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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 $\text{div}_M$ and $\text{div}_\mu$.

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

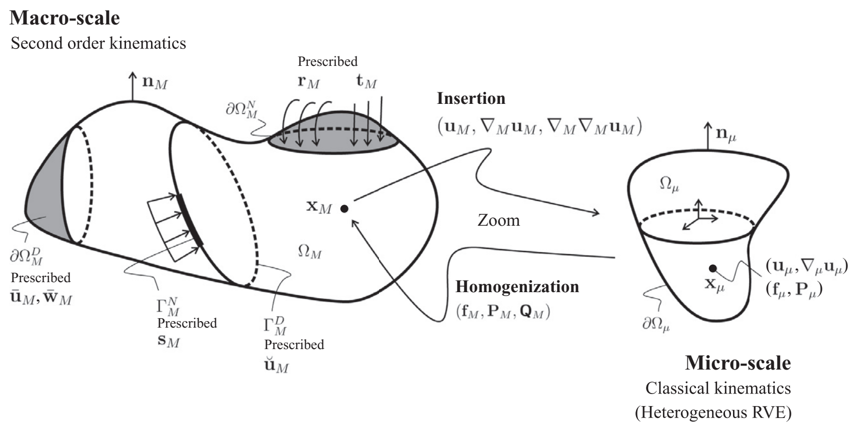


**Fig. 1.** Problem setting for the multi-scale model.

the sake of brevity, hereafter it will be assumed that the variational equations are valid $\forall t \in [0, T]$, and that proper initial conditions are defined at $t = 0$.

## 3. Macro-scale high-order formulation

At the macro-scale, a high-order model of the continuum body including inertia effects is formulated by means of the following (equilibrium) variational problem: find a displacement field $\mathbf{u}_M \in \mathcal{U}_M$ such that

$$\begin{aligned}\int_{\Omega_M} &\left[\mathbf{a}_M \cdot \hat{\mathbf{u}}_M + \mathbf{A}_M \cdot \nabla_M \hat{\mathbf{u}}_M + \mathsf{A}_M \cdot \nabla_M\nabla_M \hat{\mathbf{u}}_M\right] d\Omega_M \\ &+ \int_{\Omega_M} \left[\mathbf{S}_M \cdot \nabla_M \hat{\mathbf{u}}_M + \mathsf{R}_M \cdot \nabla_M\nabla_M \hat{\mathbf{u}}_M - \mathbf{b}_M \cdot \hat{\mathbf{u}}_M\right] d\Omega_M \\ = &\int_{\partial\Omega_M^N} \mathbf{t}_M \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N + \int_{\partial\Omega_M^N} \mathbf{r}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N \\ &+ \int_{\Gamma_M^N} \mathbf{s}_M \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N \quad \forall \hat{\mathbf{u}}_M \in \mathcal{V}_M, \end{aligned} \tag{1}$$

where $\mathbf{S}_M$ is a second order non-symmetric stress tensor, dual to the first gradient of the displacement and $\mathsf{R}_M$ is a third order stress tensor (momentum tensor) dual to the second gradient of the displacement and $\mathbf{b}_M$ is a *non-inertial* force per unit volume. Notice that we have taken into account the virtual power exerted by the inertia vector $\mathbf{a}_M$ and by the inertia high order tensors $\mathbf{A}_M$ and $\mathsf{A}_M$. In the context of a mono-scale mechanics with second order inertia, these objects take the form $\mathbf{a}_M = \rho_M \ddot{\mathbf{u}}_M$, $\mathbf{A}_M = \rho_M l_{M1}^2 \nabla_M \ddot{\mathbf{u}}_M$ and $\mathsf{A}_M = \rho_M l_{M2}^4 \nabla_M\nabla_M \ddot{\mathbf{u}}_M$, where $\rho_M$ is the material density and $l_{M1}$ and $l_{M2}$ are length scale parameters for high order inertia effects (Polizzotto, 2012, 2013). We can understand $\mathbf{a}_M$ as being an *inertial* force per unit volume, and $\mathbf{A}_M$ and *inertial* stress tensor. Also, the linear manifold $\mathcal{U}_M$, of kinematically admissible displacement fields, is defined as

$$\mathcal{U}_M = \left\{\mathbf{v} \in \mathbf{H}^2(\Omega_M),\ \mathbf{v}|_{\partial\Omega_M^D} = \bar{\mathbf{u}}_M,\ \left.\frac{\partial \mathbf{v}}{\partial n}\right|_{\partial\Omega_M^D} = \bar{\mathbf{w}}_M,\ \mathbf{v}|_{\Gamma_M^D} = \breve{\mathbf{u}}_M\right\}, \tag{2}$$

and, therefore, the space of kinematically admissible virtual actions $\hat{\mathbf{u}}_M$ is

$$\mathcal{V}_M = \left\{\mathbf{v} \in \mathbf{H}^2(\Omega_M),\ \mathbf{v}|_{\partial\Omega_M^D} = \mathbf{0},\ \left.\frac{\partial \mathbf{v}}{\partial n}\right|_{\partial\Omega_M^D} = \mathbf{0},\ \mathbf{v}|_{\Gamma_M^D} = \mathbf{0}\right\}. \tag{3}$$

