsymbol{\sigma}$ *here is the dual object of the considered strain rate – the symmetric gradient of* $\mathbf{u}$ *– and, hence, can be identified as a symmetric second-order tensor, readily recognized as the Cauchy stress.* ■

In the PVP-based formulation, the product $\langle\!\langle\cdot,\cdot\rangle\!\rangle_{\mathcal{E}'\times\mathcal{E}}$ is restricted to the reduced set $\mathcal{D}(\mathrm{Var}_u)$ of kinematically compatible generalized virtual strain actions and is known as the *internal virtual power*, denoted P^{int}. That is,

$$P^{\mathrm{int}}(\mathcal{D}(\hat{u})) = \langle \Sigma, \mathcal{D}(\hat{u})\rangle_{\mathcal{E}'\times\mathcal{E}} \quad \hat{u}\in \mathrm{Var}_u. \tag{13}$$

In summary, once the kinematics of a particular physical system model is defined, together with a corresponding duality pairing, the internal virtual power functional is defined and the nature of the generalized stresses admissible by the system in question is univocally identified. It should be noted that the internal virtual power functional must be defined such as to be invariant under changes in observer (superimposed rigid kinematical actions). We shall now see that the adoption of a specific form of duality pairing between generalized stresses and strain actions also defines the *generalized external forces*, $f\in\mathcal{U}'$, admissible by the model and the corresponding external virtual work functional. Indeed, from the definition of the *adjoint operator* [89] (also referred to as the *equilibrium operator*), we have

$$\begin{aligned} &\mathcal{D}' : \mathcal{E}' \to \mathcal{U}', \\ &\qquad \Sigma \mapsto f = \mathcal{D}'(\Sigma), \end{aligned} \tag{14}$$

where $\mathcal{D}'$ is the adjoint of $\mathcal{D}$, i.e. the operator that satisfies

$$\langle \Sigma, \mathcal{D}(u)\rangle_{\mathcal{E}'\times\mathcal{E}} = \langle \mathcal{D}'(\Sigma), u\rangle_{\mathcal{U}'\times\mathcal{U}}. \tag{15}$$

The above functional form characterizes the nature of the external load f, *admissible by the adopted kinematical model*. That is, (15) implies that

$$f \text{ has the structure of } \mathcal{D}'(\Sigma)\in\mathcal{U}'. \tag{16}$$

The form $\langle \mathcal{D}'(\Sigma), \hat{u}\rangle_{\mathcal{U}'\times\mathcal{U}}$ has the expanded representation

$$\langle \mathcal{D}'(\Sigma), \hat{u}\rangle_{\mathcal{U}'\times\mathcal{U}} = \sum_{i=1}^{n} \langle (\mathcal{D}'(\Sigma))^i, \hat{u}^i\rangle_{\mathcal{U}_i'\times\mathcal{U}_i}, \tag{17}$$

or, equivalently, by using (7),

$$\langle \mathcal{D}'(\Sigma), \hat{u}\rangle_{\mathcal{U}'\times\mathcal{U}} = \sum_{i=1}^{n}\sum_{j=1}^{m} \langle \mathcal{D}'^{ij}(\Sigma^j), \hat{u}^i\rangle_{\mathcal{U}_i'\times\mathcal{U}_i}. \tag{18}$$

As in the identification of Σ, the actual nature of f for a specific model can be identified promptly once the adjoint operator $\mathcal{D}'$ has been obtained for the model in question, as in the following.

Classical solid mechanics *In this case, the adjoint operator* $\mathcal{D}'$ *follows from integration by parts of the stress-strain rate duality pairing, i.e.* $\langle \Sigma, \mathcal{D}(u)\rangle_{\mathcal{E}'\times\mathcal{E}} = \int_\Omega \boldsymbol{\sigma}\cdot\nabla^S\mathbf{u}\,d\Omega = -\int_\Omega \mathrm{div}\,\boldsymbol{\sigma}\cdot\mathbf{u}\,d\Omega + \int_\Gamma \boldsymbol{\sigma}\mathbf{n}\cdot\mathbf{u}\,d\Gamma = \int_\Omega \mathbf{b}\cdot\mathbf{u}\,d\Omega + \int_\Gamma \mathbf{t}\cdot\mathbf{u}\,d\Gamma$, *where* $\mathbf{n}$ *is the outward unit normal to* Γ. *The admissible forces identified in this case are: a vector field, denoted* $\mathbf{b}$, *of force per unit volume acting in* Ω *and a vector field, denoted* $\mathbf{t}$, *of force per unit area acting on the boundary* Γ. ■

Having identified the nature of $f\in\mathcal{U}'$, whose structure is prescribed by (15), we can now introduce the *external virtual power* functional by restricting the evaluation of the corresponding duality pairing to the reduced space Var_u. That is, we define

$$P^{\mathrm{ext}}(\hat{u}) = \langle f, \hat{u}\rangle_{\mathcal{U}'\times\mathcal{U}} \quad \hat{u}\in\mathrm{Var}_u, \tag{19}$$

or, equivalently

$$P^{\mathrm{ext}}(\hat{u}) = \sum_{i=1}^{n} \langle f^i, \hat{u}^i\rangle_{\mathcal{U}_i'\times\mathcal{U}_i} \quad \hat{u}\in\mathrm{Var}_u. \tag{20}$$

The functional P^{ext} must also be defined such that it is invariant under changes in observer.

Finally, with the above definitions we introduce the *total virtual power* functional, defined as

$$P^{\mathrm{tot}}(\hat{u}, \mathcal{D}(\hat{u})) = P^{\mathrm{int}}(\mathcal{D}(\hat{u})) - P^{\mathrm{ext}}(\hat{u}) \quad \hat{u}\in\mathrm{Var}_u. \tag{21}$$

2.4 Second hypothesis. The Principle of Virtual Power

The **second hypothesis** in the variational formulation – the *Principle of Virtual Power* – establishes the condition under which a system of admissible generalized stresses and a system of admissible generalized external forces are in equilibrium. This is stated in the following.

Principle of Virtual Power *The generalized stress* $\Sigma\in\mathcal{E}'$ *and the generalized external force* $f\in\mathcal{U}'$ *are in equilibrium if and only if the following variational equation is satisfied:*[2]

$$P^{\mathrm{tot}}(\hat{u}, \mathcal{D}(\hat{u})) = 0 \quad \forall \hat{u} \text{ kinematically admissible.} \tag{22}$$

Equivalently, we may write

$$P^{\mathrm{int}}(\mathcal{D}(\hat{u})) = P^{\mathrm{ext}}(\hat{u}) \qquad \forall \hat{u}\in\mathrm{Var}_u, \tag{23}$$

[2] The term *equilibrium* here is not limited to *static* equilibrium. If the force system f includes generalized inertia forces associated to the physical problem at hand, then dynamic equilibrium is automatically accounted for by the Principle of Virtual Power.

or

$$\langle \Sigma, \mathcal{D}(\hat{u}) \rangle_{\mathcal{E}' \times \mathcal{E}} = \langle f, \hat{u} \rangle_{\mathcal{U}' \times \mathcal{U}} \qquad \forall \hat{u} \in \mathrm{Var}_u. \tag{24}$$

Further, from (22)*, we have that* f *must also satisfy*

$$\langle f, \hat{u} \rangle_{\mathcal{U}' \times \mathcal{U}} = 0 \qquad \forall \hat{u} \in \mathrm{Var}_u \cap \mathsf{N}(\mathcal{D}). \tag{25}$$

Application of the PVP is illustrated in the following example.

Classical solid mechanics *A Cauchy stress field* $\boldsymbol{\sigma}$ *and an external load system* $(\mathbf{b}, \mathbf{t})$ *are said to be in equilibrium if and only if* $\int_\Omega \boldsymbol{\sigma} \cdot \nabla^S \hat{\mathbf{u}}\, d\Omega = \int_\Omega \mathbf{b} \cdot \hat{\mathbf{u}}\, d\Omega + \int_\Gamma \mathbf{t} \cdot \hat{\mathbf{u}}\, d\Gamma \quad \forall \hat{u} \in \mathrm{Var}_u$*. Obviously, this equation expresses dynamic equilibrium if, for example,* $\mathbf{b}$ *is an inertia force field,* $\mathbf{b} = -\rho \ddot{\mathbf{u}}$*, with* ρ *the mass density and* $\ddot{\mathbf{u}}$ *the acceleration field. Also note that, in the present context,* (25) *implies that any system of balanced external forces (surface tractions and body forces – including inertia forces, if dynamical effects are considered) produces no virtual power under rigid virtual velocities.* ■

2.5 The equilibrium problem

To complete the description of the physical system model, a *constitutive law* must be introduced that determines Σ as a function of the history of the kinematical variables of the system. In a rather general constitutive setting, we consider the generalized stress to be a function of the *history*, denoted u^t, of the generalized displacement field to which the body was subjected up to the present time, t. Then, we write

$$\Sigma = \Sigma(u^t). \tag{26}$$

For all instants $\tau \in [0, t]$ the corresponding displacement $u(\tau)$ is kinematically admissible, i.e. $u(\tau) \in \mathrm{K}in_u$. We shall use the notation $u^t \in \mathrm{K}in_u$ to denote a history of displacements of $\mathcal{B}$ kinematically admissible at all instants in $[0, t]$.

With the above at hand, we can now state the equilibrium problem for the physical system in question as follows.

Problem 1 (The equilibrium problem) *For a given constitutive law of the type* (26) *and a given history of admissible generalized external force,* f^t*, find the history* $u^t \in \mathrm{Kin}_u$ *of kinematically admissible displacements such that*

$$\langle \Sigma(u^\tau), \mathcal{D}(\hat{u}) \rangle_{\mathcal{E}' \times \mathcal{E}} = \langle f(\tau), \hat{u} \rangle_{\mathcal{U}' \times \mathcal{U}} \qquad \forall \hat{u} \in \mathrm{Var}_u, \forall \tau \in [0, t]. \tag{27}$$

3 Method of multiscale virtual power

In this section we propose a unified variational framework, named *Method of Multiscale Virtual Power*, for the development of RVE-based multiscale models of physical systems. This is the main contribution of the present paper. The family of multiscale theories addressed here is based on the idea that any point of a macro-scale body occupying a domain Ω_M is associated with a representative volume element (RVE) with domain Ω_μ of characteristic length ℓ_μ much smaller than the characteristic length ℓ_M of Ω_M (refer to Figure 2). The domains Ω_M and Ω_μ are referred to as the macro-scale and micro-scale, respectively. Points or coordinates of the macro-scale are denoted $\mathbf{x} \in \Omega_M$, while points or coordinates ao the micro-scale are denoted $\mathbf{y} \in \Omega_\mu$. Here and in what follows we shall use the subscripts M and μ to denote, respectively, macro- and micro-scale entities.

Within the proposed framework, multiscale models are derived by following steps analogous to those described of Section 2 in the conventional (single-scale) setting. In particular, the concepts of duality and virtual power are explored and extended so that a principle of virtual power involving more than one scale – the *Principle of Multiscale Virtual Power* – can be formulated. The method lies on three fundamental principles:

(i) *Principle of Kinematical Admissibility*, whereby the macro- and micro-scale kinematics are defined and the associated variables linked across the scales. The scale-transition link is defined through appropriate definitions of *insertion* (macro-to-micro) and *homogenization* (micro-to-macro) operators, and must ensure a physically meaningful transfer of the relevant kinematical variables across the scales;

(ii) *Mathematical duality*, through which the nature of the force- and stress-like quantities are uniquely identified as the duals (power-conjugates) of the adopted kinematical variables. This concept has been used in Section 2. Here it is applied individually to each of the two scales involved; and

(iii) *Principle of Multiscale Virtual Power (PMVP)*, a generalization of the well-known Hill-Mandel Principle of Macrohomogeneity, from which equilibrium equations and homogenization relations for the force- and stress-like quantities are unequivocally obtained by straightforward variational arguments.

As we shall see, the proposed theory provides a clearly and logically structured framework within which existing formulations can be rationally justified and new, more general multiscale models can be rigorously derived in well-defined steps. The rationality of the proposed approach is entirely akin to that of the Method of

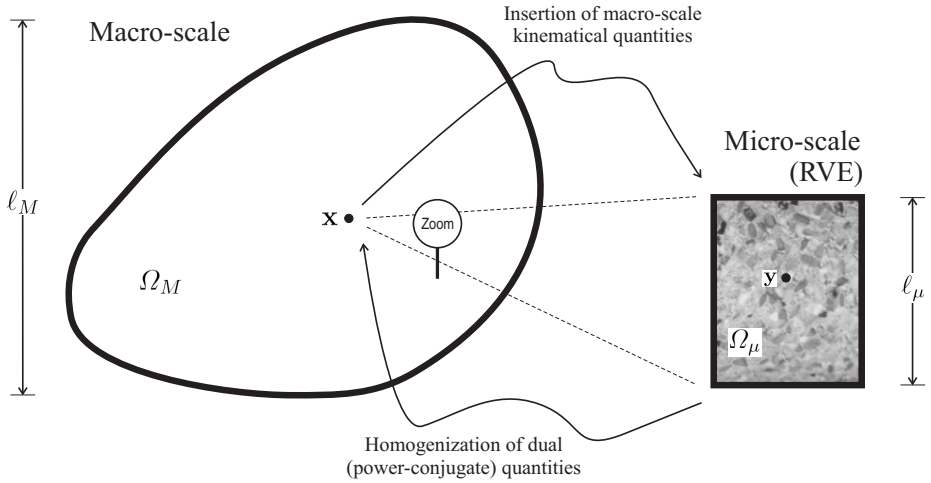

Fig. 2 RVE-based multiscale modeling. The RVE concept.

Virtual Power, reviewed in Section 2, in the derivation of single-scale physical system models. In particular, we shall see that, once the kinematical variables at the two scales are postulated, kinematical admissibility is established for the system under consideration, and the corresponding generalized force- and stress-like quantities are identified by means of duality arguments, all relevant equations of the model are derived from the PMVP following standard variational considerations.

Similiarly to the format adopted in Section 2, as the theory is presented in this section we shall show, in parallel, its specialization to the case of classical RVE-based multiscale infinitesimal solid mechanics. This should help make the newly-introduced concepts clearer.

3.1 Multiscale kinematics. Kinematical admissibility

In considering a two-scale physical system, we assume at the outset that the kinematics describing the relevant phenomena at the macro-scale may, in general, differ from the kinematics of the micro-scale. However, the ideas and definitions presented in Section 2.2 remain applicable individually to each of the two scales and analogous steps will be followed. In postulating the kinematics of a given two-scale physical system, one will, ultimately, establish a functional set of kinematically admissible micro-scale displacement fields, denoted Kin_{u_μ}, which is itself dependent upon the kinematical variables of the macro-scale.

This process of establishing Kin_{u_μ} is what we refer to as the *Principle of Kinematical Admissibility* and comprises four steps: (i) Definition the *governing kinematics* at the macro- and micro-scales; (ii) Definition of *insertion operators* that prescribe how the macro-scale kinematical variables are inserted into the micro-scale; (iii) Definition of *homogenization operators* that specify how the micro-scale kinematical fields are averaged to yield the macro-scale kinematical quantities. The kinematical homogenization process must be defined so as to ensure that the magnitude of the kinematical variables involved are, in some sense, preserved in the scale transition; and (iv) *Kinematical admissibility*. Finally, obtain the functional set Kin_{u_μ} of kinematically admissible micro-scale displacement fields.

It should be noted here that steps (i)-(iii) above are rather arbitrary with the only constraint being that the postulated kinematical transfer must ensure that the magnitude of the variables involved are preserved. The definition of the kinematical variables themselves will depend fundamentally on what phenomena (and level of detail) one is trying to capture with the model and will, also, be largely influenced by the preferences and background of the investigator. Here lies the *only* degree of arbitrariness of the proposed theory. Once kinematical admissibility has been established, the nature of the associated stress- and force-like variables at both scales will be determined from *mathematical duality* considerations and their homogenization relations together with the micro-scale equilibrium equations will be derived from the *Principle of Multiscale Virtual Power*

3.1.1 Macro-scale kinematics

Following the material presented in Section 2, the kinematics of the macro-scale is characterized by the generalized displacement $u_M \in \mathcal{U}_M$, an n_M-tuple of tensor fields, with each component u_M^i described by r_M^i scalar fields (the total number of scalar fields describing u_M is $R_M = \sum_{i=1}^{n_M} r_M^i$). These components have a domain of definition $\Omega_M^{\mathcal{U}_i} := \mathrm{Dom}(\mathcal{U}_{Mi})$, $i = 1, \ldots, n_M$, i.e.

$$\begin{aligned} u_M^i : \Omega_M^{\mathcal{U}_i} &\to \mathcal{U}_{Mi} \\ \mathbf{x} &\mapsto u_M^i(\mathbf{x}), \end{aligned} \tag{28}$$

where $\Omega_M^{\mathcal{U}_i} \subseteq \Omega_M$, with $\Omega_M^{\mathcal{U}_i}$ being a set of points, surfaces or volumes, accordingly. In compact form, we write

$$\begin{aligned} u_M : \Omega_M^{\mathcal{U}} &\to \mathcal{U}_M \\ \mathbf{x} &\mapsto u_M(\mathbf{x}), \end{aligned} \tag{29}$$

and, as in Section 2, we have $\Omega_M^{\mathcal{U}} := \mathrm{Dom}(\mathcal{U}_M) = (\mathrm{Dom}(\mathcal{U}_{M1}), \ldots, \mathrm{Dom}(\mathcal{U}_{M\,n_M}))$, or equivalently, $\Omega_M^{\mathcal{U}} = (\Omega_M^{\mathcal{U}_1}, \ldots, \Omega_M^{\mathcal{U}_{n_M}})$

The set of kinematically admissible generalized displacements is Kin_{u_M} and the associated space of kinematically admissible generalized virtual actions is Var_{u_M}. The space of generalized macro-scale strain actions is denoted $\mathcal{E}_M$. Each element $D_M \in \mathcal{E}_M$ is a m_M-tuple of tensor fields where each component D_M^i is described by s_M^i scalar fields (the total number of scalar fields describing D_M is $S_M = \sum_{i=1}^{m_M} s_M^i$). The domain of definition of these components is $\Omega_M^{\mathcal{E}_i} := \mathrm{Dom}(\mathcal{E}_{Mi})$, $i = 1, \ldots, m_M$, that is

$$\begin{aligned} D_M^i : \Omega_M^{\mathcal{E}_i} &\to \mathcal{E}_{Mi} \\ \mathbf{x} &\mapsto D_M^i(\mathbf{x}), \end{aligned} \tag{30}$$

where $\Omega_M^{\mathcal{E}_i} \subseteq \Omega_M$ can be a set of points, surfaces or volumes. In compact form, we write

$$\begin{aligned} D_M : \Omega_M^{\mathcal{E}} &\to \mathcal{E}_M \\ \mathbf{x} &\mapsto D_M(\mathbf{x}), \end{aligned} \tag{31}$$

and $\Omega_M^{\mathcal{E}} := \mathrm{Dom}(\mathcal{E}_M) = (\mathrm{Dom}(\mathcal{E}_{M1}), \ldots, \mathrm{Dom}(\mathcal{E}_{M\,m_M}))$, or equivalently $\Omega_M^{\mathcal{E}} = (\Omega_M^{\mathcal{E}_1}, \ldots, \Omega_M^{\mathcal{E}_{m_M}})$.

The macro-scale kinematically compatible generalized strain actions (and generalized virtual strain rates) are characterized by the linear operator

$$\begin{aligned} \mathcal{D}_M : \mathcal{U}_M &\to \mathcal{E}_M \\ u_M &\mapsto D_M = \mathcal{D}_M(u_M). \end{aligned} \tag{32}$$

The domain of definition of the kinematically compatible strain actions is denoted $\Omega_M^{\mathcal{E}} = \mathrm{Dom}(\mathcal{D}_M(u_M))$.

Remark 2 *As in* (7)*, since* $\mathcal{D}_M$ *is linear, we have the representation*

$$\mathcal{D}_M = \begin{pmatrix} \mathcal{D}_M^{11} & \mathcal{D}_M^{12} & \ldots & \mathcal{D}_M^{1n_M} \\ \mathcal{D}_M^{21} & \mathcal{D}_M^{22} & \ldots & \mathcal{D}_M^{2n_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_M^{m_M 1} & \mathcal{D}_M^{m_M 2} & \ldots & \mathcal{D}_M^{m_M n_M} \end{pmatrix}, \tag{33}$$

and $\Omega_M^{\mathcal{E}_i} = \mathrm{Dom}(\mathcal{D}_M^{i1}(u_M^1)) = \ldots = \mathrm{Dom}(\mathcal{D}_M^{in_M}(u_M^{n_M}))$, $i = 1, \ldots, m_M$.

Figure 3 is the counterpart of Figure 1 showing the macro-scale entities in a multiscale setting. It should be noted that additional sets and operations are introduced in the multiscale setting which relate to individual points of the macro-scale domain. The value of any entity $(\cdot)$ at an arbitrary point $\mathbf{x}$ of the macro-scale is denoted $(\cdot)|_{\mathbf{x}}$. As we shall see later, point values of relevant macro-scale entities will be associated with the problem defined at the micro-scale level (the RVE).

3.1.2 Micro-scale kinematics

The fundamental assumption in RVE-based theories is that each point $\mathbf{x}$ of the macro-scale body is associated with a micro-scale domain (an RVE). Here we shall define the kinematics of one such general RVE. The domain of the RVE is denoted Ω_μ and points of the RVE will be denoted $\mathbf{y} \in \Omega_\mu$. The space of generalized micro-scale displacements is denoted $\mathcal{U}_\mu$, with each element $u_\mu \in \mathcal{U}_\mu$ an n_μ-tuple of tensor fields, and each component u_μ^i described by r_μ^i scalar fields (the total number of scalar fields describing u_μ is $R_\mu = \sum_{i=1}^{n_\mu} r_\mu^i$). The domain of definition of each field is $\Omega_\mu^{\mathcal{U}_i} := \mathrm{Dom}(\mathcal{U}_{\mu_i})$, $i = 1, \ldots, n_\mu$, that is

$$\begin{aligned} u_\mu^i : \Omega_\mu^{\mathcal{U}_i} &\to \mathcal{U}_{\mu_i} \\ \mathbf{y} &\mapsto u_\mu^i(\mathbf{y}), \end{aligned} \tag{34}$$

with each $\Omega_\mu^{\mathcal{U}_i} \subseteq \Omega_\mu$ a set of points, surfaces or volumes. In compact notation,

$$\begin{aligned} u_\mu : \Omega_\mu^{\mathcal{U}} &\to \mathcal{U}_\mu \\ \mathbf{y} &\mapsto u_\mu(\mathbf{y}), \end{aligned} \tag{35}$$

and $\Omega_\mu^{\mathcal{U}} := \mathrm{Dom}(\mathcal{U}_\mu) = (\mathrm{Dom}(\mathcal{U}_{\mu_1}), \ldots, \mathrm{Dom}(\mathcal{U}_{\mu_{n_\mu}}))$, or alternatively, $\Omega_\mu^{\mathcal{U}} = (\Omega_\mu^{\mathcal{U}_1}, \ldots, \Omega_\mu^{\mathcal{U}_{n_\mu}})$.

Without loss of generality, it is convenient to split the generalized micro-scale displacements $u_\mu \in \mathcal{U}_\mu$ as a sum,

$$u_\mu = \bar{u}_\mu + \tilde{u}_\mu, \tag{36}$$

of a field $\bar{u}_\mu$, that depends on the macro-scale kinematics at point $\mathbf{x}$, and a field $\tilde{u}_\mu$, named the *generalized displacement fluctuation*. The field $\bar{u}_\mu$ is generally a non-uniform field (it may depend on $\mathbf{y}$). The collection of all generalized displacements $\bar{u}_\mu$ at micro-level, forms a subspace which we will denote $\bar{\mathcal{U}}_\mu$, and the collection of all $\tilde{u}_\mu$ forms the subspace $\tilde{\mathcal{U}}_\mu$, of generalized displacement fluctuations.

We also define the space $\mathcal{E}_\mu$ of micro-scale generalized strain actions. Each $D_\mu \in \mathcal{E}_\mu$ is a m_μ-tuple of tensor fields with components denoted by D_μ^i. Each component is described by s_μ^i scalar fields (the total number of scalar fields describing D_μ is $S_\mu = \sum_{i=1}^{m_\mu} s_\mu^i$).

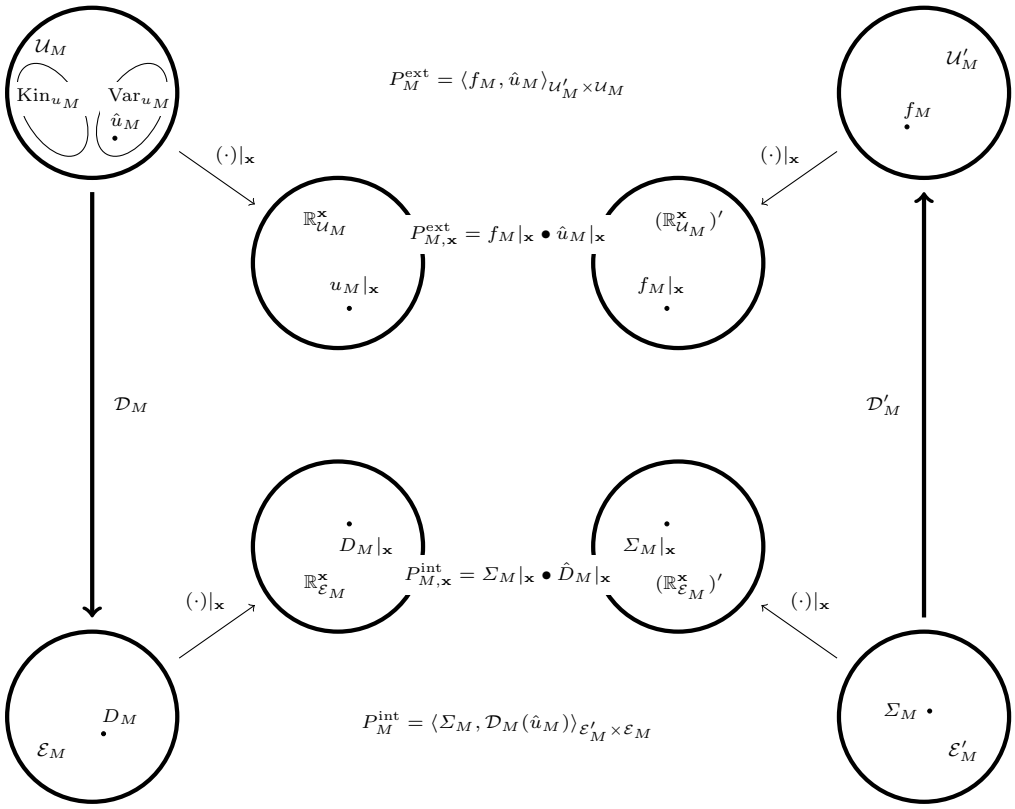

Fig. 3 Method of Multiscale Virtual Power. Basic sets and operations at the macro-scale level.

The components have a domain of definition $\Omega_\mu^{\mathcal{E}_i} := \mathrm{Dom}(\mathcal{E}_{\mu_i})$, $i = 1, \ldots, m_\mu$, i.e.

$$\begin{aligned} D_\mu^i : \Omega_\mu^{\mathcal{E}_i} &\to \mathcal{E}_{\mu_i} \\ \mathbf{y} &\mapsto D_\mu^i(\mathbf{y}), \end{aligned} \tag{37}$$

where $\Omega_\mu^{\mathcal{E}_i} \subseteq \Omega_\mu$ can be a set of points, surfaces or volumes. In compact form,

$$\begin{aligned} D_\mu : \Omega_\mu^{\mathcal{E}} &\to \mathcal{E}_\mu \\ \mathbf{y} &\mapsto D_\mu(\mathbf{y}), \end{aligned} \tag{38}$$

so $\Omega_\mu^{\mathcal{E}} := \mathrm{Dom}(\mathcal{E}_\mu) = (\mathrm{Dom}(\mathcal{E}_{\mu_1}), \ldots, \mathrm{Dom}(\mathcal{E}_{\mu_{m_\mu}}))$, or $\Omega_\mu^{\mathcal{E}} = (\Omega_\mu^{\mathcal{E}_1}, \ldots, \Omega_\mu^{\mathcal{E}_{m_\mu}})$.

Further, we define the (linear) micro-scale generalized strain action operator,

$$\begin{aligned} \mathcal{D}_\mu : \mathcal{U}_\mu &\to \mathcal{E}_\mu, \\ u_\mu &\mapsto D_\mu = \mathcal{D}_\mu(u_\mu). \end{aligned} \tag{39}$$

Its domain of definition is $\Omega_\mu^{\mathcal{E}} = \mathrm{Dom}(\mathcal{D}_\mu(u_\mu))$.

Remark 3 *Analogously to* (33) *we have the following representation for* $\mathcal{D}_\mu$*:*

$$\mathcal{D}_\mu = \begin{pmatrix} \mathcal{D}_\mu^{11} & \mathcal{D}_\mu^{12} & \ldots & \mathcal{D}_\mu^{1n_\mu} \\ \mathcal{D}_\mu^{21} & \mathcal{D}_\mu^{22} & \ldots & \mathcal{D}_\mu^{2n_\mu} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_\mu^{m_\mu 1} & \mathcal{D}_\mu^{m_\mu 2} & \ldots & \mathcal{D}_\mu^{m_\mu n_\mu} \end{pmatrix}, \tag{40}$$

and $\Omega_\mu^{\mathcal{E}_i} = \mathrm{Dom}(\mathcal{D}_\mu^{i1}(u_\mu^1)) = \ldots = \mathrm{Dom}(\mathcal{D}_\mu^{in_\mu}(u_\mu^{n_\mu}))$, $i = 1, \ldots, m_\mu$.

3.1.3 Insertion operators

As mentioned at the beginning of this section, the kinematics of an RVE (micro-scale kinematics) associated with an arbitrary point $\mathbf{x} \in \Omega_M$ of the macro-scale is linked to the kinematics at the macro-scale by means of *insertion operators*, defining the macro-to-micro kinematical transfer, and *homogenization operators*, defining the micro-to-macro kinematical transfer. These two operators are *linear* in their arguments and must be adequately constructed to account for a consistent mechanical/physical transfer of generalized displacements and strain actions between the scales. The definition of such operators will depend on the particular physical system in question.

Remark 4 *For simplicity, we shall assume in what follows that all macro-scale kinematical variables take part in the kinematical transfer between scales. In a more general scenario, we could have only a subset of the set of macro-scale kinematical variables involved in this transfer.*

Then, let us define the set $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ of elements of $\mathcal{U}_M$ evaluated at a given point $\mathbf{x} \in \Omega_M$,

$$\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} = \{w = (w^1, \dots, w^{n_M}),\ w^i \in \mathbb{R}^{r^i_M}, i = 1, \dots, n_M,\ w = u|_{\mathbf{x}},\ u \in \mathcal{U}_M\}, \quad (41)$$

where $\mathbb{R}^{r^i_M} = \overbrace{\mathbb{R} \times \cdots \times \mathbb{R}}^{r^i_M}$, with r^i_M the number of scalar descriptors in the ith tensor field within the n_M-tuple. Note that $\dim(\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}) = R_M$. We will refer to $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ as the *set of point-valued generalized macro-displacements* of $\mathbf{x}$.

Similiarly, we define the *set of point-valued generalized macro-strain actions* as the set of elements of $\mathcal{E}_M$ evaluated at point $\mathbf{x} \in \Omega_M$,

$$\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} = \{V = (V^1, \dots, V^{m_M}),\ V^i \in \mathbb{R}^{s^i_M}, i = 1, \dots, m_M,\ V = D|_{\mathbf{x}},\ D \in \mathcal{E}_M\}, \quad (42)$$

where $\mathbb{R}^{s^i_M} = \overbrace{\mathbb{R} \times \cdots \times \mathbb{R}}^{s^i_M}$, with s^i_M the number of scalar descriptors of the ith tensor field in the m_M-tuple. Note that $\dim(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}) = S_M$.

Further, within the sets of point-valued generalized macro-displacements and macro-strain actions we can distinguish the sets of point-valued virtual generalized macro-displacements, $\hat{w}$, and virtual macro-strain rates, $\hat{V}$. We denote these two sets as $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}$ and $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$, respectively. It is interesting to note that, depending on the final application of the present multiscale theory, components of such virtual macro-displacements and virtual macro-strain actions may be taken as the null element, even though the real kinematics at point $\mathbf{x}$ is not necessarily null.

Classical multiscale solid mechanics *The set of point-valued macro-displacements is defined here as* $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} = \{\mathbf{w} \in \mathbb{R}^3,\ \mathbf{w} = \mathbf{u}_M|_{\mathbf{x}},\ \mathbf{u}_M \in \mathbf{H}^1(\Omega_M)\}$*, while the set of point-valued macro-strain actions is* $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} = \{\boldsymbol{\epsilon} \in \mathbb{R}^{3\times3},\ \boldsymbol{\epsilon} = \boldsymbol{\varepsilon}_M|_{\mathbf{x}},\ \boldsymbol{\varepsilon}_M \in \mathbf{L}^2_{\mathrm{sym}}(\Omega_M)\}$. ■

At this point we introduce the concept of *insertion operator*. In the present theory, insertion operators are fundamental in that they define the way in which the macro-scale kinematical quantities contribute to the micro-scale kinematics, i.e. they define how the macro-scale kinematics is *inserted* into the micro-scale. Two insertion operators are defined:

– The u_M*-insertion operator*,

$$\mathcal{J}^{\mathcal{U}}_\mu : \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} \to \bar{\mathcal{U}}_\mu,\quad u_M|_{\mathbf{x}} \mapsto \bar{u}_\mu = \mathcal{J}^{\mathcal{U}}_\mu(u_M|_{\mathbf{x}}), \quad (43)$$

that maps the point-value $u_M|_{\mathbf{x}}$ of the macro-scale generalized displacement into a field $\bar{u}_\mu$ that contributes to the micro-scale generalized displacement field according to (36); and

– The D_M*-insertion operator*,

$$\mathcal{J}^{\mathcal{E}}_\mu : \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} \to \bar{\mathcal{U}}_\mu,\quad D_M|_{\mathbf{x}} \mapsto \bar{u}_\mu = \mathcal{J}^{\mathcal{E}}_\mu(D_M|_{\mathbf{x}}), \quad (44)$$

that maps the point-value $D_M|_{\mathbf{x}}$ of the generalized macro-strain action into another field contributing to the micro-scale generalized displacement according to (36).

Both operators are *linear* in their respective arguments.

Classical multiscale solid mechanics *The* u_M*-insertion operator in this case is postulated as* $\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{u}_M|_{\mathbf{x}}) = \mathbf{u}_M|_{\mathbf{x}}$*, i.e. it maps* $\mathbf{u}_M|_{\mathbf{x}}$ *into a uniform field over* Ω_μ*. The* D_M*-insertion operator, in turn, is postulated as* $\mathcal{J}^{\mathcal{E}}_\mu(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}) = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o)$*, where* $\mathbf{y}_o = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{y}\, d\Omega_\mu$*, i.e. it maps the macro-scale strain action (in this case, the infinitesimal strain measure) at point* $\mathbf{x}$ *into a linear displacement distributed over* Ω_μ. ■

Remark 5 *The choice of operators* $\mathcal{J}^{\mathcal{U}}_\mu$ *and* $\mathcal{J}^{\mathcal{E}}_\mu$ *is not entirely arbitrary. This lack arbitrariness stems from the fact that these operators must preserve the magnitude of the macro-scale generalized displacements/strain actions when inserted into the micro-scale. This issue will be addressed with the enforcement of an additional constraint on each operator (see, for example,* (59) *and* (60) *below).*

From (43)–(44), the kinematical variables $u_M|_{\mathbf{x}}$ and $D_M|_{\mathbf{x}}$ can be combined to deliver a non-uniform generalized displacement field which depends on $\mathbf{y}$. Particularly, we point out that the domain $\Omega^{\mathcal{U}_i}_\mu$, $i = 1, \dots, n_\mu$ is the *domain of insertion* in which component i of the image of the insertion operators $\mathcal{J}^{\mathcal{U}}_\mu$ and $\mathcal{J}^{\mathcal{E}}_\mu$ is defined.

Classical multiscale solid mechanics *The point-valued kinematical variables of the macro-scale,* $\mathbf{u}_M|_{\mathbf{x}}$ *and* $\boldsymbol{\varepsilon}_M|_{\mathbf{x}}$*, contribute to the micro-scale displacement field through* $\bar{\mathbf{u}}_\mu$*, which is contructed as follows:*

$$\bar{\mathbf{u}}_\mu = \mathcal{J}^{\mathcal{U}}_\mu(\mathbf{u}_M|_{\mathbf{x}}) + \mathcal{J}^{\mathcal{E}}_\mu(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}) = \mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o).$$

The domain of insertion at the micro-scale in this case is, obviously, the whole Ω_μ. ■

Remark 6 *The present theory allows for insertion operations far more general than those found in most existing formulations. The vast majority of existing formulations only consider an affine mapping of the macro-*

scale generalized strain action into the micro-scale generalized displacement field (such as in the classical multiscale solid mechanics case referred to above). For example, in failure multiscale analysis, a more complex insertion operation can be used [104] to account for progressive strain localization, nucleation and evolution of cracks at the macro-scale level, caused by shear bands, damage or any other possible failure mechanism at the micro-level. In this case, the micro-scale subdomain in which strain localization is taking place is embedded in the definition of the insertion operator. As shown in Section 3.4, these insertion operators are functionally essential in the characterization of the homogenization of generalized stress and body forces at macro level.

