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Research paper

# The method of multiscale virtual power for the derivation of a second order mechanical model

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ABSTRACT

A multi-scale model, based on the concept of Representative Volume Element (RVE), is proposed linking a classical continuum at RVE level to a macro-scale strain-gradient theory. The multi-scale model accounts for the effect of body forces and inertia phenomena occurring at the micro-scale. The Method of Multiscale Virtual Power recently proposed by the authors drives the construction of the model. In this context, the coupling between the macro- and micro-scale kinematical descriptors is defined by means of kinematical insertion and homogenisation operators, carefully postulated to ensure kinematical conservation in the scale transition. Micro-scale equilibrium equations as well as formulae for the homogenised (macro-scale) force- and stress-like quantities are naturally derived from the Principle of Multiscale Virtual Power – a variational extension of the Hill-Mandel Principle that enforces the balance of the virtual powers of both scales. As an additional contribution, further insight into the theory is gained with the enforcement of the RVE kinematical constraints by means of Lagrange multipliers. This approach unveils the reactive nature of homogenised force- and stress-like quantities and allows the characterisation of the homogenised stress-like quantities exclusively in terms of RVE boundary data in a straightforward manner.



## 1. Introduction

The development of second gradient theories has long been an active field of research aimed at the improvement of the predictive capabilities of mechanical models, beyond classical continuum mechanics. Such theories are developed through the enrichment of the kinematical description of continua which, in turn, yields a more complex structure of dual stress-like entities, requiring more complex constitutive models to describe the phenomenological behavior of more complex materials.

The literature in the field is vast and it is not the goal of the present work to discuss every aspect of the theory itself. The interested reader can refer to de Borst and Mühlhaus (1992); de Borst et al. (1995); Mühlhaus and Aifantis (1991); Nguyen and Andrieux (2005); Nguyen (2010); Peerlings et al. (1996); Polizzotto et al. (1997); Sunyk and Steinmann (2003), which address various theoretical and practical aspects of such formulations.

In recent years, multi-scale theories have been evolving to deal with increasingly complex materials, by linking micro-continuum mechanisms with macro-continuum theories in a myriad of contexts and applications. Particularly in the field of second gradient theories, the works by Kouznetsova et al. (2002, 2004) have provided a first link between classical micro-scale mechanics and second gradient macro-scale mechanics by means of the concept of Representative Volume Element (RVE). Similar work was later reported by Larson et al. (Larsson and Diebels, 2007; Larsson and Zhang, 2007), and also by Luscher et al. (Luscher et al., 2010, 2012). The present contribution is placed in the context of these works.

Despite such significant developments, there is still plenty of room to assess the real capabilities of muti-scale models, as well as to better understand the underlying fundamental model hypotheses and their associated consequences. Such an understanding can be achieved with the help of an appropriate variational framework. In fact, a suitable variational structure should allow a rational analysis of the model by means of a purely kinematical approach. That

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is, the definition of the kinematics at both (macro- and micro-) scales and the way in which they are coupled have a well-defined effect on the micro-scale (RVE) equilibrium problem, as well as on the homogenisation rules for the dual (force- and stress-like) quantities conjugated to the adopted kinematical descriptors. This issue deserves further discussions at present. For example, the kinematical constraints for the micro-scale fluctuation fields proposed in Kouznetsova et al. (2002) differ from that of Luscher et al. (2010). Therefore, a question naturally arises as to the possible equivalence and consistency of these boundary conditions.

Our goal in this paper, and its major novelty, is to provide a rational justification for and a rigorous derivation of the multi-scale formulation of a finite strain second-gradient macro-continuum mechanical theory arising from a classical first-order continuum theory at the micro-scale featuring body forces and inertia phenomena. In this context, the formulation is theoretically examined in detail and the consequences of the adopted kinematical assumptions are fully explored in the light of the so-called *Method of Multiscale Virtual Power* (MMVP) recently proposed by the authors in Blanco et al. (2016).

The MMVP can be seen as an extension, to multi-scale problems, of the Method of Virtual Power developed in Germain (1973), and provides a well-defined, structured framework to set the mechanical foundations of the multi-scale model addressed in the present paper. The MMVP requires firstly the definition of the kinematics of the macro- and micro-scales, as well as the way in which the two kinematics are linked. Then, through mathematical duality arguments, it is possible to identify the force- and stress-like quantities dual to the kinematical descriptors at both scales. Subsequently, the *Principle of Multiscale Virtual Power* (PMVP) also proposed in Blanco et al. (2016) is used as a generalisation of the Hill-Mandel Principle (Hill, 1965; Mandel, 1971) to provide the physical coupling between the two scales. As a variational extension of the classical Hill-Mandel principle, the PMVP postulates that the total virtual powers produced by duality pairings at both scales are balanced. As described in Blanco et al. (2016) in a rather general context, and demonstrated here in the formulation of the present higher-order multi-scale formulation, the PMVP yields a complete characterisation of the model, comprising (i) the RVE equilibrium problem with consistent boundary conditions for the micro-scale fluctuation fields, and (ii) the homogenisation formulae for body force- and stress-like quantities dual to the macro-scale kinematical descriptors. In addition, as a complementary novel aspect for the multi-scale analysis, an augmented Lagrange multiplier formulation of the PMVP allows a straightforward characterisation of the homogenised macro-scale generalised stresses which can be expressed in terms RVE boundary data alone – in line with the idea postulated by Hill in his landmark work (Hill, 1965).