Here we have considered a Dirichlet boundary $\partial\Omega_M^D$ and a Neumann $\partial\Omega_M^N$ in which there is, for simplicity, a unique edge $\Gamma_M$, which is divided into Neumann and Dirichlet counterparts $\Gamma_M^N$ and $\Gamma_M^D$ (lines in 3D, points in 2D), respectively (see Fig. 1). Essential boundary conditions are given by the displacement $\bar{\mathbf{u}}_M$, the rotation $\bar{\mathbf{w}}_M$ and the displacement $\breve{\mathbf{u}}_M$ at the edge $\Gamma_M^D$. For simplicity, we have assumed that all kinematic variables are prescribed on the Dirichlet boundary ($\bar{\mathbf{u}}_M$ and $\bar{\mathbf{w}}_M$ over $\partial\Omega_M^D$ and $\breve{\mathbf{u}}_M$ over $\Gamma_M^D$), and the Neumann boundary is the complementary part. Clearly, $\partial\Omega_M = \partial\Omega_M^N \cup \partial\Omega_M^D$ and $\Gamma_M = \Gamma_M^D \cup \Gamma_M^N \subset \partial\Omega_M$. The operator $\frac{\partial}{\partial n}$ denotes the derivative in the direction of the outward unit vector $\mathbf{n}_M$ normal to $\partial\Omega_M$. The problem setting is schematically illustrated in Fig. 1.

The variational Eq. (1) can be solved once the non-inertial force per unit volume $\mathbf{b}_M$, the force per unit surface $\mathbf{t}_M$, the moment per unit surface $\mathbf{r}_M$ and the force per unit length $\mathbf{s}_M$ are specified, and appropriate constitutive relations for $\mathbf{S}_M$ and $\mathsf{R}_M$ are given, i.e.

$$\mathbf{S}_M = \mathcal{S}_M(\nabla_M \mathbf{u}_M, \nabla_M\nabla_M \mathbf{u}_M), \tag{4}$$

$$\mathsf{R}_M = \mathcal{R}_M(\nabla_M \mathbf{u}_M, \nabla_M\nabla_M \mathbf{u}_M). \tag{5}$$

where, for the sake of notational simplicity, we shall focus on history-independent materials, with $\mathcal{S}_M$ and $\mathcal{R}_M$ denoting constitutive functionals for $\mathbf{S}_M$ and $\mathsf{R}_M$, respectively. We remark, however, that the developments presented here can be extended in a straightforward manner to consider history-dependent behavior.

In the context of multi-scale analysis, the variational problem (1) can be written simply as follows: find a displacement field $\mathbf{u}_M \in \mathcal{U}_M$ such that

$$\begin{aligned}\int_{\Omega_M} &\left[\mathbf{P}_M \cdot \nabla_M \hat{\mathbf{u}}_M + \mathsf{Q}_M \cdot \nabla_M\nabla_M \hat{\mathbf{u}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M\right] d\Omega_M \\ = &\int_{\partial\Omega_M^N} \mathbf{t}_M \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N + \int_{\partial\Omega_M^N} \mathbf{r}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N \\ &+ \int_{\Gamma_M^N} \mathbf{s}_M \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N \quad \forall \hat{\mathbf{u}}_M \in \mathcal{V}_M, \end{aligned} \tag{6}$$

where we have grouped the power exerted by quantities of the same nature introducing equivalent objects, which for the classical high order theory (Polizzotto, 2012, 2013) results

$$\mathbf{f}_M = \mathbf{b}_M - \rho_M \ddot{\mathbf{u}}_M, \tag{7}$$

$$\mathbf{P}_M = \mathbf{S}_M + \rho_M l_{M1}^2 \nabla_M \ddot{\mathbf{u}}_M, \tag{8}$$

$$\mathsf{Q}_M = \mathsf{R}_M + \rho_M l_{M2}^4 \nabla_M\nabla_M \ddot{\mathbf{u}}_M. \tag{9}$$

That is, the vector $\mathbf{f}_M$ and the tensors $\mathbf{P}_M$ and $\mathsf{Q}_M$, have inertial and non-inertial attributes.

**Remark 1.** In contrast to the classical phenomenological constitutive setting, in the context of the present multi-scale formulation the force $\mathbf{f}_M$, as well as the functionals for the stress-like quantities $\mathbf{P}_M$ and $\mathbf{Q}_M$, will be defined by means of homogenisation formulae involving fields defined over the micro-scale domain. Thus, the multi-scale model will naturally account for contributions from micro-scale level inertia effects.