Remark 7 *Since* $\mathcal{J}_\mu^{\mathcal{U}}$ *and* $\mathcal{J}_\mu^{\mathcal{E}}$ *are linear, we have the representations*

$$\mathcal{J}_\mu^{\mathcal{U}} = \begin{pmatrix} \mathcal{J}_\mu^{\mathcal{U}11} & \mathcal{J}_\mu^{\mathcal{U}12} & \dots & \mathcal{J}_\mu^{\mathcal{U}1n_M} \\ \mathcal{J}_\mu^{\mathcal{U}21} & \mathcal{J}_\mu^{\mathcal{U}22} & \dots & \mathcal{J}_\mu^{\mathcal{U}2n_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{J}_\mu^{\mathcal{U}n_\mu 1} & \mathcal{J}_\mu^{\mathcal{U}n_\mu 2} & \dots & \mathcal{J}_\mu^{\mathcal{U}n_\mu n_M} \end{pmatrix}, \tag{45}$$

and

$$\mathcal{J}_\mu^{\mathcal{E}} = \begin{pmatrix} \mathcal{J}_\mu^{\mathcal{E}11} & \mathcal{J}_\mu^{\mathcal{E}12} & \dots & \mathcal{J}_\mu^{\mathcal{E}1m_M} \\ \mathcal{J}_\mu^{\mathcal{E}21} & \mathcal{J}_\mu^{\mathcal{E}22} & \dots & \mathcal{J}_\mu^{\mathcal{E}2m_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{J}_\mu^{\mathcal{E}n_\mu 1} & \mathcal{J}_\mu^{\mathcal{E}n_\mu 2} & \dots & \mathcal{J}_\mu^{\mathcal{E}n_\mu m_M} \end{pmatrix}, \tag{46}$$

We now introduce the following definition. We say that $u_\mu \in \mathcal{U}_\mu$ is *linked to the macro-kinematics at point* $\mathbf{x} \in \Omega_M$ if there exist a $u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and a $D_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$ such that

$$u_\mu = \bar{u}_\mu + \tilde{u}_\mu = \mathcal{J}_\mu^{\mathcal{U}}(u_M|_{\mathbf{x}}) + \mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}}) + \tilde{u}_\mu. \tag{47}$$

Then, for any micro-scale generalized displacement, $u_\mu \in \mathcal{U}_\mu$, linked to the macro-kinematics, the corresponding kinematically compatible micro-scale generalized strain action is given by

$$\begin{aligned} D_\mu = \mathcal{D}_\mu(u_\mu) = \mathcal{D}_\mu(\bar{u}_\mu) + \mathcal{D}_\mu(\tilde{u}_\mu) = \\ \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{U}}(u_M|_{\mathbf{x}})) + \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}})) + \mathcal{D}_\mu(\tilde{u}_\mu). \end{aligned} \tag{48}$$

On physical grounds, we impose the following constraint on the operator $\mathcal{J}_\mu^{\mathcal{U}}$ to prevent the insertion of u_M from causing generalized straining actions at the micro-scale,

$$\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{U}}(u_M|_{\mathbf{x}})) = 0 \qquad \forall u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}. \tag{49}$$

From the mechanical point of view, this constraint infers that the inserted generalized displacement from the macro scale must belong to the kernel of $\mathcal{D}_\mu$, $\mathsf{N}(\mathcal{D}_\mu)$, i.e. the image of the operator $\mathcal{J}_\mu^{\mathcal{U}}$ is in the space of rigid generalized micro-displacements fields.

Classical multiscale solid mechanics *By writing* $\mathbf{u}_\mu = \mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu$*, we ensure that the micro-scale displacement,* $\mathbf{u}_\mu$*, is linked with the macro-kinematics at point* $\mathbf{x}$*. Then, since* $\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}}) = \mathbf{u}_M|_{\mathbf{x}}$ *is a uniform field, the corresponding micro-scale strain action is* $\boldsymbol{\varepsilon}_\mu = \nabla^S_{\mathbf{y}}(\mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{u}}_\mu) = \boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu$. ■

Remark 8 *From* (48)*, the generalized micro-scale strain action can be written as*

$$D_\mu = \bar{D}_\mu + \tilde{D}_\mu, \tag{50}$$

where $\bar{D}_\mu$ *is a contribution from the macro-scale kinematics to the micro-scale strain action, and* $\tilde{D}_\mu$*, the micro-scale strain action* fluctuation*, depends only on micro-scale entities, that is*

$$\begin{aligned} \bar{D}_\mu &= \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}})), \\ \tilde{D}_\mu &= \mathcal{D}_\mu(\tilde{u}_\mu). \end{aligned} \tag{51}$$

Remark 9 *The contribution of the macro-scale generalized strain action to its micro-scale counterpart field can be obtained directly by applying the combined insertion operator, defined as* $\mathcal{I}_\mu = \mathcal{D}_\mu\mathcal{J}_\mu^{\mathcal{E}}$*, to the point-value* $D_M|_{\mathbf{x}}$*, i.e. we may write*

$$\begin{aligned} &\mathcal{I}_\mu : \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} \to \mathcal{E}_\mu, \\ &\quad D_M|_{\mathbf{x}} \mapsto D_\mu = \mathcal{I}_\mu(D_M|_{\mathbf{x}}). \end{aligned} \tag{52}$$

3.1.4 Kinematical homogenization operators

Kinematical homogenization operators also play a fundamental role in the present multiscale theory. These operators must be postulated when devising an RVE-based model, according to the physical nature of the system/model in question. They define how the micro-scale kinematical fields are homogenized (averaged) to yield the corresponding macro-scale point-valued kinematical variables. There are two such operators. The u_μ*-homogenization operator*, mapping the micro-scale generalized displacement field into the point-value of the macro-scale generalized displacement,

$$\begin{aligned} &\mathcal{H}_\mu^{\mathcal{U}} : \mathcal{U}_\mu \to \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}, \\ &\quad u_\mu \mapsto \mathcal{H}_\mu^{\mathcal{U}}(u_\mu) \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}, \end{aligned} \tag{53}$$

and the D_μ*-homogenization operator*, that maps the micro-scale generalized strain action field into the point-value of the macro-scale generalized strain action,

$$\begin{aligned} &\mathcal{H}_\mu^{\mathcal{E}} : \mathcal{E}_\mu \to \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}, \\ &\quad D_\mu \mapsto \mathcal{H}_\mu^{\mathcal{E}}(D_\mu) \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}. \end{aligned} \tag{54}$$

Both operators are *linear* and involve average measures over the corresponding domains of insertion, $\Omega_\mu^{\mathcal{U}_i}, i = 1,\dots,n_\mu$, and $\Omega_\mu^{\mathcal{E}_i}, i = 1,\dots,m_\mu$.

Classical multiscale solid mechanics *The u_μ-homogenization operator is defined as $\mathcal{H}_\mu^{\mathcal{U}}(\mathbf{u}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{u}_\mu\,d\Omega_\mu$, while the D_μ-homogenization operator is defined as $\mathcal{H}_\mu^{\mathcal{E}}(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\varepsilon}_\mu\,d\Omega_\mu$. That is, $\mathbf{u}_M|_{\mathbf{x}}$ and $\boldsymbol{\varepsilon}_M|_{\mathbf{x}}$ are simple* volume averages *of their micro-scale counterpart fields over the RVE.* ■

Remark 10 *From the linearity of operator $\mathcal{H}_\mu^{\mathcal{U}}$, the following matrix representations hold*

$$\mathcal{H}_\mu^{\mathcal{U}} = \begin{pmatrix} \mathcal{H}_\mu^{\mathcal{U}^{11}} & \mathcal{H}_\mu^{\mathcal{U}^{12}} & \dots & \mathcal{H}_\mu^{\mathcal{U}^{1n_\mu}} \\ \mathcal{H}_\mu^{\mathcal{U}^{21}} & \mathcal{H}_\mu^{\mathcal{U}^{22}} & \dots & \mathcal{H}_\mu^{\mathcal{U}^{2n_\mu}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{H}_\mu^{\mathcal{U}^{n_M1}} & \mathcal{H}_\mu^{\mathcal{U}^{n_M2}} & \dots & \mathcal{H}_\mu^{\mathcal{U}^{n_Mn_\mu}} \end{pmatrix}, \tag{55}$$

and

$$\mathcal{H}_\mu^{\mathcal{E}} = \begin{pmatrix} \mathcal{H}_\mu^{\mathcal{E}^{11}} & \mathcal{H}_\mu^{\mathcal{E}^{12}} & \dots & \mathcal{H}_\mu^{\mathcal{E}^{1m_\mu}} \\ \mathcal{H}_\mu^{\mathcal{E}^{21}} & \mathcal{H}_\mu^{\mathcal{E}^{22}} & \dots & \mathcal{H}_\mu^{\mathcal{E}^{2m_\mu}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{H}_\mu^{\mathcal{E}^{m_M1}} & \mathcal{H}_\mu^{\mathcal{E}^{m_M2}} & \dots & \mathcal{H}_\mu^{\mathcal{E}^{m_Mm_\mu}} \end{pmatrix}. \tag{56}$$

Now, let us go back to the issue posed in Remark 5 about the constraints on the insertion operators $\mathcal{J}_\mu^{\mathcal{U}}$ and $\mathcal{J}_\mu^{\mathcal{E}}$, defined in (43) and (44), respectively. On physical grounds, we must require that these operators are defined such that the magnitude of the kinematical variables involved in the transfer across the scales are, in some sense, preserved. This can be understood as a principle of *conservation of macro-scale generalized displacements* and *conservation of macro-scale generalized strain actions*. Effectively, we want to ensure that the homogenization of the insertion of each component $u_M^i|_{\mathbf{x}}$ of $u_M|_{\mathbf{x}}$ results in $u_M^i|_{\mathbf{x}}$ itself. The same applying to the components $D_M^i|_{\mathbf{x}}$. To formally state this requirement, we define $u_M^{\{i\}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and $D_M^{\{i\}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$ such that

$$(u_M^{\{i\}})^j = \begin{cases} u_M^i|_{\mathbf{x}} & \text{if } j = i \\ 0 & \text{if } j \neq i, \end{cases} \tag{57}$$

$$(D_M^{\{i\}})^j = \begin{cases} D_M^i|_{\mathbf{x}} & \text{if } j = i \\ 0 & \text{if } j \neq i. \end{cases} \tag{58}$$

Then, the postulated kinematics conservation principle holds if $\mathcal{J}_\mu^{\mathcal{U}}$ and $\mathcal{J}_\mu^{\mathcal{E}}$ satisfy the constraints

$$\mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}(u_M^{\{i\}})) = u_M^{\{i\}}, \quad i = 1,\dots,n_M, \tag{59}$$

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(D_M^{\{i\}}))) = D_M^{\{i\}}, \quad i = 1,\dots,m_M. \tag{60}$$

Remark 11 *If not all macro-scale kinematical variables are inserted into the micro-scale (refer to Remark 4), then the constraints* (59) *and* (60) *must hold only for the inserted variables.*

Classical multiscale solid mechanics *In this case, $\mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}})) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{u}_M|_{\mathbf{x}}\,d\Omega_\mu = \mathbf{u}_M|_{\mathbf{x}}$. Also, $\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\nabla^S_{\mathbf{y}}(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o))\,d\Omega_\mu = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}$. Hence, constraints* (59) *and* (60) *are satisfied in the context of the classical theory.* ■

Remark 12 *From* (59) *we observe that the compound operation $\mathcal{H}_\mu^{\mathcal{U}}\mathcal{J}_\mu^{\mathcal{U}}$ is the identity map in $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$. Similarly, the compound operation $\mathcal{H}_\mu^{\mathcal{E}}\mathcal{D}_\mu\mathcal{J}_\mu^{\mathcal{E}}$ is the identity map in $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$.*

3.1.5 Kinematical admissibility

Let us now introduce the fundamental concept of *kinematical admissibility* of the kinematical transfer between scales. A micro-scale generalized displacement $u_\mu \in \mathcal{U}_\mu$, linked to the macro-kinematics, and its generalized strain action $\mathcal{D}_\mu(u_\mu) \in \mathcal{E}_\mu$ are *kinematically admissible* with respect to $u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and $D_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$ if the following relations are satisfied

$$\mathcal{H}_\mu^{\mathcal{U}}(u_\mu) = \mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}(u_M|_{\mathbf{x}})), \tag{61}$$

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(u_\mu)) = \mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}}))). \tag{62}$$

The above definition implies additional constraints. Since $u_\mu \in \mathcal{U}_\mu$ is linked to the macro-scale kinematics, (47) holds and, therefore, the left hand side of (61) yields

$$\mathcal{H}_\mu^{\mathcal{U}}(u_\mu) = \mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}(u_M|_{\mathbf{x}})) + \mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}})) + \mathcal{H}_\mu^{\mathcal{U}}(\tilde{u}_\mu). \tag{63}$$

Here, we shall impose the following further constraint on the operator $\mathcal{J}_\mu^{\mathcal{E}}$:

$$\mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{E}}(D_M|_{\mathbf{x}})) = 0. \tag{64}$$

As consequence of (61), (63) and (64), $\tilde{u}_\mu$ must satisfy the following kinematical constraint:

$$\mathcal{H}_\mu^{\mathcal{U}}(\tilde{u}_\mu) = 0. \tag{65}$$

Since $\mathcal{H}_\mu^{\mathcal{U}}$ represents an averaging operation involving the measure of the domain related to each component of the insertion operators, then equations (59) and (61) establish a relation between $u_M|_{\mathbf{x}}$ and the homogenization of the micro-displacements u_μ. In addition, equation (65) embodies n_M tensorial constraints (i.e. R_M

scalar constraints) that must be satisfied by the generalized displacement fluctuation $\tilde{u}_\mu$ to link the micro-kinematics to the macro-kinematics.

Classical multiscale solid mechanics *With the definition of the u_μ-homogenization operator, the kinematical admissibility of $\mathbf{u}_\mu$ implies that $\mathcal{H}^{\mathcal{U}}_\mu(\mathbf{u}_\mu) = \mathcal{H}^{\mathcal{U}}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{u}_M|_{\mathbf{x}})) = \mathbf{u}_M|_{\mathbf{x}}$. Since, by construction, the operator $\mathcal{J}^{\mathcal{E}}_\mu$ is such that $\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)\,d\Omega_\mu = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}\big(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbf{y}-\mathbf{y}_o)\,d\Omega_\mu\big) = \mathbf{0}$, we have $\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{u}}_\mu)\,d\Omega_\mu = \mathbf{u}_M|_{\mathbf{x}} + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{u}_M|_{\mathbf{x}}$. This is satisfied if $\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0}$.* ■

We can proceed in an analogous manner with equation (62). By taking equation (49) into account, we have

$$\begin{aligned}&\mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(u_\mu)) = \\ &\mathcal{H}^{\mathcal{E}}_\mu(\underbrace{\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(u_M|_{\mathbf{x}}))}_{=0}) + \mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(D_M|_{\mathbf{x}}))) \\ &\quad + \mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\tilde{u}_\mu)) = \mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(D_M|_{\mathbf{x}}))). \quad (66)\end{aligned}$$

This yields

$$\mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\tilde{u}_\mu)) = 0. \quad (67)$$

Then, equations (60) and (62) determine a relation between $D_M|_{\mathbf{x}}$ and the homogenization of the micro-scale strain action D_μ.

In summary, any kinematically admissible generalized micro-scale displacement field u_μ must be such that its fluctuation component, $\tilde{u}_\mu$, satisfies the kinematical constraints (65) and (67). This motivates the definition of the space of *kinematically admissible generalized micro-scale displacement fluctuations*:

$$\mathrm{Kin}_{\tilde{u}_\mu} = \{\tilde{u}_\mu \in \mathcal{U}_\mu,\ \mathcal{H}^{\mathcal{U}}_\mu(\tilde{u}_\mu) = 0,\ \mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\tilde{u}_\mu)) = 0\}. \quad (68)$$

Elements $\tilde{u}_\mu \in \mathrm{Kin}_{\tilde{u}_\mu}$ satisfy the *minimal* kinematical constraints that render the kinematical transfer between scales admissible. Further kinematical constraints may be added leading, in general, to different multiscale models. Also note that, since the constraints over $\tilde{u}_\mu$ are linear and homogeneous, it follows that the space of *kinematically admissible virtual micro-scale generalized fluctuation displacements* is given by

$$\mathrm{Var}_{\tilde{u}_\mu} = \mathrm{Kin}_{\tilde{u}_\mu}. \quad (69)$$

Classical multiscale solid mechanics *With the definition of the D_μ-homogenization operator, the kinematical admissibility of D implies that $\mathcal{H}^{\mathcal{E}}_\mu(\nabla^S_{\mathbf{y}}\mathbf{u}_\mu) = \mathcal{H}^{\mathcal{E}}_\mu(\nabla^S_{\mathbf{y}}(\mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{u}}_\mu)) = \mathcal{H}^{\mathcal{E}}_\mu(\boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu) = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}$. Then, $\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu)\,d\Omega_\mu = \boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}$, which is satisfied if $\int_{\Omega_\mu}\nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0}$. Equivalently, after integration by parts, $\int_{\Gamma_\mu}\tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0}$, with $\mathbf{n}_\mu$ the unit outward normal to the boundary Γ_μ of Ω_μ. Therefore, the space of kinematically admissible fluctuation displacements at micro scale and the associated space of admissible virtual variations are $\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{u}}_\mu} = \{\tilde{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0},\ \int_{\Gamma_\mu}\tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0}\}$.* ■

Remark 13 *The constraints imposed by the kinematical admissibility between macro- and micro-scales reduces to n_M tensorial constraints given by* (65) *plus m_M tensorial constraints given by* (67)*. Note that, since the kinematics at the two scales are allowed to be different, the kinematical fields at micro-scale may not be properly controlled. That is, some micro-scale kinematical descriptors may not be visible to the macro-scale. In such cases, further constraints over $\tilde{u}_\mu$ will be required to ensure the mathematical well-posedness of the micro-scale problem. Such extra constraints must be homogeneous and depend on the modeling hypotheses based on physical considerations for the micro-scale problem.*

Remark 14 *As we will show later, the space* $\mathrm{Kin}_{\tilde{u}_\mu}$ *plays a fundamental role in the definition of the micro-scale equilibrium state. If further kinematical constraints are added to* $\mathrm{Kin}_{\tilde{u}_\mu}$*, the response produced by the multiscale model will change in general. An easy way to construct a more constrained space of admissible generalized micro-scale displacement fluctuations is to force $\tilde{u} \equiv 0$. This leads to the model known as* Taylor Model *(or rule of mixtures) in classical multiscale solid mechanics. Here, in the general context of the present paper, we shall refer to the space so constrained as the* Taylor Fluctuations Space*. It contains only the zero element of* $\mathrm{Kin}_{\tilde{u}_\mu}$*:*

$$\mathrm{Kin}^{Taylor}_{\tilde{u}_\mu} = \{\tilde{u}_\mu \in \mathcal{U}_\mu,\ \tilde{u}_\mu = 0 \in \mathcal{U}^{\mathcal{U}}_\mu\} = \{0\}. \quad (70)$$

This is obviously the maximally *constrained space of kinematically admissible generalized micro-scale fluctuations. It is possible to adopt other (less constrained) subspaces of* $\mathrm{Kin}_{\tilde{u}_\mu}$*, each choice delivering, in general, a different model behaviour as illustrated in the following example.*

Classical multiscale solid mechanics *In addition to* $\mathrm{Kin}^{Taylor}_{\tilde{\mathbf{u}}_\mu}$*, other choices of subspaces of* $\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$ *can be considered. For example, null boundary condition subspace, denoted by* $\mathrm{Kin}^{nbc}_{\tilde{\mathbf{u}}_\mu}$*, which is obtained prescribing $\tilde{\mathbf{u}}_\mu = 0$, $\forall \mathbf{y} \in \Gamma_\mu$. Another subspace,* $\mathrm{Kin}^{pbc}_{\tilde{\mathbf{u}}_\mu}$*, could be easily constructed for RVEs with periodic geometry (typical of periodic media). Periodic RVEs have anti-periodic unit normal vector field $\mathbf{n}_\mu$ to the boundary*

Γ_μ. In this case, any $\mathbf{y} \in \Gamma_\mu$ has a one-to-one correspondance a point $\mathbf{y}^* \in \Gamma_\mu$ lying on the opposite side of Γ_μ and such that $\mathbf{n}_\mu(\mathbf{y}) = -\mathbf{n}_\mu(\mathbf{y}^*)$. Kinematical admissibility is guaranteed if the fluctuation field $\tilde{\mathbf{u}}_\mu$ is periodic on Γ_μ, i.e. $\tilde{\mathbf{u}}_\mu(\mathbf{y}) = \tilde{\mathbf{u}}_\mu(\mathbf{y}^*)$. It is easy to verify that $\mathrm{Kin}^{Taylor}_{\tilde{\mathbf{u}}_\mu} \subset \mathrm{Kin}^{nbc}_{\tilde{\mathbf{u}}_\mu} \subset \mathrm{Kin}^{pbc}_{\tilde{\mathbf{u}}_\mu} \subset \mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$. From a mechanical viewpoint, this means that the RVE-based model produces the stiffest behavior for the choice $\mathrm{Kin}^{Taylor}_{\tilde{\mathbf{u}}_\mu}$ and the most compliant behavior with the choice $\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$. ■

It is now possible to characterize the subspace Kin_{u_μ} of kinematically admissible generalized micro-scale displacements. This subspace is formed by all generalized displacements, $u_\mu \in \mathcal{U}_\mu$, linked to the macro-kinematics at point $\mathbf{x} \in \Omega_M$ and kinematically admissible with respect to $u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and $D_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$, i.e.

$$\mathrm{Kin}_{u_\mu} = \{u_\mu \in \mathcal{U}_\mu,\, u_\mu = \mathcal{J}^{\mathcal{U}}_\mu(u_M|_{\mathbf{x}}) + \mathcal{J}^{\mathcal{E}}_\mu(D_M|_{\mathbf{x}}) + \tilde{u}_\mu, \quad u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M},\, D_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}, \tilde{u}_\mu \in \mathrm{Kin}_{\tilde{u}_\mu}\}. \quad (71)$$

The corresponding space of kinematically admissible generalized micro-scale virtual displacements, Var_{u_μ}, is given by

$$\mathrm{Var}_{u_\mu} = \{\hat{u}_\mu \in \mathcal{U}_\mu; \hat{u}_\mu = u^1_\mu - u^2_\mu,\, u^1_\mu, u^2_\mu \in \mathrm{Kin}_{u_\mu}\} \quad (72)$$

or, in view of (69),

$$\mathrm{Var}_{u_\mu} = \mathrm{Kin}_{u_\mu}. \quad (73)$$

3.2 Multiscale duality

In this section we proceed to explore the duality concepts reviewed in Section 2.3 in each of the two scales. In the present multiscale setting, particular attention is focused on the assessment of the virtual power at a generic point $\mathbf{x}$ of the macro-scale. At the micro-scale, special attention is given the identification of admissible genralized forces and stresses.

3.2.1 Macro-scale virtual power

Following Section 2, the macro-scale internal virtual power is given by

$$P^{\mathrm{int}}_M(\mathcal{D}_M(\hat{u}_M)) = \langle \Sigma_M, \mathcal{D}_M(\hat{u}_M)\rangle_{\mathcal{E}'_M \times \mathcal{E}_M} \qquad \hat{u}_M \in \mathrm{Var}_{u_M} \quad (74)$$

or

$$P^{\mathrm{int}}_M(\mathcal{D}_M(\hat{u}_M)) = \sum_{k=1}^{m_M} \langle \Sigma^k_M, (\mathcal{D}_M(\hat{u}_M))^k\rangle_{\mathcal{E}'_{Mk} \times \mathcal{E}_{Mk}} \qquad \hat{u}_M \in \mathrm{Var}_{u_M}. \quad (75)$$

In the present context, we are interested in evaluating the virtual power associated with a generic point $\mathbf{x}$ of the macro-scale, so that it can be related to the virtual power of the corresponding RVE by means of the Principle of Multiscale Virtual Power that will be established later. Then, note that at a point $\mathbf{x} \in \Omega_M$, the kinematical quantity associated with internal power is $\mathcal{D}_M(\hat{u}_M)|_{\mathbf{x}}$. With the notation $\hat{D}_M|_{\mathbf{x}} = \mathcal{D}_M(\hat{u}_M)|_{\mathbf{x}}$, the macro-scale internal virtual power, $P^{\mathrm{int}}_{M,\mathbf{x}}(\hat{D}_M|_{\mathbf{x}})$, at a point $\mathbf{x}$ can be expressed as

$$P^{\mathrm{int}}_{M,\mathbf{x}}(\hat{D}_M|_{\mathbf{x}}) = \sum_{k=1}^{m_M} \omega_k (\Sigma_M|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k =: \Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} \qquad \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (76)$$

where ω_k, $k = 1, \ldots, m_M$, are dimensional scalars (see Remark 18) that guarantee the dimensional compatibility of the products $(\Sigma_M|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k$, $k = 1, \ldots, m_M$, taking part in the summation of internal power contributions above. It should be noted here that (76) has unit of *power*, whereas each product $(\Sigma_M|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k$ is a power *density*, i.e. power per unit measure of a corresponding RVE subset whose measure is ω_k. Each such subset may be of a different dimensionality (e.g. a volume, surface or point). We remark that this level of generality is crucial to model physical systems that feature simultaneously phenomena defined over distinct RVE subdomains, such as continuum straining, strain localization, cohesive cracks or even discrete phenomena. The operation denoted $(\cdot) \bullet (\cdot)$ above is then a duality product defined as

$$\begin{aligned} (\cdot) \bullet (\cdot) : (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} &\to \mathbb{R}, \\ (\Sigma_M|_{\mathbf{x}}, D_M|_{\mathbf{x}}) &\mapsto \Sigma_M|_{\mathbf{x}} \bullet D_M|_{\mathbf{x}} = \\ &\sum_{k=1}^{m_M} \omega_k \, (\Sigma_M|_{\mathbf{x}})^k \cdot (D_M|_{\mathbf{x}})^k. \end{aligned} \quad (77)$$

Classical multiscale solid mechanics *The internal macro-scale virtual power is, as usual, given by the product between the virtual strain action (a virtual strain rate in this case) and the Cauchy stress fields: $P^{\mathrm{int}}_M = \int_{\Omega_M} \boldsymbol{\sigma}_M \cdot \nabla^S_{\mathbf{x}} \hat{\mathbf{u}}_M \, d\Omega_M$. The virtual power of a point $\mathbf{x}$ (which is to be linked to an RVE) is $P^{\mathrm{int}}_{M,\mathbf{x}} = \boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \omega_1 \boldsymbol{\sigma}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}$.* ■

Similarly, we define the macro-scale external virtual power as

$$P^{\mathrm{ext}}_M(\hat{u}_M) = \langle f_M, \hat{u}_M\rangle_{\mathcal{U}'_M \times \mathcal{U}_M} \quad \hat{u}_M \in \mathrm{Var}_{u_M}, \quad (78)$$

where f_M has the structure of $\mathcal{D}'_M(\Sigma_M)$. The external virtual power at point $\mathbf{x}$ is expressed by

$$P^{\text{ext}}_{M,\mathbf{x}}(\hat{u}_M|_{\mathbf{x}}) = \sum_{k=1}^{n_M} \gamma_k \, (f_M|_{\mathbf{x}})^k \cdot (\hat{u}_M|_{\mathbf{x}})^k =: f_M|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} \qquad \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \quad (79)$$

The dimensional parameters γ_k, $k = 1, \ldots, n_M$, are entirely analogous to the parameters ω_k of (76). Note that in (79) we have used the same pairing product notation, $(\cdot) \bullet (\cdot)$, as in (76) but the exact meaning of the product will be dictated by the context. In this case, the duality product $(\cdot) \bullet (\cdot)$ is defined as

$$\begin{aligned} (\cdot) \bullet (\cdot) : (\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} &\to \mathbb{R}, \\ (f_M|_{\mathbf{x}}, u_M|_{\mathbf{x}}) &\mapsto f_M|_{\mathbf{x}} \bullet u_M|_{\mathbf{x}} = \\ &\sum_{k=1}^{n_M} \gamma_k \, (f_M|_{\mathbf{x}})^k \cdot (u_M|_{\mathbf{x}})^k. \end{aligned} \quad (80)$$

Classical multiscale solid mechanics *The external macro-scale virtual power is* $P^{\text{ext}}_M = \int_{\Omega_M} \mathbf{f}_M \cdot \hat{\mathbf{u}}_M \, d\Omega_M + \int_{\Gamma_M} \mathbf{t}_M \cdot \hat{\mathbf{u}}_M \, d\Gamma_M$. *The external virtual power of a point* $\mathbf{x} \in \Omega_M$ *is* $P^{\text{ext}}_{M,\mathbf{x}} = \mathbf{f}_M|_{\mathbf{x}} \bullet \hat{\mathbf{u}}_M|_{\mathbf{x}} = \gamma_1 \mathbf{f}_M|_{\mathbf{x}} \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}}$. ■

With the above definitions at hand, we can now define the *total macro-scale virtual power at point* $\mathbf{x}$. Using (76) and (79), we define

$$P^{\text{tot}}_{M,\mathbf{x}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}) = \Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} - f_M|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} \qquad \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}, \; \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (81)$$

The schematic diagram of Figure 3 shows a representation of the various concepts used in the definition of the macro-scale variational setting that is part of the present multiscale theory.

Remark 15 *Point* $\mathbf{x}$ *is a point belonging to some geometrical object of the macro-scale body. In general, it can be a point in a volume, a point on a surface or simply a point on its own. Thus, the external virtual power,* $P^{\text{ext}}_{M,\mathbf{x}}$*, of that point is associated to generalized external forces defined over the geometric object the point belongs to, and is characterized by means of duality. In the case of a point in the bulk of a three-dimensional solid body, we will have the notion of generalized body forces. This notion includes generalized passive body forces per unit volume (e.g. force due to gravity in classical mechanics) and generalized inertia forces (e.g. due to acceleration in classical mechanics). The term* generalized body force *will be used here to refer to these two kinds of generalized forces (passive and inertia). Hence, dynamic phenomena are automatically taken into account within the present framework. Note, however, that in the present theory the macro- and micro-scale share the same time scale.*

3.2.2 Micro-scale virtual power

With the duality concepts already presented in Section 2, the *internal micro-scale virtual power* can be expressed as

$$P^{\text{int}}_\mu(\mathcal{D}_\mu(\hat{u}_\mu)) = \langle \Sigma_\mu, \mathcal{D}_\mu(\hat{u}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \quad \hat{u}_\mu \in \text{Var}_{u_\mu}. \quad (82)$$

By considering (47) and (49), and with a slight abuse of notation, we obtain the equivalent expression

$$P^{\text{int}}_\mu(\hat{D}_M|_{\mathbf{x}}, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)) = \langle \Sigma_\mu, \mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}}) + \hat{\tilde{u}}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \qquad \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}, \; \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}, \quad (83)$$

in terms of virtual macro-scale strain actions, $\hat{D}_M|_{\mathbf{x}}$, and virtual micro-scale displacement fluctuations, $\hat{\tilde{u}}_\mu$. The macro-scale kinematics is mapped into the micro-scale by the insertion operator $\mathcal{J}^{\mathcal{E}}_\mu$. The schematic diagram of Figure 4 illustrates the basic concepts of the variational formulation at the micro-level, which are fundamental within the proposed unified variational multiscale formulation.

Classical multiscale solid mechanics *By taking into account the split of the micro-scale virtual strain action, the micro-scale virtual power can be expressed as* $P^{\text{int}}_\mu = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\mathbf{u}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} + \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu) \, d\Omega_\mu = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$. ■

The *external macro-scale virtual power* is defined as a linear functional on the subspace $\text{Var}_{u_\mu} = \text{Kin}_{u_\mu}$:

$$P^{\text{ext}}_\mu(\hat{u}_\mu) = \langle f_\mu, \hat{u}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \quad \hat{u}_\mu \in \text{Var}_{u_\mu}. \quad (84)$$

From (82) and the definition of the adjoint operator $\mathcal{D}'_\mu$ we can fully characterize the nature of the admissible generalized micro-scale external force $f_\mu \in \mathcal{U}'_\mu$. Indeed, we have

$$\begin{aligned} &\langle \Sigma_\mu, \mathcal{D}_\mu(\hat{u}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} = \langle \mathcal{D}'_\mu(\Sigma_\mu), \hat{u}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = \\ &\langle f_\mu, \mathcal{J}^{\mathcal{U}}_\mu(\hat{u}_M|_{\mathbf{x}}) + \mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}}) + \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\ &\qquad\qquad \hat{u}_\mu \in \text{Var}_{u_\mu}, \end{aligned} \quad (85)$$

that is,

$$\begin{aligned} &P^{\text{ext}}_\mu(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) = \\ &\langle f_\mu, \mathcal{J}^{\mathcal{U}}_\mu(\hat{u}_M|_{\mathbf{x}}) + \mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}}) + \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\ &\qquad \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}, \; \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}, \; \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}. \end{aligned} \quad (86)$$

Again, note the contributions from kinematical entities defined at the macro-scale and kinematical entities of the micro-scale to the micro-scale external virtual power.

Classical multiscale solid mechanics *The micro-scale external virtual power in this case reads* $P_\mu^{\text{ext}} = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot (\hat{\mathbf{u}}_M|_{\mathbf{x}} + \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o) + \hat{\tilde{\mathbf{u}}}_\mu) \, d\Omega_\mu = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$. ■

With the above at hand, we can now define the *total micro-scale virtual power*,

$$
\begin{aligned}
&P_\mu^{\text{tot}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) = \\
&P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)) - P_\mu^{\text{ext}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \\
&\qquad \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}, \; \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}, \; \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}, \quad (87)
\end{aligned}
$$

given as a sum of (linear) functionals in Var_{u_μ}.

The contribution of the macro-scale virtual quantities, $\hat{u}_M|_{\mathbf{x}}$ and $\hat{D}_M|_{\mathbf{x}}$, to the micro-scale total virtual power (87) has fundamental implications to the present theory. To see this, we begin by evaluating P_μ^{tot} for $\hat{\tilde{u}}_\mu = 0$,

$$
\begin{aligned}
&P_\mu^{\text{tot}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, 0) = \\
&P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, 0) - P_\mu^{\text{ext}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, 0) = \\
&= \langle \Sigma_\mu, \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}})) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \\
&- \langle f_\mu, \mathcal{J}_\mu^{\mathcal{U}}(\hat{u}_M|_{\mathbf{x}}) + \mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = \\
&= \langle (\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\
&\qquad - \langle f_\mu, \mathcal{J}_\mu^{\mathcal{U}}(\hat{u}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu}. \quad (88)
\end{aligned}
$$

From this expression, dual (stress- and force-like) entities, which we shall denote $\Sigma_M^\mu|_{\mathbf{x}} \in (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})'$ and $f_M^\mu|_{\mathbf{x}} \in (\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})'$, associated respectively with the macro-scale virtual actions $\hat{u}_M|_{\mathbf{x}}$ and $\hat{D}_M|_{\mathbf{x}}$, can be promptly identified as follows. By making use of the adjoint operators $(\mathcal{J}_\mu^{\mathcal{E}})' : \mathcal{U}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})'$ and $(\mathcal{J}_\mu^{\mathcal{U}})' : \mathcal{U}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})'$, from (88) we obtain

$$
\begin{aligned}
\Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} &= \sum_{k=1}^{m_M} \omega_k \, (\Sigma_M^\mu|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k \\
&:= \langle (\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\
&= \langle (\mathcal{J}_\mu^{\mathcal{E}})'(\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \hat{D}_M|_{\mathbf{x}} \rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}, \quad (89)
\end{aligned}
$$

$$
\begin{aligned}
f_M^\mu|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} &= \sum_{k=1}^{n_M} \gamma_k \, (f_M^\mu|_{\mathbf{x}})^k \cdot (\hat{u}_M|_{\mathbf{x}})^k \\
&:= \langle f_\mu, \mathcal{J}_\mu^{\mathcal{U}}(\hat{u}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\
&= \langle (\mathcal{J}_\mu^{\mathcal{U}})' f_\mu, \hat{u}_M|_{\mathbf{x}} \rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \quad (90)
\end{aligned}
$$

Then, by substituting expressions (89) and (90) into (88) we have

$$
\begin{aligned}
&P_\mu^{\text{tot}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, 0) = \\
&\qquad \Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} - f_M^\mu|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}}. \quad (91)
\end{aligned}
$$

In summary, by means of duality considerations it has been shown in the above that as a result of the kinematical admissibility link postulated between the macro- and micro-scales, the micro-scale total virtual power has contributions from the macro-scale virtual actions. Comparison between (91) and (81) suggests that a further link – between the macro- and micro-scale virtual powers – can be postulated. This is addressed in the following.

3.3 Principle of Multiscale Virtual Power

The *Principle of Multiscale Virtual Power*, stated in this section, establishes a consistency link between the macro- and micro-scale virtual powers. This principle lies at the heart of the *Method of Multiscale Virtual Power* proposed in this paper and, as we shall see, yields the following consequences:

- Micro-scale variational equilibrium equation (n_μ variational equations);
- Homogenization formulae for the macro-scale internal generalized stresses (m_M homogenization formulae); and
- Homogenization formulae for the macro-scale external generalized forces (n_M homogenization formulae).

The principle itself can be regarded as a variational statement of an extended version of the well-known Hill-Mandel Principle of Macrohomogeneity [45,72]. It is postulated in the following.