Fundamentally, the theoretical framework based on the MMVP employed in the present work yields a multi-scale model that in some aspects differs from, and in many cases generalises, those available in previous contributions, such as (Kouznetsova et al., 2002, 2004; Luscher et al., 2010, 2012). The specific differences between the present approach and the existing literature will be highlighted throughout the manuscript, and we should stress that the definition of the micro-scale kinematics in the present paper leads to different kinematical constraints for the micro-scale fluctuation fields. Since the RVE mechanical equilibrium is subordinated to these constraints, homogenisation of dual quantities will ultimately differ. These issues are essential for a deeper understanding of the resulting multi-scale model and will be discussed in detail throughout the text.

The paper is organised as follows. Section 2 presents fundamental aspects of the methodology and basic ingredients of the multi-scale problem. The macro-scale second gradient mechanical model is reviewed in Section 3. Kinematical relations coupling both scales are presented in Section 4, and the corresponding Principle of Multiscale Virtual Power is formulated in Section 5. In Section 6, the RVE equilibrium equations as well as the homogenisation formulae for the macro-scale force- and stress-like quantities are derived from the PMVP by means of straightforward variational arguments. A discussion on the reactive nature of such homogenised quantities is also presented. Tangent operators for the present model are derived in Section 7. The paper closes in Section 8, where a discussion on the model hypotheses and their corresponding consequences is presented together with some concluding remarks.

## 2. Preliminaries

### 2.1. Method of Multiscale Virtual Power (MMVP)

In this work we employ the so-called Method of Multiscale Virtual Power (MMVP) proposed in Blanco et al. (2016). The method relies on three fundamental principles:

- Principle of *kinematical admissibility*: whereby the macro- and micro-kinematics are properly defined and the link between them is established by means of suitable assumptions concerning the procedures of *kinematical insertion* (i.e. how macro-scale kinematical quantities contribute to the micro-scale kinematics) and *kinematical homogenisation* (i.e. how micro-scale kinematical quantities are averaged in some sense to produce corresponding macro-scale counterparts).
- *Mathematical duality*: which allows a straightforward identification of force- and stress-like quantities compatible with the theory as power-conjugates of the kinematical descriptors adopted in each scale.
- The *Principle of Multiscale Virtual Power (PMVP)*: a variational generalisation of the Hill-Mandel Principle of Macrohomogeneity, from which the micro-scale equilibrium problem, as well as the homogenisation formulae for macro-scale force- and stress-like quantities, can be univocally derived by means of straightforward variational arguments.

### 2.2. Notation

The indices $M$ and $\mu$ are used to denote quantities belonging to the macro- and micro-scale, respectively. Then, the macro- and micro-scale reference domains (open sets in $\mathbb{R}^3$) are denoted, respectively, $\Omega_M$ and $\Omega_\mu$, with corresponding boundaries $\partial\Omega_M$ and $\partial\Omega_\mu$. Macro- and micro-scale reference coordinates are denoted $\mathbf{x}_M$ and $\mathbf{x}_\mu$. Let $\mathbf{u}_M$ and $\mathbf{u}_\mu$ be the macro- and micro-scale displacement vector fields, respectively. The reference gradient operators are denoted $\nabla_M$ in the macro-scale and $\nabla_\mu$ in the micro-scale, with corresponding divergence operators $\mathrm{div}_M$ and $\mathrm{div}_\mu$.

Second-order kinematics is adopted at the macro-scale. Hence, the kinematical descriptors that play a role in the characterisation of the macro-scale problem are $\mathbf{u}_M$, $\nabla_M\mathbf{u}_M$ and $\nabla_M\nabla_M\mathbf{u}_M$. Each point $\mathbf{x}_M$ of the macro-scale is associated to a Representative Volume Element (RVE) at the micro-scale. Within the micro-scale, only a first-order (classical) kinematics is considered. Hence, the kinematical descriptors of the micro-scale are simply $\mathbf{u}_\mu$ and $\nabla_\mu\mathbf{u}_\mu$.

Finally, a super-imposed hat $\hat{(\cdot)}$ is used in variational equations to denote kinematically admissible virtual actions in both scales. Tensor algebra operations (some of them non-conventional) are used throughout the paper and are represented using intrinsic tensor notation. These are defined in Appendix A.

Inertia effects will be considered throughout the manuscript, and $\ddot{(\cdot)}$ will be used to denote the second time derivative. It is important to remark that the multi-scale analysis considers that the time-scale is the same for both spatial scales. In addition, and for