The Euler-Lagrange equations associated to the variational Eq. (6) are obtained by means of the following procedure. First, integration by parts in (6) is required

$$\begin{aligned}\int_{\Omega_M} [-\mathrm{div}_M \mathbf{P}_M \cdot \hat{\mathbf{u}}_M + \mathrm{div}_M \mathrm{div}_M \mathbf{Q}_M \cdot \hat{\mathbf{u}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M]\, d\Omega_M \\ + \int_{\partial\Omega_M^N} \mathbf{P}_M \mathbf{n}_M \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N - \int_{\partial\Omega_M} (\mathrm{div}_M \mathbf{Q}_M)\mathbf{n}_M \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ + \int_{\partial\Omega_M^N} \mathbf{Q}_M \mathbf{n}_M \cdot \nabla_M \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ = \int_{\partial\Omega_M^N} \mathbf{t}_M \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N + \int_{\partial\Omega_M^N} \mathbf{r}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N \\ + \int_{\Gamma_M^N} \mathbf{s}_M \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N \qquad \forall \hat{\mathbf{u}}_M \in \mathcal{V}_M. \end{aligned} \tag{10}$$

Eq. (10) can be reorganised, yielding

$$\begin{aligned}\int_{\Omega_M} [-\mathrm{div}_M \mathbf{P}_M + \mathrm{div}_M \mathrm{div}_M \mathbf{Q}_M - \mathbf{f}_M] \cdot \hat{\mathbf{u}}_M \, d\Omega_M \\ + \int_{\partial\Omega_M^N} ([\mathbf{P}_M - \mathrm{div}_M \mathbf{Q}_M]\mathbf{n}_M - \mathbf{t}_M) \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ + \int_{\partial\Omega_M^N} \mathbf{Q}_M \mathbf{n}_M \cdot \nabla_M \hat{\mathbf{u}}_M \, d\partial\Omega_M^N - \int_{\partial\Omega_M^N} \mathbf{r}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N \\ - \int_{\Gamma_M^N} \mathbf{s}_M \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N = 0 \quad \forall\ \hat{\mathbf{u}}_M \in \mathcal{V}_M. \end{aligned} \tag{11}$$

Now note that, given a vector $\mathbf{v}$ and the surface $\partial\Omega_M^N$ with normal $\mathbf{n}_M$, we can decompose the gradient $\nabla_M \mathbf{v}$ as

$$\nabla_M \mathbf{v} = (\nabla_M^\partial \mathbf{v})\boldsymbol{\Pi}_M + \frac{\partial \mathbf{v}}{\partial n} \otimes \mathbf{n}_M, \tag{12}$$

where $\boldsymbol{\Pi}_M = \mathbf{I} - \mathbf{n}_M \otimes \mathbf{n}_M$ is the orthogonal projection operator onto the tangent plane at the considered point of the surface $\partial\Omega_M^N$, and $\nabla_M^\partial$ stands for the surface gradient operator (partial derivative operator with respect to the surface coordinates). Then, the product $\mathbf{Q}_M \mathbf{n}_M \cdot \nabla_M \hat{\mathbf{u}}_M$ is equivalently written as

$$\begin{aligned}\mathbf{Q}_M \mathbf{n}_M \cdot \nabla_M \hat{\mathbf{u}}_M &= \mathbf{Q}_M \mathbf{n}_M \cdot \left[ (\nabla_M^\partial \hat{\mathbf{u}}_M)\boldsymbol{\Pi}_M + \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \otimes \mathbf{n}_M \right] \\ &= (\mathbf{Q}_M \mathbf{n}_M)\boldsymbol{\Pi}_M \cdot \nabla_M^\partial \hat{\mathbf{u}}_M + (\mathbf{Q}_M \mathbf{n}_M)\mathbf{n}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n}. \end{aligned} \tag{13}$$

Integrating by parts over the surface $\partial\Omega_M^N$ the third term on the left hand side of (11), we obtain

$$\begin{aligned}\int_{\partial\Omega_M^N} \mathbf{Q}_M \mathbf{n}_M \cdot \nabla_M \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ = \int_{\partial\Omega_M^N} (\mathbf{Q}_M \mathbf{n}_M)\boldsymbol{\Pi}_M \cdot \nabla_M^\partial \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ + \int_{\partial\Omega_M^N} (\mathbf{Q}_M \mathbf{n}_M)\mathbf{n}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N \\ = -\int_{\partial\Omega_M^N} \mathrm{div}_M^\partial \left[ (\mathbf{Q}_M \mathbf{n}_M)\boldsymbol{\Pi}_M \right] \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ + \int_{\Gamma_M^N} [\![ (\mathbf{Q}_M \mathbf{n}_M)\mathbf{m}_M ]\!] \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N \\ + \int_{\partial\Omega_M^N} (\mathbf{Q}_M \mathbf{n}_M)\mathbf{n}_M \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N, \end{aligned} \tag{14}$$

where $\mathbf{m}_M = \boldsymbol{\tau}_M \times \mathbf{n}_M$, $\boldsymbol{\tau}_M$ is the unit vector tangent to the edge $\Gamma_M^N$, $\mathrm{div}_M^\partial$ is the surface divergence operator and $[\![\bullet]\!]$ denotes the jump of $\bullet$.