Principle of Multiscale Virtual Power *The total macro-scale virtual power at a point* $\mathbf{x}$ *must be equal to the total micro-scale virtual power at the corresponding RVE for all kinematically admissible macro- and micro-scale virtual actions. That is,*

$$
\begin{aligned}
&P_{M,\mathbf{x}}^{\text{tot}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}) = P_\mu^{\text{tot}}(\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \\
&\qquad \forall (\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \textit{ kinematically admissible.} \quad (92)
\end{aligned}
$$

or, equivalently, in a more explicit form

$$
\begin{aligned}
&\Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} - f_M|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} = \\
&\langle \Sigma_\mu, \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}}) + \hat{\tilde{u}}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \\
&- \langle f_\mu, \mathcal{J}_\mu^{\mathcal{U}}(\hat{u}_M|_{\mathbf{x}}) + \mathcal{J}_\mu^{\mathcal{E}}(\hat{D}_M|_{\mathbf{x}}) + \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\
&\qquad \forall (\hat{u}_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \text{Var}_{\tilde{u}_\mu}. \quad (93)
\end{aligned}
$$

At variance with the classical Hill-Mandel Principle, where only internal powers are considered, the PMVP

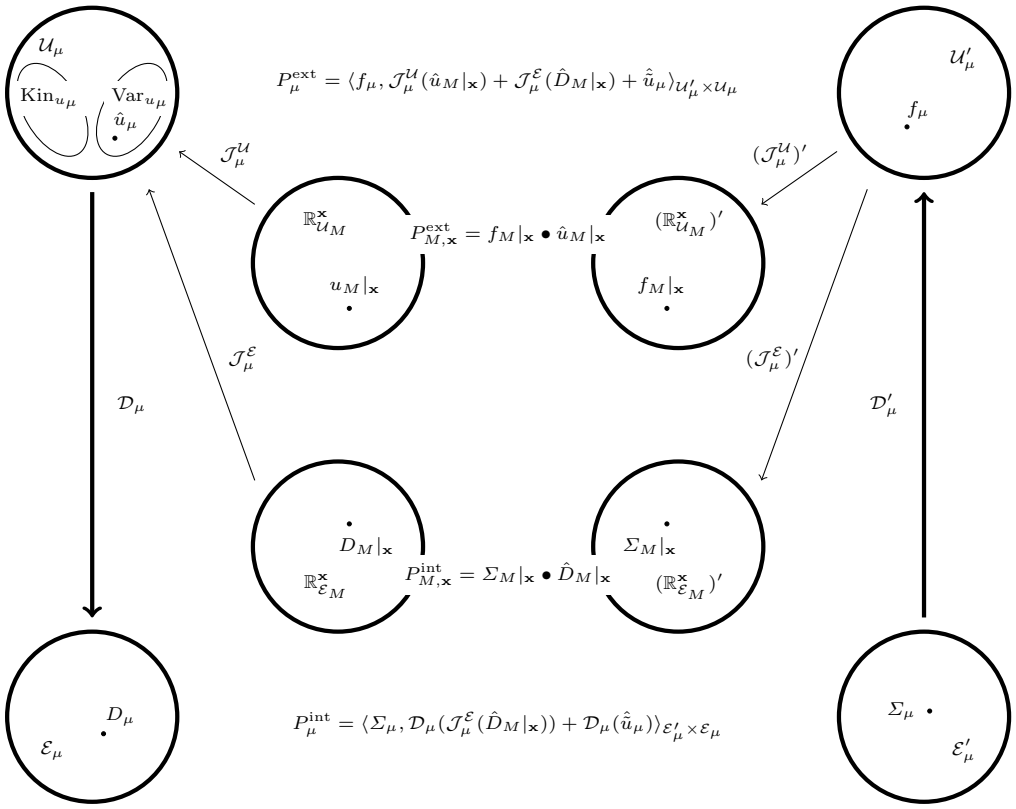

Fig. 4 Method of Multiscale Virtual Power. Basic sets and operations at the micro-scale level.

implies a balance of both the internal and external virtual powers at a point $\mathbf{x}$ of the macro-scale with the total virtual power of the associated RVE.

Classical multiscale solid mechanics *The Principle of Multiscale Virtual Power in this case states that: The macro-scale stress and body force* $(\boldsymbol{\sigma}_M|_{\mathbf{x}}, \mathbf{f}_M|_{\mathbf{x}})$ *and their micro-scale counterpart fields* $(\boldsymbol{\sigma}_\mu, \mathbf{f}_\mu)$ *satisfy the Principle of Multiscale Virtual Power if and only if the following variational equation holds:* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} - \mathbf{f}_M|_{\mathbf{x}} \bullet \hat{\mathbf{u}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}\, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}}\, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu \ \forall (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\tilde{\mathbf{u}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$. ■

Remark 16 *The Principle of Multiscale Virtual Power will also provide the definition of the scalars* $\omega_k, k = 1, \ldots, m_M$ *and* $\gamma_k, k = 1, \ldots, n_M$*, which appear in the left hand side of* (93) *(following the identities* (77) *and* (80)*).*

3.4 Dual homogenization operators and micro-scale equilibrium

The dual homogenization operators (for the macro-scale generalized stresse- and force-like quantities) and the micro-scale equilibrium equations are derived here as natural consequences of the Principle of Multiscale Virtual Power. As we shall see, they are the Euler-Lagrange equations associated with the variational statement (93).

3.4.1 Micro-scale equilibrium

By setting $\hat{D}_M|_{\mathbf{x}} = 0$ and $\hat{u}_M|_{\mathbf{x}} = 0$ in (93), we obtain the variational form of the *micro-scale equilibrium equation*:

$$\langle \Sigma_\mu, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} - \langle f_\mu, \hat{\tilde{u}}_\mu\rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = 0 \quad \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu}. \quad (94)$$

Obviously, this equation has the same format as the standard equilibrium of a general physical system written as the Principle of Virtual Power, here applied to an RVE with the corresponding generalized applied external forces and kinematical constraints embedded in the definition of $\mathrm{Var}_{\tilde{u}_\mu}$.

Classical multiscale solid mechanics *In this xase, when we choose* $\hat{\mathbf{u}}_M|_{\mathbf{x}} = \mathbf{0}$ *and* $\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \mathbf{0}$ *in the corresponding PMVP, the RVE equilibrium is obtained as the following variational equation:* $\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu = 0 \ \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$. ■

By making use of the adjoint operator $\mathcal{D}'_\mu$ in (94), we obtain the alternative form

$$\langle \mathcal{D}'_\mu(\Sigma_\mu) - f_\mu, \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = 0 \qquad \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu}, \tag{95}$$

or, equivalently,

$$\mathcal{D}'_\mu(\Sigma_\mu) - f_\mu \in (\mathrm{Var}_{\tilde{u}_\mu})^\perp \subset \mathcal{U}_\mu{}'. \tag{96}$$

Further, we recall that f_μ must satisfy (25), i.e.

$$\langle f_\mu, \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = 0 \qquad \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu} \bigcap \mathsf{N}(\mathcal{D}_\mu), \tag{97}$$

which implies

$$f_\mu \in (\mathrm{Var}_{\tilde{u}_\mu} \bigcap \mathsf{N}(\mathcal{D}_\mu))^\perp, \tag{98}$$

where $(\cdot)^\perp$ denotes the orthogonal complement of $(\cdot)$. That is, the system f_μ of generalized forces is orthogonal to micro-scale rigid admissible virtual fluctuations of the RVE.

Classical multiscale solid mechanics *If we decompose* $\mathbf{f}_\mu = \bar{\mathbf{f}}_\mu + \tilde{\mathbf{f}}_\mu$, *where* $\bar{\mathbf{f}}_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{f}_\mu \, d\Omega_\mu$, *and* $\tilde{\mathbf{f}}_\mu = \mathbf{f}_\mu - \bar{\mathbf{f}}_\mu$, *we have that* $\int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \tilde{\mathbf{f}}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$. *Hence, only fluctuations of the body force,* $\tilde{\mathbf{f}}_\mu$, *which are not orthogonal to* $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$, *play a role in the micro-scale equilibrium problem.* ■

Finally, we remark that the *micro-scale equilibrium problem* is completely defined by the variational equation (94) once the external load f_μ is known (a given datum) and a constitutive law $\Sigma_\mu = \Sigma_\mu(u^t_\mu)$, expressing the stress Σ_μ as a function of the history u^t_μ of the field u_μ, is assigned to each point of the RVE. The problem is stated in the following.

Problem 2 (Micro-scale equilibrium) *For a given constitutive law* $\Sigma_\mu = \Sigma_\mu(u^t_\mu)$, *a given history* $u^t_M|_{\mathbf{x}}$ *and* $D^t_M|_{\mathbf{x}}$, *of macro-scale generalized displacement and strain actions, and a given history of micro-scale admissible generalized external force,* f^t_μ, *find the history* $u^t_\mu \in \mathrm{Kin}_{u_\mu}$ *of kinematically admissible generalized micro-scale displacements such that*

$$\langle \Sigma_\mu(u^\tau_\mu), \mathcal{D}_\mu(\hat{u}_\mu) \rangle_{\mathcal{E}' \times \mathcal{E}} = \langle f(\tau), \hat{u}_\mu \rangle_{\mathcal{U}' \times \mathcal{U}} \qquad \forall \hat{u}_\mu \in \mathrm{Var}_{u_\mu}, \forall \tau \in [0,t]. \tag{99}$$

3.4.2 Generalized stress homogenization formulae

Now, we set $\hat{u}_M|_{\mathbf{x}} = 0$ and $\hat{\tilde{u}}_\mu = 0$ in (93) (see also (89)) and obtain

$$\begin{aligned} \Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} &= \langle \Sigma_\mu, \mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}})) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \\ &\quad - \langle f_\mu, \mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\ &= \langle \mathcal{D}'_\mu \Sigma_\mu - f_\mu, \mathcal{J}^{\mathcal{E}}_\mu(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\ &= \langle (\mathcal{J}^{\mathcal{E}}_\mu)'(\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \hat{D}_M|_{\mathbf{x}} \rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \\ &= \Sigma^\mu_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} \quad \forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \end{aligned} \tag{100}$$

From the above, we can promptly identify the general (linear) *Σ_M-homogenization operator* as

$$\begin{aligned} &\mathfrak{H}_\Sigma : \mathcal{U}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \\ &(\mathcal{D}'_\mu \Sigma_\mu - f_\mu) \mapsto \Sigma^\mu_M|_{\mathbf{x}} = \mathfrak{H}_\Sigma(\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \end{aligned} \tag{101}$$

such that

$$\begin{aligned} &\langle (\mathcal{J}^{\mathcal{E}}_\mu)'(\mathcal{D}'_\mu \Sigma_\mu - f_\mu), \hat{D}_M|_{\mathbf{x}} \rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \\ &\quad = \mathfrak{H}_\Sigma(\mathcal{D}'_\mu \Sigma_\mu - f_\mu) \bullet \hat{D}_M|_{\mathbf{x}} \quad \forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \end{aligned} \tag{102}$$

From (100) and the above definition, we have

$$(\Sigma_M|_{\mathbf{x}} - \mathfrak{H}_\Sigma(\mathcal{D}'_\mu \Sigma_\mu - f_\mu)) \bullet \hat{D}_M|_{\mathbf{x}} = 0 \qquad \forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \tag{103}$$

This gives the homogenization formula for the macro-scale generalized stress:

$$\Sigma_M|_{\mathbf{x}} - \mathfrak{H}_\Sigma(\mathcal{D}'_\mu \Sigma_\mu - f_\mu) \in (\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}})^\perp \subseteq (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})'. \tag{104}$$

Remark 17 *The Σ_M-homogenization operator and the corresponding homogenization formula for stress-like quantities is consistently* derived *here as a consequence of the proposed PMVP. This is in contrast with most of the existing literature in the field, where stress homogenization formulae are postulated a priori instead.*

Classical multiscale solid mechanics *In this case, by setting* $\hat{\mathbf{u}}_M|_{\mathbf{x}} = \mathbf{0}$ *and* $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$ *in the PMVP, we obtain:* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \; \forall \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$. *The homogenization formula is obtained by first identifying* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = |\Omega_\mu| \, \boldsymbol{\sigma}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}$, *which results in* $\boldsymbol{\sigma}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu - (\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)) \, d\Omega_\mu$. *In this case, we have identified* $\omega_1 = |\Omega_\mu|$ *so that the stress homogenization is physically consistent. Note that this is the Σ_M-homogenization formula that naturally results from the formulation. This was found using a shortcut. To see this the long way, we consider the operator* $\mathcal{D}_\mu = \nabla^S_{\mathbf{y}}$ *explicitly as follows:* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}}(\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o)) \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \; \forall \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$. *Then, integration by parts of the first term on the right hand side gives* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} [-\operatorname{div}_{\mathbf{y}} \boldsymbol{\sigma}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)] \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Gamma_\mu} [\boldsymbol{\sigma}_\mu \mathbf{n}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)] \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Gamma_\mu - \int_{\Omega_\mu} [\mathbf{f}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o)] \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \; \forall \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$. *Now, by using the strong form of the micro-scale equilibrium, we have that* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \big(\int_{\Gamma_\mu} \boldsymbol{\sigma}_\mu \mathbf{n}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o) \, d\Gamma_\mu \big) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \; \forall \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$. *Then, by proceeding in the same way as before, we conclude that the Σ_M-homogenization formula reads* $\boldsymbol{\sigma}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \boldsymbol{\sigma}_\mu \mathbf{n}_\mu \otimes^S (\mathbf{y} - \mathbf{y}_o) \, d\Omega_\mu$. *This form is completely analogous to the previous one. The advantage of the latter formula over the former is that the*

homogenized variable depends only on RVE boundary fields – something that has been pointed out by Hill [45] as of fundamental practical importance in RVE-based theories. However, note that the former formula is requires less regularity of the fields involved and, as such, is better suited for problems tackled in weak form at all levels. ■

Remark 18 *According to expression* (100)*, the coefficients* ω_k*,* $k = 1\ldots,m_M$*, appearing on its left hand side (refer to* (77)*), are identified from the homogenization procedure given by operator* $\mathfrak{H}_\Sigma$ *so as to render the homogenization operation physically consistent (refer to the above example of classical multiscale solid mechanics). In Section 6 this is illustrated in further practical examples.*

3.4.3 Generalized force homogenization formulae

Now, we specialize (93) by choosing $\hat{D}_M|_{\mathbf{x}} = 0$ and $\hat{\tilde{u}}_\mu = 0$ (see also (90)). This gives

$$\begin{aligned} f_M|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} &= \langle f_\mu, \mathcal{J}_\mu^{\mathcal{U}}(\hat{u}_M|_{\mathbf{x}})\rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} \\ &= \langle (\mathcal{J}_\mu^{\mathcal{U}})'(f_\mu), \hat{u}_M|_{\mathbf{x}}\rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \\ &= f_M^\mu|_{\mathbf{x}} \bullet \hat{u}_M|_{\mathbf{x}} \quad \forall \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \end{aligned} \tag{105}$$

Similarly to the derivation of the stress homogenization operator, from the above variational equation we identify the f_M*-homogenization operator*,

$$\begin{aligned} &\mathfrak{H}_f : \mathcal{U}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})', \\ &\quad f_\mu \mapsto f_M^\mu|_{\mathbf{x}} = \mathfrak{H}_f(f_\mu), \end{aligned} \tag{106}$$

such that

$$\begin{aligned} &\langle (\mathcal{J}_\mu^{\mathcal{U}})'(f_\mu), \hat{u}_M|_{\mathbf{x}}\rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \\ &\quad = \mathfrak{H}_f(f_\mu) \bullet \hat{u}_M|_{\mathbf{x}} \quad \forall \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \end{aligned} \tag{107}$$

With the above defined $\mathfrak{H}_f$, (105) gives

$$(f_M|_{\mathbf{x}} - \mathfrak{H}_f(f_\mu)) \bullet \hat{u}_M|_{\mathbf{x}} = 0 \qquad \forall \hat{u}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \tag{108}$$

Then, we arrive at the homogenization formula for the generalized macro-scale force:

$$f_M|_{\mathbf{x}} - \mathfrak{H}_f(f_\mu) \in (\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}})^\perp \subseteq (\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M})'. \tag{109}$$

Classical multiscale solid mechanics *By considering* $\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \mathbf{0}$ *and* $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$ *in the corresponding PMVP, we get* $\mathbf{f}_M|_{\mathbf{x}} \bullet \hat{\mathbf{u}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}}\, d\Omega_\mu \ \forall \hat{\mathbf{u}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}$*. Here we identify:* $\mathbf{f}_M|_{\mathbf{x}} \bullet \hat{\mathbf{u}}_M|_{\mathbf{x}} = |\Omega_\mu|\, \mathbf{f}_M|_{\mathbf{x}} \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}}$*, so that we have* $\mathbf{f}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{f}_\mu\, d\Omega_\mu$*. This defines the* f_M*-homogenization operator. Note that* γ_1 *has been identified here as* $\gamma_1 = |\Omega_\mu|$ *so as to guarantee the physical consistency of the homogenization operation.* ■

Remark 19 *According to* (105)*, the coefficients* γ_k*,* $k = 1\ldots,n_M$*, taking part in its left hand side (refer to*(80)*), are identified from the homogenization process defined by* $\mathfrak{H}_f$ *so as to make the operation physically consistent (refer to the above example on classical multiscale solid mechanics). This will be further illustrated in other examples presented in Section 6.*

3.5 Summary and discussion

In summary, we have established in the above a complete variational theory of RVE-based multiscale modeling of physical systems. Within the proposed theory, RVE-based models are devised in a systematic way by means of well-defined steps according to the proposed *Method of Multiscale Virtual Power*. Once the kinematics at both macro- and micro-scales are established, and the link between kinematical variables across the scales is defined, the nature of stress- and force-like quantities at both scales is identified through mathematical duality and the micro-scale equilibrium equation and homogenization relations for the stress- and force-like quantities are univocally derived from the *Principle of Multiscale Virtual Power* entirely by means of straightforward variational arguments. The overall procedure is summarized in Box 1 where a *recipe* for the consistent derivation of general RVE-based multiscale models is presented.

An interesting point to note, made clear when the theory is presented within the proposed framework, is that the concepts of internal and external virtual powers are not entirely distinct form each other as in the conventional single-scale theory. That is, in general, the macro-scale internal stress, Σ_M, which produces macro-scale *internal* virtual power, has contributions from both the micro-scale internal stress Σ_μ (that produces micro-scale internal virtual power), *and* the micro-scale *external* force f_μ (that produces *external* micro-scale virtual power). The effects of Σ_μ and f_μ on Σ_M are combined in a non-linear way, through the micro-scale equilibrium problem defined by (92). These interactions alter the standard notion of *constitutiveness* of the *material behavior* in that internal forces (e.g. micro-scale inertia forces in dynamical problems) may contribute to the macro-scale stress. However, one situation where the standard notion of constitutiveness of the RVE-based model is retained is when the physical transfer between scales involves *only* the balance of *internal* virtual power. That is, when only $P^{\text{int}}_{M,\mathbf{x}}$ and P^{int}_μ are considered in the Principle of Multiscale Virtual Power and the macro- and micro-scale external virtual powers are disregarded. In this case, a *purely constitutive* modeling framework is obtained. This is the case of all multiscale

models based on the Hill-Mandel Principle of Macrohomogeneity [72,45]. The interesting aspect in this case is that the generalized macro-scale stress, $\Sigma_M|_{\mathbf{x}}$, derives only from micro-scale constitutive and mechanical interactions, for which only the generalized micro-scale stress Σ_μ is responsible. While f_μ can exist, it is orthogonal to the corresponding space of admissible virtual generalized displacements and hence does not generate virtual power. That is, f_μ in this case is a *reactive* force to the kinematical constraints embedded in the definition of $\mathrm{Var}_{\tilde{u}_\mu}$ [112]. As such, f_μ cannot be arbitrarily modeled. This particular case will be considered in detail in Section 4.

4 Multiscale constitutive modeling

Following the above discussion, we present here the specialization of the general MMVP to the case where only the virtual powers of the macro- and micro-scale generalized stresses are accounted for in the PMVP. The motivation to present this specialization in detail is that the vast majority of publications on multiscale modeling falls into this category of RVE-based theories. For example, the classical RVE-based theories in continuum solid mechanics do fall into this category. In this case, the multiscale model defines a macro-scale *constitutive model* where the macro-scale stress $\Sigma_M|_{\mathbf{x}}$ is a function (implicitly defined by means of the operations of kinematical insertion, micro-scale equilibrium solution and stress homogenization) of the history $D^t_M|_{\mathbf{x}}$ of the macro-strain actions. That is, $\Sigma_M|_{\mathbf{x}}{=}\Sigma_M|_{\mathbf{x}}(D^t_M|_{\mathbf{x}})$.

4.1 On the insertion operators

As in the general case of Section 3, the insertion of elements $u_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ into the micro-scale $\mathcal{U}_\mu$ is performed by the insertion operator $\mathcal{J}^{\mathcal{U}}_\mu$ defined in (43).

For the present case, where external virtual powers play no role, the insertion of elements $D_M|_{\mathbf{x}} \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$ into the micro-scale is understood to be directly performed into $\mathcal{E}_\mu$, by means of the linear operator

$$\begin{aligned}\mathcal{I}_\mu = \mathcal{D}_\mu \mathcal{J}^{\mathcal{E}}_\mu : \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} &\to \mathcal{E}_\mu,\\ D_M|_{\mathbf{x}} &\mapsto \bar{D}_\mu = \mathcal{I}_\mu(D_M|_{\mathbf{x}}),\end{aligned} \tag{110}$$

which is the composition $\mathcal{D}_\mu\mathcal{J}^{\mathcal{E}}_\mu$ of operators (defined by (39) and (44), respectively), as highlighted in Remark 9 (see (52)). The mapping of $D_M|_{\mathbf{x}}$ through $\mathcal{I}_\mu$ may result in a non-uniform field (dependent on $\mathbf{y}$) in the micro-scale.

From the developments of Section 3 we observe that in the present case micro-scale generalized strain actions are the sum of a macro-scale contribution inserted through the operator $\mathcal{I}_\mu$ and a strain action fluctuation field intrinsically related to the kinematics and equilibrium of the micro-scale. That is,

$$D_\mu = \mathcal{I}_\mu(D_M|_{\mathbf{x}}) + \mathcal{D}_\mu(\tilde{u}_\mu). \tag{111}$$

Remark 20 *The linearity of operator $\mathcal{I}_\mu$ allows matrix the representation*

$$\mathcal{I}_\mu = \begin{pmatrix} \mathcal{I}_\mu^{11} & \mathcal{I}_\mu^{12} & \dots & \mathcal{I}_\mu^{1m_M} \\ \mathcal{I}_\mu^{21} & \mathcal{I}_\mu^{22} & \dots & \mathcal{I}_\mu^{2m_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{I}_\mu^{m_\mu 1} & \mathcal{I}_\mu^{m_\mu 2} & \dots & \mathcal{I}_\mu^{m_\mu m_M} \end{pmatrix}, \tag{112}$$

where

$$\begin{pmatrix} \mathcal{I}_\mu^{11} & \mathcal{I}_\mu^{12} & \dots & \mathcal{I}_\mu^{1m_M} \\ \mathcal{I}_\mu^{21} & \mathcal{I}_\mu^{22} & \dots & \mathcal{I}_\mu^{2m_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{I}_\mu^{m_\mu 1} & \mathcal{I}_\mu^{m_\mu 2} & \dots & \mathcal{I}_\mu^{m_\mu m_M} \end{pmatrix} = \begin{pmatrix} \mathcal{D}_\mu^{11} & \mathcal{D}_\mu^{12} & \dots & \mathcal{D}_\mu^{1n_\mu} \\ \mathcal{D}_\mu^{21} & \mathcal{D}_\mu^{22} & \dots & \mathcal{D}_\mu^{2n_\mu} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{D}_\mu^{m_\mu 1} & \mathcal{D}_\mu^{m_\mu 2} & \dots & \mathcal{D}_\mu^{m_\mu n_\mu} \end{pmatrix} \begin{pmatrix} \mathcal{J}_\mu^{\mathcal{E}\,11} & \mathcal{J}_\mu^{\mathcal{E}\,12} & \dots & \mathcal{J}_\mu^{\mathcal{E}\,1m_M} \\ \mathcal{J}_\mu^{\mathcal{E}\,21} & \mathcal{J}_\mu^{\mathcal{E}\,22} & \dots & \mathcal{J}_\mu^{\mathcal{E}\,2m_M} \\ \vdots & \vdots & \ddots & \vdots \\ \mathcal{J}_\mu^{\mathcal{E}\,n_\mu 1} & \mathcal{J}_\mu^{\mathcal{E}\,n_\mu 2} & \dots & \mathcal{J}_\mu^{\mathcal{E}\,n_\mu m_M} \end{pmatrix}. \tag{113}$$

The concepts involved in the kinematical transition between scales (i.e. the kinematical admissibility concept) follow those presented in the general context of Section 3.

4.2 Multiscale duality

The internal virtual powers at macro- and micro-scales are exactly as defined in Section 3.2. For the macro-scale we then have

$$P^{\mathrm{int}}_M(\mathcal{D}_M(\hat{u}_M)) = \langle \Sigma_M, \mathcal{D}_M(\hat{u}_M)\rangle_{\mathcal{E}'_M \times \mathcal{E}_M} \qquad \hat{u}_M \in \mathrm{Var}_{u_M}. \tag{114}$$

At point $\mathbf{x} \in \Omega_M$, we have

$$P^{\mathrm{int}}_{M,\mathbf{x}}(\hat{D}_M|_{\mathbf{x}}) = \sum_{k=1}^{m_M} \omega_k (\Sigma_M|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k = \Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} \qquad \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \tag{115}$$

For the micro-scale, the internal virtual power is given by

$$P_\mu^{\text{int}}(\hat{D}_\mu) = \langle \Sigma_\mu, \hat{D}_\mu \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \quad \hat{D}_\mu \text{ given by (111)}, \quad (116)$$

or, equivalently, with a slight abuse of notation, we write

$$P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)) = \langle \Sigma_\mu, \mathcal{I}_\mu(\hat{D}_M|_{\mathbf{x}}) + \mathcal{D}_\mu(\hat{\tilde{u}}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu}$$
$$\hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}, \ \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}. \quad (117)$$

As in Section 3.2.2, we now set $\hat{\tilde{u}}_\mu = 0$ in the above formula to assess the contribution of the macro-scale quantity $\hat{D}_M|_{\mathbf{x}}$ to the micro-scale internal virtual power. Then, we obtain

$$P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, 0) = \langle \Sigma_\mu, \mathcal{I}_\mu(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu}. \quad (118)$$

Further, by making use of the adjoint operator $(\mathcal{I}_\mu)' : \mathcal{E}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})'$ we obtain (see also (77))

$$\begin{aligned} \Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} &= \sum_{k=1}^{m_M} \omega^k \, (\Sigma_M^\mu|_{\mathbf{x}})^k \cdot (\hat{D}_M|_{\mathbf{x}})^k \\ &:= \langle \Sigma_\mu, \mathcal{I}_\mu(\hat{D}_M|_{\mathbf{x}}) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \\ &= \langle (\mathcal{I}_\mu)'(\Sigma_\mu), \hat{D}_M|_{\mathbf{x}} \rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \end{aligned} \quad (119)$$

Finally, by substituting (119) into (118) we arrive at the particularization of expression (91) for the purely constitutive multiscale formulation, in which external forces play no role in the scale transition,

$$P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, 0) = \Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}}. \quad (120)$$

4.3 Principle of Constitutive Multiscale Virtual Power

In the present case we state a *Principle of Constitutive Multiscale Virtual Power*, whose consequences will be:

- Micro-scale variational equilibrium problem (n_μ variational equations); and
- Homogenization formulae for the macro-scale internal generalized stresses (m_M homogenization formulae).

Principle of Constitutive Multiscale Virtual Power *The internal macro-scale virtual power at a point* $\mathbf{x}$ *must be equal to the internal micro-scale virtual power at the corresponding RVE for all kinematically admissible macro- and micro-scale virtual actions. That is,*

$$P_{M,\mathbf{x}}^{\text{int}}(\hat{D}_M|_{\mathbf{x}}) = P_\mu^{\text{int}}(\hat{D}_M|_{\mathbf{x}}, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu))$$
$$\forall (\hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \text{ kinematically admissible}, \quad (121)$$

or, equivalently, in a more explicit form,

$$\Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} = \langle \Sigma_\mu, \mathcal{I}_\mu(\hat{D}_M|_{\mathbf{x}}) + \mathcal{D}_\mu(\hat{\tilde{u}}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu}$$
$$\forall (\hat{D}_M|_{\mathbf{x}}, \hat{\tilde{u}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \text{Var}_{\tilde{u}_\mu}. \quad (122)$$

The above principle is a generalized form of the Hill-Mandel Principle of Macro-Homogeneity which preserves the idea that only internal virtual powers are to be balanced in the scale transition.

Classical multiscale solid mechanics *The PMVP in this case is stated as follows: The macro-scale stress* $\boldsymbol{\sigma}_M|_{\mathbf{x}}$ *and the micro-scale stress field* $\boldsymbol{\sigma}_\mu$ *satisfy the Principle of Multiscale Virtual Power if and only if the following variational equation holds:* $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \ \forall (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\tilde{\mathbf{u}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \text{Var}_{\tilde{\mathbf{u}}_\mu}$. *This is the variational statement of the classical Hill-Mandel Principle for RVE-based multiscale solid mechanics, widely invoked in the current literature on the subject.* ■

4.4 Stress homogenization and micro-scale equilibrium

Analogously to Section 3.4, the stress homogenization relation and the micro-scale equilibrium are derived here as the Euler-Lagrange equations associated to the variational statement (122).

4.4.1 Micro-scale equilibrium

By setting, in particular, $\hat{D}_M|_{\mathbf{x}} = 0$ in (122), we obtain the micro-scale variational equilibrium equation:

$$\langle \Sigma_\mu, \mathcal{D}_\mu(\hat{\tilde{u}}_\mu) \rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} = 0 \qquad \forall \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}. \quad (123)$$

This equation is a particular case of (94) when f_μ is orthogonal to the space $\text{Var}_{\tilde{u}_\mu}$. Equivalently, by using the adjoint operator $\mathcal{D}'_\mu$ we have

$$\langle \mathcal{D}'_\mu(\Sigma_\mu), \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = 0 \qquad \forall \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}, \quad (124)$$

which implies

$$\mathcal{D}'_\mu(\Sigma_\mu) \in (\text{Var}_{\tilde{u}_\mu})^\perp \subset \mathcal{U}_\mu{}'. \quad (125)$$

The micro-scale external forces, f_μ, can be identified from the above as having the structure of $\mathcal{D}'_\mu(\Sigma_\mu)$, as usual. It should be noted, however, that, in the present case, they must be purely *reactive* forces (they do not generate virtual power) as they are orthogonal to $\text{V}ar_{\tilde{u}_\mu}$. That is,

$$\langle f_\mu, \hat{\tilde{u}}_\mu \rangle_{\mathcal{U}'_\mu \times \mathcal{U}_\mu} = 0 \qquad \forall \hat{\tilde{u}}_\mu \in \text{Var}_{\tilde{u}_\mu}. \quad (126)$$

The *micro-scale equilibrium problem* is completely defined by the variational equation (94) once a constitutive law $\Sigma_\mu = \Sigma_\mu(u_\mu^t)$, expressing the generalized micro-scale stress Σ_μ as a function of the history u_μ^t of the field u_μ, is assigned to each point of the RVE. The problem is analogous to Problem 2.

4.4.2 Generalized stress homogenization formula

If we choose $\hat{\tilde{u}}_\mu = 0$ in (122), we obtain (see also (119))

$$\begin{aligned}\Sigma_M|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} &= \langle \Sigma_\mu, \mathcal{I}_\mu(\hat{D}_M|_{\mathbf{x}})\rangle_{\mathcal{E}'_\mu \times \mathcal{E}_\mu} \\ &= \langle (\mathcal{I}_\mu)'(\Sigma_\mu), \hat{D}_M|_{\mathbf{x}}\rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \\ &= \Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} \quad \forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \end{aligned} \tag{127}$$

The (linear) constitutive Σ_M*-homogenization operator* is identified from the above variational equation as

$$\begin{aligned} &\mathfrak{H}^c_\Sigma : \mathcal{E}'_\mu \to (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \\ &\quad \Sigma_\mu \mapsto \Sigma_M^\mu|_{\mathbf{x}} = \mathfrak{H}^c_\Sigma(\Sigma_\mu), \end{aligned} \tag{128}$$

such that

$$\begin{aligned} \langle \mathfrak{H}^c_\Sigma(\Sigma_\mu), \hat{D}_M|_{\mathbf{x}}\rangle_{(\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})' \times \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} &= \Sigma_M^\mu|_{\mathbf{x}} \bullet \hat{D}_M|_{\mathbf{x}} \\ &\forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \end{aligned} \tag{129}$$

With the above defined operator $\mathfrak{H}^c_\Sigma$, equation (127) gives

$$(\Sigma_M|_{\mathbf{x}} - \mathfrak{H}^c_\Sigma(\Sigma_\mu)) \bullet \hat{D}_M|_{\mathbf{x}} = 0 \quad \forall \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \tag{130}$$

This yields the homogenization formula for the macro-scale generalized stress,

$$\Sigma_M|_{\mathbf{x}} - \mathfrak{H}^c_\Sigma(\Sigma_\mu) \in (\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}})^\perp \subseteq (\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M})'. \tag{131}$$

Remark 21 *When the given micro-scale constitutive function is of the type $\Sigma_\mu(\mathbf{y}) = \Sigma_\mu(D_\mu^t(\mathbf{y}))$ – a standard local constitutive law (in the strict sense of the word), where the stress depends solely on the local history of the generalized strain actions – the multiscale model above defines a macro-scale constitutive function of the same type, i.e. $\Sigma_M|_{\mathbf{x}} = \Sigma_M|_{\mathbf{x}}(D_M^t|_{\mathbf{x}})$. That this is indeed true can be established as follows. According to* (111)*, micro-scale strain actions are a sum of a contribution from the macro-scale strain actions (inserted by the operator $\mathcal{I}_\mu$) and a contribution from the micro-scale generalized displacement fluctuation $\tilde{u}_\mu$ (the solution of the micro-scale equilibrium problem). Once the micro-equilibrium problem is solved (for the history u_μ^t), with the micro-scale stress field delivered by the given micro-scale constitutive equation, the macro-scale stress $\Sigma_M|_{\mathbf{x}}$ is obtained by means of the homogenization operation* (131)*.*

5 Multiscale tangent constitutive operators

The linearization of non-linear problems plays an important role both in theoretical and computational continuum mechanics. This issue is particulary relevant in non-linear solid mechanics [73]. In the theoretical context, linearization can be essential in the determination of crucial properties, such as the stability of solutions, for instance. In the computational setting, linearization becomes especially important in the solution of approximate (discretized) non-linear problems – typically undertaken by iterative numerical methods relying on the sequential solution of linearized problems. In particular, the widely used Newton-Raphson iterative algorithm, whose key advantage is the quadratic rate of asymptotic convergence, requires the exact linearization of the problem at each iteration.

Our main concern here is the derivation of an exact canonical form for the constitutive tangent operators arising in multiscale theories of the type discussed in Section 4, i.e. theories classed here as *purely constitutive*, for which only the internal virtual powers play a role in the scale transition. More specifically, the formulae derived here will be restricted to the case alluded in Remark 21, where the micro-scale constitutive law is such that the micro-scale generalized stresses at each point of the RVE are functions of the history of the corresponding generalized strain actions at that point. The tangent operators will be derived by consistently linearizing the corresponding problems in the continuum setting, i.e. before any temporal or spatial discretization is introduced. The specific format taken by the tangent operators under different discretization schemes can be determined by simply introducing the relevant numerical aproximations into the continuum canonical expressions.

Firstly, let us briefly review the notion of tangent operator. To this end, consider a generic functional $\mathfrak{F}$ which, for example, depends on a field D and consider the perturbation

$$D_\epsilon = D + \epsilon\, \Delta D, \tag{132}$$

given by a scalar factor ϵ, in the direction of an *admissible* perturbation ΔD. Then, for sufficiently smooth functionals, the value of $\mathfrak{F}$ at D_ϵ can be expressed as

$$\mathfrak{F}(D_\epsilon) = \mathfrak{F}(D) + \epsilon\, \mathfrak{D}\mathfrak{F}(D)\Delta D + o(\epsilon), \tag{133}$$

where

$$\mathfrak{D}\mathfrak{F}(D)\Delta D \equiv \frac{d}{d\epsilon}\mathfrak{F}(D_\epsilon)\bigg|_{\epsilon=0} \tag{134}$$

denotes the *directional derivative* of the functional $\mathfrak{F}$ at D in the direction of ΔD and $o(\cdot)$ denotes a term such

that, for any scalar a,

$$\lim_{a\to 0}\frac{o(a)}{a}=0. \tag{135}$$

The first two terms on the right hand side of (133) define the linearization of functional $\mathfrak{F}$ at D in the direction of ΔD. If the representation (133) is valid for any ΔD, then the functional $\mathfrak{F}$ is said to be differentiable at D and the operator $\mathfrak{DF}$ defined by (134) is the *gradient* – or *tangent operator* - of $\mathfrak{F}$ at D.

5.1 Homogenized macro-scale constitutive functional

To start with let us recall that the generalized strain actions D_μ are related to macro-scale generalized strain actions $D_M|_{\mathbf{x}}$ and micro-scale generalized displacement fields u_μ by means of (111). Also, in the present case (alluded to in Remark 21), we shall limit ourselves to local micro-scale constitutive descriptions, represented by constitutive functions $\mathfrak{F}_\mu$ such that

$$\Sigma_\mu(\mathbf{y})=\mathfrak{F}_\mu(D^t_\mu(\mathbf{y})), \tag{136}$$

or, in view of (111), with an obvious notation,

$$\Sigma_\mu=\mathfrak{F}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})+\mathcal{D}(\tilde{u}^t_\mu)). \tag{137}$$

With the above considerations, the micro-scale equilibrium problem (Problem 2), reduces in the present case to the following: Given a constitutive function $\mathfrak{F}_\mu$, of the above type, and a history $D^t_M|_{\mathbf{x}}$ of the macro-scale generalized strain actions at point $\mathbf{x}$, find the history $\tilde{u}^t_\mu\in \mathrm{Kin}_{\tilde{u}_\mu}$ of kinematically admissible micro-scale generalized displacement fluctuations such that

$$\langle \mathfrak{F}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})+\mathcal{D}(\tilde{u}^t_\mu)),\mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu\times\mathcal{E}_\mu}=0 \quad \forall\hat{\tilde{u}}_\mu\in \mathrm{Var}_{\tilde{u}_\mu},\forall\tau\in[0,t]. \tag{138}$$

Clearly, the solution of the above problem defines a mapping between histories of generalized macro-scale displacements $D^t_M|_{\mathbf{x}}$ and histories $\tilde{u}^t_\mu$ of generalized micro-scale displacements. This will be represented by a (generally non-linear) operator, $\mathfrak{C}_\mu$, i.e.

$$\tilde{u}^t_\mu=\mathfrak{C}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})) \tag{139}$$

By replacing this definition into (137), we have

$$\Sigma_\mu=\mathfrak{F}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})+\mathcal{D}_\mu(\mathfrak{C}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})))). \tag{140}$$

Further, by taking into account the generalized stress homogenization operator $\mathfrak{H}^c_\Sigma$ introduced in (128), we obtain

$$\begin{aligned}\Sigma^\mu_M|_{\mathbf{x}} =\ & \mathfrak{H}^c_\Sigma(\mathfrak{F}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}})+\mathcal{D}_\mu(\mathfrak{C}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}}))))\\ =:\ & \mathfrak{F}^{hom}(D^t_M|_{\mathbf{x}}),\end{aligned} \tag{141}$$

where we have defined the *homogenized constitutive functional*, $\mathfrak{F}^{hom}$, that maps the history the of macro-scale generalized strain actions at point $\mathbf{x}$ into $\Sigma^\mu_M|_{\mathbf{x}}$.