Replacing (14) into (11) yields

$$\begin{aligned}\int_{\Omega_M} \left[ -\mathrm{div}_M \mathbf{P}_M + \mathrm{div}_M \mathrm{div}_M \mathbf{Q}_M - \mathbf{f}_M \right] \cdot \hat{\mathbf{u}}_M \, d\Omega_M \\ + \int_{\partial\Omega_M^N} \left( \left[ \mathbf{P}_M - \mathrm{div}_M \mathbf{Q}_M \right]\mathbf{n}_M - \mathbf{t}_M \right) \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ - \int_{\partial\Omega_M^N} \mathrm{div}_M^\partial \left[ (\mathbf{Q}_M \mathbf{n}_M)\boldsymbol{\Pi}_M \right] \cdot \hat{\mathbf{u}}_M \, d\partial\Omega_M^N \\ + \int_{\Gamma_M^N} \left( [\![ (\mathbf{Q}_M \mathbf{n}_M)\mathbf{m}_M ]\!] - \mathbf{s}_M \right) \cdot \hat{\mathbf{u}}_M \, d\Gamma_M^N \\ + \int_{\partial\Omega_M^N} \left[ (\mathbf{Q}_M \mathbf{n}_M)\mathbf{n}_M - \mathbf{r}_M \right] \cdot \frac{\partial \hat{\mathbf{u}}_M}{\partial n} \, d\partial\Omega_M^N = 0 \\ \forall \hat{\mathbf{u}}_M \in \mathcal{V}_M. \end{aligned} \tag{15}$$

Finally, by using standard variational arguments we obtain the Euler-Lagrange equations associated to the variational Eq. (6)

$$-\mathrm{div}_M \mathbf{P}_M + \mathrm{div}_M \mathrm{div}_M \mathbf{Q}_M = \mathbf{f}_M \qquad \text{in } \Omega_M, \tag{16}$$

$$\left[ \mathbf{P}_M - \mathrm{div}_M \mathbf{Q}_M \right]\mathbf{n}_M - \mathrm{div}_M^\partial \left[ (\mathbf{Q}_M \mathbf{n}_M)\boldsymbol{\Pi}_M \right] = \mathbf{t}_M \qquad \text{on } \partial\Omega_M^N, \tag{17}$$

$$(\mathbf{Q}_M \mathbf{n}_M)\mathbf{n}_M = \mathbf{r}_M \qquad \text{on } \partial\Omega_M^N, \tag{18}$$

$$[\![ (\mathbf{Q}_M \mathbf{n}_M)\mathbf{m}_M ]\!] = \mathbf{s}_M \qquad \text{on } \Gamma_M^N, \tag{19}$$

which, together with the following essential boundary conditions,

$$\mathbf{u}_M = \bar{\mathbf{u}}_M \qquad \text{on } \partial\Omega_M^D, \tag{20}$$

$$\frac{\partial \mathbf{u}_M}{\partial n} = \bar{\mathbf{w}}_M \qquad \text{on } \partial\Omega_M^D, \tag{21}$$

$$\mathbf{u}_M = \breve{\mathbf{u}}_M \qquad \text{on } \Gamma_M^D, \tag{22}$$

fully characterise the boundary value problem associated to the variational principle (6).

Note that by introducing (7), (8) and (9) in (16), (17), (18) and (19), the equilibrium equations for high order continua with inertia effects are recovered. The reader is referred to Polizzotto (2013) for further details.

In what follows, we denote $\mathbf{G}_M = \nabla_M \mathbf{u}_M$, $\mathbb{G}_M = \nabla_M \nabla_M \mathbf{u}_M$ and, accordingly, we define $\hat{\mathbf{G}}_M = \nabla_M \hat{\mathbf{u}}_M$ and $\hat{\mathbb{G}}_M = \nabla_M \nabla_M \hat{\mathbf{u}}_M$. Note that the third-order tensor $\mathbb{G}_M$ is such that $\mathbb{G}_M = \mathbb{G}_M^T$ (symmetric in the last two indices, see Appendix A for details).

## 4. Multi-scale kinematics

In the context of the Method of Multiscale Virtual Power proposed in Blanco et al. (2016), the definition of the kinematics of the macro- and micro-scales, as well as how they are linked, is the only degree of arbitrariness one has in developing a multi-scale model. Once such kinematical relations are postulated, mathematical duality will define the associated force- and stress-like quantities compatible with each scale of the model, and the Principle of Multiscale Virtual Power will univocally lead to the RVE equilibrium equations as well as to the homogenisation relations linking the micro- and macro-scale force- and stress-like quantities. The kinematics of the macro-continuum has already been established in Section 3. Here we shall proceed to postulate the kinematics of the micro-scale as well as the operations of *kinematical insertion*and *kinematical homogenisation*, that link the kinematics of the two scales. These will completely characterise the kinematical description of the proposed multi-scale model.