5.2 Homogenized macro-scale constitutive tangent

The *homogenized (macro-scale) constitutive tangent operator* is a tangent operator associated with the functional $\mathfrak{F}^{hom}$. To derive it, we first apply the directional derivative formula (134) to (141), noting that, except for $\mathfrak{F}_\mu$ and $\mathfrak{C}_\mu$, all operators involved in the definition of $\mathfrak{F}^{hom}$ are linear. This gives,

$$\begin{aligned}&\mathfrak{DF}^{hom}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]=\\ &\frac{d}{d\epsilon}\mathfrak{F}^{hom}(D^t_M|_{\mathbf{x}}+\epsilon\Delta D_M|_{\mathbf{x}})\Big|_{\epsilon=0}=\\ &=\mathfrak{H}^c_\Sigma\{\mathfrak{DF}_\mu(D^t_\mu)(\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}})+\\ &\qquad\mathcal{D}_\mu(\mathfrak{DC}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}}))\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}})))\},\end{aligned} \tag{142}$$

or, due to the linearity of all operators involved in the above linearized expression,

$$\begin{aligned}&\mathfrak{DF}^{hom}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]=\\ &\mathfrak{H}^c_\Sigma\{\mathfrak{DF}_\mu(D^t_\mu)\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}})\}+\\ &\quad\mathfrak{H}^c_\Sigma\{\mathfrak{DF}_\mu(D^t_\mu)\mathcal{D}_\mu(\mathfrak{DC}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}}))\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}}))\}.\end{aligned} \tag{143}$$

The first term on the right hand side of the above expression is the contribution to the directional derivative when $\tilde{u}_\mu$ is held fixed. This corresponds to the linearization of the macro-scale generalized stress response under the assumption of generalized Taylor kinematical constraint (referred to in Remark 14). This motivates the following definition:

$$\begin{aligned}&\mathfrak{DF}^{Taylor}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]=\\ &\qquad\mathfrak{H}^c_\Sigma\{\mathfrak{DF}_\mu(D^t_\mu)\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}})\}.\end{aligned} \tag{144}$$

With this notation we re-write expression (143) as

$$\begin{aligned}&\mathfrak{DF}^{hom}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]=\\ &\quad\mathfrak{DF}^{Taylor}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]+\mathfrak{L}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}],\end{aligned} \tag{145}$$

where $\mathfrak{L}(D^t_M|_{\mathbf{x}})$ is the linear operator defined by

$$\begin{aligned}&\mathfrak{L}(D^t_M|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]=\\ &\quad\mathfrak{H}^c_\Sigma\{\mathfrak{DF}_\mu(D^t_\mu)\mathcal{D}_\mu(\mathfrak{DC}_\mu(\mathcal{I}_\mu(D^t_M|_{\mathbf{x}}))\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}}))\}.\end{aligned} \tag{146}$$

This term is the contribution to the directional derivative stemming from the linearization of the (generally

non-linear) operator $\mathfrak{C}_\mu$, defined by (139) and associated with the solution of the (generally non-linear) variational equation (138). Further insight into this contribution can be gained by looking into the linearization of (138) about an RVE equilibrium state with given macro-scale generalized strain actions history D_M^t. The linearized problem reads: Given a field $\Delta D_M|_{\mathbf{x}}$, find the field $\Delta\tilde{u}_\mu \in \mathrm{Var}_{\tilde{u}_\mu}$ that solves the following *linear* variational equation:

$$\begin{aligned}\langle \mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{D}_\mu(\Delta\tilde{u}_\mu), \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu\times\mathcal{E}_\mu} = \\ - \langle \mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}}), \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu\times\mathcal{E}_\mu} \\ \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu}. \quad (147)\end{aligned}$$

The above equation defines the linear (tangent) operator $\mathfrak{D}\mathfrak{C}_\mu(D_M^t|_{\mathbf{x}})$ associated to the operator introduced in equation (139). Clearly, $\mathfrak{D}\mathfrak{C}_\mu(D_M^t|_{\mathbf{x}})$ also depends on the choice of the space $\mathrm{Var}_{\tilde{u}_\mu}$, i.e. on the chosen kinematical constraints imposed on the RVE-based model. In the case of the generalized Taylor constraint ($\tilde{u}_\mu \equiv 0$), the tangent operator $\mathfrak{D}\mathfrak{C}_\mu(D_M^t|_{\mathbf{x}})$ is the null operator. Moreover, the above equation has an appealing interpretation. In fact, its right hand side can be seen as a virtual power associated to a *reactive body force* field b_μ^r defined by

$$\begin{aligned}\langle b_\mu^r, \hat{\tilde{u}}_\mu\rangle_{\mathcal{U}'_\mu\times\mathcal{U}_\mu} = \\ - \langle \mathcal{D}'_\mu\mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}}), \hat{\tilde{u}}_\mu\rangle_{\mathcal{U}'_\mu\times\mathcal{U}_\mu} \\ \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu} \quad (148)\end{aligned}$$

that would result if the RVE (with linearized constitutive equation) were subjected to a prescribed generalized strain action $\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}})$. With use of a generalized tensorial canonical basis E_i, $i = 1, \ldots, m_M$, of $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$, $\Delta D_M|_{\mathbf{x}}$ can be expressed as

$$\Delta D_M|_{\mathbf{x}} = (\Delta D_M|_{\mathbf{x}})_i\, E_i, \quad (149)$$

with implied summation on the repeated index. Then, the solution $\Delta\tilde{u}_\mu$ of the linear variational equation (147) can be expressed as

$$\Delta\tilde{u}_\mu = (\Delta D_M|_{\mathbf{x}})_i \Delta\tilde{u}_\mu^i, \quad (150)$$

where $\Delta\tilde{u}_\mu^i$, here referred to as *tangential generalized displacement fluctuations*, are the solutions of the linear variational problems

$$\begin{aligned}\langle \mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{D}_\mu(\Delta\tilde{u}_\mu^i), \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu\times\mathcal{E}_\mu} = \\ - \langle \mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{I}_\mu(E_i), \mathcal{D}_\mu(\hat{\tilde{u}}_\mu)\rangle_{\mathcal{E}'_\mu\times\mathcal{E}_\mu} \\ \forall \hat{\tilde{u}}_\mu \in \mathrm{Var}_{\tilde{u}_\mu}, \quad (151)\end{aligned}$$

for $i = 1, \ldots, m_M$.

Now, note that the linearization of (139) gives

$$\Delta\tilde{u}_\mu = \mathfrak{D}\mathfrak{C}_\mu(\mathcal{I}_\mu(D_M^t|_{\mathbf{x}}))\mathcal{I}_\mu(\Delta D_M|_{\mathbf{x}}). \quad (152)$$

Then, with the solutions of (151) at hand, the contribution $\mathfrak{L}(D_M^t|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}]$ to (145) can now be easily evaluated through the expression

$$\mathfrak{L}(D_M^t|_{\mathbf{x}})[\Delta D_M|_{\mathbf{x}}] = \mathfrak{H}^c_\Sigma\{\mathfrak{D}\mathfrak{F}_\mu(D_\mu^t)\mathcal{D}_\mu(\Delta\tilde{u}_\mu)\}, \quad (153)$$

with $\Delta\tilde{u}_\mu$ given by (150). The linearized operator $\mathfrak{D}\mathfrak{F}^{hom}$ can be assembled according to (145).

Finally, by linearizing (154) we find that the *homogenized tangent constitutive operator* at the macro-scale point $\mathbf{x}$, is the operator $\mathfrak{D}\Sigma_M|_{\mathbf{x}}$ that satisfies

$$\begin{aligned}(\mathfrak{D}\Sigma_M|_{\mathbf{x}} - \mathfrak{D}\mathfrak{F}^{hom}(D_M^t|_{\mathbf{x}}))[\Delta D_M|_{\mathbf{x}}] \bullet \hat{D}_M|_{\mathbf{x}} = 0 \\ \forall \Delta D_M|_{\mathbf{x}}, \hat{D}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (154)\end{aligned}$$

Remark 22 *The derivation of the tangent operator has been limited here to what we refer to as the* purely constitutive case*, i.e. when the macro-scale generalized stress response functional obeys a standard local constitutive law. This has been motivated by the fact that the vast majority of multiscale theories reported in the literature falls into this category. We remark, however, that the derivation of more general tangent stress-response operators, within the broader setting of the theory proposed in Section 3, can be carried out by following the same steps.*

6 Applications

In this section, the *Method of Multiscale Virtual Power* is applied to formulate a range of multiscale models. In this context, some existing models already reported in the literature are cast within the proposed framework and new multiscale models, incorporating more complex phenomena, are newly derived. Our main aim here is to demonstrate by means of practical examples that the methodology proposed in the present paper offers indeed a very robust theoretical framework whereby existing multiscale models can be rigorously justified and new models can be systematically devised in a clear manner. In particular, it becomes obvious in the examples presented here that RVE boundary conditions as well as the dual homogenization operators (for the stress- and force-like quantities) – issues that may easily lead to theoretical inconsistencies if not addressed properly – can be derived in a most natural way as a result of duality considerations and the Principle of Multiscale Virtual Power. Each of the multiscale models is

discussed in an individual subsection and models are derived by following identical steps: We start with a brief description of the underlying micro- and macro-scale kinematics, followed by the definition of kinematical admissibility and application of the Principle of Multiscale Virtual Power.

At last, the mathematical setting employed in the presentation of the mechanical models throughout this section follows the standard choice of Sobolev function spaces.

6.1 Classical finite strain solid mechanics with dynamic effects

This section derives a multiscale model of a classical solid undergoing finite straining, subjected to dynamic forces. At variance with the vast majority of published articles on multiscale solid mechanics, we shall consider here the presence of dynamic forces at the micro-scale and their link to their macro-scale counterpart (assumed to share the same time scale). In the context of the framework proposed in this paper, this will require that the virtual power of dynamic forces at both macro- and micro-scales be accounted for in the definition of the Principle of Multiscale Virtual Power.

The model will be formulated in terms of the reference configurations (taken as the initial configurations) both at macro- and micro-scales. To start with, let the open subset $\Omega_M \subset \mathbb{R}^3$ be the reference domain occupied by the macro-scale solid body, with smooth boundary Γ_M and outward unit boundary normal $\mathbf{N}_M$. Points of the body will be described by their reference coordinates $\mathbf{X}$. The set of generalized displacements in the present case contains only the displacement vector field: $u_M = \mathbf{U}_M$. The space of generalized displacements in this case is $\mathcal{U}_M = \mathbf{H}^1(\Omega_M)$. The strain action operator here is the reference gradient operator, $\mathcal{D}_M(\cdot) = \nabla_{\mathbf{X}}(\cdot)$, so that the generalized strain action is the displacement gradient, that is, $D_M = \mathbf{G}_M(\mathbf{U}_M) = \nabla_{\mathbf{X}}\mathbf{U}_M$. Hence, the space of generalized strain actions reads $\mathcal{E}_M = \mathbf{L}^2(\Omega_M)$. In this case, we have $n_M = 1$ ($R_M = 3$) and $m_M = 1$ ($S_M = 9$).

At the micro-scale the finite strain regime also holds, and the RVE domain is $\Omega_\mu \subset \mathbb{R}^3$, with smooth boundary Γ_μ (outward unit normal $\mathbf{N}_\mu$), and coordinates $\mathbf{Y}$. The generalized displacements are the micro-scale displacement vector field $u_\mu = \mathbf{U}_\mu = \bar{\mathbf{U}}_\mu + \tilde{\mathbf{U}}_\mu$. The corresponding function space is $\mathcal{U}_\mu = \mathbf{H}^1(\Omega_\mu)$. Analogously to the macro-scale we have $\mathcal{D}_\mu(\cdot) = \nabla_{\mathbf{Y}}(\cdot)$, so that $D_\mu = \mathbf{G}_\mu(\mathbf{U}_\mu) = \nabla_{\mathbf{Y}}\mathbf{U}_\mu$, and $\mathbf{G}_\mu \in \mathcal{E}_\mu = \mathbf{L}^2(\Omega_\mu)$. The strain action and displacement are also defined over the entire RVE domain so that $n_\mu = 1$ ($R_\mu = 3$) and $m_\mu = 1$ ($S_\mu = 9$).

The space of point-valued macro-scale displacements is given by $\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M} = \{\mathbf{W} \in \mathbb{R}^3, \mathbf{W} = \mathbf{U}_M|_{\mathbf{X}}, \mathbf{U}_M \in \mathcal{U}_M\}$, and the space of point-valued macro-scale strain actions is $\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M} = \{\mathbf{H} \in \mathbb{R}^{3\times 3}, \mathbf{H} = \mathbf{G}_M|_{\mathbf{X}}, \mathbf{G}_M \in \mathcal{E}_M\}$. In this case we have $\widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}} = \mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}$ and $\widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} = \mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}$.

The displacement insertion operator here is defined as

$$\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}}) = \mathbf{U}_M|_{\mathbf{X}}, \tag{155}$$

while the macro-scale strain action is inserted into the micro-scale according to

$$\mathcal{J}^{\mathcal{E}}_\mu(\mathbf{G}_M|_{\mathbf{X}}) = \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y} - \mathbf{Y}_o), \tag{156}$$

with $\mathbf{Y}_o$ the geometrical center of the RVE, i.e. $\mathbf{Y}_o = \frac{1}{\Omega_\mu}\int_{\Omega_\mu} \mathbf{Y}\, \Omega_\mu$. Having defined the above kinematical insertion operations, we then have for the micro-scale displacement field:

$$\mathbf{U}_\mu = \mathbf{U}_M|_{\mathbf{x}} + \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y} - \mathbf{Y}_o) + \tilde{\mathbf{U}}_\mu. \tag{157}$$

Since $\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}})) = \nabla_{\mathbf{Y}}\mathbf{U}_M|_{\mathbf{x}} = \mathbf{0}$, it follows that

$$\mathbf{G}_\mu = \mathbf{G}_M|_{\mathbf{X}} + \nabla_{\mathbf{Y}}\tilde{\mathbf{U}}_\mu. \tag{158}$$

In addition, we have trivially,

$$\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\mathbf{G}_M|_{\mathbf{X}})) = \mathbf{G}_M|_{\mathbf{X}}. \tag{159}$$

We now proceed to postulate the kinematical homogenization operators. For the displacement, we define

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathbf{U}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{U}_\mu\, d\Omega_\mu, \tag{160}$$

and, for the strain action,

$$\mathcal{H}^{\mathcal{E}}_\mu(\mathbf{G}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_\mu\, d\Omega_\mu. \tag{161}$$

Note that, by construction of the above operators, the principle of conservation of macro-scale displacements (59) is automatically satisfied, that is, we have

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}})) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}})\, d\Omega_\mu = \mathbf{U}_M|_{\mathbf{X}}. \tag{162}$$

In order to define kinematical admissibility in the present case, we begin by specializing (61) with the above operators. Then, a micro-scale displacement field is said to be admissible if

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{U}_\mu\, d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}})\, d\Omega_\mu. \tag{163}$$

Further, by observing (157), the above definition of $\mathcal{J}_\mu^{\mathcal{U}}$ and the fact that

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o)\,d\Omega_\mu = \mathbf{0}, \tag{164}$$

we find that kinematically admissible micro-scale displacement fields must satisfy

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{U}}_\mu\,d\Omega_\mu = \mathbf{0}. \tag{165}$$

The principle of conservation of macro-scale strain actions (60) is, in turn, guaranteed here by the definition of the above strain action insertion and homogenization operators. Indeed, we have

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(G_M|_{\mathbf{X}}))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\mathbf{G}_M|_{\mathbf{X}}))\,d\Omega_\mu = \mathbf{G}_M|_{\mathbf{X}}. \tag{166}$$

The strain action is linked between scales by considering (see (62))

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_\mu\,d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\mathbf{G}_M|_{\mathbf{X}}))\,d\Omega_\mu, \tag{167}$$

which is met by doing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_{\mathbf{Y}}\tilde{\mathbf{U}}_\mu\,d\Omega_\mu = \mathbf{0}, \tag{168}$$

and integrating by parts gives

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu \otimes \mathbf{N}_\mu\,d\Gamma_\mu = \mathbf{0}. \tag{169}$$

Hence, the space of kinematically admissible displacement fields at micro scale is defined as

$$\mathrm{Kin}_{\tilde{\mathbf{U}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{U}}_\mu} = \Big\{\tilde{\mathbf{U}}_\mu \in \mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu}\tilde{\mathbf{U}}_\mu\,d\Omega_\mu = \mathbf{0},\ \int_{\Gamma_\mu}\tilde{\mathbf{U}}_\mu\otimes\mathbf{N}_\mu\,d\Gamma_\mu = \mathbf{0}\Big\}. \tag{170}$$

The internal virtual power at macro scale is the product between the virtual strain rate and the first Piola-Kirchhoff stress tensor, that is $P_M^{\mathrm{int}} = \int_{\Omega_M}\mathbf{P}_M\cdot\nabla_{\mathbf{X}}\hat{\mathbf{U}}_M\,d\Omega_M$. The internal power at point $\mathbf{X}$ (posteriorly linked with a RVE) is $P_{M,\mathbf{X}}^{\mathrm{int}} = \mathbf{P}_M|_{\mathbf{X}}\bullet\hat{\mathbf{G}}_M|_{\mathbf{X}}$, still to be defined. The external virtual power is $P_M^{\mathrm{ext}} = \int_{\Omega_M}\mathbf{f}_M\cdot\hat{\mathbf{U}}_M\,d\Omega_M$, and at point $\mathbf{X}$ it is $P_{M,\mathbf{X}}^{\mathrm{ext}} = \mathbf{f}_M|_{\mathbf{X}}\bullet\hat{\mathbf{U}}_M|_{\mathbf{X}}$. We note that $\mathbf{f}_M$ can be formed by a passive external load $\mathbf{f}_M^p$ (e.g. due to the gravity) and/or by an active dynamic load $\mathbf{f}_M^a$. We can write $\mathbf{f}_M = \mathbf{f}_M^p - \mathbf{f}_M^a$.

In turn, the internal virtual power at micro scale results

$$P_\mu^{\mathrm{int}} = \int_{\Omega_\mu}\mathbf{P}_\mu\cdot\nabla_{\mathbf{Y}}\hat{\mathbf{U}}_\mu\,d\Omega_\mu = \int_{\Omega_\mu}\mathbf{P}_\mu\cdot(\hat{\mathbf{G}}_M|_{\mathbf{X}}+\nabla_{\mathbf{Y}}\hat{\tilde{\mathbf{U}}}_\mu)\,d\Omega_\mu = \int_{\Omega_\mu}\mathbf{P}_\mu\cdot\hat{\mathbf{G}}_M|_{\mathbf{X}}\,d\Omega_\mu + \int_{\Omega_\mu}\mathbf{P}_\mu\cdot\nabla_{\mathbf{Y}}\hat{\tilde{\mathbf{U}}}_\mu\,d\Omega_\mu. \tag{171}$$

Dynamic phenomena is considered through the classical characterization of acceleration forces $\mathbf{f}_\mu^a = \rho_\mu\mathbf{A}_\mu$. Then, we can write

$$\mathbf{f}_\mu^a = \rho_\mu\mathbf{A}_\mu = \rho_\mu\ddot{\mathbf{U}}_\mu = \rho_\mu(\ddot{\mathbf{U}}_M|_{\mathbf{X}} + \ddot{\mathbf{F}}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o) + \ddot{\tilde{\mathbf{U}}}_\mu). \tag{172}$$

As well, passive forces are considered in the model and denoted by $\mathbf{f}_\mu^p$. Thus, the external virtual power can be expressed as

$$\begin{aligned} P_\mu^{\mathrm{ext}} &= \int_{\Omega_\mu}\mathbf{f}_\mu^p\cdot\hat{\mathbf{U}}_\mu\,d\Omega_\mu - \int_{\Omega_\mu}\rho_\mu\ddot{\mathbf{U}}_\mu\cdot\hat{\mathbf{U}}_\mu\,d\Omega_\mu = \\ &\int_{\Omega_\mu}\mathbf{f}_\mu^p\cdot(\hat{\mathbf{U}}_M|_{\mathbf{X}}+\hat{\mathbf{G}}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o)+\hat{\tilde{\mathbf{U}}}_\mu)\,d\Omega_\mu \\ &-\int_{\Omega_\mu}\rho_\mu\ddot{\mathbf{U}}_\mu\cdot(\hat{\mathbf{U}}_M|_{\mathbf{X}}+\hat{\mathbf{G}}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o)+\hat{\tilde{\mathbf{U}}}_\mu)\,d\Omega_\mu = \\ &\int_{\Omega_\mu}\mathbf{f}_\mu^p\cdot\hat{\mathbf{U}}_M|_{\mathbf{X}}\,d\Omega_\mu + \int_{\Omega_\mu}(\mathbf{f}_\mu^p\otimes(\mathbf{Y}-\mathbf{Y}_o))\cdot\hat{\mathbf{G}}_M|_{\mathbf{X}}\,d\Omega_\mu \\ &+\int_{\Omega_\mu}\mathbf{f}_\mu^p\cdot\hat{\tilde{\mathbf{U}}}_\mu\,d\Omega_\mu - \int_{\Omega_\mu}\rho_\mu\ddot{\mathbf{U}}_\mu\cdot\hat{\mathbf{U}}_M|_{\mathbf{X}}\,d\Omega_\mu \\ &-\int_{\Omega_\mu}\rho_\mu(\ddot{\mathbf{U}}_\mu\otimes(\mathbf{Y}-\mathbf{Y}_o))\cdot\hat{\mathbf{G}}_M|_{\mathbf{X}}\,d\Omega_\mu \\ &-\int_{\Omega_\mu}\rho_\mu\ddot{\mathbf{U}}_\mu\cdot\hat{\tilde{\mathbf{U}}}_\mu\,d\Omega_\mu. \end{aligned} \tag{173}$$

The Principle of Multiscale Virtual Power for the present case is enunciated next. In the remaining of this section recall that $\ddot{\mathbf{U}}_\mu = \ddot{\mathbf{U}}_M|_{\mathbf{X}} + \ddot{\mathbf{F}}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o) + \ddot{\tilde{\mathbf{U}}}_\mu$.

PMVP. *It is said that* $(\mathbf{P}_M|_{\mathbf{X}}, \mathbf{f}_M|_{\mathbf{X}})$ *and* $(\mathbf{P}_\mu, \mathbf{f}_\mu)$ *are equilibrated if the following variational equation is sat-*

isfied

$$\mathbf{P}_M|_{\mathbf{X}} \bullet \hat{\mathbf{G}}_M|_{\mathbf{X}} - \mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu + \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}^p_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}\, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}^p_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}^p_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu + \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{U}}_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}\, d\Omega_\mu + \int_{\Omega_\mu} \rho_\mu (\ddot{\mathbf{U}}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu + \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{U}}_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu \quad \forall (\hat{\mathbf{U}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\tilde{\mathbf{U}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} \times \mathrm{Var}_{\tilde{\mathbf{U}}_\mu}. \quad (174)$$

■

The consequences of the principle formulated above are the following.

Equilibrium problem at micro scale. Take $\hat{\mathbf{U}}_M|_{\mathbf{X}} = \mathbf{0}$ and $\hat{\mathbf{G}}_M|_{\mathbf{X}} = \mathbf{0}$. The equilibrium problem at the micro scale can be stated as follows

$$\int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}^p_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu + \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{U}}_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu\, d\Omega_\mu = 0 \quad \forall \hat{\tilde{\mathbf{U}}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{U}}_\mu}. \quad (175)$$

Stress homogenization at macro scale. Let now $\hat{\mathbf{U}}_M|_{\mathbf{X}} = \mathbf{0}$ and $\hat{\tilde{\mathbf{U}}}_\mu = \mathbf{0}$. Then

$$\mathbf{P}_M|_{\mathbf{X}} \bullet \hat{\mathbf{G}}_M|_{\mathbf{X}} = \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}^p_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu + \int_{\Omega_\mu} \rho_\mu (\ddot{\mathbf{U}}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}\, d\Omega_\mu \quad \forall \hat{\mathbf{G}}_M|_{\mathbf{X}} \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} \quad (176)$$

Therefore, the homogenization formula is

$$\mathbf{P}_M|_{\mathbf{X}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu - (\mathbf{f}^p_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o))\, d\Omega_\mu + \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \rho_\mu (\ddot{\mathbf{U}}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o))\, d\Omega_\mu. \quad (177)$$

Here, we have identified the operation $\mathbf{P}_M|_{\mathbf{X}} \bullet \hat{\mathbf{G}}_M|_{\mathbf{X}} = |\Omega_\mu|\, \mathbf{P}_M|_{\mathbf{X}} \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}}$, from which it is $\omega_1 = |\Omega_\mu|$.

Body force homogenization at macro scale. Now, consider $\hat{\mathbf{G}}_M|_{\mathbf{X}} = \mathbf{0}$ and $\hat{\tilde{\mathbf{U}}}_\mu = \mathbf{0}$, then

$$\mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = \int_{\Omega_\mu} \mathbf{f}^p_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}\, d\Omega_\mu - \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{U}}_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}\, d\Omega_\mu \quad \forall \hat{\mathbf{U}}_M|_{\mathbf{X}} \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}}. \quad (178)$$

and then

$$\mathbf{f}_M|_{\mathbf{X}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}^p_\mu - \rho_\mu \ddot{\mathbf{U}}_\mu)\, d\Omega_\mu. \quad (179)$$

Here, also the operation is identified as $\mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = |\Omega_\mu|\, \mathbf{f}_M|_{\mathbf{X}} \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}$, resulting in $\gamma_1 = |\Omega_\mu|$.

Remark 23 *This model considers continuum media at both scales. A fully analogous development could be carried out for a micro scale including molecular dynamics or even atomistic models. In such cases, the present theory leads to models similar to those presented in [4, 5, 131].*

6.2 Bar model at macro scale - Classical micro mechanics

This section presents a very simple mechanical model at the macro scale consisting of a bar (one dimensional) model for which it is desired to obtain constitutive multiscale information from a micro scale model consisting of a full (three-dimensional) model. For simplicity we consider infinitesimal strain hypothesis at both scales. Notice that the model at micro scale is kinematically richer than the model at the macro scale. Thus, this example illustrates a typical case of a multiscale formulation having dimensional heterogeneity in the kinematical description at macro and micro scales.

The domain in the macro scale is an open subset $\Omega_M \subset \mathbb{R}$, that is, a straight segment representing the configuration of the bar, for which axial coordinates are x, being $\mathbf{e}_x$ the unit vector in $\mathbb{R}^3$ in the axial direction. The generalized displacements is a scalar field $u_M = u_M$, standing for the displacement in the axial direction of the bar. Then the structure of the underlying space is $\mathcal{U}_M = H^1(\Omega_M)$. The strain action operator is simply $\mathcal{D}_M(\cdot) = \frac{d}{dx}(\cdot)$, so $D_M = d_M(u_M) = \frac{du_M}{dx}$, and therefore $D_M \in \mathcal{E}_M = L^2(\Omega_M)$. All fields are defined in Ω_M. Then, it is $n_M = 1$ ($R_M = 1$) and $m_M = 1$ ($S_M = 1$).

At the micro-scale we have full three-dimensional kinematics, so the RVE domain is $\Omega_\mu \subset \mathbb{R}^3$, with smooth

boundary Γ_μ (outward unit normal $\mathbf{n}_\mu$). Coordinates in the micro scale are $\mathbf{y}$. In this case, generalized displacements at micro scale are displacements vector fields, expressed as $u_\mu = \mathbf{u}_\mu = \bar{\mathbf{u}}_\mu + \tilde{\mathbf{u}}_\mu$, with an underlying structure given by $\mathcal{U}_\mu = \mathbf{H}^1(\Omega_\mu)$. The strain action operator is the classical symmetric gradient $\mathcal{D}_\mu(\cdot) = \nabla^S_{\mathbf{y}}(\cdot)$, so it is $D_\mu = \boldsymbol{\varepsilon}_\mu(\mathbf{u}_\mu) = \nabla^S_{\mathbf{y}}\mathbf{u}_\mu$, and then $\mathcal{E}_\mu = \{\boldsymbol{\varepsilon}_\mu \in \mathbf{L}^2(\Omega_\mu),\, \boldsymbol{\varepsilon}_\mu = \boldsymbol{\varepsilon}_\mu^T\}$. All fields are defined in Ω_μ. Here $n_\mu = 1$ ($R_\mu = 3$) and $m_\mu = 1$ ($S_\mu = 6$).

The intermediate space of point-valued displacements at macro scale is $\mathbb{R}^x_{\mathcal{U}_M} = \{w \in \mathbb{R},\, w = u_M|_x,\, u_M \in \mathcal{U}_M\}$, and for the strain actions we have $\mathbb{R}^x_{\mathcal{E}_M} = \{g \in \mathbb{R},\, g = d_M|_x,\, d_M \in \mathcal{E}_M\}$. In this case it is $\widehat{\mathbb{R}^x_{\mathcal{U}_M}} = \mathbb{R}^x_{\mathcal{U}_M}$ and $\widehat{\mathbb{R}^x_{\mathcal{E}_M}} = \mathbb{R}^x_{\mathcal{E}_M}$. The operator that inserts the displacement into the RVE domain is

$$\mathcal{J}^{\mathcal{U}}_\mu(u_M|_x) = u_M|_x \mathbf{e}_x, \tag{180}$$

resulting in a constant vector field over the entire RVE pointing in the axial direction of the bar. In turn, the strain rate from the macro scale is inserted into the micro scale as

$$\mathcal{J}^{\mathcal{E}}_\mu(d_M|_x) = d_M|_x(\mathbf{e}_x \otimes \mathbf{e}_x)(\mathbf{y} - \mathbf{y}_o), \tag{181}$$

with $\mathbf{y}_o$ the geometrical center of the RVE, i.e. $\mathbf{y}_o = \frac{1}{\Omega_\mu}\int_{\Omega_\mu} \mathbf{y}\, \Omega_\mu$. Then, the composition of the displacement field at micro scale is

$$\mathbf{u}_\mu = u_M|_x \mathbf{e}_x + d_M|_x(\mathbf{e}_x \otimes \mathbf{e}_x)(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu. \tag{182}$$

Since $\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(u_M|_x)) = \nabla^S_{\mathbf{y}}(u_M|_x \mathbf{e}_x) = \mathbf{0}$, it results

$$\boldsymbol{\varepsilon}_\mu = d_M|_x(\mathbf{e}_x \otimes \mathbf{e}_x) + \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu, \tag{183}$$

and also

$$\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(d_M|_x)) = d_M|_x(\mathbf{e}_x \otimes \mathbf{e}_x). \tag{184}$$

The homogenization operator for the displacement field is defined as follows

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathbf{u}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \cdot \mathbf{e}_x \, d\Omega_\mu, \tag{185}$$

and for the strain rate field the homogenization operator is

$$\mathcal{H}^{\mathcal{E}}_\mu(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Omega_\mu. \tag{186}$$

By construction, the insertion operator satisfies (i.e. equation (59) is satisfied)

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(u_M|_x)) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}^{\mathcal{U}}_\mu(u_M|_x) \cdot \mathbf{e}_x \, d\Omega_\mu = u_M|_x. \tag{187}$$

Then, the kinematical admissibility for the displacement field (see (61)) states that

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \cdot \mathbf{e}_x \, d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}^{\mathcal{U}}_\mu(u_M|_x) \cdot \mathbf{e}_x \, d\Omega_\mu. \tag{188}$$

Since it is

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} d_M|_x(\mathbf{e}_x \otimes \mathbf{e}_x)(\mathbf{y} - \mathbf{y}_o)\, d\Omega_\mu = \mathbf{0}, \tag{189}$$

we have that the condition (188) is satisfied by doing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \cdot \mathbf{e}_x \, d\Omega_\mu = 0. \tag{190}$$

However, this condition is not enough to control all the kinematic fields at the micro scale. Observe that components on the direction of y and z of the fluctuation field are not controled from the macro scale. In this case, further restrictions are necessary to have a mathematically well-posed problem. This can be accomplished by incorporating the following restrictions

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \cdot \mathbf{e}_y \, d\Omega_\mu = 0, \tag{191}$$

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \cdot \mathbf{e}_z \, d\Omega_\mu = 0. \tag{192}$$

Regarding strain actions, the insertion operator by definition satisfies the following identity (i.e. equation (60) is satisfied)

$$\mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(d_M|_x))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(d_M|_x)) \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Omega_\mu = d_M|_x. \tag{193}$$

Hence, the kinematical admissibility is met if we have (see (62))

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(d_M|_x)) \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Omega_\mu. \tag{194}$$

which is fulfilled by enforcing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Omega_\mu = 0. \tag{195}$$

Integrating by parts it is

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} (\tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu) \cdot (\mathbf{e}_x \otimes \mathbf{e}_x)\, d\Gamma_\mu = 0. \tag{196}$$

Then, the space of kinematically admissible displacement fields at micro scale is

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{u}}_\mu} = \Big\{ \tilde{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \int_{\Gamma_\mu} (\tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu) \cdot (\mathbf{e}_x \otimes \mathbf{e}_x) \, d\Gamma_\mu = 0 \Big\}. \quad (197)$$

In this case the internal virtual power at macro scale is given by the product $P_M^{\mathrm{int}} = \int_{\Omega_M} A_M \sigma_M \frac{d\hat{u}_M}{dx} \, d\Omega_M$, where recall that Ω_M is the one-dimensional domain of the bar, and A_M is the cross sectional area of the bar. In addition we called σ_M to the uniaxial stress in the bar, that is $\sigma_M = \frac{1}{A_M} \int_{A_M} \sigma_M \, dA_M$. The internal power at any macro scale point (which is to be linked with a RVE) is denoted by $P_{M,x}^{\mathrm{int}} = \sigma_M|_x \bullet \hat{d}_M|_x$. In turn, the external virtual power is $P_M^{\mathrm{ext}} = \int_{\Omega_M} A_M f_M \cdot \hat{u}_M \, d\Omega_M$, where f_M is the uniaxial load, and at a point in the macro scale is $P_{M,x}^{\mathrm{ext}} = f_M|_x \bullet \hat{u}_M|_x$.

At the micro scale, the internal virtual power results

$$P_\mu^{\mathrm{int}} = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\mathbf{u}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\hat{d}_M|_x (\mathbf{e}_x \otimes \mathbf{e}_x) + \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu) \, d\Omega_\mu = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu. \quad (198)$$

and, the external virtual power is written as

$$P_\mu^{\mathrm{ext}} = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot (\hat{u}_M|_x \mathbf{e}_x + \hat{d}_M|_x (\mathbf{e}_x \otimes \mathbf{e}_x)(\mathbf{y} - \mathbf{y}_o) + \hat{\tilde{\mathbf{u}}}_\mu) \, d\Omega_\mu = \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x) \hat{u}_M|_x \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x)((\mathbf{y} - \mathbf{y}_o) \cdot \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu + \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu. \quad (199)$$

Therefore, the formulation of the Principle of Multiscale Virtual Power is given by the following sentence.

PMVP. *It is said that* $(\sigma_M|_x, f_M|_x)$ *and* $(\boldsymbol{\sigma}_\mu, \mathbf{f}_\mu)$ *satisfy the Principle of Multiscale Virtual Power if the following variational equation is satisfied*

$$\sigma_M|_x \bullet \hat{d}_M|_x - f_M|_x \bullet \hat{u}_M|_x = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x) \hat{u}_M|_x \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x)((\mathbf{y} - \mathbf{y}_o) \cdot \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$$
$$\forall (\hat{u}_M|_x, \hat{d}_M|_x, \hat{\tilde{\mathbf{u}}}_\mu) \in \widehat{\mathbb{R}^x_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^x_{\mathcal{E}_M}} \times \mathrm{Var}_{\tilde{\mathbf{u}}_\mu} \quad (200)$$

■

The consequences of the principle enunciated above are listed below.

Equilibrium problem at micro scale. Now, consider $\hat{u}_M|_x = 0$ and $\hat{d}_M|_x = 0$. The equilibrium problem at the micro scale is defined by the following variational equation

$$\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu = 0 \quad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \quad (201)$$

Stress homogenization at macro scale. Let $\hat{u}_M|_x = 0$ and $\hat{\tilde{\mathbf{u}}}_\mu = 0$, then

$$\sigma_M|_x \bullet \hat{d}_M|_x = \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x)((\mathbf{y} - \mathbf{y}_o) \cdot \mathbf{e}_x) \hat{d}_M|_x \, d\Omega_\mu \quad \forall \hat{d}_M|_x \in \widehat{\mathbb{R}^x_{\mathcal{E}_M}} \quad (202)$$

And the homogenization formula results

$$\sigma_M|_x = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\mathbf{e}_x \otimes \mathbf{e}_x) \, d\Omega_\mu - \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}_\mu \cdot \mathbf{e}_x)((\mathbf{y} - \mathbf{y}_o) \cdot \mathbf{e}_x) \, d\Omega_\mu \quad (203)$$

As before, the duality operation is identified to be $\sigma_M|_x \bullet \hat{d}_M|_x = |\Omega_\mu| \, \sigma_M|_x \hat{d}_M|_x$, and it is $\omega_1 = |\Omega_\mu|$.

Body force homogenization at macro scale. Now, consider $\hat{d}_M|_x = 0$ and $\hat{\tilde{\mathbf{u}}}_\mu = 0$, which yields

$$f_M|_x \bullet \hat{u}_M|_x = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \mathbf{e}_x \hat{u}_M|_x \, d\Omega_\mu \quad \forall \hat{u}_M|_x \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \quad (204)$$

and then

$$f_M|_x = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{f}_\mu \cdot \mathbf{e}_x \, d\Omega_\mu. \tag{205}$$

Here the duality operation is defined to be $f_M|_x \bullet \hat{u}_M|_x = |\Omega_\mu| \; f_M|_x \hat{u}_M|_x$, and it is $\gamma_1 = |\Omega_\mu|$.

Remark 24 *Other models can be derived from the very same framework presented here. In fact, the model derived from considering the kinematical constrain* (196) *results in a model with null traction over the boundary of the micro scale domain in many of the components. Suppose that additional constraints are considered inspired in* (196)*, i.e.*

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} (\tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu) \, d\Gamma_\mu = 0. \tag{206}$$

Such model is kinematically more restricted, and results in a model with uniform traction over the entire boundary of the RVE, part of which is purely reactive.

6.3 High order macro mechanics - Classical micro mechanics

In this section we work with the multiscale modeling in solid mechanics applied to higher order continua at the macro scale, while keeping the classical first order continuum in the micro scale. That is, unlike the previous section, here the model at macro scale is kinematically richer than the model at the micro scale. At both scales we consider the finite strain mechanical regime.

The domain at macro scale (reference or material configuration) is an open subset $\Omega_M \subset \mathbb{R}^3$, with smooth boundary Γ_M (outward unit normal $\mathbf{N}_M$), and coordinates $\mathbf{X}$. Like in the classical setting, the generalized displacement is the displacement vector field described in the material configuration $u_M = \mathbf{U}_M$ (structure given by the space $\mathcal{U}_M = \mathbf{H}^1(\Omega_M)$). The strain action operator is given by $\mathcal{D}_M(\cdot) = (\nabla_{\mathbf{X}}(\cdot), \frac{1}{2}\nabla_{\mathbf{X}}\nabla_{\mathbf{X}}(\cdot))$. Thus, the structure of the strain action results $D_M = (\mathbf{G}_M(\mathbf{U}_M), \mathbf{G}_M(\mathbf{U}_M)) = (\nabla_{\mathbf{X}}\mathbf{U}_M, \frac{1}{2}\nabla_{\mathbf{X}}\nabla_{\mathbf{X}}\mathbf{U}_M)$. All fields are defined in Ω_M. The kinematics in the macro scale is such that $n_M = 1$ ($R_M = 3$) and $m_M = 2$ ($s^1_M = 9$, $s^2_M = 18$ and $S_M = 27$).

Further, given a third order tensor $\mathbf{H}$, we define a transpose operation as follows $(\mathbf{H}\mathbf{m})\mathbf{n} = (\mathbf{H}^{\mathsf{T}}\mathbf{n})\mathbf{m}$. Such transpose operation T can be more clearly written: being $\mathbf{H} = \mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c}$, we have $(\mathbf{H}\mathbf{m})\mathbf{n} = ((\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})\mathbf{m})\mathbf{n} = (\mathbf{c}\cdot\mathbf{m})(\mathbf{b}\cdot\mathbf{n})\mathbf{a}$. It follows that $(\mathbf{H}^{\mathsf{T}}\mathbf{n})\mathbf{m} = ((\mathbf{a}\otimes\mathbf{c}\otimes\mathbf{b})\mathbf{n})\mathbf{m} = (\mathbf{b}\cdot\mathbf{n})(\mathbf{c}\cdot\mathbf{m})\mathbf{a}$. Hence, it results $\mathbf{H}^{\mathsf{T}} = \mathbf{a}\otimes\mathbf{c}\otimes\mathbf{b}$. Finally, a symmetrization operation can be defined as $\mathbf{H}^{\mathsf{S}} = \frac{1}{2}(\mathbf{H} + \mathbf{H}^{\mathsf{T}})$. Therefore, it is $\mathcal{E}_M = \{(\mathbf{G}_M, \mathbf{G}_M) \in \mathbf{L}^2(\Omega_M)\times \boldsymbol{L}^2(\Omega_M),\, \mathbf{G}_M = \mathbf{G}_M^{\mathsf{T}}\}$.

At the micro-scale we adopt classic kinematical description. The RVE domain is $\Omega_\mu \subset \mathbb{R}^3$, with smooth boundary Γ_μ (outward unit normal $\mathbf{N}_\mu$) and coordinates $\mathbf{Y}$. The generalized displacements are displacements in the material configuration $u_\mu = \mathbf{U}_\mu = \bar{\mathbf{U}}_\mu + \tilde{\mathbf{U}}_\mu$, with structure $\mathcal{U}_\mu = \mathbf{H}^1(\Omega_\mu)$. The strain action operator is $\mathcal{D}_\mu(\cdot) = \nabla_{\mathbf{Y}}(\cdot)$, so $D_\mu = \mathbf{G}_\mu(\mathbf{U}_\mu) = \nabla_{\mathbf{Y}}\mathbf{U}_\mu$, from which $D_\mu \in \mathcal{E}_\mu = \mathbf{L}^2(\Omega_\mu)$. Here, the fields are defined in the entire RVE. So, $n_\mu = 1$ ($R_\mu = 3$) and $m_\mu = 1$ ($S_\mu = 9$).

The intermediate space of point-valued displacements at macro scale is given by $\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M} = \{\mathbf{W} \in \mathbb{R}^3, \mathbf{W} = \mathbf{U}_M|_{\mathbf{X}}, \mathbf{U}_M \in \mathcal{U}_M\}$, and for the strain actions $\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M} = \{(\mathbf{H},\mathbf{H}) \in \mathbb{R}^{3\times3}\times\mathbb{R}^{3\times3\times3},\quad (\mathbf{H},\mathbf{H}) = (\mathbf{G}_M|_{\mathbf{X}}, \mathbf{G}_M|_{\mathbf{X}}), (\mathbf{G}_M,\mathbf{G}_M) \in \mathcal{E}_M\}$. As in previous sections, here it is $\widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}} = \mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}$ and $\widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} = \mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}$. The insertion of the displacement field is given by the following operator

$$\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}}) = \mathbf{U}_M|_{\mathbf{X}}, \tag{207}$$

and the insertion of the strain action results

$$\mathcal{J}^{\mathcal{E}}_\mu((\mathbf{G}_M|_{\mathbf{X}}, \mathbf{G}_M|_{\mathbf{X}})) = \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o) + \frac{1}{2}\mathbf{G}_M|_{\mathbf{X}}\big[(\mathbf{Y}-\mathbf{Y}_o)\otimes(\mathbf{Y}-\mathbf{Y}_o) - \mathbf{J}\big], \tag{208}$$

where $\mathbf{Y}_o$ is the geometrical center of the RVE, that is $\mathbf{Y}_o = \frac{1}{\Omega_\mu}\int_{\Omega_\mu}\mathbf{Y}\, d\Omega_\mu$, and $\mathbf{J}$ is defined as

$$\mathbf{J} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbf{Y}-\mathbf{Y}_o)\otimes(\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu. \tag{209}$$

As a consequence, at micro scale it results

$$\mathbf{U}_\mu = \mathbf{U}_M|_{\mathbf{x}} + \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o) + \frac{1}{2}\mathbf{G}_M|_{\mathbf{X}}\big[(\mathbf{Y}-\mathbf{Y}_o)\otimes(\mathbf{Y}-\mathbf{Y}_o) - \mathbf{J}\big] + \tilde{\mathbf{U}}_\mu, \tag{210}$$

Since $\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{U}_M|_{\mathbf{X}})) = \nabla_{\mathbf{Y}}\mathbf{U}_M|_{\mathbf{x}} = \mathbf{0}$ and $\mathbf{J}$ is constant, we have

$$\mathbf{G}_\mu = \mathbf{G}_M|_{\mathbf{X}} + \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o) + \nabla_{\mathbf{Y}}\tilde{\mathbf{U}}_\mu. \tag{211}$$

where

$$\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\mathbf{G}_M|_{\mathbf{X}}, \mathbf{G}_M|_{\mathbf{X}})) = \mathbf{G}_M|_{\mathbf{X}} + \mathbf{G}_M|_{\mathbf{X}}(\mathbf{Y}-\mathbf{Y}_o). \tag{212}$$

Regarding the homogenization of the displacement field we define

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathbf{U}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{U}_\mu\, d\Omega_\mu. \tag{213}$$

The homogenization of the strain action is a more sensible step, but equally treated within the current framework. Observe that the homogenization operator maps

the strain action from micro scale into the macro scale. So, the present homogenization procedure is represented by a rectangular matrix operation (two rows, one column, see Remark 10). These two rows are

$$\mathcal{H}_\mu^{\mathcal{E}\,11}(\mathbf{G}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_\mu \, d\Omega_\mu, \tag{214}$$

$$\mathcal{H}_\mu^{\mathcal{E}\,21}(\mathbf{G}_\mu) = \frac{1}{|\Omega_\mu|}\left(\left[\int_{\Omega_\mu} \mathbf{G}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}}. \tag{215}$$

where the $(\cdot)^{\mathsf{S}}$ operation implies the symmetrization operation as introduced at the beginning of the section.

By construction, the insertion operator satisfies (equation (59) is verified)

$$\mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{U}_M|\mathbf{x})) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}_\mu^{\mathcal{U}}(\mathbf{U}_M|\mathbf{x})\, d\Omega_\mu = \mathbf{U}_M|\mathbf{x}. \tag{216}$$

As well, we must satisfy (see constraint (61))

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{U}_\mu \, d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{J}_\mu^{\mathcal{U}}(\mathbf{U}_M|\mathbf{x})\, d\Omega_\mu. \tag{217}$$

Trivially, we have

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_M|\mathbf{x}(\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu = \mathbf{0}. \tag{218}$$

and also

$$\frac{1}{2|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_M|\mathbf{x}\big[(\mathbf{Y}-\mathbf{Y}_o)\otimes(\mathbf{Y}-\mathbf{Y}_o)-\mathbf{J}\big]\, d\Omega_\mu = \mathbf{0}. \tag{219}$$

Therefore, by forcing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{U}}_\mu \, d\Omega_\mu = \mathbf{0}. \tag{220}$$

it is possible to guarantee the kinematical admissibility in (217) in terms of displacements. The operator which inserts the strain action in this case satisfies by definition (expression (60) is verified)

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{G}_M|\mathbf{x},\mathbf{0})))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{G}_M|\mathbf{x},\mathbf{0})))\, d\Omega_\mu = \mathbf{G}_M|\mathbf{x}, \tag{221}$$

and also it satisfies

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{0},\mathbf{G}_M|\mathbf{x})))) = \frac{1}{|\Omega_\mu|}\left(\left[\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{0},\mathbf{G}_M|\mathbf{x})))\otimes(\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}} = \mathbf{G}_M|\mathbf{x}. \tag{222}$$

In turn, kinematical admissibility concept concerning the strain action is satisfied if (see (62))

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{G}_\mu \, d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{G}_M|\mathbf{x},\mathbf{G}_M|\mathbf{x})))\, d\Omega_\mu, \tag{223}$$

$$\frac{1}{|\Omega_\mu|}\left(\left[\int_{\Omega_\mu} \mathbf{G}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}} = \frac{1}{|\Omega_\mu|}\left(\left[\int_{\Omega_\mu} \mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}(\mathbf{G}_M|\mathbf{x},\mathbf{G}_M|\mathbf{x}))\otimes(\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}}. \tag{224}$$

Observe that (223) is met by doing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_{\mathbf{Y}}\tilde{\mathbf{U}}_\mu \, d\Omega_\mu = \mathbf{0}, \tag{225}$$

which after integration by parts gives

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu \otimes \mathbf{N}_\mu \, d\Gamma_\mu = \mathbf{0}. \tag{226}$$

By exploiting the form of $\mathbf{G}_\mu$ we have that (224) is satisfied if

$$\frac{1}{|\Omega_\mu|}\left(\left[\int_{\Omega_\mu} \nabla_{\mathbf{Y}}\tilde{\mathbf{U}}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)\, d\Omega_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}} = \mathbf{0}, \tag{227}$$

which after integration by parts gives

$$\frac{1}{|\Omega_\mu|}\left(\left[\int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu\otimes\mathbf{N}_\mu\otimes(\mathbf{Y}-\mathbf{Y}_o)\, d\Gamma_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}} = \mathbf{0}. \tag{228}$$

Thus, the space of kinematically admissible displacement fields at micro scale is therefore defined as

$$\mathrm{Kin}_{\tilde{\mathbf{U}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{U}}_\mu} = \Big\{\tilde{\mathbf{U}}_\mu \in \mathbf{H}^1(\Omega_\mu), \int_{\Omega_\mu} \tilde{\mathbf{U}}_\mu \, d\Omega_\mu = \mathbf{0}, \int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu \otimes \mathbf{N}_\mu \, d\Gamma_\mu = \mathbf{0}, \left(\left[\int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu \otimes \mathbf{N}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o)\, d\Gamma_\mu\right]\mathbf{J}^{-1}\right)^{\mathsf{S}} = \mathbf{0}\Big\}. \tag{229}$$

Remark 25 *In the case of a square geometry (in two dimensional space) representing the micro scale domain, with length ℓ_μ, we have $\mathbf{J} = \frac{\ell_\mu}{12}\mathbf{I}$. Then,* (228) *simplifies to*

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \tilde{\mathbf{U}}_\mu \otimes \mathbf{N}_\mu \otimes^{S} (\mathbf{Y}-\mathbf{Y}_o)\, d\Gamma_\mu = \mathbf{0}. \tag{230}$$

which is consistent with the boundary condition postulated in [58], and slightly different to that one postulated

in [71]. However, boundary condition (228) *has been derived systematically within the present multiscale framework, and provides a robust argumentation for boundary conditions previously proposed in the literature.*

The internal virtual power at macro scale is the product between the generalized virtual strain action and the dual stresses, which in the present case turns to be $P_M^{\text{int}} = \int_{\Omega_M} [\mathbf{P}_M \cdot \nabla_{\mathbf{X}} \hat{\mathbf{U}}_M + \mathbf{Q}_M \cdot \nabla_{\mathbf{X}} \nabla_{\mathbf{X}} \hat{\mathbf{U}}_M] \, d\Omega_M$. This internal virtual power at a given point $\mathbf{X}$ is $P_{M,\mathbf{X}}^{\text{int}} = (\mathbf{P}_M|_{\mathbf{X}}, \mathbf{Q}_M) \bullet (\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}})$, which is specified later on. As before, the external virtual power results $P_M^{\text{ext}} = \int_{\Omega_M} \mathbf{f}_M \cdot \hat{\mathbf{U}}_M \, d\Omega_M$, and at a point $\mathbf{X}$ is $P_{M,\mathbf{X}}^{\text{ext}} = \mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}}$.

Differently, for the micro scale, the internal virtual power is

$$
\begin{aligned}
P_\mu^{\text{int}} &= \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\mathbf{U}}_\mu \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{P}_\mu \cdot (\hat{\mathbf{G}}_M|_{\mathbf{X}} + \hat{\mathbf{G}}_M|_{\mathbf{X}} (\mathbf{Y} - \mathbf{Y}_o) + \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu) \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{P}_\mu \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{P}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&\qquad + \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu. \quad (231)
\end{aligned}
$$

And the external virtual power is expressed as

$$
\begin{aligned}
P_\mu^{\text{ext}} &= \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{U}}_\mu \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{f}_\mu \cdot \Big(\hat{\mathbf{U}}_M|_{\mathbf{X}} + \hat{\mathbf{G}}_M|_{\mathbf{X}} (\mathbf{Y} - \mathbf{Y}_o) \\
&+ \frac{1}{2} \hat{\mathbf{G}}_M|_{\mathbf{X}} [(\mathbf{Y} - \mathbf{Y}_o) \otimes (\mathbf{Y} - \mathbf{Y}_o) - \mathbf{J}] + \hat{\tilde{\mathbf{U}}}_\mu \Big) \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}} \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&+ \frac{1}{2} \int_{\Omega_\mu} \big(\mathbf{f}_\mu \otimes [(\mathbf{Y} - \mathbf{Y}_o) \otimes (\mathbf{Y} - \mathbf{Y}_o) - \mathbf{J}] \big) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&\qquad + \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu. \quad (232)
\end{aligned}
$$

Then, the Principle of Multiscale Virtual Power for the present case is formulated as follows.

PMVP. *It is said that* $(\mathbf{P}_M|_{\mathbf{X}}, \mathbf{Q}_M|_{\mathbf{X}}, \mathbf{f}_M|_{\mathbf{X}})$ *and* $(\mathbf{P}_\mu, \mathbf{f}_\mu)$ *are equilibrated if the following variational equation is satisfied*

$$
\begin{aligned}
&(\mathbf{P}_M|_{\mathbf{X}}, \mathbf{Q}_M|_{\mathbf{X}}) \bullet (\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) - \mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = \\
&\int_{\Omega_\mu} \mathbf{P}_\mu \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{P}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&+ \int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu \\
&- \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}} \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&- \frac{1}{2} \int_{\Omega_\mu} \big(\mathbf{f}_\mu \otimes [(\mathbf{Y} - \mathbf{Y}_o) \otimes (\mathbf{Y} - \mathbf{Y}_o) - \mathbf{J}] \big) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&- \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu \\
&\forall (\hat{\mathbf{U}}_M|_{\mathbf{X}}, (\hat{\mathbf{F}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}), \hat{\tilde{\mathbf{U}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} \times \text{Var}_{\tilde{\mathbf{U}}_\mu}. \quad (233)
\end{aligned}
$$

■

The consequences of the principle formulated above are the following.

Equilibrium problem at micro scale. At first, take $\hat{\mathbf{U}}_M|_{\mathbf{X}} = \mathbf{0}$ and $(\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) = (\mathbf{0}, \mathbf{0})$. The equilibrium problem at the micro scale is formulated as follows

$$
\int_{\Omega_\mu} \mathbf{P}_\mu \cdot \nabla_{\mathbf{Y}} \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{U}}}_\mu \, d\Omega_\mu = 0 \quad \forall \hat{\tilde{\mathbf{U}}}_\mu \in \text{Var}_{\tilde{\mathbf{U}}_\mu}. \quad (234)
$$

Stress homogenization at macro scale. Consider $\hat{\mathbf{U}}_M|_{\mathbf{X}} = \mathbf{0}$ and $\hat{\tilde{\mathbf{U}}}_\mu = \mathbf{0}$. Then

$$
\begin{aligned}
&(\mathbf{P}_M|_{\mathbf{X}}, \mathbf{Q}_M|_{\mathbf{X}}) \bullet (\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) = \\
&\int_{\Omega_\mu} \mathbf{P}_\mu \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&+ \int_{\Omega_\mu} (\mathbf{P}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&- \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&- \frac{1}{2} \int_{\Omega_\mu} \big(\mathbf{f}_\mu \otimes [(\mathbf{Y} - \mathbf{Y}_o) \otimes (\mathbf{Y} - \mathbf{Y}_o) - \mathbf{J}] \big) \cdot \hat{\mathbf{G}}_M|_{\mathbf{X}} \, d\Omega_\mu \\
&\qquad \forall (\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}} \quad (235)
\end{aligned}
$$

Considering now $(\hat{\mathbf{G}}_M|_{\mathbf{X}}, \mathbf{0})$ we obtain the homogenization formula for the Piola-Kirchhoff stress tensor

$$
\mathbf{P}_M|_{\mathbf{X}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu - (\mathbf{f}_\mu \otimes (\mathbf{Y} - \mathbf{Y}_o)) \, d\Omega_\mu. \quad (236)
$$

In turn, taking $(\mathbf{0}, \hat{\mathbf{G}}_M|_{\mathbf{X}})$ we obtain the homogenization formula for the third order stress tensor

$$\mathbf{Q}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} (\mathbf{P}_\mu \otimes (\mathbf{Y}-\mathbf{Y}_o))^{\mathsf{S}}\, d\Omega_\mu - \frac{1}{2}\int_{\Omega_\mu} \mathbf{f}_\mu \otimes [(\mathbf{Y}-\mathbf{Y}_o)\otimes(\mathbf{Y}-\mathbf{Y}_o) - \mathbf{J}]\, d\Omega_\mu. \tag{237}$$

The symmetrization operation acting on the first term above derives from the orthogonality condition with respect to the symmetric third order tensor $\hat{\mathbf{G}}_M|_{\mathbf{X}}$ (see definition of $\widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{E}_M}}$). For this case, the duality operation is $(\mathbf{P}_M|_{\mathbf{X}}, \mathbf{Q}_M|_{\mathbf{X}}) \bullet (\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) = |\Omega_\mu|\mathbf{P}_M|_{\mathbf{X}}\cdot\hat{\mathbf{G}}_M|_{\mathbf{X}} + |\Omega_\mu|\mathbf{Q}_M|_{\mathbf{X}}\cdot\hat{\mathbf{G}}_M|_{\mathbf{X}}$ following that $\omega_1 = \omega_2 = |\Omega_\mu|$.

Body force homogenization at macro scale. Now, let us consider $(\hat{\mathbf{G}}_M|_{\mathbf{X}}, \hat{\mathbf{G}}_M|_{\mathbf{X}}) = (\mathbf{0}, \mathbf{0})$ and $\hat{\tilde{\mathbf{U}}}_\mu = \mathbf{0}$, then

$$\mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}\, d\Omega_\mu \quad \forall \hat{\mathbf{U}}_M|_{\mathbf{X}} \in \widehat{\mathbb{R}^{\mathbf{X}}_{\mathcal{U}_M}}. \tag{238}$$

therefore

$$\mathbf{f}_M|_{\mathbf{X}} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{f}_\mu\, d\Omega_\mu. \tag{239}$$

The duality operation for the external power results $\mathbf{f}_M|_{\mathbf{X}} \bullet \hat{\mathbf{U}}_M|_{\mathbf{X}} = |\Omega_\mu|\ \mathbf{f}_M|_{\mathbf{X}} \cdot \hat{\mathbf{U}}_M|_{\mathbf{X}}$, following that $\gamma_1 = |\Omega_\mu|$.

6.4 Cohesive macro cracks - Strain localization at micro

In this section we present a multiscale model that accounts for nucleation and evolution of cohesive surfaces at the macro-scale level as a way to characterize the degradation phenomena taking place at the micro-scale. In the RVE, some mechanical processes can lead to the material failure, such as strain localization, damage, shear band formation, and so on. For simplicity, the model is developed considering infinitesimal strain hypothesis at both scales, however its extension to finite strain theory is straightforward. Body force effects are also neglected for the sake of simplicity. Furthermore, the application of the present multiscale model is restricted to a point $\mathbf{x}$ after the nucleation of a macro-cohesive crack $\mathcal{S}_M$. The interested reader can follow [104,123] for a detailed description of a very simmilar to that presented here. In such contributions this approach has been called Failure-Oriented Multiscale Formulation (FOMF).

The domain at macro scale is $\Omega_M \in \mathbb{R}^3$, with boundary Γ_M (outward unit normal $\mathbf{n}_M$) and coordinates $\mathbf{x}$. At such scale, a crack has been nucleated due to material degradation, generating a surface $\mathcal{S}_M$ (with normal $\mathbf{n}_{\mathcal{S}}^M$). The kinematics at point $\mathbf{x}$ in the macro scale but not on the surface $\mathcal{S}_M$ is given by a displacement field $u_M = \mathbf{u}_M$ which is continuous, while on the surface $\mathcal{S}_M$ it is characterized by the pair $u_M = (\mathbf{u}_M, \boldsymbol{\beta}_M)$, where $\boldsymbol{\beta}_M$ is the displacement jump on the surface at the macro scale. So, the structure of the kinematics at the such scale is $\mathcal{U}_M = \mathbf{H}^1(\Omega_M) \times \mathbf{L}^2(\mathcal{S}_M)$. The strain action operator is $\mathcal{D}_M(\cdot) = (\nabla^S_{\mathbf{x}}(\cdot), \cdot)$. So, over the surface the strain is given by the pair $D_M = (\boldsymbol{\varepsilon}_M(\bar{\mathbf{u}}_M), \boldsymbol{\beta}_M) = (\nabla^S_{\mathbf{x}}\bar{\mathbf{u}}_M, \boldsymbol{\beta}_M)$. Thus, it is $\mathcal{E}_M = \{(\boldsymbol{\varepsilon}_M, \boldsymbol{\beta}_M) \in \mathbf{L}^2(\Omega_M) \times \mathbf{L}^2(\mathcal{S}_M),\ \boldsymbol{\varepsilon}_M = \boldsymbol{\varepsilon}_M^T\}$. Observe that while the continuous displacement and strain action are defined in Ω_M, the displacement jump is defined in $\mathcal{S}_M$. Hence, at macro scale we have $n_M = 2$ ($R_M = 6$) and $m_M = 2$ ($s^1_M = 6$, $s^2_M = 3$ and $S_M = 9$).

At the micro scale, the RVE is denoted as $\Omega_\mu \in \mathbb{R}^3$ (boundary Γ_μ, unit normal $\mathbf{n}_\mu$, coordinates $\mathbf{y}$). Due to material degradation mechanisms, a failure zone (where strain localization takes place) is identified, and denoted by $\Omega^L_\mu \subseteq \Omega_\mu$ (boundary Γ^L_μ, unit normal $\mathbf{n}^L_\mu$). This domain can be regarded as constructed by the product of a middle surface $\mathcal{S}_\mu$ (generally tortuous at the micro scale, with coordinates $\mathbf{y}_0$ and normal $\mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0)$) and a length $l_\mu(\mathbf{y}_0)$ representing the thickness of the strain localization zone. Note that $\mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}) = \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0)$ and $l_\mu(\mathbf{y}) = l_\mu(\mathbf{y}_0)$ because of the property which states that $\Pi^\mu_{\mathcal{S}}\mathbf{y} = \mathbf{y}_0$, being $\Pi^\mu_{\mathcal{S}}$ the orthogonal projection operator over the middle surface $\mathcal{S}_\mu$. At this scale, the displacement is characterized by the pair $u_\mu = (\mathbf{u}_\mu, \boldsymbol{\beta}_\mu)$, where $\mathbf{u}_\mu$ is defined in Ω_μ and is a continuous component of the displacement field, and $\boldsymbol{\beta}_\mu$ is a displacement field defined in Ω^L_μ. Then the structure of the kinematics at this scale is

$$\mathcal{U}_\mu = \mathbf{H}^1(\Omega_\mu) \times \mathbf{L}^2(\Omega^L_\mu). \tag{240}$$

The strain action operator at this scale is given by

$$\mathcal{D}_\mu(\cdot) = \left(\nabla^S_{\mathbf{y}}(\cdot), \phi^L_\mu(\mathbf{y})\, \frac{(\cdot)\otimes^S \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0)}{l_\mu(\mathbf{y}_0)}\right), \tag{241}$$

where

$$\phi^L_\mu(\mathbf{y}) = \begin{cases} 1 & \text{if } \mathbf{y} \in \Omega^L_\mu \\ 0 & \text{otherwise} \end{cases} \tag{242}$$

Then, we have

$$\mathcal{D}_\mu((\mathbf{u}_\mu, \boldsymbol{\beta}_\mu)) = \nabla^S_{\mathbf{y}}\mathbf{u}_\mu + \phi^L_\mu(\mathbf{y})\, \frac{\boldsymbol{\beta}_\mu \otimes^S \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0)}{l_\mu(\mathbf{y}_0)} \tag{243}$$

from which it is $\mathcal{E}_\mu = \{\boldsymbol{\varepsilon}_\mu \in \mathbf{L}^2(\Omega_\mu),\ \boldsymbol{\varepsilon}_\mu = \boldsymbol{\varepsilon}_\mu^T\}$. With this structure we have $n_\mu = 2$ ($r_\mu^1 = 3$, $r_\mu^2 = 3$ and $R_\mu = 6$) and $m_\mu = 1$ ($S_\mu = 6$).

For the intermediate point-valued spaces it is $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} = \{\mathbf{w} \in \mathbb{R}^3,\ \mathbf{w} = \mathbf{u}_M|_{\mathbf{x}},\ \mathbf{u}_M \in \mathcal{U}_M\}$ and $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} = \{(\boldsymbol{\epsilon}, \mathbf{b}) \in \mathbb{R}^{3\times 3} \times \mathbb{R}^3,\ (\boldsymbol{\epsilon}, \mathbf{b}) = (\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\beta}_M|_{\mathbf{x}}),\ (\boldsymbol{\varepsilon}_M, \boldsymbol{\beta}_M) \in \mathcal{E}_M\}$. Note here that not all the kinematic fields from the macro scale play a role in the kinematic transfer, i.e. field $\boldsymbol{\beta}_M$ is not considered as part of the generalized displacement to be inserted into the micro scale, but it is considered as a generalized strain action. For this case it is $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} = \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and, unlike previous examples, we have now $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} = \{(\boldsymbol{\epsilon}, \mathbf{b}) \in \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M},\ \boldsymbol{\epsilon} = 0\}$.

The insertion operator for the generalized macro displacement is

$$\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}}) = (\mathbf{u}_M|_{\mathbf{x}}, \mathbf{0}) \tag{244}$$

i.e only $\mathbf{u}_M|_{\mathbf{x}}$ is uniformly inserted in the entire domain Ω_μ. The generalized strain actions provided from the macro scale is inserted as follows

$$\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\beta}_M|_{\mathbf{x}})) = \left(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o), \frac{\boldsymbol{\beta}_M|_{\mathbf{x}}}{\theta}\right), \tag{245}$$

where the first component is the displacement at micro scale obtained through an affine insertion of the macro deformation ($\boldsymbol{\varepsilon}_M|_{\mathbf{x}}$) over the entire RVE, and the second component is a displacement field ($\boldsymbol{\beta}_\mu$) obtained from a uniform insertion over Ω_μ^L of the jump displacement at macro scale $\boldsymbol{\beta}_M|_{\mathbf{x}}$, which is also a component of the generalized strain action at point $\mathbf{x}$ of the macro crack $\mathcal{S}_M$. In addition, $\mathbf{y}_o = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{y}\, d\Omega_\mu$ (the geometric center of the RVE), and θ is a non-dimensional parameter given by

$$\theta = \frac{1}{|\mathcal{S}_\mu|}\left\| \int_{\Omega_\mu^L} \frac{\mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)}{l_\mu(\mathbf{y}_0)}\, d\Omega_\mu^L \right\|, \tag{246}$$

where $|\mathcal{S}_\mu|$ means the measure of the middle surface $\mathcal{S}_\mu$. Taking into account the above definitions and that $l_\mu(\mathbf{y}_0)$ measures the thickness of the localization domain Ω_μ^L at point $\mathbf{y}_0$, the parameter θ could be rewritten as follows

$$\theta = \frac{1}{|\mathcal{S}_\mu|}\left\| \int_{\Omega_\mu^L} \frac{\mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)}{l_\mu(\mathbf{y}_0)}\, d\Omega_\mu^L \right\| = \frac{1}{|\mathcal{S}_\mu|}\left\| \int_{\mathcal{S}_\mu} \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)\, d\mathcal{S}_\mu \right\|. \tag{247}$$

Hence, θ can be interpreted as a *tortuosity index* of the surface $\mathcal{S}_\mu$. In fact, if $\mathcal{S}_\mu$ is a plane we have $\theta = 1$, see [104] where this approach was adopted. With the introduction of the tortuosity index the model in [104] is extended to take into account more complex situations. The need to introduce the factor θ has a strict kinematical justification in order to preserve the magnitude of the inserted macro-displacement jump $\boldsymbol{\beta}_M|_{\mathbf{x}}$, which becomes evident later (see (260)).

Besides, it is defined $\overline{\mathbf{n}_{\mathcal{S}}^\mu}$ as a unit vector given by

$$\overline{\mathbf{n}_{\mathcal{S}}^\mu} = \frac{\int_{\mathcal{S}_\mu} \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)\, d\mathcal{S}_\mu}{\left\| \int_{\mathcal{S}_\mu} \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)\, d\mathcal{S}_\mu \right\|}. \tag{248}$$

Moreover, we assume that the fluctuation related to the field $\boldsymbol{\beta}_\mu$, denoted by $\tilde{\boldsymbol{\beta}}_\mu$ is null. Then, at micro scale we have

$$(\mathbf{u}_\mu, \boldsymbol{\beta}_\mu) = \left(\mathbf{u}_M|_{\mathbf{x}} + \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o) + \tilde{\mathbf{u}}_\mu, \frac{\boldsymbol{\beta}_M|_{\mathbf{x}}}{\theta}\right). \tag{249}$$

And the strain action at micro scale results

$$\boldsymbol{\varepsilon}_\mu = \mathcal{D}_\mu((\mathbf{u}_\mu, \boldsymbol{\beta}_\mu)) = \boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \nabla_{\mathbf{y}}^S \tilde{\mathbf{u}}_\mu + \phi_\mu^L(\mathbf{y}) \frac{\boldsymbol{\beta}_M|_{\mathbf{x}} \otimes^S \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)}{\theta\, l_\mu(\mathbf{y}_0)}. \tag{250}$$

In view of the characteristics of space $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}$, we have that the virtual strain action (or kinematically admissible variations of the strain) becomes

$$\hat{\boldsymbol{\varepsilon}}_\mu = \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu + \phi_\mu^L(\mathbf{y}) \frac{\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} \otimes^S \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)}{\theta\, l_\mu(\mathbf{y}_0)}. \tag{251}$$

Here, it is verified that

$$\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}})) = \mathbf{0}, \tag{252}$$

and

$$\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\beta}_M|_{\mathbf{x}}))) = \boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \phi_\mu^L(\mathbf{y})\, \frac{\boldsymbol{\beta}_M|_{\mathbf{x}} \otimes^S \mathbf{n}_{\mathcal{S}}^\mu(\mathbf{y}_0)}{\theta\, l_\mu(\mathbf{y}_0)}. \tag{253}$$

We now define the homogenization of the generalized micro displacement fields. This linear aplication maps generalized displacements from $\mathcal{U}_\mu$ to $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$, so the operator can be represented by a 2×1 rectangular matrix where the only component to be characterized is

$$\mathcal{H}_\mu^{\mathcal{U}\,11}((\mathbf{u}_\mu, \boldsymbol{\beta}_\mu)) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu\, d\Omega_\mu, \tag{254}$$

while the remainder component is zero, since only $\mathbf{u}_M|_{\mathbf{x}}$ was inserted, see (244).

In turn, the homogenization of the strain action is performed through a linear rectangular operator (represented by a 2×1 matrix). We postulate the following block homogenization operators

$$\mathcal{H}_\mu^{\mathcal{E}\,11}(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu\, d\Omega_\mu, \quad \text{for } \mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \mathbf{0})) \tag{255}$$

$$\mathcal{H}_\mu^{\mathcal{E}\,21}(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\mathcal{S}_\mu|}\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Omega_\mu^L}\boldsymbol{\varepsilon}_\mu\, d\Omega_\mu^L\Big], \quad \text{for } \mathcal{J}_\mu^{\mathcal{E}}((\mathbf{0},\boldsymbol{\beta}_M|_{\mathbf{x}})) \quad (256)$$

where $\boldsymbol{\Pi}(\cdot)[\cdot]$ is a projection defined through the following operation

$$\boldsymbol{\Pi}(\mathbf{c})[\mathbf{a}\otimes^S\mathbf{b}] = (\mathbf{b}\cdot\mathbf{c})\mathbf{a} \quad \text{for any } \mathbf{a},\mathbf{b},\mathbf{c}. \quad (257)$$

Observe that, as stated by (59), the insertion operator $\mathcal{J}_\mu^{\mathcal{U}}$ satisfies

$$\mathcal{H}_\mu^{\mathcal{U}\,11}(\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}})) = \mathcal{H}_\mu^{\mathcal{U}\,11}((\mathbf{u}_M|_{\mathbf{x}},\mathbf{0})) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{u}_M|_{\mathbf{x}}d\Omega_\mu = \mathbf{u}_M|_{\mathbf{x}}. \quad (258)$$

Now we show that expression (60) (which constraints the choice of $\mathcal{J}_\mu^{\mathcal{E}}$) also holds. First note that applying (255) to (253), the definition of $\mathcal{J}_\mu^{\mathcal{E}}$ satisfies

$$\mathcal{H}_\mu^{\mathcal{E}\,11}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\mathbf{0})))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\varepsilon}_M|_{\mathbf{x}}\,d\Omega_\mu = \boldsymbol{\varepsilon}_M|_{\mathbf{x}}. \quad (259)$$

Second, applying (256) to (253), and using the definitions (247)-(248), $\mathcal{J}_\mu^{\mathcal{E}}$ satisfies

$$\mathcal{H}_\mu^{\mathcal{E}\,21}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\mathbf{0},\boldsymbol{\beta}_M|_{\mathbf{x}})))) = \frac{1}{|\mathcal{S}_\mu|}\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Omega_\mu^L}\frac{\boldsymbol{\beta}_M|_{\mathbf{x}}\otimes^S\mathbf{n}_{\mathcal{S}}^{\mu}(\mathbf{y}_0)}{\theta l_\mu(\mathbf{y}_0)}\,d\Omega_\mu^L\Big] = \boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\boldsymbol{\beta}_M|_{\mathbf{x}}\otimes^S\frac{1}{\theta|\mathcal{S}_\mu|}\int_{\mathcal{S}_\mu}\mathbf{n}_{\mathcal{S}}^{\mu}(\mathbf{y}_0)\,d\mathcal{S}_\mu\Big] = \boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\big[\boldsymbol{\beta}_M|_{\mathbf{x}}\otimes^S\overline{\mathbf{n}_{\mathcal{S}}^{\mu}}\big] = \boldsymbol{\beta}_M|_{\mathbf{x}}. \quad (260)$$

Let us apply the kinematical admissibility concept for generalized displacements. We require that (see (61))

$$\mathcal{H}_\mu^{\mathcal{U}\,11}((\mathbf{u}_\mu,\boldsymbol{\beta}_\mu)) = \mathcal{H}_\mu^{\mathcal{U}\,11}(\mathcal{J}_\mu^{\mathcal{U}}(\mathbf{u}_M|_{\mathbf{x}})). \quad (261)$$

Constraint (261) is accomplished by forcing

$$\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0}. \quad (262)$$

Concerning the kinematical admissibility for strain actions, we must satisfy (see expression (62))

$$\mathcal{H}_\mu^{\mathcal{E}\,11}(\boldsymbol{\varepsilon}_\mu) = \mathcal{H}_\mu^{\mathcal{E}\,11}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\boldsymbol{\beta}_M|_{\mathbf{x}})))), \quad (263)$$

$$\mathcal{H}_\mu^{\mathcal{E}\,21}(\boldsymbol{\varepsilon}_\mu) = \mathcal{H}_\mu^{\mathcal{E}\,21}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\boldsymbol{\beta}_M|_{\mathbf{x}})))). \quad (264)$$

From the structure of the $\mathcal{H}_\mu^{\mathcal{E}\,11}$-component, given by (255), constraint (263) yields the following definition of kinematical admissibility

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\varepsilon}_\mu\,d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\boldsymbol{\beta}_M|_{\mathbf{x}})))\,d\Omega_\mu \quad (265)$$

Then, since (259) holds, and considering (250), expression (265) is fulfilled if

$$\int_{\Omega_\mu}\nabla_{\mathbf{y}}^S\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0}, \quad (266)$$

which is equivalent to

$$\int_{\Gamma_\mu}\tilde{\mathbf{u}}_\mu\otimes^S\mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0}. \quad (267)$$

On the other hand, from the $\mathcal{H}_\mu^{\mathcal{E}\,21}$-component of the homogenization operator, see (256), the kinematical admissibility requirement (264) results in

$$\frac{1}{|\mathcal{S}_\mu|}\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Omega_\mu^L}\boldsymbol{\varepsilon}_\mu\,d\Omega_\mu^L\Big] = \frac{1}{|\mathcal{S}_\mu|}\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Omega_\mu^L}\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\boldsymbol{\beta}_M|_{\mathbf{x}})))\,d\Omega_\mu^L\Big]. \quad (268)$$

Using (250) and (260), we get that condition (268) is satisfied whenever

$$\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Omega_\mu^L}\nabla_{\mathbf{y}}^S\tilde{\mathbf{u}}_\mu\,d\Omega_\mu^L\Big] = \mathbf{0}, \quad (269)$$

which, after integration by parts, results equivalent to

$$\boldsymbol{\Pi}(\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\Big[\int_{\Gamma_\mu^L}\tilde{\mathbf{u}}_\mu\otimes^S\mathbf{n}_\mu\,d\Gamma_\mu^L\Big] = \mathbf{0}, \quad (270)$$

and from definition (257), it yields

$$\int_{\Gamma_\mu^L}(\mathbf{n}_\mu\cdot\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\tilde{\mathbf{u}}_\mu\,d\Gamma_\mu^L = \mathbf{0}. \quad (271)$$

Thus, the space of kinematically admissible fluctuations for the $\mathbf{u}_\mu$-component of the displacement field at micro scale is defined as

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{u}}_\mu} = \Big\{\tilde{\mathbf{u}}_\mu\in\mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\,d\Omega_\mu = \mathbf{0},\ \int_{\Gamma_\mu}\tilde{\mathbf{u}}_\mu\otimes^S\mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0},\ \int_{\Gamma_\mu^L}\tilde{\mathbf{u}}_\mu(\mathbf{n}_\mu\cdot\overline{\mathbf{n}_{\mathcal{S}}^{\mu}})\,d\Gamma_\mu^L = \mathbf{0}\Big\}. \quad (272)$$

We recall here that $\tilde{\boldsymbol{\beta}}_\mu = \mathbf{0}$.