### 4.1. Kinematical insertion

Without loss of generality, we consider the origin of the coordinate system of an RVE associated to a point $\mathbf{x}_M$ of the macro-scale to be located at the geometric center of the micro-scale domain $\Omega_\mu$, that is

$$\int_{\Omega_\mu} \mathbf{x}_\mu \, d\Omega_\mu = \mathbf{0}. \tag{23}$$

*Kinematical insertion* (Blanco et al., 2016) defines how the macro-scale kinematics at a given point of the macro-continuum contributes to the kinematics of the micro-scale. In the present case, the operation of *insertion*of the macro-scale kinematical descriptors – the triad $(\mathbf{u}_M, \mathbf{G}_M, \mathbb{G}_M)$ – into the micro-scale kinematics is postulated as follows:

$$\mathbf{u}_\mu = \mathbf{u}_M + \mathbf{G}_M \mathbf{x}_\mu + \frac{1}{2}\mathbb{G}_M[(\mathbf{x}_\mu \otimes \mathbf{x}_\mu) - \mathbf{J}] + \tilde{\mathbf{u}}_\mu, \tag{24}$$

where $\mathbf{J}$ is the RVE second-order moment of volume tensor defined by

$$\mathbf{J} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\Omega_\mu, \tag{25}$$

and $\tilde{\mathbf{u}}_\mu$ is named the micro-scale displacement *fluctuation* field.

Note that, by construction, $\mathbf{J}$ is an invertible second-order tensor. The reason for the tensor $\mathbf{J}$ to take part in expression (24) will be clear later. For the moment, we anticipate that the macro-scale kinematics inserted this way allows (along with the kinematically admissibility concept of Section 4.3) the conservation of kinematical quantities in the multi-scale transition process.

It is important to highlight that in expansion (24) the triad $(\mathbf{u}_M, \mathbf{G}_M, \mathbb{G}_M)$ represents the value of the macro-scale fields $\mathbf{u}_M$, $\nabla_M \mathbf{u}_M$ and $\nabla_M \nabla_M \mathbf{u}_M$ at a point $\mathbf{x}_M$ of the macro-scale, associated to a given RVE, that is to say $(\mathbf{u}_M, \nabla_M \mathbf{u}_M, \nabla_M \nabla_M \mathbf{u}_M)|_{\mathbf{x}_M} = (\mathbf{u}_M, \mathbf{G}_M, \mathbb{G}_M)$. Thus, $(\mathbf{u}_M, \mathbf{G}_M, \mathbb{G}_M) \in \mathbb{R}^3 \times \mathbb{R}^{3\times3} \times (\mathbb{R}^{3\times3\times3})^S$, where $(\mathbb{R}^{3\times3\times3})^S$ denotes the set of third order matrices satisfying $\mathbb{A}^\top = \mathbb{A}$ in the sense defined in Appendix A.

**Remark 2.** The decomposition of the micro-scale displacement field $\mathbf{u}_\mu$ considered in (24) differs from the ones proposed in Kouznetsova et al. (2002, 2004); Luscher et al. (2010, 2012) since in the present work the contribution of the macro-scale displacement $\mathbf{u}_M$ is added as it will be fundamental for the characterisation of the external power exerted per unit volume that must be considered at the RVE level when general micro-scale body and inertia forces are present. This was actually not required in Kouznetsova et al. (2002, 2004) because external body forces were not considered in the micro-scale analysis presented by these authors. In Luscher et al. (2010, 2012), however, such forces were incorporated in the analysis, but the macro-scale displacement contribution to the micro-scale displacement was not accounted for. Another difference between the present paper and these contributions is the form of the second-order term. While in Kouznetsova et al. (2002, 2004); Luscher et al. (2010, 2012) the second-order term features the form $\frac{1}{2}\mathbb{G}_M(\mathbf{x}_\mu \otimes \mathbf{x}_\mu)$, in (24) we have incorporated the term $-\frac{1}{2}\mathbb{G}_M\mathbf{J}$ (not present in previous contributions) which is fundamental for a correct characterisation of the homogenised part of the micro-scale external power per unit volume. In fact, this contribution to the homogenisation is obtained in duality with the constant component of the micro-scale displacement field $\mathbf{u}_\mu$.

### 4.2. Kinematical homogenisation

The operations of *kinematical homogenisation*define how macro-scale kinematical descriptors are related to averages (in some sense) of micro-scale kinematical descriptors. In the present context, we postulate that the homogenisation of the micro-scale kinematical fields is given by the following formulae:

- Homogenisation related to the macro-scale displacement vector

$$\mathbf{u}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \, d\Omega_\mu. \tag{26}$$

- Homogenisation related to the first gradient of the macro-scale displacement vector

$$\mathbf{G}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_\mu \mathbf{u}_\mu \, d\Omega_\mu. \tag{27}$$

- Homogenisation related to the second gradient of the macro-scale displacement vector

$$\mathbb{G}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} [(\nabla_\mu \mathbf{u}_\mu \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}]^S \, d\Omega_\mu, \tag{28}$$

where the $(\cdot)^S$ and $(\cdot \circ \cdot)$ operations are defined in Appendix A.

We remark that the postulated averaging relations (26), (27) and (28) guarantee the conservation of kinematical quantities. In the case that the micro-scale kinematics is exclusively described in terms of the macro-scale quantities, i.e. $\tilde{\mathbf{u}}_\mu = \mathbf{0}$ in (24), it is a simple exercise to prove that (26), (27) and (28) hold trivially. This sense of kinematical conservation implies that if a certain macro-scale kinematical quantity is inserted into the micro-scale domain, the same quantity must be retrieved by the homogenisation process. As a result, we shall see that the fluctuation of the micro-scale displacement field can in general be non-zero, but cannot be entirely arbitrary. That is, additional constraints must be imposed upon displacement fluctuation fields in order to preserve the macro-scale kinematics in the homogenisation process. This motivates the introduction of the so-called *kinematical admissibility* requirement, explained below.

**Remark 3.** The conservation of kinematical quantities is a novel concept introduced in the present framework that establishes the need for homogenisation rules connecting $\mathbf{u}_M$, $\mathbf{G}_M$ and $\mathbb{G}_M$ to the micro-scale field $\mathbf{u}_\mu$. While averaging relation (27) is standard and has been employed in Kouznetsova et al. (2002, 2004); Luscher et al. (2010, 2012), (26) and (28) are postulated here in order to establish such a connection between macro- and micro-scale kinematical fields. Differently from the aforementioned papers, in the present approach the resulting kinematical micro-scale level constraints are entirely dependent on the definition of these averaging relations.

### 4.3. Kinematical admissibility

Following the above discussion, we class as *kinematically admissible* all micro-scale displacement fields $\mathbf{u}_\mu \in \mathcal{V}_\mu$, where

$$\begin{aligned}\mathcal{V}_\mu = \Big\{\mathbf{v} \in \mathbf{H}^1(\Omega_\mu),\ &\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{v}\, d\Omega_\mu = \mathbf{u}_M,\\ &\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_\mu \mathbf{v}\, d\Omega_\mu = \mathbf{G}_M,\\ &\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \left[(\nabla_\mu \mathbf{v} \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}\right]^S d\Omega_\mu = \mathbb{G}_M\Big\},\end{aligned} \tag{29}$$

is the linear manifold of kinematically admissible micro-scale displacements. The kinematical admissibility concept can be expressed equivalently in terms of the fluctuation of the micro-scale displacement field $\tilde{\mathbf{u}}_\mu$ as follows.

First, by introducing (24) into the right hand side of (26), and using (23), we readily obtain

$$\mathbf{u}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\left[\mathbf{u}_M + \mathbf{G}_M\mathbf{x}_\mu + \frac{1}{2}\mathbb{G}_M[(\mathbf{x}_\mu\otimes\mathbf{x}_\mu)-\mathbf{J}] + \tilde{\mathbf{u}}_\mu\right]d\Omega_\mu = \mathbf{u}_M + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\, d\Omega_\mu. \quad (30)$$

Then, (26) is satisfied provided that

$$\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\, d\Omega_\mu = \mathbf{0}. \quad (31)$$

Next, by replacing (24) in (27), we get

$$\mathbf{G}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\left[\mathbf{G}_M + \mathbb{G}_M\mathbf{x}_\mu + \nabla_\mu\tilde{\mathbf{u}}_\mu\right]d\Omega_\mu = \mathbf{G}_M + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\nabla_\mu\tilde{\mathbf{u}}_\mu\, d\Omega_\mu. \quad (32)$$

Then, (27) is satisfied provided that

$$\int_{\Omega_\mu}\nabla_\mu\tilde{\mathbf{u}}_\mu\, d\Omega_\mu = \mathbf{0}, \quad (33)$$

or, equivalently,

$$\int_{\partial\Omega_\mu}\tilde{\mathbf{u}}_\mu\otimes\mathbf{n}_\mu\, d\partial\Omega_\mu = \mathbf{0}, \quad (34)$$

where $\mathbf{n}_\mu$ is the outward unit vector normal to $\partial\Omega_\mu$. Further, by introducing (24) into (28), and using (23) and (25), we obtain

$$\mathbb{G}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\left[((\mathbf{G}_M + \mathbb{G}_M\mathbf{x}_\mu + \nabla_\mu\tilde{\mathbf{u}}_\mu)\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\Omega_\mu = \mathbb{G}_M + \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\left[(\nabla_\mu\tilde{\mathbf{u}}_\mu\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\Omega_\mu. \quad (35)$$

Then, (28) is satisfied provided that

$$\int_{\Omega_\mu}\left[(\nabla_\mu\tilde{\mathbf{u}}_\mu\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\Omega_\mu = \mathbb{0}. \quad (36)$$

For any vector $\mathbf{v}$, and recalling that $\mathbf{J}^{-1}$ is symmetric, the following holds

$$\begin{aligned}(\nabla_\mu\mathbf{v}\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1} &= (\nabla_\mu\mathbf{v}\otimes(\mathbf{J}^{-1}\mathbf{x}_\mu)) \\ &= (\nabla_\mu((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\mathbf{v}))^t - \mathbf{v}\otimes(\mathbf{J}^{-1}\nabla_\mu\mathbf{x}_\mu)^T \\ &= (\nabla_\mu((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\mathbf{v}))^t - \mathbf{v}\otimes\mathbf{J}^{-1}. \end{aligned} \quad (37)$$