Remark 26 *In [104, 123], a slightly different kinematical formulation was derived. This remark describes such model. Only the kinematical ingredients which are different between the proposal of [104, 123] and the present approach are discussed here.*

The kinematical counterpart in terms of macro generalized strain actions, D_M, on the cohesive crack, was reinterpreted in the cited contributions. The strain action operator is defined as $\mathcal{D}_M(\cdot) = (\nabla^S_{\mathbf{x}}(\cdot), (\cdot) \otimes^S \overline{\mathbf{n}^{\mu}_{\mathcal{S}}})$. So, D_M is given by the pair $(\boldsymbol{\varepsilon}_M(\mathbf{u}_M), \boldsymbol{\varepsilon}^L_M(\boldsymbol{\beta}_M)) = (\nabla^S_{\mathbf{x}}\mathbf{u}_M, \boldsymbol{\beta}_M \otimes^S \overline{\mathbf{n}^{\mu}_{\mathcal{S}}})$. Then, it is $\mathcal{E}_M = \{(\boldsymbol{\varepsilon}_M, \boldsymbol{\varepsilon}^L_M) \in \mathbf{L}^2(\Omega_M) \times \mathbf{L}^2(\mathcal{S}_M), \boldsymbol{\varepsilon}_M = \boldsymbol{\varepsilon}^T_M, \boldsymbol{\varepsilon}^L_M = (\boldsymbol{\varepsilon}^L_M)^T\}$. Observe that the term $\boldsymbol{\varepsilon}^L_M$ has a very intuitive physical interpretation: a strain-like action, or a localized strain-like mode, induced by the displacement jump $\boldsymbol{\beta}_M$ acting on the macro cohesive surface $\mathcal{S}_M$, with unit normal vector $\overline{\mathbf{n}^{\mu}_{\mathcal{S}}}$.

The structure of the micro-scale generalized displacement vector space results in: $\mathcal{U}_\mu = \mathbf{H}^1(\Omega_\mu) \times \mathbf{H}^1(\Omega_\mu) \times \mathbf{L}^2(\Omega^L_\mu)$. As before we have: $u_\mu = (\mathbf{u}_\mu, \boldsymbol{\gamma}_\mu, \boldsymbol{\beta}_\mu) \in \mathcal{U}_\mu$. The insertion operator for the generalized macro strain actions is the following

$$\mathcal{J}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}})) = \left(\mathbf{0}, \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y} - \mathbf{y}_o), \frac{\boldsymbol{\beta}_M|_{\mathbf{x}}}{\theta}\right). \quad (273)$$

Instead of (256)*, the following alternative homogenization operator is considered*

$$\mathcal{H}^{\mathcal{E}\,21}_\mu(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\mathcal{S}_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu \, d\Omega_\mu, \quad \text{for } \mathcal{J}^{\mathcal{E}}_\mu((\mathbf{0}, \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}})). \quad (274)$$

From (274)*, equation* (60) *is now verified as seen next*

$$\mathcal{H}^{\mathcal{E}\,21}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu((\mathbf{0}, \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}})))) = \frac{1}{|\mathcal{S}_\mu|}\int_{\Omega^L_\mu} \frac{\boldsymbol{\beta}_M|_{\mathbf{x}} \otimes^S \mathbf{n}^{\mu}_{\mathcal{S}}(\mathbf{y}_0)}{\theta\, l_\mu(\mathbf{y}_0)}\, d\Omega^L_\mu = \boldsymbol{\beta}_M|_{\mathbf{x}} \otimes^S \overline{\mathbf{n}^{\mu}_{\mathcal{S}}} = \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}} \quad (275)$$

In this case, the kinematical admissibility concept for strain actions can be written as

$$\mathcal{H}^{\mathcal{E}\,11}_\mu(\boldsymbol{\varepsilon}_\mu) = \mathcal{H}^{\mathcal{E}\,11}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}})))), \quad (276)$$

$$\mathcal{H}^{\mathcal{E}\,21}_\mu(\boldsymbol{\varepsilon}_\mu) = \mathcal{H}^{\mathcal{E}\,21}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \boldsymbol{\varepsilon}^L_M|_{\mathbf{x}})))). \quad (277)$$

Fulfillment of expressions (276)-(277) *requires that*

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \quad (278)$$

$$\frac{1}{|\mathcal{S}_\mu|}\int_{\Omega^L_\mu} \nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu \, d\Omega^L_\mu = \mathbf{0}, \quad (279)$$

or integrating by parts

$$\int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu \, d\Gamma_\mu = \mathbf{0}, \quad (280)$$

$$\int_{\Gamma^L_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}^L_\mu \, d\Gamma^L_\mu = \mathbf{0}. \quad (281)$$

The previous discussion leads to the following space of kinematically admissible fluctuations of the displacement field at the micro scale

$$\mathrm{Kin}^{\circ}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}^{\circ}_{\tilde{\mathbf{u}}_\mu} = \Big\{\tilde{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu), \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu \, d\Gamma_\mu = \mathbf{0}, \int_{\Gamma^L_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}^L_\mu \, d\Gamma^L_\mu = \mathbf{0}\Big\}. \quad (282)$$

It is now clear that $\mathrm{Var}^{\circ}_{\tilde{\mathbf{u}}_\mu} \subset \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$. Then, the multiscale model developed in [104, 123], which results from the use of $\mathrm{Var}^{\circ}_{\tilde{\mathbf{u}}_\mu}$ given by (282)*, is kinematically more restricted than the model developed in the body of this section, which results from using $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$ given by* (272)*.*

The internal virtual power associated to point $\mathbf{x}$ over a macro-cohesive crack (which is to be linked with the RVE) is given by the product $\mathbf{T}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} = \omega_1\, \mathbf{T}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}}$, where $\mathbf{T}_M|_{\mathbf{x}}$ represent the traction vector acting on the crack, at point $\mathbf{x}$. The cohesive traction $\mathbf{T}_M|_{\mathbf{x}}$ is identified as a dual quantity (power-conjugate) respect to $\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}}$ and its constitutive characterization will be obtained from the homogenization of a micro-mechanical problem. At the RVE-level, after exploiting the form of the admissible variations $\hat{\boldsymbol{\varepsilon}}_\mu$ (see (251)), the internal virtual power results

$$P^{\mathrm{int}}_\mu = \int_{\Omega^L_\mu} \boldsymbol{\sigma}_\mu \cdot \frac{\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} \otimes^S \mathbf{n}^{\mu}_{\mathcal{S}}(\mathbf{y})}{\theta\, l_\mu(\mathbf{y})}\, d\Omega^L_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}}\hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \quad (283)$$

Therefore, the formulation of the Principle of Multiscale Virtual Power for the present application is given by the following statement.

PMVP. *It is said that $\mathbf{T}_M|_{\mathbf{x}}$ and $\boldsymbol{\sigma}_\mu$ are equilibrated if the following variational equation is satisfied*

$$\mathbf{T}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} = \int_{\Omega^L_\mu} \boldsymbol{\sigma}_\mu \cdot \frac{\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} \otimes^S \mathbf{n}^{\mu}_{\mathcal{S}}(\mathbf{y})}{\theta\, l_\mu(\mathbf{y})}\, d\Omega^L_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}}\hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \quad \forall((\mathbf{0}, \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}}), \hat{\tilde{\mathbf{u}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \quad (284)$$

The consequences of the principle formulated above are the following.

Equilibrium problem at micro scale. Consider $\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} = \mathbf{0}$ then, the equilibrium problem at the micro scale is formulated as follows

$$\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla^S_{\mathbf{y}} \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu = 0 \qquad \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \quad (285)$$

Traction homogenization at macro scale. Let $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$, then

$$\mathbf{T}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} = \int_{\Omega^L_\mu} \boldsymbol{\sigma}_\mu \cdot \frac{\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} \otimes^S \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y})}{\theta \, l_\mu(\mathbf{y})} \, d\Omega^L_\mu \qquad \forall (\mathbf{0}, \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}}) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (286)$$

Working on the right hand side of the above expression we obtain

$$\int_{\Omega^L_\mu} \boldsymbol{\sigma}_\mu \cdot \frac{\hat{\boldsymbol{\beta}}_M|_{\mathbf{x}} \otimes^S \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y})}{\theta \, l_\mu(\mathbf{y})} \, d\Omega^L_\mu = \left[\int_{\mathcal{S}_\mu} \frac{1}{\theta} \overline{\boldsymbol{\sigma}_\mu}(\mathbf{y}_0) \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0) \, d\mathcal{S}_\mu \right] \cdot \hat{\boldsymbol{\beta}}_M|_{\mathbf{x}}, \quad (287)$$

where $\overline{\boldsymbol{\sigma}_\mu}(\mathbf{y}_0)$ is the mean value of $\boldsymbol{\sigma}_\mu$ over the thickness of the domain of localization Ω^L_μ at point $\mathbf{y}_0$. Therefore, the homogenization formula for $\mathbf{T}_M|_{\mathbf{x}}$ results

$$\mathbf{T}_M|_{\mathbf{x}} = \frac{1}{\theta |\mathcal{S}_\mu|} \int_{\mathcal{S}_\mu} \overline{\boldsymbol{\sigma}_\mu}(\mathbf{y}_0) \mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0) \, d\mathcal{S}_\mu. \quad (288)$$

Observe that the dimensional parameter ω_1 involved in the duality product $(\cdot) \bullet (\cdot)$ can be easily identified from (287) being, in this problem, $\omega_1 = |\mathcal{S}_\mu|$. Consider the particular case where $\mathcal{S}_\mu$ is a plane ($\mathbf{n}^\mu_{\mathcal{S}}(\mathbf{y}_0) = \mathbf{n}^\mu_{\mathcal{S}}$) and $l_\mu(\mathbf{y}_0) = l_\mu$ are constants, then we have $\theta = 1$, and the above homogenization formula (288) agrees with that proposed in [104], which is repeated here

$$\mathbf{T}_M|_{\mathbf{x}} = \frac{1}{|\Omega^L_\mu|} \int_{\Omega^L_\mu} \boldsymbol{\sigma}_\mu \mathbf{n}^\mu_{\mathcal{S}} \, d\Omega^L_\mu. \quad (289)$$

Numerical simulations obtained using a very similar model to the one presented here are discussed in detail in Section 7.2.

■

6.5 Convective/dissipative macro effects - Classical micro fluidics

In what follows we consider the multiscale modeling in fluid mechanics for a steady state problem. At the micro scale the fluid is considered to behave as Newtonian, and the focus is on the interplay between forces due to convective effects (acceleration forces) and constitutive (viscous) effects phenomena. In addition, incompressibility constraint is considered at both scales. That is, the materials of the domain at micro scale are all incompressible, resulting in an incompressible behavior at macro scale.

At macro scale, the domain (configuration of the body) is an open subset $\Omega_M \subset \mathbb{R}^3$, with smooth boundary Γ_M (outward unit normal $\mathbf{n}_M$), and whose coordinates are $\mathbf{x}$. We consider an Eulerian description of the physical phenomena. The generalized displacement is the velocity vector field $u_M = \mathbf{v}_M$, with structure given by $\mathcal{U}_M = \{\mathbf{v}_M \in \mathbf{H}^1(\Omega_M), \mathrm{div}_{\mathbf{x}} \mathbf{v}_M = 0\}$. The strain action operator is not the classical symmetric gradient, but the full gradient, which will allow us to retrieve non-symmetric stress tensors due to convective effects at micro scale, so $\mathcal{D}_M(\cdot) = \boldsymbol{g}_M(\cdot) = \nabla_{\mathbf{x}}(\cdot)$. Thus, it is $D_M = \boldsymbol{g}_M(\mathbf{v}_M) = \nabla_{\mathbf{x}} \mathbf{v}_M$, and therefore $D_M \in \mathcal{E}_M = \{\boldsymbol{g}_M \in \mathbb{L}^2(\Omega_M), \mathrm{tr}(\boldsymbol{g}_M) = 0\}$. All fields are defined in Ω_M. Then, we have $n_M = 1$ ($R_M = 3$) and $m_M = 1$ ($S_M = 9$).

At the micro-scale we have a similar model to the one used at the macro scale, so the RVE domain is $\Omega_\mu \subset \mathbb{R}^3$, with smooth boundary Γ_μ (outward unit normal $\mathbf{n}_\mu$), whose coordinates are $\mathbf{y}$. This RVE is a representative element standing for a fixed window in the micro scale (Eulerian approach). As well, the generalized displacement is a velocity field, expressed as $u_\mu = \mathbf{v}_\mu = \bar{\mathbf{v}}_\mu + \tilde{\mathbf{v}}_\mu$, with structure given by $\mathcal{U}_\mu = \{\mathbf{v}_\mu \in \mathbf{H}^1(\Omega_\mu), \mathrm{div}_{\mathbf{y}} \mathbf{v}_\mu = 0\}$. Equivalently, the strain action operator is the full gradient $\mathcal{D}_\mu(\cdot) = \nabla_{\mathbf{y}}(\cdot)$, so $D_\mu = \boldsymbol{g}_\mu(\mathbf{v}_\mu) = \nabla_{\mathbf{y}} \mathbf{v}_\mu$, so $D_\mu \in \mathcal{E}_\mu = \{\boldsymbol{g}_\mu \in \mathbb{L}^2(\Omega_\mu), \mathrm{tr}(\boldsymbol{g}_\mu) = 0\}$. In this case, the strain action and velocity are distributed throughout the entire RVE domain, implying that $\Omega^{\boldsymbol{g}}_\mu = \Omega^{\mathbf{v}}_\mu = \Omega_\mu$. Here, it is $n_\mu = 1$ ($R_\mu = 3$) and $m_\mu = 1$ ($S_\mu = 9$).

The definition of the intermediate space of point-valued velocities at macro scale is given by $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M} = \{\mathbf{w} \in \mathbb{R}^3, \mathbf{w} = \mathbf{v}_M|_{\mathbf{x}}, \mathbf{v}_M \in \mathcal{U}_M\}$, and for the strain action we have $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M} = \{\boldsymbol{d} \in \mathbb{R}^{3\times 3}, \boldsymbol{d} = \boldsymbol{g}_M|_{\mathbf{x}}, \boldsymbol{g}_M \in \mathcal{E}_M\}$. Note that tensors in $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$ are such that $\mathrm{tr}(\boldsymbol{d}) = 0$. Here, it is $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} = \mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} = \mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$.

The insertion operator for the velocity field is defined as follows

$$\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{v}_M|_{\mathbf{x}}) = \mathbf{v}_M|_{\mathbf{x}}, \quad (290)$$

and the insertion operator for the strain action is proposed to be

$$\mathcal{J}^{\mathcal{E}}_{\mu}(\boldsymbol{g}_M|_{\mathbf{x}}) = \boldsymbol{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o), \tag{291}$$

with $\mathbf{y}_o$ being the geometrical center of the RVE, i.e. $\mathbf{y}_o = \frac{1}{\Omega_\mu}\int_{\Omega_\mu}\mathbf{y}\,\Omega_\mu$. Then, at micro scale we have

$$\mathbf{v}_\mu = \mathbf{v}_M|_{\mathbf{x}} + \boldsymbol{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{v}}_\mu. \tag{292}$$

Considering the divergence of $\mathbf{v}_\mu$, taking into account that $\mathbf{v}_M|_{\mathbf{x}}$ is constant with respect to $\mathbf{y}$ and that $\boldsymbol{g}_M|_{\mathbf{x}}$ is trace free, we obtain

$$\operatorname{div}_{\mathbf{y}}\mathbf{v}_\mu = \operatorname{div}_{\mathbf{y}}(\mathbf{v}_M|_{\mathbf{x}} + \boldsymbol{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{v}}_\mu) = \operatorname{div}_{\mathbf{y}}\tilde{\mathbf{v}}_\mu, \tag{293}$$

so, the velocity field at micro scale is divergence free provided that

$$\operatorname{div}_{\mathbf{y}}\tilde{\mathbf{v}}_\mu = 0. \tag{294}$$

Besides, since $\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{v}_M|_{\mathbf{x}})) = \nabla_{\mathbf{y}}\mathbf{v}_M|_{\mathbf{x}} = \mathbf{0}$, we have

$$\boldsymbol{g}_\mu = \boldsymbol{g}_M|_{\mathbf{x}} + \nabla_{\mathbf{y}}\tilde{\mathbf{v}}_\mu. \tag{295}$$

Regarding homogenization, we define the following homogenization operator for the velocity field

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathbf{v}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{v}_\mu\,d\Omega_\mu, \tag{296}$$

and for the strain action field

$$\mathcal{H}^{\mathcal{E}}_\mu(\boldsymbol{\varepsilon}_\mu) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{g}_\mu\,d\Omega_\mu. \tag{297}$$

By definition of the insertion operator, it is verified that equation (59) is satisfied, i.e.

$$\mathcal{H}^{\mathcal{U}}_\mu(\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{v}_M|_{\mathbf{x}})) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{v}_M|_{\mathbf{x}})\,d\Omega_\mu = \mathbf{v}_M|_{\mathbf{x}}. \tag{298}$$

In addition, the kinematical admissibility concept (see equation (61)) states that

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{v}_\mu\,d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathcal{J}^{\mathcal{U}}_\mu(\mathbf{v}_M|_{\mathbf{x}})\,d\Omega_\mu. \tag{299}$$

By construction it is

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)\,d\Omega_\mu = \mathbf{0}. \tag{300}$$

So, (299) is satisfied by ensuring

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\tilde{\mathbf{v}}_\mu\,d\Omega_\mu = \mathbf{0}. \tag{301}$$

For the insertion of the strain action, by construction we have that equation (60) is satisfied, in fact

$$\mathcal{H}^{\mathcal{E}}_\mu(\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\boldsymbol{g}_M|_{\mathbf{x}}))) = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\boldsymbol{g}_M|_{\mathbf{x}}))\,d\Omega_\mu = \boldsymbol{g}_M|_{\mathbf{x}}, \tag{302}$$

while the linkage between strain action at macro and micro scales is performed by the kinematical admissibility concept (see (62)), which states that

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{g}_\mu\,d\Omega_\mu = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu(\boldsymbol{g}_M|_{\mathbf{x}}))\,d\Omega_\mu. \tag{303}$$

Expression (303) is fulfilled by enforcing

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\nabla_{\mathbf{y}}\tilde{\mathbf{v}}_\mu\,d\Omega_\mu = \mathbf{0}. \tag{304}$$

After integrating by parts we reach

$$\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu}\tilde{\mathbf{v}}_\mu\otimes\mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0}. \tag{305}$$

Thus, we define the space of kinematically admissible velocity fluctuation fields at micro scale as being

$$\operatorname{Kin}_{\tilde{\mathbf{v}}_\mu} = \operatorname{Var}_{\tilde{\mathbf{v}}_\mu} = \Big\{\tilde{\mathbf{v}}_\mu\in\mathbf{H}^1(\Omega_\mu),\ \operatorname{div}_{\mathbf{y}}\tilde{\mathbf{v}}_\mu = 0,\ \int_{\Omega_\mu}\tilde{\mathbf{v}}_\mu\,d\Omega_\mu = \mathbf{0},\ \int_{\Gamma_\mu}\tilde{\mathbf{v}}_\mu\otimes\mathbf{n}_\mu\,d\Gamma_\mu = \mathbf{0}\Big\}. \tag{306}$$

The internal virtual power at macro scale is given by $P^{\text{int}}_M = \int_{\Omega_M}\boldsymbol{\sigma}_M\cdot\nabla_{\mathbf{x}}\hat{\mathbf{v}}_M\,d\Omega_M$. This internal power at a given point $\mathbf{x}$ is $P^{\text{int}}_{M,\mathbf{x}} = \boldsymbol{\sigma}_M|_{\mathbf{x}}\bullet\hat{\boldsymbol{g}}_M|_{\mathbf{x}}$. The external virtual power in this case is given by acceleration forces, particularly the convective acceleration forces $P^{\text{ext}}_M = \int_{\Omega_M}\mathbf{c}_M\cdot\hat{\mathbf{v}}_M\,d\Omega_M$. Here we slightly modified the notation, using $\mathbf{c}_M$ instead of $\mathbf{f}_M$. In the classical single scale scenario the convective force is $\mathbf{c}_M = \rho(\nabla_{\mathbf{x}}\mathbf{v}_M)\mathbf{v}_M$, but in the present multiscale setting we will retrieve such term from the micro scale. This external power at a given point $\mathbf{x}$ is $P^{\text{ext}}_{M,\mathbf{x}} = \mathbf{c}_M|_{\mathbf{x}}\bullet\hat{\mathbf{v}}_M|_{\mathbf{x}}$.

After exploiting the composition of the strain action, and introducing the hypothesis about the Newtonian behavior of the fluid at micro scale, i.e. $\boldsymbol{\sigma}_\mu =$

$2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu$, being μ the fluid viscosity, the internal virtual power at micro scale results

$$P^{\text{int}}_\mu = \int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \nabla_{\mathbf{y}}\hat{\mathbf{v}}_\mu \, d\Omega_\mu =$$
$$\int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot (\hat{\boldsymbol{g}}_M|_{\mathbf{x}} + \nabla_{\mathbf{y}}\hat{\tilde{\mathbf{v}}}_\mu) \, d\Omega_\mu =$$
$$\int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \nabla_{\mathbf{y}}\hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu. \quad (307)$$

The external virtual power accounting for the convective effects is expressed as

$$P^{\text{ext}}_\mu = \int_{\Omega_\mu} \mathbf{c}_\mu \cdot \hat{\mathbf{v}}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\mathbf{v}}_\mu \, d\Omega_\mu =$$
$$\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot (\hat{\mathbf{v}}_M|_{\mathbf{x}} + \hat{\boldsymbol{g}}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \hat{\tilde{\mathbf{v}}}_\mu) \, d\Omega_\mu =$$
$$\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\mathbf{v}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} (\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu. \quad (308)$$

The formulation of the Principle of Multiscale Virtual Power for the present case is the following.

PMVP. *It is said that* $(\boldsymbol{\sigma}_M|_{\mathbf{x}}, \mathbf{c}_M|_{\mathbf{x}})$ *and* $(\boldsymbol{\sigma}_\mu, \mathbf{c}_\mu) = (2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu, (\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu)$ *are equilibrated if the following variational equation is satisfied*

$$\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{g}}_M|_{\mathbf{x}} + \mathbf{c}_M|_{\mathbf{x}} \bullet \hat{\mathbf{v}}_M|_{\mathbf{x}} =$$
$$\int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \nabla_{\mathbf{y}}\hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\mathbf{v}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} (\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu$$
$$\forall (\hat{\mathbf{v}}_M|_{\mathbf{x}}, \hat{\boldsymbol{g}}_M|_{\mathbf{x}}, \hat{\tilde{\mathbf{v}}}_\mu) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \text{Var}_{\tilde{\mathbf{v}}_\mu}. \quad (309)$$

■

The consequences of the principle enunciated above are listed below.

Equilibrium problem at micro scale. At first, consider $\hat{\mathbf{v}}_M|_{\mathbf{x}} = \mathbf{0}$ and $\hat{\boldsymbol{g}}_M|_{\mathbf{x}} = \mathbf{0}$. The equilibrium problem at the micro scale is defined by the following variational equation

$$\int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \nabla_{\mathbf{y}}\hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\tilde{\mathbf{v}}}_\mu \, d\Omega_\mu = 0$$
$$\forall \hat{\tilde{\mathbf{v}}}_\mu \in \text{Var}_{\tilde{\mathbf{v}}_\mu}. \quad (310)$$

Stress homogenization at macro scale. Consider now $\hat{\mathbf{v}}_M|_{\mathbf{x}} = \mathbf{0}$ and $\hat{\tilde{\mathbf{v}}}_\mu = \mathbf{0}$. Then it results

$$\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{g}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$+ \int_{\Omega_\mu} (\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$\forall \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (311)$$

Therefore, we have that the element $\boldsymbol{\sigma}_M|_{\mathbf{x}} - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu + (\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o))] \, d\Omega_\mu$ is in $(\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}})^\perp$. Since in the macro scale the internal power is performed by $\boldsymbol{\sigma}_M$ against the space of divergence free velocity fields, it turns out that the relevant part of the stress, from the internal power point of view, is the deviatoric component of $\boldsymbol{\sigma}_M$, called $\boldsymbol{\sigma}^{\text{dev}}_M$. Then the homogenization for this component is

$$\boldsymbol{\sigma}^{\text{dev}}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu$$
$$+ \rho((\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o))^{\text{dev}}] \, d\Omega_\mu, \quad (312)$$

where dev denotes deviatoric operation. The duality operation is $\boldsymbol{\sigma}_M|_{\mathbf{x}} \bullet \hat{\boldsymbol{g}}_M|_{\mathbf{x}} = |\Omega_\mu|\boldsymbol{\sigma}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} = |\Omega_\mu|\boldsymbol{\sigma}^{\text{dev}}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}}$, so, it is $\omega_1 = |\Omega_\mu|$.

In this expression, it is clear the contribution of the different phenomena from the micro scale onto the homogenized macro scale stress tensor, which is clearly non-symmetric because of the last term in (312).

Convective force homogenization at macro scale. Now, consider $\hat{\boldsymbol{g}}_M|_{\mathbf{x}} = \mathbf{0}$ and $\hat{\tilde{\mathbf{v}}}_\mu = \mathbf{0}$, which yields

$$\mathbf{c}_M|_{\mathbf{x}} \bullet \hat{\mathbf{v}}_M|_{\mathbf{x}} = \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\mathbf{v}}_M|_{\mathbf{x}} \, d\Omega_\mu$$
$$\forall \hat{\mathbf{v}}_M|_{\mathbf{x}} \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}, \quad (313)$$

from where we obtain

$$\mathbf{c}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu \, d\Omega_\mu. \quad (314)$$

Notice that the duality operation is $\mathbf{c}_M|_{\mathbf{x}} \bullet \hat{\mathbf{v}}_M|_{\mathbf{x}} = |\Omega_\mu| \mathbf{c}_M|_{\mathbf{x}} \cdot \hat{\mathbf{v}}_M|_{\mathbf{x}}$, and then $\gamma_1 = |\Omega_\mu|$.

Further manipulation of the above expression by introducing the form of the velocity field at micro scale, leads to

$$\begin{aligned}
&\mathbf{c}_M|_{\mathbf{x}} = \\
&\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \rho \nabla_{\mathbf{y}} \mathbf{v}_\mu (\mathbf{v}_M|_{\mathbf{x}} + \boldsymbol{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \tilde{\mathbf{v}}_\mu)\, d\Omega_\mu = \\
&\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \rho\, d\Omega_\mu\right) \boldsymbol{g}_M|_{\mathbf{x}} \mathbf{v}_M|_{\mathbf{x}} \\
&+ \frac{1}{|\Omega_\mu|} \boldsymbol{g}_M|_{\mathbf{x}} \boldsymbol{g}_M|_{\mathbf{x}} \int_{\Omega_\mu} \rho(\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu \\
&+ \frac{1}{|\Omega_\mu|} \boldsymbol{g}_M|_{\mathbf{x}} \int_{\Omega_\mu} \rho \tilde{\mathbf{v}}_\mu\, d\Omega_\mu \\
&+ \frac{1}{|\Omega_\mu|}\left(\int_{\Omega_\mu} \rho \nabla_{\mathbf{y}} \tilde{\mathbf{v}}_\mu\, d\Omega_\mu\right) \mathbf{v}_M|_{\mathbf{x}} \\
&+ \frac{1}{|\Omega_\mu|}\left(\int_{\Omega_\mu} \rho \nabla_{\mathbf{y}} \tilde{\mathbf{v}}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu\right) \boldsymbol{g}_M|_{\mathbf{x}} + \\
&\qquad \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \rho (\nabla_{\mathbf{y}} \tilde{\mathbf{v}}_\mu) \tilde{\mathbf{v}}_\mu\, d\Omega_\mu. \quad (315)
\end{aligned}$$

For the particular case of a fluid in the micro scale with constant density it simplifies to

$$\begin{aligned}
&\mathbf{c}_M|_{\mathbf{x}} = \rho\Big[\boldsymbol{g}_M|_{\mathbf{x}} \mathbf{v}_M|_{\mathbf{x}} \\
&+ \frac{1}{|\Omega_\mu|}\left(\int_{\Omega_\mu} \nabla_{\mathbf{y}} \tilde{\mathbf{v}}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu\right) \boldsymbol{g}_M|_{\mathbf{x}} \\
&\qquad + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} (\nabla_{\mathbf{y}} \tilde{\mathbf{v}}_\mu) \tilde{\mathbf{v}}_\mu\, d\Omega_\mu\Big]. \quad (316)
\end{aligned}$$

Remark 27 *The model will deliver, as an internal reactive force, a certain pressure field in the macro scale and a micro pressure field. These are reactions with respect to the macro and micro incompressibility. More general situations can be thought of if we consider, for example, the interaction of an incompressible flow with compressible objects at micro scale, delivering an effective compressible response.*

Remark 28 *Considering* $\tilde{\mathbf{v}}_\mu = \mathbf{0}$ *in the expressions derived above, and assuming constant density and viscosity, we obtain a simplified multiscale model for fluid flow whose homogenized form for the stress becomes*

$$\begin{aligned}
&\boldsymbol{\sigma}_M^{\mathrm{dev}}|_{\mathbf{x}} = 2\mu \boldsymbol{g}_M^S|_{\mathbf{x}} \\
&+\rho\left[\boldsymbol{g}_M|_{\mathbf{x}} \boldsymbol{g}_M|_{\mathbf{x}}\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} (\mathbf{y}-\mathbf{y}_o)\otimes(\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu\right)\right]^{\mathrm{dev}}. \quad (317)
\end{aligned}$$

Therefore, the stress loses symmetry, while accounts for second order terms due to the convective phenomena at micro scale. In turn, under the same assumptions as before, for the convective force, from (316)*, we obtain*

$$\mathbf{c}_M|_{\mathbf{x}} = \rho \boldsymbol{g}_M|_{\mathbf{x}} \mathbf{v}_M|_{\mathbf{x}}. \quad (318)$$

That is, such simple model contributes with high order terms in the behavior of stresses, while does not affect the convective force.

Remark 29 *In fluid mechanics, it is customary to have obstacles at the micro scale. Consider the case in which obstacles are fixed and a no-slip condition is considered over the boundaries. In such case, obstacles introduce external forces, which are the reactive forces to the no-slip condition the flow must comply. These reactive forces are put in evidence through the corresponding Lagrange multipliers. The external virtual power at the micro scale changes in this case to account for such external forces. Consider that* Γ^i_{obs}, $i = 1, \ldots, N_{\mathrm{obs}}$, *are the boundaries corresponding to the micro scale obstacles. Lagrange multipliers are denoted by* $\boldsymbol{\lambda}^i_\mu \in \boldsymbol{\Lambda}^i$ *(*$\boldsymbol{\Lambda}^i$ *a proper functional space),* $i = 1, \ldots, N_{\mathrm{obs}}$. *Then it is*

$$\begin{aligned}
&P^{\mathrm{ext}}_\mu = \int_{\Omega_\mu} \mathbf{c}_\mu \cdot \hat{\mathbf{v}}_\mu\, d\Omega_\mu + \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu \cdot \hat{\mathbf{v}}_\mu\, d\Gamma^i_{\mathrm{obs}} = \\
&\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}} \mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\mathbf{v}}_\mu\, d\Omega_\mu + \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu \cdot \hat{\mathbf{v}}_\mu\, d\Gamma^i_{\mathrm{obs}} = \\
&\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}} \mathbf{v}_\mu)\mathbf{v}_\mu \cdot (\hat{\mathbf{v}}_M|_{\mathbf{x}} + \hat{\boldsymbol{g}}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \hat{\tilde{\mathbf{v}}}_\mu)\, d\Omega_\mu \\
&+ \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu \cdot (\hat{\mathbf{v}}_M|_{\mathbf{x}} + \hat{\boldsymbol{g}}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \hat{\tilde{\mathbf{v}}}_\mu)\, d\Gamma^i_{\mathrm{obs}} = \\
&\left[\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}} \mathbf{v}_\mu)\mathbf{v}_\mu\, d\Omega_\mu + \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu\, d\Gamma^i_{\mathrm{obs}}\right] \cdot \hat{\mathbf{v}}_M|_{\mathbf{x}} \\
&+ \left[\int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}} \mathbf{v}_\mu)\mathbf{v}_\mu \otimes (\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu \right. \\
&\left. + \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu \otimes (\mathbf{y}-\mathbf{y}_o)\, d\Gamma^i_{\mathrm{obs}}\right] \cdot \hat{\boldsymbol{g}}_M|_{\mathbf{x}} \\
&+ \int_{\Omega_\mu} \rho(\nabla_{\mathbf{y}} \mathbf{v}_\mu)\mathbf{v}_\mu \cdot \hat{\tilde{\mathbf{v}}}_\mu\, d\Omega_\mu \\
&\qquad + \sum_{i=1}^{N_{\mathrm{obs}}} \int_{\Gamma^i_{\mathrm{obs}}} \boldsymbol{\lambda}^i_\mu \cdot \hat{\tilde{\mathbf{v}}}_\mu\, d\Gamma^i_{\mathrm{obs}}. \quad (319)
\end{aligned}$$

Thus, the equilibrium problem at the micro scale is

$$\int_{\Omega_\mu} 2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu\cdot\nabla_{\mathbf{y}}\hat{\tilde{\mathbf{v}}}_\mu\,d\Omega_\mu+\int_{\Omega_\mu}\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu\cdot\hat{\tilde{\mathbf{v}}}_\mu\,d\Omega_\mu$$
$$+\sum_{i=1}^{N_{\rm obs}}\int_{\Gamma^i_{\rm obs}}\boldsymbol{\lambda}^i_\mu\cdot\hat{\tilde{\mathbf{v}}}_\mu\,d\Gamma^i_{\rm obs}+\sum_{i=1}^{N_{\rm obs}}\int_{\Gamma^i_{\rm obs}}\hat{\boldsymbol{\lambda}}^{\,i}_\mu\cdot\mathbf{v}_\mu\,d\Gamma^i_{\rm obs}=0$$
$$\forall(\hat{\tilde{\mathbf{v}}}_\mu,\hat{\boldsymbol{\lambda}}^1_\mu,\ldots,\hat{\boldsymbol{\lambda}}^{N_{\rm obs}}_\mu)\in{\rm Var}_{\tilde{\mathbf{v}}_\mu}\times\boldsymbol{\Lambda}^1\times\ldots\times\boldsymbol{\Lambda}^{N_{\rm obs}}. \tag{320}$$

The homogenization form for the (deviatoric component of the) stress results

$$\boldsymbol{\sigma}^{\rm dev}_M|_{\mathbf{x}}=\frac{1}{|\Omega_\mu|}\Big[\int_{\Omega_\mu}[2\mu\nabla^S_{\mathbf{y}}\mathbf{v}_\mu+\rho((\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu\otimes(\mathbf{y}-\mathbf{y}_o))^{\rm dev}]\,d\Omega_\mu$$
$$+\sum_{i=1}^{N_{\rm obs}}\int_{\Gamma^i_{\rm obs}}(\boldsymbol{\lambda}^i_\mu\otimes(\mathbf{y}-\mathbf{y}_o))^{\rm dev}\,d\Gamma^i_{\rm obs}\Big], \tag{321}$$

and that of the convective acceleration forces is

$$\mathbf{c}_M|_{\mathbf{x}}=\frac{1}{|\Omega_\mu|}\Big[\int_{\Omega_\mu}\rho(\nabla_{\mathbf{y}}\mathbf{v}_\mu)\mathbf{v}_\mu\,d\Omega_\mu$$
$$+\sum_{i=1}^{N_{\rm obs}}\int_{\Gamma^i_{\rm obs}}\boldsymbol{\lambda}^i_\mu\,d\Gamma^i_{\rm obs}\Big]. \tag{322}$$

6.6 Thermo-mechanics with temperature fluctuations

This section is devoted to the problem of modeling multiscale phenomena in the field of thermomechanics. For simplicity, we consider infinitesimal strain theory at both scales.

The domain in the macro scale is an open subset $\Omega_M\subset\mathbb{R}^3$, with smooth boundary Γ_M (outward unit normal $\mathbf{n}_M$) and with coordinates $\mathbf{x}$. The generalized displacements is now the displacement-temperature pair $u_M=(\mathbf{u}_M,\theta_M)$, and then the structure of the space of generalized displacements is $\mathcal{U}_M=\mathbf{H}^1(\Omega_M)\times H^1(\Omega_M)$. The generalized strain action operator is $\mathcal{D}_M(\cdot)=(\nabla^S_{\mathbf{x}}(\cdot),\nabla_{\mathbf{x}}(\cdot))$, where ∇^S is the symmetric gradient. Thus, we have $D_M=(\nabla^S_{\mathbf{x}}\mathbf{u}_M,\nabla_{\mathbf{x}}\theta_M)$, and therefore $D_M\in\mathcal{E}_M=\{(\boldsymbol{\varepsilon}_M,\mathbf{g}_M)\in\mathbb{L}^2(\Omega_M)\times\mathbf{L}^2(\Omega_M),\,\boldsymbol{\varepsilon}_M=\boldsymbol{\varepsilon}^T_M\}$. All the kinematic fields are defined in Ω_M. It is then $n_M=2$ ($R_M=4$), and $m_M=2$ ($S_M=9$).

At the micro-scale we have classical thermomechanics with the RVE domain being $\Omega_\mu\subset\mathbb{R}^3$, with smooth boundary Γ_μ (outward unit normal $\mathbf{n}_\mu$) and coordinates $\mathbf{y}$. Generalized displacements at this scale are also displacement-temperature pairs, i.e. $u_\mu=(\mathbf{u}_\mu,\theta_\mu)=(\bar{\mathbf{u}}_\mu+\tilde{\mathbf{u}}_\mu,\bar{\theta}_\mu+\tilde{\theta}_\mu)$, with underlying structure given by $\mathcal{U}_\mu=\mathbf{H}^1(\Omega_\mu)\times H^1(\Omega_\mu)$. Analogously, it is $\mathcal{D}_\mu(\cdot)=(\nabla^S_{\mathbf{y}}(\cdot),\nabla_{\mathbf{y}}(\cdot))$, so $D_\mu=(\nabla^S_{\mathbf{y}}\mathbf{u}_\mu,\nabla_{\mathbf{y}}\theta_\mu)$, and thus $D_\mu\in\mathcal{E}_\mu=\{(\boldsymbol{\varepsilon}_\mu,\mathbf{g}_\mu)\in\mathbb{L}^2(\Omega_\mu)\times\mathbf{L}^2(\Omega_\mu),\,\boldsymbol{\varepsilon}_\mu=\boldsymbol{\varepsilon}^T_\mu\}$. At micro scale the fields are defined in the entire RVE domain. As for the macro scale, we have $n_\mu=2$ ($R_\mu=4$) and $m_\mu=2$ ($S_\mu=9$).

The intermediate space of point-valued generalized displacements at macro scale is $\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}=\{(\mathbf{w},\tau)\in\mathbb{R}^3\times\mathbb{R},\,(\mathbf{w},\tau)=(\mathbf{u}_M|_{\mathbf{x}},\theta_M|_{\mathbf{x}}),\,(\mathbf{u}_M,\theta_M)\in\mathcal{U}_M\}$, and for the generalized strain actions $\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}=\{(\boldsymbol{\epsilon},\mathbf{h})\in\mathbb{R}^{3\times3}\times\mathbb{R}^3,\,(\boldsymbol{\epsilon},\mathbf{h})=(\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\mathbf{g}_M|_{\mathbf{x}}),\,(\boldsymbol{\varepsilon}_M,\mathbf{g}_M)\in\mathcal{E}_M\}$. In this case it is $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}=\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}$ and $\widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}=\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}$. The operator which makes the insertion of the pair displacement-temperature into the RVE domain is postulated to be

$$\mathcal{J}^{\mathcal{U}}_\mu((\mathbf{u}_M|_{\mathbf{x}},\theta_M|_{\mathbf{x}}))=(\mathbf{u}_M|_{\mathbf{x}},\theta_M|_{\mathbf{x}}), \tag{323}$$

resulting in uniform fields over the entire RVE. In turn, the generalized strain action from the macro scale is postulated to be inserted into the micro scale as

$$\mathcal{J}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\mathbf{g}_M|_{\mathbf{x}}))=$$
$$(\boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o),\mathbf{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)), \tag{324}$$

with $\mathbf{y}_o$ being the geometrical center of the RVE, i.e. $\mathbf{y}_o=\frac{1}{\Omega_\mu}\int_{\Omega_\mu}\mathbf{y}\,\Omega_\mu$. Then, at micro scale we have the following expansion of the generalized displacement field

$$\mathbf{u}_\mu=\mathbf{u}_M|_{\mathbf{x}}+\boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)+\tilde{\mathbf{u}}_\mu, \tag{325}$$
$$\theta_\mu=\theta_M|_{\mathbf{x}}+\mathbf{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)+\tilde{\theta}_\mu. \tag{326}$$

Naturally, it is $\mathcal{D}_\mu(\mathcal{J}^{\mathcal{U}}_\mu((\mathbf{u}_M|_{\mathbf{x}},\theta_M|_{\mathbf{x}})))=(\mathbf{0},\mathbf{0})$, from which it results

$$\boldsymbol{\varepsilon}_\mu=\boldsymbol{\varepsilon}_M|_{\mathbf{x}}+\nabla^S_{\mathbf{y}}\tilde{\mathbf{u}}_\mu, \tag{327}$$
$$\mathbf{g}_\mu=\mathbf{g}_M|_{\mathbf{x}}+\nabla_{\mathbf{y}}\tilde{\theta}_\mu. \tag{328}$$

Further, by construction the insertion operator $\mathcal{J}^{\mathcal{E}}_\mu$ is such that

$$\mathcal{D}_\mu(\mathcal{J}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\mathbf{g}_M|_{\mathbf{x}})))=(\boldsymbol{\varepsilon}_M|_{\mathbf{x}},\mathbf{g}_M|_{\mathbf{x}})$$
$$\forall\mathbf{y}\in\Omega_\mu. \tag{329}$$

Now, we define the following homogenization operator for the generalized displacement field

$$\mathcal{H}^{\mathcal{U}}_\mu((\mathbf{u}_\mu,\theta_\mu))=$$
$$\Big(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{u}_\mu\,d\Omega_\mu,\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\theta_\mu\,d\Omega_\mu\Big), \tag{330}$$

and for the generalized strain action field

$$\mathcal{H}^{\mathcal{E}}_\mu((\boldsymbol{\varepsilon}_\mu,\mathbf{g}_\mu))=$$
$$\Big(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\boldsymbol{\varepsilon}_\mu\,d\Omega_\mu,\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbf{g}_\mu\,d\Omega_\mu\Big). \tag{331}$$

By construction, the operator $\mathcal{J}_\mu^{\mathcal{U}}$ satisfies (see (59))

$$\mathcal{H}_\mu^{\mathcal{U}}(\mathcal{J}_\mu^{\mathcal{U}}((\mathbf{u}_M|_{\mathbf{x}}, \theta_M|_{\mathbf{x}}))) = \left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_M|_{\mathbf{x}}\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \theta_M|_{\mathbf{x}}\, d\Omega_\mu\right) = (\mathbf{u}_M|_{\mathbf{x}}, \theta_M|_{\mathbf{x}}). \quad (332)$$

To put the kinematical admissibility into action let us consider the generalized displacement field first. Then we must fullfil (see constraint (61))

$$\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \theta_\mu\, d\Omega_\mu\right) = \left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_M|_{\mathbf{x}}\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \theta_M|_{\mathbf{x}}\, d\Omega_\mu\right). \quad (333)$$

In addition, observe that by construction it is

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu = \mathbf{0}, \quad (334)$$

$$\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{g}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o)\, d\Omega_\mu = \mathbf{0}. \quad (335)$$

So the expression (333) is met by enforcing

$$\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \tilde{\theta}_\mu\, d\Omega_\mu\right) = (\mathbf{0}, 0). \quad (336)$$

Regarding the linkage between strain action at macro and micro scales, first we have that the operator $\mathcal{J}_\mu^{\mathcal{E}}$ satisfies by construction (see requirement (60))

$$\mathcal{H}_\mu^{\mathcal{E}}(\mathcal{D}_\mu(\mathcal{J}_\mu^{\mathcal{E}}((\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \mathbf{g}_M|_{\mathbf{x}})))) = \left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_M|_{\mathbf{x}}\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{g}_M|_{\mathbf{x}}\, d\Omega_\mu\right) = (\boldsymbol{\varepsilon}_M|_{\mathbf{x}}, \mathbf{g}_M|_{\mathbf{x}}). \quad (337)$$

Second, we have that the kinematical admissibility condition for generalized strain actions establishes (see constraint (62))

$$\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_\mu\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{g}_\mu\, d\Omega_\mu\right) = \left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \boldsymbol{\varepsilon}_M|_{\mathbf{x}}\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{g}_M|_{\mathbf{x}}\, d\Omega_\mu\right), \quad (338)$$

which is fulfilled by enforcing

$$\left(\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_{\mathbf{y}}^S \tilde{\mathbf{u}}_\mu\, d\Omega_\mu, \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_{\mathbf{y}} \tilde{\theta}_\mu\, d\Omega_\mu\right) = (\mathbf{0}, \mathbf{0}). \quad (339)$$

Integrating by parts yields in the expression above we obtain

$$\left(\frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu\, d\Gamma_\mu, \frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \tilde{\theta}_\mu \mathbf{n}_\mu\, d\Gamma_\mu\right) = (\mathbf{0}, \mathbf{0}), \quad (340)$$

where $\otimes^S$ is the symmetric tensor product. Thus, we define the space of kinematically admissible fluctuation displacement fields at micro scale as being

$$\mathrm{Kin}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)} = \mathrm{Var}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)} = \Big\{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu) \in [H^1(\Omega_\mu)]^3 \times H^1(\Omega_\mu),\ \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu\, d\Omega_\mu = \mathbf{0},\ \int_{\Omega_\mu} \tilde{\theta}_\mu\, d\Omega_\mu = 0,\ \int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu\, d\Gamma_\mu = \mathbf{0},\ \int_{\Gamma_\mu} \tilde{\theta}_\mu \mathbf{n}_\mu\, d\Gamma_\mu = \mathbf{0}\Big\}. \quad (341)$$

The internal virtual power at macro scale is given by the contribution of the mechanical and thermal powers $P_M^{\mathrm{int}} = \int_{\Omega_M} \boldsymbol{\sigma}_M \cdot \nabla_{\mathbf{x}}^S \hat{\mathbf{u}}_M\, d\Omega_M + \chi \int_{\Omega_M} \mathbf{q}_M \cdot \nabla_{\mathbf{x}} \hat{\theta}_M\, d\Omega_M$ (χ is a dimensional scalar to make the sum of powers dimensionally consistent, therefore, it has the units of [temperature]$^{-1}$). At a point $\mathbf{x}$ (linked to the RVE) we then have $P_{M,\mathbf{x}}^{\mathrm{int}} = (\boldsymbol{\sigma}_M|_{\mathbf{x}}, \chi \mathbf{q}_M|_{\mathbf{x}}) \bullet (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}})$. The external virtual power is $P_M^{\mathrm{ext}} = \int_{\Omega_M} \mathbf{f}_M \cdot \hat{\mathbf{u}}_M\, d\Omega_M + \chi \int_{\Omega_M} h_M \cdot \hat{\theta}_M\, d\Omega_M$, and at a point $\mathbf{x}$ it is $P_{M,\mathbf{x}}^{\mathrm{ext}} = (\mathbf{f}_M|_{\mathbf{x}}, \chi h_M|_{\mathbf{x}}) \bullet (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}})$. Observe that in the external virtual power the macro scale model allows for classical body forces, $\mathbf{f}_M$, and sources of heat per unit volume, h_M.

The internal virtual power at micro scale, after exploiting the composition of the generalized strain action at micro scale, results

$$\begin{aligned} P_\mu^{\mathrm{int}} &= \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\mathbf{u}}_\mu\, d\Omega_\mu + \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \nabla_{\mathbf{y}} \hat{\theta}_\mu\, d\Omega_\mu = \\ &\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} + \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu)\, d\Omega_\mu \\ &+ \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot (\hat{\mathbf{g}}_M|_{\mathbf{x}} + \nabla_{\mathbf{y}} \hat{\tilde{\theta}}_\mu)\, d\Omega_\mu = \\ &\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}\, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu \\ &+ \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}}\, d\Omega_\mu + \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \nabla_{\mathbf{y}} \hat{\tilde{\theta}}_\mu\, d\Omega_\mu. \end{aligned} \quad (342)$$

In turn, the external virtual power in the present model incorporates body forces $\mathbf{f}_\mu$ and sources of heat per unit of volume h_μ, both defined in the micro scale domain.

It can be written as follows

$$
\begin{aligned}
&P_\mu^{\text{ext}} = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_\mu \, d\Omega_\mu + \chi \int_{\Omega_\mu} h_\mu \cdot \hat{\theta}_\mu \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{f}_\mu \cdot (\hat{\mathbf{u}}_M|_{\mathbf{x}} + \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \hat{\tilde{\mathbf{u}}}_\mu) \, d\Omega_\mu \\
&+ \chi \int_{\Omega_\mu} h_\mu \cdot (\hat{\theta}_M|_{\mathbf{x}} + \hat{\mathbf{g}}_M|_{\mathbf{x}}(\mathbf{y}-\mathbf{y}_o) + \hat{\tilde{\theta}}_\mu) \, d\Omega_\mu = \\
&\int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&+ \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \\
&+ \chi \int_{\Omega_\mu} h_\mu \hat{\theta}_M|_{\mathbf{x}} \, d\Omega_\mu + \chi \int_{\Omega_\mu} h_\mu (\mathbf{y}-\mathbf{y}_o) \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&\qquad + \chi \int_{\Omega_\mu} h_\mu \hat{\tilde{\theta}}_\mu \, d\Omega_\mu. \quad (343)
\end{aligned}
$$

The formulation of the Principle of Multiscale Virtual Power for the present case is the following.

PMVP. *It is said that* $((\boldsymbol{\sigma}_M|_{\mathbf{x}}, \mathbf{q}_M|_{\mathbf{x}}), (\mathbf{f}_M|_{\mathbf{x}}, h_M|_{\mathbf{x}}))$ *and* $((\boldsymbol{\sigma}_\mu, \mathbf{q}_\mu), (\mathbf{f}_\mu, h_\mu))$ *are at equilibrium if the following variational equation is satisfied*

$$
\begin{aligned}
&(\boldsymbol{\sigma}_M|_{\mathbf{x}}, \chi \mathbf{q}_M|_{\mathbf{x}}) \bullet (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) \\
&- (\mathbf{f}_M|_{\mathbf{x}}, \chi h_M|_{\mathbf{x}}) \bullet (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) = \\
&\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \\
&+ \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}} \, d\Omega_\mu + \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \nabla_{\mathbf{y}} \hat{\tilde{\theta}}_\mu \, d\Omega_\mu \\
&- \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}} \, d\Omega_\mu - \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&- \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \\
&- \chi \int_{\Omega_\mu} h_\mu \hat{\theta}_M|_{\mathbf{x}} \, d\Omega_\mu - \chi \int_{\Omega_\mu} h_\mu (\mathbf{y}-\mathbf{y}_o) \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&- \chi \int_{\Omega_\mu} h_\mu \hat{\tilde{\theta}}_\mu \, d\Omega_\mu \\
&\forall ((\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}), (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}), (\hat{\tilde{\mathbf{u}}}_\mu, \hat{\tilde{\theta}}_\mu)) \in \\
&\qquad \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}} \times \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}} \times \text{Var}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)} \quad (344)
\end{aligned}
$$

■

The consequences of the principle enunciated above are listed below.

Equilibrium problem at micro scale. Firstly, take $(\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) = (\mathbf{0}, 0)$ and $(\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) = (\mathbf{0}, \mathbf{0})$. The equilibrium problem at the micro scale is defined by the following variational equations

$$
\begin{aligned}
&\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu + \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \nabla_{\mathbf{y}} \hat{\tilde{\theta}}_\mu \, d\Omega_\mu \\
&- \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu - \chi \int_{\Omega_\mu} h_\mu \cdot \hat{\tilde{\theta}}_\mu \, d\Omega_\mu = 0 \\
&\qquad \forall (\hat{\tilde{\mathbf{u}}}_\mu, \hat{\tilde{\theta}}_\mu) \in \text{Var}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)}. \quad (345)
\end{aligned}
$$

That is, we obtain the classical variational formulations for the mechanical

$$
\begin{aligned}
&\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \nabla_{\mathbf{y}}^S \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu - \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu = 0 \\
&\qquad \forall (\hat{\tilde{\mathbf{u}}}_\mu, 0) \in \text{Var}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)}, \quad (346)
\end{aligned}
$$

and thermal subsystems of the body

$$
\begin{aligned}
&\int_{\Omega_\mu} \mathbf{q}_\mu \cdot \nabla_{\mathbf{y}} \hat{\tilde{\theta}}_\mu \, d\Omega_\mu - \int_{\Omega_\mu} h_\mu \cdot \hat{\tilde{\theta}}_\mu \, d\Omega_\mu = 0 \\
&\qquad \forall (\mathbf{0}, \hat{\tilde{\theta}}_\mu) \in \text{Var}_{(\tilde{\mathbf{u}}_\mu, \tilde{\theta}_\mu)}. \quad (347)
\end{aligned}
$$

Generalized stress homogenization at macro scale. Consider $(\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) = (\mathbf{0}, 0)$ and $(\hat{\tilde{\mathbf{u}}}_\mu, \hat{\tilde{\theta}}_\mu) = (\mathbf{0}, 0)$. Then it results

$$
\begin{aligned}
&(\boldsymbol{\sigma}_M|_{\mathbf{x}}, \chi \mathbf{q}_M|_{\mathbf{x}}) \bullet (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) = \\
&\int_{\Omega_\mu} \boldsymbol{\sigma}_\mu \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu + \chi \int_{\Omega_\mu} \mathbf{q}_\mu \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&- \int_{\Omega_\mu} (\mathbf{f}_\mu \otimes^S (\mathbf{y}-\mathbf{y}_o)) \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&- \chi \int_{\Omega_\mu} h_\mu (\mathbf{y}-\mathbf{y}_o) \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}} \, d\Omega_\mu \\
&\qquad \forall (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{E}_M}}. \quad (348)
\end{aligned}
$$

Therefore, the homogenization formulae for the stress and the heat flux is obtained from identifying that $(\boldsymbol{\sigma}_M|_{\mathbf{x}}, \chi \mathbf{q}_M|_{\mathbf{x}}) \bullet (\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) = |\Omega_\mu| \, \boldsymbol{\sigma}_M|_{\mathbf{x}} \cdot \hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}} + \chi |\Omega_\mu| \, \mathbf{q}_M|_{\mathbf{x}} \cdot \hat{\mathbf{g}}_M|_{\mathbf{x}}$, resulting in

$$
\begin{aligned}
&\boldsymbol{\sigma}_M|_{\mathbf{x}} = \\
&\qquad \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \boldsymbol{\sigma}_\mu - (\mathbf{f}_\mu \otimes^S (\mathbf{y}-\mathbf{y}_o)) \, d\Omega_\mu, \quad (349)
\end{aligned}
$$

and

$$
\mathbf{q}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{q}_\mu - h_\mu (\mathbf{y}-\mathbf{y}_o) \, d\Omega_\mu. \quad (350)
$$

Note that in this case it is $\omega_1 = \omega_2 = |\Omega_\mu|$.

Generalized body force homogenization at macro scale. Now, it is considered $(\hat{\boldsymbol{\varepsilon}}_M|_{\mathbf{x}}, \hat{\mathbf{g}}_M|_{\mathbf{x}}) = (\mathbf{0}, \mathbf{0})$ and $(\hat{\tilde{\mathbf{u}}}_\mu, \hat{\tilde{\theta}}_\mu) = (\mathbf{0}, 0)$, which yields

$$(\mathbf{f}_M|_{\mathbf{x}}, \chi h_M|_{\mathbf{x}}) \bullet (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) = \int_{\Omega_\mu} \mathbf{f}_\mu \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}}\, d\Omega_\mu + \chi \int_{\Omega_\mu} h_\mu \cdot \hat{\theta}_M|_{\mathbf{x}}\, d\Omega_\mu \quad \forall (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) \in \widehat{\mathbb{R}^{\mathbf{x}}_{\mathcal{U}_M}}. \tag{351}$$

and from the fact that the product $(\mathbf{f}_M|_{\mathbf{x}}, \chi h_M|_{\mathbf{x}}) \bullet (\hat{\mathbf{u}}_M|_{\mathbf{x}}, \hat{\theta}_M|_{\mathbf{x}}) = |\Omega_\mu|\, \mathbf{f}_M|_{\mathbf{x}} \cdot \hat{\mathbf{u}}_M|_{\mathbf{x}} + \chi |\Omega_\mu|\, h_M|_{\mathbf{x}} \cdot \hat{\theta}_M|_{\mathbf{x}}$, we have

$$\mathbf{f}_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{f}_\mu\, d\Omega_\mu, \tag{352}$$

and

$$h_M|_{\mathbf{x}} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} h_\mu\, d\Omega_\mu. \tag{353}$$

Here, it is $\gamma_1 = \gamma_2 = |\Omega_\mu|$.

Remark 30 *Let us consider that at micro scale the material exhibits a classical linear constitutive response in the thermomechanic setting, i.e.*

$$\boldsymbol{\sigma}_\mu = \mathbb{C}_\mu \boldsymbol{\varepsilon}_\mu - \mathbf{B}_\mu \theta_\mu, \tag{354}$$

with $\mathbb{C}_\mu$ and $\mathbf{B}_\mu$ the elasticity tensor and the thermal expansion tensor, respectively. Now, due to the splitting of fields we have

$$\boldsymbol{\sigma}_\mu = \mathbb{C}_\mu(\boldsymbol{\varepsilon}_M|_{\mathbf{x}} + \nabla^S_{\mathbf{y}} \tilde{\mathbf{u}}_\mu) - \mathbf{B}_\mu(\theta_M|_{\mathbf{x}} + \mathbf{g}_M|_{\mathbf{x}} \cdot (\mathbf{y} - \mathbf{y}_o) + \tilde{\theta}_\mu). \tag{355}$$

Beyond standard functional dependencies, in this case $\boldsymbol{\sigma}_\mu$ depends on $\mathbf{g}_M|_{\mathbf{x}}$, which implies that $\boldsymbol{\sigma}_M|_{\mathbf{x}}$ depends on $\mathbf{g}_M|_{\mathbf{x}}$. As pointed out in [15], even having considered a standard thermodynamic setting at micro scale, the multiscale formulation results in an extended thermodynamics setting at the macro scale.

7 Numerical Applications

7.1 A plasticity-like multiscale model of martensitic transformation

In this section we present a multiscale model of stress-induced martensitic transformation. The model relies on a multiplicative plasticity-like description of the phase transformation phenomenon that occurs at grain level – here taken as the micro-scale – accounting for the accompanying large transformational strains. The overall behaviour of the alloy is predicted by means of the homogenization of an RVE containing a sufficient number of randomly oriented grains. A crucial feature of the model presented here is that the mechanical dissipation associated with the martensitic transformation above the temperature of spontaneous austenite-martensite transformation is rigorously accounted for in a newly proposed plasticity-like criterion that incorporate the ideas of Patel and Cohen [95] in a thermodynamically consistent finite strain framework. We remark that the multiscale class within which the present model is developed is standard in the sense that no discontinuities or higher-order kinematics are present. In particular, the model is an instance of the purely constitutive approach referred to in Section 4. The main contribution here is the level of refinement of the constitutive model used at the micro-scale and our main aim is to show that higher levels of micro-scale constitutive refinement can lead to macro-scale material behaviour descriptions capable of capturing the effects of rather complex phenomena – phase transformation in the present case – usually not easily captured by standard phenomenological (macro-scale) constitutive theories. Such levels of refinement are, in our view, essential in order to move towards truly predictive (rather than simply descriptive) multi-scale models with potential use in application-tailored micro-structure design – an important area of current research in materials engineering and science.

7.1.1 Martensitic transformation kinematics

Crucial in development of the constitutive model to be used at the micro-scale is the description of the kinematics of the phase transformation under consideration. The transformation of metastable austenite into martensite is a diffusionless transformation that at any one point of the transforming crystal can be described in continuum terms by a shear deformation and an expansion normal to a so-called *habit plane*. The potential habit planes and the possible shear directions within each such a plane are entirely determined by the geometry of the crystal lattice under consideration, according to the theory of Wechsler-Lieberman-Read/Bowles-Mackenzie [16,127]. With ξ denoting the transformational shear, δ the accompanying normal expansion, $\mathbf{m}^i$ the unit normal to the habit plane and $\mathbf{s}^i$ the relevant shear direction for the *variant* i, the transformation is characterized by a deformation gradient

$$\mathbf{F}^{\mathrm{tr}} = \mathbf{I} + \mathbf{d}^i \otimes \mathbf{m}^i, \tag{356}$$

where

$$\mathbf{d}^i = \xi \mathbf{s}^i + \delta \mathbf{m}^i, \tag{357}$$

with no summation on repeated indices.

Typically, stress-induced martensitic transformation occurs as part of a process involving elastic lattice deformations and possibly plastic slip prior to the onset of the transformation. In this context, we shall adopt a multiplicative kinematics whereby the total deformation gradient $\mathbf{F}$ at any point of the crystal is given as a product of elastic, plastic and transformational contributions:

$$\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A}, \tag{358}$$

where $\mathbf{F}^{\mathrm{e}}$ denotes the elastic deformation gradient, $\mathbf{F}^{\mathrm{p}}_{A}$ the plastic deformation gradient associated with plastic slip of the meta-stable austenite phase (prior to the transformation). If plastic slip of the newly-formed martensite is to be considered, then the corresponding plastic deformation gradient $\mathbf{F}^{\mathrm{p}}_{M}$ can be accounted for by augmenting the above decomposition according to

$$\mathbf{F} = \mathbf{F}^{\mathrm{e}}\mathbf{F}^{\mathrm{p}}_{M}\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A}. \tag{359}$$

Martensite plasticity, however, will not be considered here. We remark that the above multiplicative splits of the deformation gradient can be rigorously justified as a continuum model of the kinematics associated with the lattice geometry changes associated with the elastic, plastic and transformational phenomena under consideration. It extends the now standard multiplicative kinematics adopted in finite strain elasto-plasticity [111].

7.1.2 Thermodynamical considerations. Plasticity-like model

It is widely accepted [14,96,116] that external mechanical work is required for the martensitic transformation to occur at temperatures above the temperature M_s at which martensite forms spontaneously. This idea appears to have been formally explored firstly in the seminal paper by Patel and Cohen [95] and is illustrated in Figure 5. It suggests that the total energy density dissipated by the transformation is a constant. Below or at M_s the difference between the chemical free-energy density of the (unstable) austenite and (stable) matensite phases is sufficient to allow the transformation to occur spontaneously, without external energy input into the lattice. At temperatures above M_s and below T_0 (the austenite-martensite equilibrium temperature), where the chemical free-energy drop during transformation is smaller than the energy dissipated by the transformation itself, the transformation may only occur if additional energy is injected into the lattice. When the transformation does occur under such circumstances, this additional energy density,

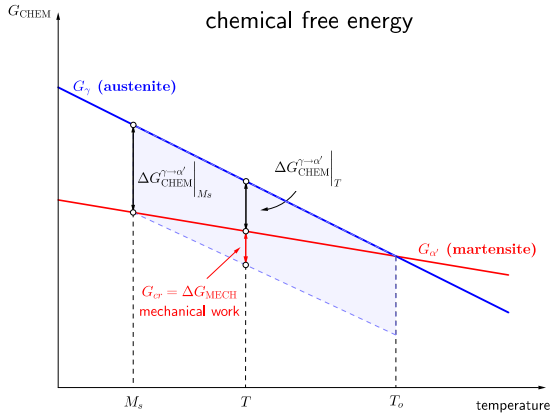

Fig. 5 Martensitic transformation. Energies involved.

denoted ΔG_{MEC}, is provided by mechanical work. The parameter ΔG_{MEC} can be regarded as a (temperature-dependent) material property. In summary, we want to model a mechanism that dissipates a given energy density ΔG_{MEC} (at a given temperature) and whose phenomenological manifestation is a deformation gradient $\mathbf{F}^{\mathrm{tr}}$, in the context of a multiplicative split (358) of the total deformation gradient.

The situation here is analogous to finite multiplicative plasticity and, as such, the underlying phenomenon can be modelled in the very same way. Assuming the mechanical free-energy density ψ to be a function solely of the elastic deformation gradient $\mathbf{F}^{\mathrm{e}}$, and accounting for the split (358), we have

$$\begin{aligned}\dot{\psi} &= \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}} : \dot{\mathbf{F}}^{\mathrm{e}} \\ &= \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}\,(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T} : \dot{\mathbf{F}} \\ &\quad - \mathbf{F}^{\mathrm{e}T}\,\frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T} : (\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{\cdot},\end{aligned} \tag{360}$$

or, since the rate of plastic slip vanishes during the transformation,

$$\dot{\psi} = \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}\,(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T} : \dot{\mathbf{F}} - \mathbf{F}^{\mathrm{e}T}\,\frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T} : \dot{\mathbf{F}}^{\mathrm{tr}}. \tag{361}$$

The dissipation inequality,

$$\dot{D} \equiv \mathbf{P} : \dot{\mathbf{F}} - \dot{\psi} > 0, \tag{362}$$

then reads

$$\left[\mathbf{P} - \frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}\,(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T}\right] : \dot{\mathbf{F}} + \mathbf{F}^{\mathrm{e}T}\,\frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}(\mathbf{F}^{\mathrm{tr}}\mathbf{F}^{\mathrm{p}}_{A})^{-T} : \dot{\mathbf{F}}^{\mathrm{tr}} > 0. \tag{363}$$

From the above we identify the constitutive equation for the first Piola-Kirchhoff stress,

$$\mathbf{P} = \frac{\partial \psi}{\partial \mathbf{F}^{\mathrm{e}}} (\mathbf{F}^{\mathrm{tr}} \mathbf{F}_A^{\mathrm{p}})^{-T}, \tag{364}$$

and the dissipation inequality during the martensitic transformation reduces to

$$\dot{D} = \mathbf{T} : \dot{\mathbf{F}}^{\mathrm{tr}} > 0, \tag{365}$$

where

$$\mathbf{T} \equiv \mathbf{F}^{\mathrm{e}T} \mathbf{P} \tag{366}$$

is the work-conjugate stress to the transformational deformation gradient.

A plasticity-like constitutive model that dissipates exactly the additional energy density ΔG_{MEC} over a transformation on a variant i can be devised by firstly postulating a transformation function Φ_i^{tr}, analogous to a plastic yield function, of the type

$$\Phi_i^{\mathrm{tr}}(\mathbf{T}) \equiv \mathbf{T} : (\mathbf{d}^i \otimes \mathbf{s}^i) - \Delta G_{\mathrm{MEC}}. \tag{367}$$

The model is completed by further postulating an associative transformation rule (c.f. associative plastic flow rule)

$$\dot{\mathbf{F}}^{\mathrm{tr}} = \dot{\gamma} \frac{\partial \Phi_i^{\mathrm{tr}}}{\partial \mathbf{T}} = \dot{\gamma}\, \mathbf{d}^i \otimes \mathbf{s}^i, \tag{368}$$

where the multiplier $\dot{\gamma}$ satisfies

$$\begin{cases} \Phi_i^{\mathrm{tr}} \leq 0;\ \dot{\gamma} \geq 0;\ \Phi_i^{\mathrm{tr}} \dot{\gamma} = 0 & \text{if } \gamma < 1, \\ \dot{\gamma} = 0 & \text{if } \gamma = 1. \end{cases} \tag{369}$$

Note that with initial conditions $\gamma = 0$ and $\mathbf{F}^{\mathrm{tr}} = \mathbf{I}$ at the onset of transformation, the evolution problem defined by (368) and (369) ensures that $\mathbf{F}^{\mathrm{tr}} = \mathbf{I} + \mathbf{d}^i \otimes \mathbf{s}^i$ upon completion of the transformation (when $\gamma = 1$).

The consistency of the model with the ideas illustrated in Figure 5 can be trivially demonstrated as follows. In view of the transformation rule (368) the dissipation rate (365) can be expressed as

$$\dot{D} = \dot{\gamma}\, \mathbf{T} : \mathbf{d}^i \otimes \mathbf{s}^i. \tag{370}$$

Further, note that (369) requires that $\Phi_i^{\mathrm{tr}} = 0$ during the transformation (when $\dot{\gamma} > 0$) or, equivalently, $\mathbf{T} : \mathbf{d}^i \otimes \mathbf{s}^i = \Delta G_{\mathrm{MEC}}$. Substituting this into (370) renders

$$\dot{D} = \dot{\gamma}\, \Delta G_{\mathrm{MEC}}, \tag{371}$$

so that the total mechanical energy density dissipated during the transformation reads

$$D = \int_0^1 d\gamma \Delta G_{\mathrm{MEC}} = \Delta G_{\mathrm{MEC}}. \tag{372}$$

That is, the total mechanical energy density dissipated by the martensitic transformation mechanism coincides with the (temperature-dependent) parameter ΔG_{MEC} alluded to in Figure 5.

7.1.3 Elastic and austenite plasticity descriptions

As a first approximation to the description of the elastic behaviour of the crystal lattices, a regularized neo-Hookean model is adopted for both the austenite and the transformed martensite phases. The plasticity of the meta-stable austenite, in turn, is described by a rather conventional (time-dependent) crystal plasticity approach of the type described in [111]. The austenitic plastic flow is assumed governed by the rule

$$\dot{\mathbf{F}}_A^{\mathrm{p}} = \left[\sum_{\alpha=1}^{n_{\mathrm{syst}}} \dot{\gamma}^\alpha (\mathbf{r}^\alpha \otimes \mathbf{m}^\alpha) \right], \tag{373}$$

where n_{syst} is the total number of slip systems, $\mathbf{r}^\alpha$ and $\mathbf{m}^\alpha$ are, respectively, the unit vectors in the slip direction and normal to the slip plane of slip system α. The multiplier $\dot{\gamma}^\alpha$ – the slip-rate on slip system α – is given by

$$\dot{\gamma}^\alpha = \begin{cases} \frac{1}{\mu} \left[\left(\frac{|\tau^\alpha|}{\tau_y} \right)^{\frac{1}{\epsilon}} - 1 \right] \mathrm{sign}(\tau^\alpha) & \text{if } |\tau^\alpha| \geq \tau_y \\ 0 & \text{if } |\tau^\alpha| < \tau_y, \end{cases} \tag{374}$$

with τ^α the Kirchhoff resolved Schmid shear stress on slip system α and μ, ϵ and τ_y material constants.

7.1.4 Integration algorithm

The numerical integration of the coupled elastic-plastic-transformation constitutive equations described in the above follows a procedure analogous to those of crystal plasticity described in [111]. Before the start of the transformation the material behaviour is given by a multiplicative elasto-viscoplatic crystal model with slip-rate given by (374). The integration algorithm adopted at this stage is that based on the exponential map as described in [111]. The transformation begins within a time interval $[t_n, t_{n+1}]$ if the corresponding elastic trial stress $\mathbf{T}_{n+1}^{\mathrm{trial}}$ obtained by the elasto-viscoplastic crystal model integration algorithm is such that $\Phi_j^{\mathrm{tr}}(\mathbf{T}_{n+1}^{\mathrm{trial}}) > 0$ for some variant j. In this case, a variant selection procedure – determining the transformation actual system i in which the transformation occurs – will select the most favourable system (the one with highest transformation function value) and the stress will be updated by means of a return mapping-type algorithm for the transformation rule. For the transformation, however, the return mapping-type algorithm is simpler than that of crystal plasticity in that: (a) It only accounts for plastic flow originating from one system – the transforming variant; and, (b) The transformation rule is discretized by a *standard* backward-Euler scheme (as opposed to the more complex exponential map-based

scheme of crystal plasticity), i.e. (368) has the following time-discrete counterpart,

$$\mathbf{F}^{\mathrm{tr}}_{n+1} = \Delta\gamma\, \mathbf{d}^i \otimes \mathbf{s}^i, \tag{375}$$

where $\Delta\gamma \equiv \gamma_{n+1} - \gamma_n$ satisfies

$$\Phi^{\mathrm{tr}}_i(\mathbf{T}_{n+1}) \leq 0;\ \Delta\gamma \geq 0;\ \Phi^{\mathrm{tr}}(\mathbf{T}_{n+1})\Delta\gamma = 0, \tag{376}$$

when $\gamma_{n+1} < 1$. The overall algorithm is described in the following in pseudo-code format, with $\mathbf{F}_\Delta$ denoting the incremental deformation gradient between times t_n and t_{n+1} and ψ the regularized neo-Hookean free-energy function.