Hence, from (36), and bearing in mind that (31) must hold, we obtain

$$\begin{aligned}&\int_{\Omega_\mu}\left[(\nabla_\mu\tilde{\mathbf{u}}_\mu\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\Omega_\mu \\ &= \int_{\Omega_\mu}\left[(\nabla_\mu((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\tilde{\mathbf{u}}_\mu))^t - \tilde{\mathbf{u}}_\mu\otimes\mathbf{J}^{-1}\right]^S d\Omega_\mu \\ &= \int_{\Omega_\mu}\left[(\nabla_\mu((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\tilde{\mathbf{u}}_\mu))^t\right]^S d\Omega_\mu - \left[\left(\int_{\Omega_\mu}\tilde{\mathbf{u}}_\mu\, d\Omega_\mu\right)\otimes\mathbf{J}^{-1}\right]^S \\ &= \int_{\Omega_\mu}\left[(\nabla_\mu((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\tilde{\mathbf{u}}_\mu))^t\right]^S d\Omega_\mu \\ &= \int_{\partial\Omega_\mu}\left[((\mathbf{J}^{-1}\mathbf{x}_\mu)\otimes\tilde{\mathbf{u}}_\mu\otimes\mathbf{n}_\mu))^t\right]^S d\partial\Omega_\mu \\ &= \int_{\partial\Omega_\mu}[\tilde{\mathbf{u}}_\mu\otimes\mathbf{n}_\mu\otimes(\mathbf{J}^{-1}\mathbf{x}_\mu)]^S d\partial\Omega_\mu = \mathbb{0},\end{aligned} \quad (38)$$

where $(\cdot)^t$ is a transpose operation defined in Appendix A.

Then, (36) can be equivalently expressed as a boundary constraint as follows:

$$\int_{\partial\Omega_\mu}\left[(\tilde{\mathbf{u}}_\mu\otimes\mathbf{n}_\mu\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\partial\Omega_\mu = \mathbb{0}. \quad (39)$$

It is important to highlight that in the derivation of (39) we have made use of the fact that (31) is satisfied. That is, constraint (36) can be written as a boundary constraint only if the field $\tilde{\mathbf{u}}_\mu$ has zero mean value over the entire micro-scale domain.

**Remark 4.** It is important to point out that the derivation of the boundary conditions comes naturally as a consequence of the conservation of homogenised kinematic quantities in the transition between scales. A different approach to obtain boundary conditions for a high-order model is proposed in Luscher et al. (2010, 2012), where orthogonality conditions are postulated to derive independent boundary constraints at the RVE level.

**Remark 5.** Comparing to previous works, the kinematical constraint given by (31) was not considered in Kouznetsova et al. (2002, 2004); but it was acknowledged in Luscher et al. (2010, 2012) for the displacement fluctuation field. Nonetheless, it is not clear in the latter works whether the constraint (31) is effectively considered for the admissible variations of the fluctuation field in the principle of virtual power. In turn, constraint (36), which leads to (39), is completely new. Specifically, constraint (31) allows a correct characterisation, through duality, of homogenised forces; and, constraint (39) provides a general form to ensure the conservation of second-order kinematics in the transition between scales. In Kouznetsova et al. (2002, 2004) the argument to construct a boundary condition resembling (39) is similar to the one employed here; however, it is not the same, because for the derivation of boundary conditions from these constraints it is necessary to make use of (31), which, as already mentioned, is not considered in Kouznetsova et al. (2002, 2004). Differently, the criterion to construct boundary conditions in Luscher et al. (2010, 2012) is based on orthogonality arguments, which yield different kinematical constraints.

Hence, the micro-scale displacement $\mathbf{u}_\mu$, given by (24), is kinematically admissible for a given triad $(\mathbf{u}_M, \mathbf{G}_M, \mathbb{G}_M)$, if it satisfies (31), (34) and (39), that is if $\tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{V}}_\mu$, where

$$\tilde{\mathcal{V}}_\mu = \left\{\mathbf{v}\in\mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu}\mathbf{v}\, d\Omega_\mu = \mathbf{0},\ \int_{\partial\Omega_\mu}\mathbf{v}\otimes\mathbf{n}_\mu\, d\partial\Omega_\mu = \mathbf{0},\ \int_{\partial\Omega_\mu}\left[(\mathbf{v}\otimes\mathbf{n}_\mu\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\partial\Omega_\mu = \mathbb{0}\right\}. \quad (40)$$

Note that space $\tilde{\mathcal{V}}_\mu$ can be equivalently defined using only volume constraints:

$$\tilde{\mathcal{V}}_\mu = \left\{\mathbf{v}\in\mathbf{H}^1(\Omega_\mu),\ \int_{\Omega_\mu}\mathbf{v}\, d\Omega_\mu = \mathbf{0},\ \int_{\Omega_\mu}\nabla_\mu\mathbf{v}\, d\Omega_\mu = \mathbf{0},\ \int_{\Omega_\mu}\left[(\nabla_\mu\mathbf{v}\otimes\mathbf{x}_\mu)\circ\mathbf{J}^{-1}\right]^S d\Omega_\mu = \mathbb{0}\right\}. \quad (41)$$