(i) Compute elastic trial state

$$\mathbf{F}^{\mathrm{e\,trial}}_{n+1} = \mathbf{F}_\Delta \mathbf{F}^{\mathrm{e}}_n;\ \mathbf{T}^{\mathrm{trial}}_{n+1} = (\mathbf{F}^{\mathrm{e\,trial}}_{n+1})^T \left.\frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}\right|^{\mathrm{trial}}_{n+1} (\mathbf{F}^{\mathrm{tr}}_n \mathbf{F}^{\mathrm{p}}_{A\,n})^{-T}$$

(ii) Transformation update
IF a variant i has been selected, THEN
IF $\Phi^{\mathrm{tr}}_i(\mathbf{T}^{\mathrm{trial}}_{n+1}) > 0$ THEN
GOTO **transformation return mapping** to update $\mathbf{F}^{\mathrm{tr}}_{n+1}$ and $\mathbf{T}_{n+1}$
ELSE
update $(\cdot)_{n+1} := (\cdot)^{\mathrm{trial}}$ and EXIT
ELSE
variant selection:
Set $i := \arg\{\max_{j=1,\cdots,n_v}\{\Phi^{\mathrm{trial}}_j : \Phi^{\mathrm{trial}}_j > 0\}\}$
IF $i = \emptyset$ THEN
GOTO **elasto-plastic algorithm** and EXIT
ELSE GOTO (ii)

The *elasto-plastic algorithm* referred to in the above is that of conventional time-dependent crystal plasticity with exponential map plastic flow integrator [111] – here with slip-rate governed by (374) and material parameters corresponding to the metastable austenite phase in question. The *transformation return mapping*, in turn, is given by:

(a) Solve the scalar equation
$\Phi^{\mathrm{tr}}(\mathbf{T}(\Delta\gamma)) = 0$
for the unknown $\Delta\gamma$, where

$$\mathbf{T}(\Delta\gamma) \equiv [\mathbf{F}^{\mathrm{e}}(\Delta\gamma)]^T \left.\frac{\partial\psi}{\partial\mathbf{F}^{\mathrm{e}}}\right|_{\mathbf{F}^{\mathrm{e}}(\Delta\gamma)} [\mathbf{F}^{\mathrm{tr}}(\Delta\gamma)\mathbf{F}^{\mathrm{p}}_{A\,n}]^{-T},$$

with $\mathbf{F}^{\mathrm{tr}}(\Delta\gamma) \equiv (\gamma_n + \Delta\gamma)\mathbf{d}^i \otimes \mathbf{s}^i$
and $\mathbf{F}^{\mathrm{e}}(\Delta\gamma) \equiv \mathbf{F}_{n+1}(\mathbf{F}^{\mathrm{p}}_{A\,n})^{-1}[\mathbf{F}^{\mathrm{tr}}(\Delta\gamma)]^{-1}$

(b) Update γ_{n+1}, $\mathbf{F}^{\mathrm{e}}_{n+1}$ and $\mathbf{F}^{\mathrm{tr}}_{n+1}$
$\gamma_{n+1} := \gamma_n + \Delta\gamma$
IF $\gamma_{n+1} > 1$ THEN
set $\gamma_{n+1} := 1$; $\Delta\gamma := \gamma_{n+1} - \gamma_n$
ENDIF
$\mathbf{F}^{\mathrm{e}}_{n+1} := \mathbf{F}^{\mathrm{e}}(\Delta\gamma)$; $\mathbf{F}^{\mathrm{tr}}_{n+1} := \mathbf{F}^{\mathrm{tr}}(\Delta\gamma)$

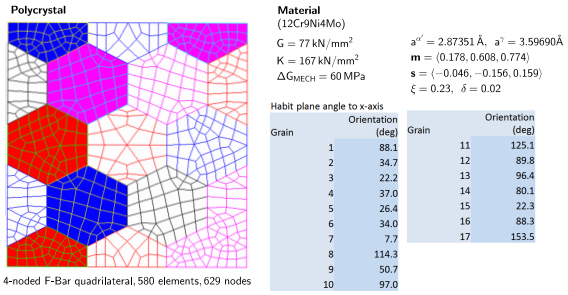

Fig. 6 Polycrystalline aggregate RVE. Geometry, mesh and material parameters

Finally, we remark that, for use within an implicit finite element framework (adopted in the numerical example described below), linearization of the time-discrete constitutive model resulting from the above numerical integration scheme and the corresponding constitutive tangent operators can be obtained in exact form in the same way as in conventional crystal plasticity [111].

7.1.5 RVE-based simulations

In the simulations presented in this section, the above constitutive model/algorithm is used to model the material behaviour at the micro-scale, taken here to be the crystal scale of a polycrystalline aggregate. That is, the RVE is formed by representative sample of crystals assumed to be perfectly bonded together within the aggregate – each crystal having its own crystallographic orientation. The specific material modelled here is 12Cr9Ni4Mo – a low carbon austenitic stainless steel whose retained austenitic phase can fully transform into martensite at room temperature under the action of external mechanical loading [60,61]. A simplified two-dimensional model is used whereby the twenty four variants of the three-dimensional fcc austenite crystal are reduced to a total of four in-plane variants. Crystals are assumed to be in their metastable austenitic phase at first and then will be subjected to a mechanical loading process leading to martensitic transformation according to the proposed rule. The RVE representing the polycrystalline aggregate is shown in Fig. 6 together with the material parameters published in [34,96]. The grains are oriented randomly. It should be noted that the transformation in this case is accompanied by a 2% dilation normal to the habit plane and 26% shear deformation in the corresponding shear direction.

The first test presented here consists of the numerical prediction of the *transformation surface* in stress space, i.e. the locus in stress space containing combinations of stresses at the onset of martensitic transformation. The procedure is analogous to that used in

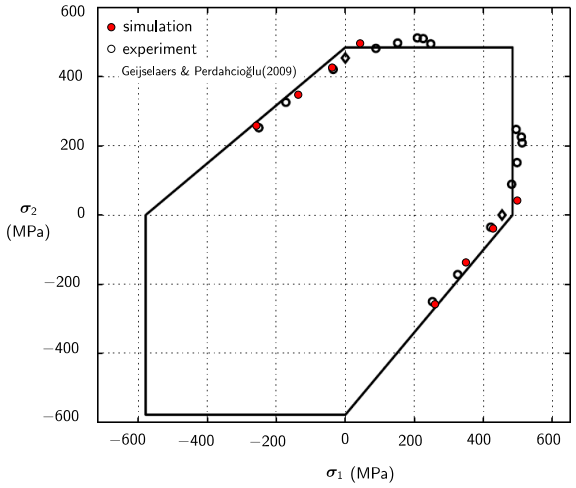

Fig. 7 Numerically predicted transformation surface in stress space.

[38] in the determination of a plastic yield surface for a porous metal (see also [32,94]). Deformation gradient histories (linear in time) are applied to the RVE so as to produce a wide range of homogenized stress paths. For any path for which martensitic transformation occurs, the homogenized stress is recorded at the onset of transformation and the stress point plotted in stress space. The collection of all such points will provide a numerical approximation for the transformation locus in stress space. Due to the assumed randomness of grain orientation, the aggregate may be regarded as macroscopically isotropic. Under this assumption, the transformation surface can be plotted in principal stress space. The numerical results are shown in Fig. 7. It can be seen that the present multiscale model is able to capture quite accurately the experimental results produced by Geijselaers and Perdahcioğlu [34]. Interestingly, the experimental transformation surface resembles a Mohr-Coulomb yield surface (typical in the modelling of geomaterials) in stress space. It is worth remarking that, in fact, the proposed criterion based on the transformation function (367) is entirely analogous to a Mohr-Coulomb plasticity criterion, the main difference being that in the criterion proposed here the critical combination of normal and shear stresses must occur with respect to one plane (the transforming habit plane) whereas in the Mohr-Coulomb criterion critical combinations may occur at any plane. Obviously with increasing numbers of randomly oriented planes in an RVE, the predicted locus here will converge to a Mohr-Coulomb-type locus. In particular, we should point out that the horizontal and vertical lines of the Mohr-Coulomb-type surface plotted in Fig. 7 (not captured by the present 2D model) will be trivially captured by a three-dimensional version of the present model.

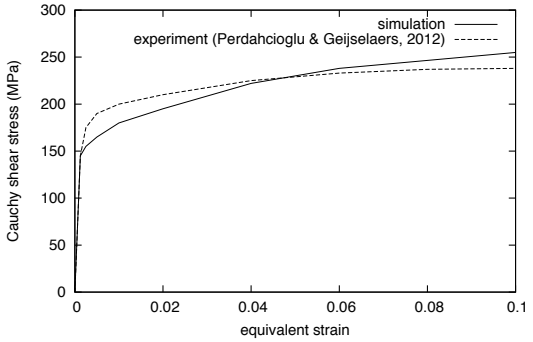

Fig. 8 Stress-strain response under monotonic shearing.

Finally, in Fig. 8 we plot the results evolution of the homogenized Cauchy shear stress over a loading programme consisting of a monotonic shearing of the RVE. A macro-scale (in-plane) deformation gradient,

$$\mathbf{F} = \begin{bmatrix} 1 & \eta \\ 0 & 1 \end{bmatrix},$$

is imposed with η monotonically increasing in time. The RVE is subjected to the minimal kinematical constraint (uniform boundary traction). The model is able to capture the experimental results of Perdahcioglu & Geijselaers [96] with reasonable accuracy. We remark that further refinements of the model, such as the use of a full three-dimensional RVE and incorporation of martensite plasticity are likely to improve the predictive capability of the model. These are currently under investigation and shall be the subject of a future publication.

7.2 Failure modeling in heterogeneous materials

7.2.1 Preliminaries

One of the main motivations to develop an abstract generalization of the concepts behind multiscale formulations has been the modeling of failure in complex heterogeneous materials. This kind of problems forced us to realize a very critical reinterpretation about the underlying foundations of conventional RVE-based multiscale approaches, in order to be able to model mechanical scenarios ruled by strain localization phenomena leading, ultimately, to complete material exhaustion. Such problems cannot be addressed by using conventional multiscale procedures because its mechanical consistency is lost during the unstable macroscopic material regime [37,87,104]. In this context, the particular multiscale model exposed in Section 6.4, called Failure-Oriented Multiscale Formulation (FOMF) (see

also [103,104]), could be considered as one of the most representative branches of the unified variational theory debated in this document. Indeed, the FOMF approach exploits (at maximum) the potentialities of the generalized framework of Section 3. Hence, the introduction of a numerical simulation showing the behavior and capabilities of such class of multiscale model adapts perfectly to the objectives of this contribution.

The FOMF approach considers crack nucleation in the macro scale (i.e displacement discontinuities) and strain localization in the micro scale domain. Thus, once the failure mechanism is activated in the macro scale, the proposed multiscale technique has to deal with *kinematical heterogeneity* between the involved physical length scales, since it establishes a kinematical/constitutive link between a macro cohesive *"interface"* and a *"volumetric"* RVE. Furthermore, the mechanics at the level of the micro scale features different mechanical regimes with localization phenomena taking place in certain regions of the RVE. In such case, the role of the insertion operators is of the utmost relevance.

This part of the manuscript focuses around a mechanical scenario that becomes intrinsically discontinuous after the nucleation of a macro cohesive crack. The main mechanism that needs to be captured here is the intricate interplay between micro degradation phenomena and its influence at macro-scale level. Therefore, subsidiary effects such as for example, the consideration of finite strain kinematics or the incorporation of external body forces, are disregarded in the subsequent analysis.

The numerical implementation of the FOMF approach is based on a nested (coupled) macro-micro finite element scheme, which is not described here. In [123], a detailed description of the numerical and algorithmic aspects can be found.

7.2.2 General description

The numerical example we incorporate in this section deals with damage, degradation, strain localization and material failure. See [123] for more details. In particular, we are interested in the assessment of the multiscale model performance and accuracy to estimate the (effective) fracture energy at the macro-scale as a result of the dissipative processes and complex interactions taking place at the microscopic level.

To this end we choose a classical problem in the *"phenomenological"* fracture mechanics community, which has been adapted here to a *"multiscale"* (two-scale) setting. It consists in the so-called Single-Edge Notched Beam Test at the macro scale (SENBT), undergoing a vertical descendant displacement which is prescribed in the upper mid-span point, $\mathrm{P_I}$, see Figs. 9-(e)-(g). The beam has a very marked heterogeneous microstructure. Actually three different microstructural patterns have been considered for modeling purposes, as we explain in this section.

Two important features are highlighted about the proposed problem setting: (i) the strain localization pattern in the microstructure, leading to failure, is preinduced to be vertical by means of the material definitions in each RVE, and (ii) the cohesive macro-crack path can be easily predicted, indeed it will be a vertical crack which propagates from the notch up to the top mid-span point of the beam (i.e. towards the point $\mathrm{P_I}$ where the vertical descendant displacement is imposed). These two features permit us to estimate, a priori and with sufficient precision, the macro fracture energy through simple analytical computations and then, we can compare it with the predictions of the multiscale model.

In spite of the previous simplifying hypotheses, the proposed test is complex enough to consider all the fundamental (and novel) ingredients which are present in the FOMF methodology, namely: (i) non-linear damage and strain localization in the micro scale, (ii) the irreversible degradation mechanisms, taking place in the RVE, trigger a critical material state or *material instability* in the macro point linked to such RVE, (iii) the critical condition is evaluated performing a spectral analysis on the homogenized tangent constitutive tensor, (iv) when material instability is reached, in some point of the macro scale, a cohesive crack is nucleated (thus we determine the nucleation time t_N), (v) the constitutive response of the macro crack is evaluated from specific homogenization rules, naturally provided by the variational formulation presented in this work, and (vi) new kinematical restrictions are applied over the boundary Γ_μ^L of the strain localization domain Ω_μ^L in the RVE (an original ingredient derived from our unified variational formulation) which are the responsible of preserving objectivity of the mechanical response with respect to the RVE size.

7.2.3 Test configuration

The characteristic dimensions of the macro structure (the beam) is displayed in Figs. 9-(d)-(e)-(g). Three beams with identical macro-geometries and boundary conditions but with different microstructures are simulated. The topology of each micro structure (the RVEs), together with their characteristic dimensions, are showed in Figs. 9-(a)-(b)-(c). In all cases, plain strain condition has been considered for both scales.

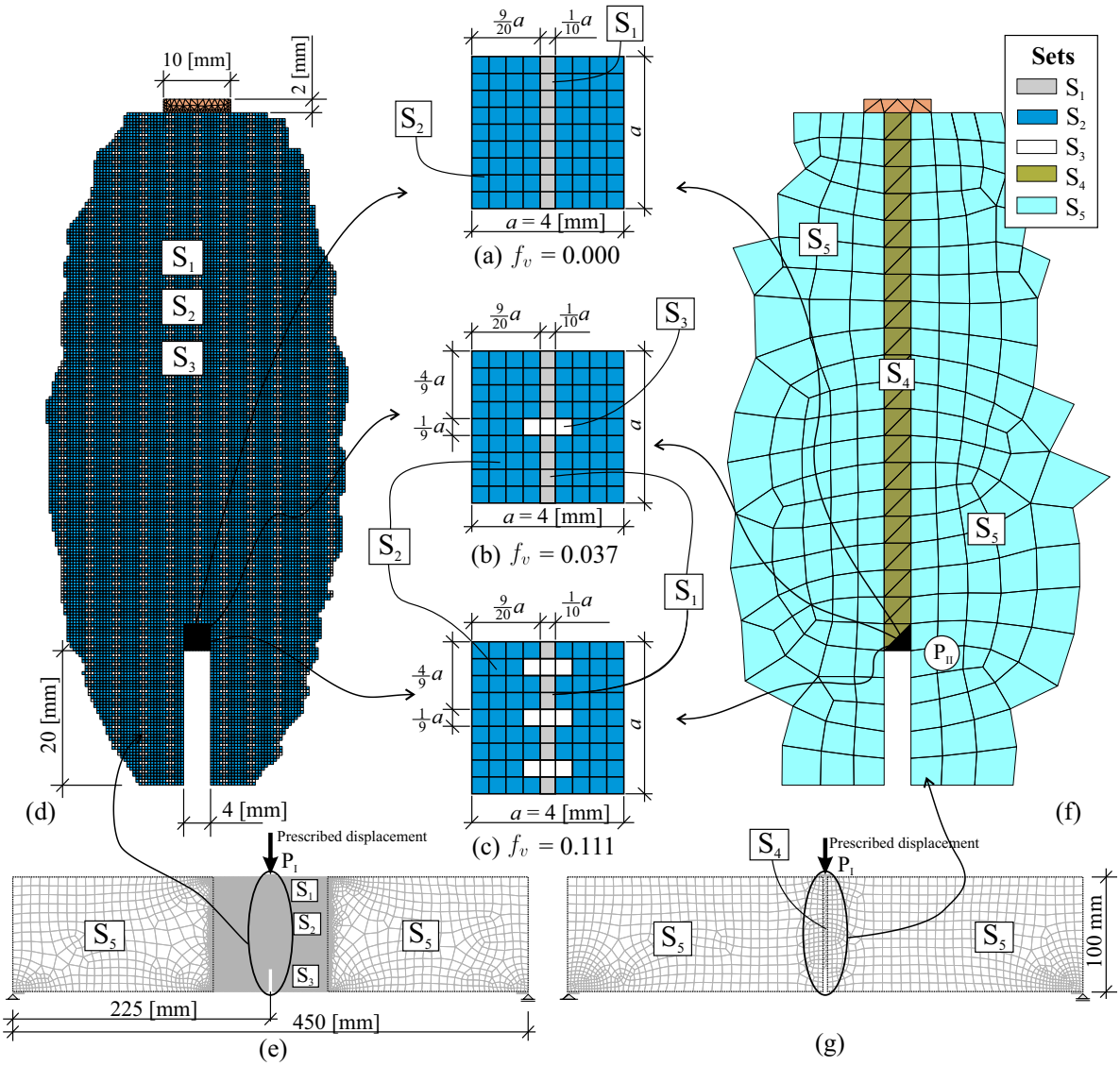

Fig. 9 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Geometrical definitions, material distributions and finite element meshes.

The domains of the macro and the micro scales are partitioned into several patches or finite element sets, see Fig. 9. Each set is characterized by its constitutive behavior and by the finite element technology employed. There are two categories of constitutive models: (i) the classical or "*Phenomenological*" material, where the constitutive response is obtained from standard, generally non-linear, mono-scale return-mapping schemes, and (ii) "*Multiscale RVE-based*" constitutive model, where the mechanical response is recovered after homogenization of a micro-mechanical problem. Table 1 gives the required specifications for each set, where the following terminology has been introduced: E_μ is the Young's Modulus, ν_μ is the Poisson's ratio, $G_{\mu F}$ is the fracture energy and σ_μ^u is the ultimate tensile limit stress; all quantities related to the micro scale domain, thence the sub-index $(\cdot)_\mu$.

Three types of periodic microstructures, containing a regular arrangement of voids, are modeled. Figs. 9-(a)-(b)-(c) show a sketch of the adopted microstructural patterns. The void volume fraction, f_v, in each one of the three cases is: $f_v = 0$, $f_v = 0.037$ and $f_v = 0.111$, respectively (quantities referred to the total RVE measure $|\Omega_\mu|$). The micro pores (see set S_3 in Fig. 9-(b)) are modeled by means of an extremely soft (phenomenological) elastic material (i.e. $E_\mu^{S_3} \to 0$)[3]. An additional

[3] This treatment simplifies the algorithmic procedure used for detecting the localization sub-domain Ω_μ^L, where the strain field localizes in the RVE, and thus the boundary Γ_μ^L of Ω_μ^L, where new kinematical restrictions must be prescribed after the cohesive crack nucleation.

SET Number	Constitutive Model	E_μ [GPa]	ν_μ	$G_{\mu F}$ [N/m]	σ_μ^u [MPa]	Finite element
S_1	Phenomenological Damage	20	0.20	100	2.40	Bilinear quadrilateral
S_2	Phenomenological Elasticity	20	0.20	-	-	Bilinear quadrilateral
S_3	Phenomenological Elasticity (voids)	0	0	-	-	Bilinear quadrilateral
S_4	Multiscale RVE-based	-	-	-	-	Strong discontinuity linear triangle
S_5	Phenomenological Elasticity (homogenized)	-	-	-	-	Bilinear quadrilateral

Table 1 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Material properties and finite element description according to the nomenclature introduced in Fig. 9.

heterogeneity introduced in the material definition of the RVE is a central vertical band of finite thickness, ℓ_μ, which is characterized in terms of a (phenomenological) isotropic damage model with softening that degrades under tensile stress states. The softening behavior is regularized by using the "*Smeared Crack Approach*" to fracture [90,102]. This set is denoted as S_1 in Fig. 9-(a)-(b)-(c). The softening band is surrounded by the set S_2, made of a (phenomenological) elastic material, see Figs. 9-(a)-(b)-(c). Considering all previous definitions, the strain localization mode in the micro scale domain will develop along the vertical central band, crossing the pores.

The element set S_4, defined at the macrostructural level, has a complex material behavior which is obtained through the RVE-based multiscale formulation, via the homogenization approach developed in the present work, see Figs. 9-(f)-(g).

Finally, the set S_5, also defined for the macro scale, behaves as a (phenomenological) elastic material. However, its elasticity tensor is actually a *homogenized* tensor, obtained from off-line microstructural analysis for each RVE, during an elastic loading process. This set S_5 permits us to take into account the complex elastic material behavior, due to the underlying heterogeneous microstructure, in large sub-domains of the beam where we know, a priori, that no dissipative mechanisms will occur, see Figs. 9-(e)-(f)-(g). Computational effort is drastically decreased following such a simple modeling assumption.

7.2.4 Numerical approaches

For each one of the three beam tests, two different numerical strategies have been considered:

Multiscale Simulation (MS). It is based on the proposed FOMF methodology. In this case, the finite element meshes used in the macro scale are shown in Figs. 9-(f)-(g). Note that in correspondence with the vertical zone where the macro cohesive crack is able to propagate (i.e. from the notch up to the point P_I), the set S_4 is considered. A total of 40 multiscale strong-discontinuity triangular finite elements compose this set. The macroscopic integration points of such finite element list are linked with their corresponding RVEs. Outside the fracture zone the set S_5 is used, composed of about 1130 standard bilinear quadrilateral finite elements. The discrete models for each RVE are depicted in Figs. 9-(a)-(b)-(c). These micro cells are composed by the sets $\{S_1, S_2, S_3\}$ and consider standard bilinear quadrilateral finite elements.

Direct Numerical Simulation (DNS). In this approach, the microstructural heterogeneities are explicitly embedded into the macro scale domain, thus no technique for scale transition is required. The discrete models use very refined meshes to capture the details of the microstructure. In our simulation, the DNS approach only represents the central part of the beam, such as shown in Figs. 9-(e)-(d). The remaining part of the beam is modeled by using the set S_5, previously described. A total of about 53700 standard bilinear quadrilateral finite elements compose the beam models. The pattern adopted to define the central zone, where failure is expected to occur, is based on a periodic repetition of micro-cells, identical in size and geometry, to those used for the RVEs of the MS analysis, see Fig. 9-(d) and Figs. 9-(a)-(b)-(c). Also, the material distributions corresponding to the sets $\{S_1, S_2, S_3\}$ are identical to those defined for the MS models.

Remark 31 *The most remarkable difference between* MS *and* DNS *approaches lies on the fact that* MS *models utilize strong discontinuity kinematics for simulat-*

ing crack propagation in the macro scale. On the other hand in the DNS *method the failure zone is simulated within a classical continuum kinematical description, where the softening response is regularized through the smeared crack approach.*

Remark 32 *The results obtained with* DNS *are taken as reference solutions to validate the material response predicted by the* MS *approach. It is worthwhile to note that such a comparison represents a consistent, and probably the most rigorous, form to evaluate the numerical performance of any multiscale formulation.*

Next we describe the kinematical restrictions applied to the RVEs in MS models, differentiating between the pre-critical and post-critical material regime. Recall that the underlying finite element technology used to simulate the failure zone in MS model is a strong discontinuity linear triangle. Thus, a unique integration point is required during the stable macro material response, which is called Regular Gauss Point (RGP). The so-called *Minimal Kinematical Restrictions* are prescribed on the RVE-boundaries linked to the RGP, it is

$$\int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes^S \mathbf{n}_\mu \, d\Gamma_\mu = \int_{\Gamma_\mu} \tilde{\boldsymbol{\varepsilon}}^*_\mu \, d\Gamma_\mu = \mathbf{0}. \tag{377}$$

In a two-dimensional problem, as the present case, the previous constraint imposes three independent linear and homogeneous equations, one for each component of the symmetric tensor $\tilde{\boldsymbol{\varepsilon}}^*_\mu$ (i.e. $\tilde{\varepsilon}^*_{\mu\, y_1 y_1}$, $\tilde{\varepsilon}^*_{\mu\, y_2 y_2}$ and $\tilde{\varepsilon}^*_{\mu\, y_1 y_2}$), see the sketch in Fig. 10-(a).

Once detected the material bifurcation condition in a macroscopic regular integration point ($t = t_N$), a new quadrature point is activated into the finite element under study, which we call Singular Gauss Point (SGP). At t_N, the SGP is cloned from the RGP, i.e. their mechanical states are identical. For $t > t_N$, the RGP and SGP evolve following different equilibrium branches. The RVE related to the RGP is forced to respond elastically during the postcritical regime, preserving their initial boundary conditions already explained[4]. On the other hand, the RVE associated to the SGP is endowed with new kinematical restrictions, according to FOMF approach. In the present case, we adopt a sub-model with zero displacement fluctuation increments in the boundary Γ^L_μ of Ω^L_μ, such as sketched in Fig. 10-(b). Observe that the kinematical restrictions applied on the RVE associated with the SGP can be identified as particular case of the minimally constrained model proposed in Section (6.4), Remark 26.

[4] The idea of forcing an elastic unloading behavior in those integration points located outside the cohesive crack in a strong discontinuity finite element, is a standard technique widely used in the phenomenological approach to fracture. We have adapted this procedure to the multiscale modeling context.

7.2.5 Numerical results

Fig. 11 plots the (macro) structural responses of the SENB tests in terms of the homogenized vertical loads vs. the vertical (imposed) displacements of point $\mathrm{P_I}$. Remarkably, observe that the DNS and MS models provide almost the same macroscopic solutions for the three microstructures and during the complete loading history, involving the pre-critical as well as the post-critical regime. As expected, microstructures with larger void volume fraction, f_v, have less elastic stiffness, less peak load and require less dissipation energy to completely exhaust the macro structure.

Fig. 12-(a) features the contours of homogenized cohesive traction vs. displacement jump for the singular integration point (SGP), where the bifurcation condition is first satisfied during the loading history, i.e. at point $\mathrm{P_{II}}$ (see Fig. 12-(b)). The plots of Fig. 12-(a) represent the normal components of both vector fields, the tractions (T_n) and the displacement jumps (β_n), where the sub-index $(\cdot)_n$ refers to the normal projection with respect to the crack path. The tangential components of both quantities, the tractions (T_s) and the displacement jumps (β_s), are almost zero (the sub-index $(\cdot)_s$ refers to the tangential projection with respect to the crack path). Then, as expected, the macro cohesive crack opening mode is a pure Mode I of fracture. The numerically obtained unit vector field, normal to the macroscopic discontinuity surface, is depicted in Fig. 12-(b). In the FOMF approach this result is obtained from a discontinuous bifurcation analysis.

The cohesive responses observed in Fig. 12-(a) allow us to evaluate the effective fracture energy (G_F) which is put into play to fully exhaust the macroscopic cohesive crack, nucleated at point $\mathrm{P_{II}}$. The effective fracture energy can be simply computed by determining the area under the plots in Fig. 12-(a):

$$G_F = \int_{t_N}^{\infty} (\boldsymbol{T} \cdot \dot{\boldsymbol{\beta}}) \, dt \tag{378}$$

This parameter is reported in Table 2 (column 3). Alternatively, we can also "*estimate*" the fracture energy available in each RVE via an average value of the fracture energy for those finite elements that belong to the strain localization band Ω^L_μ, including the voids:

$$G_F^{est} = \frac{1}{|\Omega^L_\mu|} \int_{\Omega^L_\mu} G_{\mu F} \, d\Omega_\mu \tag{379}$$

where $G^{S_1}_{\mu F} = 100$ [N/m], for the set $\mathrm{S_1}$, and $G^{S_3}_{\mu F} = 0$ [N/m], for the set $\mathrm{S_3}$, as shown in Table 1. The so

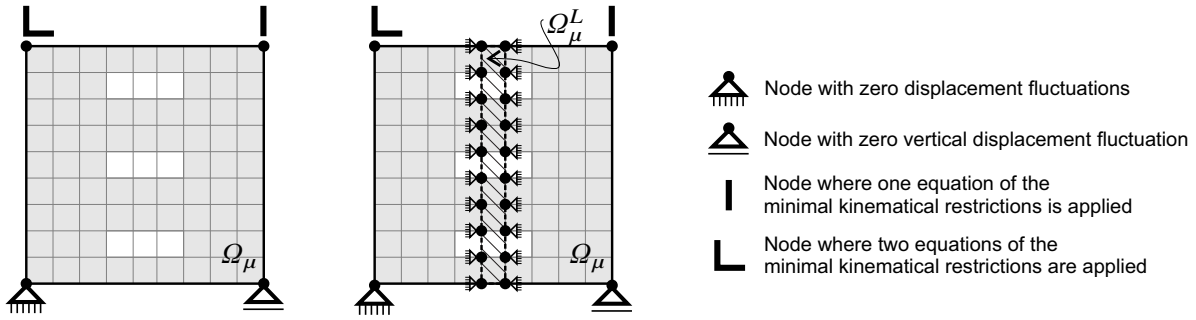

Fig. 10 Single-Edge Notched Beam Test with inner heterogeneous microstructure. RVE kinematical restrictions. (a) Standard Boundary Conditions for the stable macroscopic regime ($t < t_N$). (b) Non-Standar Boundary Conditions for the unstable macroscopic regime ($t > t_N$).

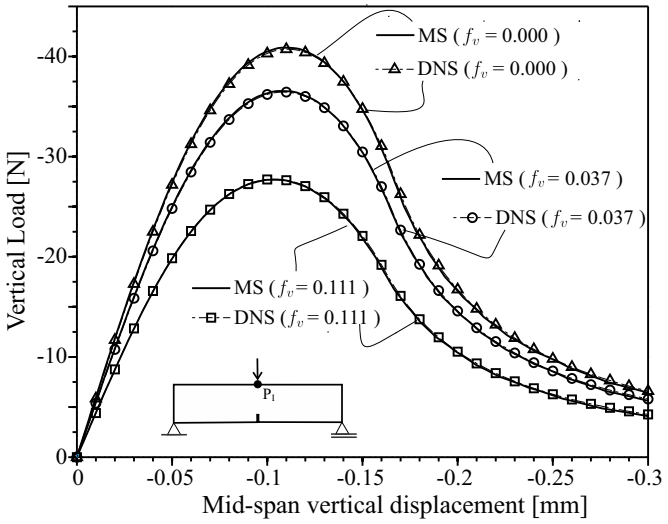

Fig. 11 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Vertical load vs. vertical displacement curve for point P_I. Comparison between MS and DNS approaches for different void volume fractions.

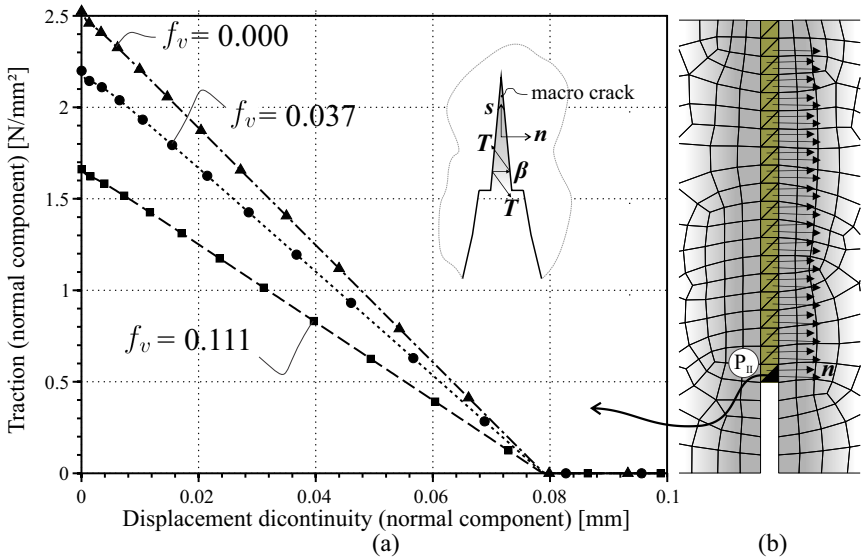

Fig. 12 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Homogenized cohesive responses (T_n vs. β_n) obtained using the Failure-Oriented Multi-Scale Formulation. Curves evaluated at point P_{II} (see picture-(b)), for different void volume fractions.

estimated macro fracture energies, G_F^{est}, are shown in Table 2 (column 4) for each microstructure. Note the well marked effect that the variable f_v has on both, the effective fracture energy G_F as well as the estimated fracture energy G_F^{est}.

Comparing the values of G_F and G_F^{est} it is noticed that, for the RVE without pores, the agreement between both quantities is almost exact. A slightly larger disagreement is observed for the microstructures with one and three voids. This result has a rational/physical explanation. From expression (379), the value G_F^{est} is computed by assuming that, during the macroscopic stable regime (i.e. previous to the crack nucleation at macro scale: $t < t_N$), energy dissipation has not occurred. In the case of the RVE without pores, the problem is homogeneous before bifurcation because all materials have the same elastic constants, see Table 1. In this case, macroscopic bifurcation detection happens just at the same time (t_N) that the central band, described with the damage model, reaches its limit ultimate strength. Then, the assumption that there is no dissipation before bifurcation, is correct. However, in the micro structures with pores damage during the stable regime happens. Therefore, the assumption that the fracture energy can be evaluated by equation (379) is no longer correct and the parameter G_F^{est} overestimates the actual fracture energy.

Fig. 13 shows structural responses similar to those explained in Fig. 11. This time we demostrate the mechanical consistency of the multiscale response modifying the macroscopic finite element size (mesh size independence). Just the problem with void volume fraction $f_v = 0.111$ has been considered. The finite element mesh of Case 2 (Mesh_2) displays smaller elements with respect to Case 1 (Mesh_1) in the zone where the multiscale set S_4 is simulated.

8 Concluding remarks

A unified variational theory has been proposed for a general class of multiscale models based on the concept of Representative Volume Element. The entire theory lies on three fundamental principles: (i) *kinematical admissibility*, whereby the macro- and micro-scale kinematics are defined and linked in a physically meanigful way; (ii) *duality*, through which the natures of the force- and stress-like quantities are uniquely identified as the duals (power-conjugates) of the adopted kinematical variables at the two scales; and (iii) the *Principle of Multiscale Virtual Power*, requiring the total virtual powers of the macro- and micro-scales to coincide. This is a generalization of a variational statement of the well-known Hill-Mandel Principle of Macrohomogeneity and allows the RVE equilibrium equations and homogenization relations for the force- and stress-like quantities to be unequivocally derived as Euler-Lagrange equations.

The proposed theory leads to a clear, logically structured method – named here the *Method of Multiscale Virtual Power* – whereby general multiscale models of complex physical systems can be rigorously derived in well-defined steps. The method is well-suited for the treatment of problems involving phenomena as diverse as dynamics, higher order strain effects, material failure with kinematical discontinuities, fluid mechanics and coupled multi-physics, among others.

Particularly noteworthy is the fact that the proposed methodology allows the development of multiscale models in an intuitive manner without ambiguities. In fact, the *only* degree of arbitrariness one has in the development of a multiscale model lies in postulating its kinematics. This consists in defining: (a) the kinematical variables adopted at macro- and micro-scales; and (b) how these kinematical variables are linked, subject to the condition that their magnitudes are preserved in the micro-macro kinematical transfer – this amounts solely to the definition of physically sound kinematical *insertion* and *homogenization operators*. Once the kinematics has been postulated, the function space of admissible micro-scale generalized displacements is automatically defined and all remaining model equations will be unequivocally derived on the basis of the principles of *duality* and *multiscale virtual power*. This is in sharp contrast with most of the work currently published in the field, where various such equations are postulated *a priori* – a procedure that can potentially lead to serious inconsistencies in the resulting model.

The theory has been presented in a rather abstract setting, which allows its use in the modeling of a very wide range of physical systems. However, practical examples of its use with several well-known multiscale formulations have been presented. In our view, casting known models within the proposed framework has made the distinction between their kinematics and their consequences very clear, allowing a better understanding of the limitations of each model and showing directions for possible improvements that can be incorporated in a consistent manner. In addition, application of the theory to the modeling of more complex, less conventional physical systems – including higher order kinematics, dynamical effects, material failure with dissimilar kinematics across scales, thermomechanics and even fluid mechanics – has also been presented. This provides very strong evidence of how powerful and useful the proposed variational framework can be as a tool for the rigorous and consistent development of new multiscale models.

Void volume fraction: f_v (referred to $\|\Omega_\mu\|$)	Void volume fraction: f_v^* (referred to $\|\Omega_\mu^L\|$)	Effective fracture energy: G_F [N/m]	Estimated fracture energy: G_F^{est} [N/m]
0.0	0.0	99.90	100
0.037	0.111	88.42	88.89
0.111	0.333	66.16	66.67

Table 2 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Comparison between the Effective fracture energy "G_F" (obtained by using the mutiscale approach) vs. the Estimated fracture energy "G_F^{est}"(computed from simple analytical considerations).

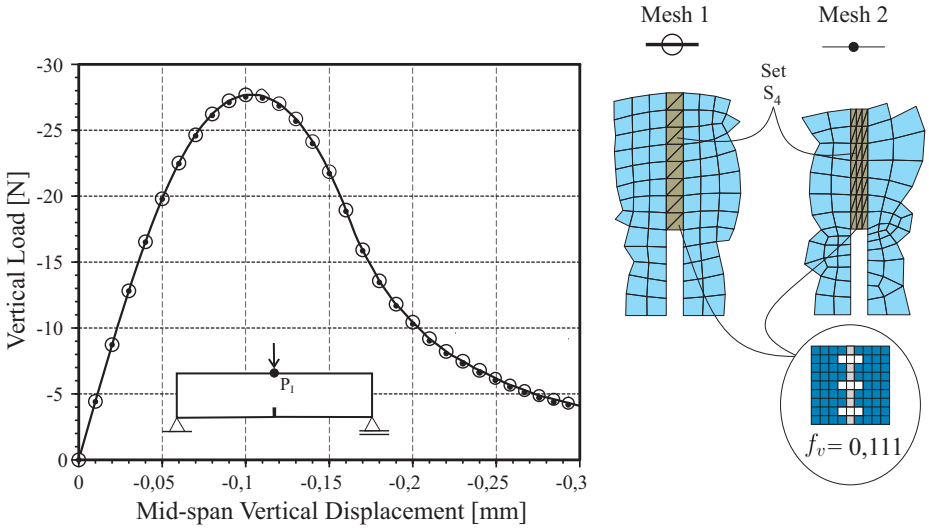

Fig. 13 Single-Edge Notched Beam Test with inner heterogeneous microstructure. Mesh-size independence of the FOMF approach.

We believe that the proposed systematization of RVE-based multiscale modeling is particularly relevant at present when there is a clear need to further combine more complex models of continua describing phenomena that take place at different scales in order to improve predictive capabilities. Our experience has shown that this appears to be even more relevant when resorting to kinematical descriptions for the different scales that are a priori heterogeneous.

Finally, we remark that the variational format in which model equations are presented within the present framework is naturally well-suited for numerical approximation by means of schemes such as the Finite Element Method. In this context, examples of practical numerical computations were presented, including the use of a non-conventional failure-oriented multiscale model with discontinuous kinematics.

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