Clearly, the set of constraints (31), (34) and (39) that defines $\tilde{\mathcal{V}}_\mu$ in (40) is equivalent to the set (31), (33) and (36) that defines $\tilde{\mathcal{V}}_\mu$ in (41). In fact, these two sets of constraints over the fluctuation field $\tilde{\mathbf{u}}_\mu$ are equivalent to the original relations between macro-scale and micro-scale kinematical descriptors given by the set of Eq. (26), (27) and (28) which define the linear manifold $\mathcal{V}_\mu$ in (29). That is, assuming that $\mathbf{u}_\mu$ is expanded as in (24), then $\mathbf{u}_\mu \in \mathcal{V}_\mu$ if and only if $\tilde{\mathbf{u}}_\mu \in \tilde{\mathcal{V}}_\mu$.

**Remark 6.** The complete characterisation of the space of admissible displacement fluctuation fields, $\tilde{\mathcal{V}}_\mu$, provides the kinematical foundation upon which the principle of multi-scale virtual power is to be regarded. That is, the constraints that play a role in (40) (or, equivalently, in (41)) inevitably affect the micro-scale mechanical equilibrium problem. Therefore, since novel kinematical constraints are derived in the present work, they will result in a novel multi-scale model.

**Remark 7.** The space $\tilde{\mathcal{V}}_\mu$ introduced above is the *space of minimally constrained displacement fluctuations* such that the kinematical relations between both scales are satisfied. Any subspace, $\tilde{\mathcal{V}}^*_\mu \subset \tilde{\mathcal{V}}_\mu$ can be adopted as a *kinematically admissible space of displacement fluctuations* and should serve, in this sense, to derive more kinematically constrained multi-scale submodels (e.g. models based on the assumption of null RVE kinematical boundary conditions for the displacement fluctuation field, or on suitable generalisations to this high order setting of periodic boundary constraints). This choice of "working" space of kinematically admissible displacement fluctuations is rather arbitrary and, if a realistic model is to be derived, should be made so as to capture the real kinematics of the physical problem in question as closely as possible.

Finally, it should be noted that, since all the kinematical constraints on $\tilde{\mathbf{u}}_\mu$ are homogeneous, it follows that the corresponding virtual actions, denoted $\hat{\tilde{\mathbf{u}}}_\mu$, satisfy $\hat{\tilde{\mathbf{u}}}_\mu \in \tilde{\mathcal{V}}_\mu$.

## 5. Principle of Multiscale Virtual Power (PMVP)

Having completely characterised the kinematics of the multi-scale model in question, we shall now proceed to state the *Principle of Multiscale Virtual Power*– one of the pillars of the multi-scale variational framework developed in Blanco et al. (2016). This principle effectively postulates that the total virtual power is conserved across scales and, by means of standard variational arguments, leads univocally to the homogenisation formulae for the relevant force- and stress-like quantities, as well as to the micro-scale equilibrium equations appropriate for the present model.

For the sake of completeness, and to gain further insight into the theory, two equivalent forms of this principle are discussed here, namely the *Primal Variational Statement* and the *Lagrange Multiplier Variational Statement*, presented respectively in Sections 5.1 and 5.2.

### 5.1. Primal variational statement

This version of the Principle of Multiscale Virtual Power is established by considering that the kinematical constraints, discussed in Section 4, are embedded in the definition of the kinematical functional space $\tilde{\mathcal{V}}_\mu$ defined by (40) or (41).

Let us firstly introduce the total virtual power at a macro-scale point $\mathbf{x}_M$, according to the macro-scale problem (1). The total virtual power is a linear functional of the triad $(\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathbb{G}}_M)$ whose form is

$$P^{\text{tot}}_{M,\mathbf{x}_M}(\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathbb{G}}_M) = |\Omega_\mu|(\mathbf{P}_M \cdot \hat{\mathbf{G}}_M + \mathbb{Q}_M \cdot \hat{\mathbb{G}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M). \quad (42)$$

Since our aim here is to describe the micro-scale mechanics by means of the classical continuum theory with inertia effects, the total virtual power of the RVE is, in turn, a linear functional of only the virtual micro-scale displacement field, $\hat{\mathbf{u}}_\mu$, and its first gradient, $\nabla_\mu \hat{\mathbf{u}}_\mu$. Its classical form is

$$P^{\text{tot}}_\mu(\hat{\mathbf{u}}_\mu, \nabla_\mu \hat{\mathbf{u}}_\mu) = \int_{\Omega_\mu} (\mathbf{P}_\mu \cdot \nabla_\mu \hat{\mathbf{u}}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \cdot \hat{\mathbf{u}}_\mu)\, d\Omega_\mu, \quad (43)$$

where $\mathbf{P}_\mu$ is the first Piola-Kirchhoff stress tensor, $\mathbf{f}_\mu$ and $\rho_\mu$ are, respectively, the micro-scale body force and mass density fields.

The Principle of Multiscale Virtual Power for the present case states that the total virtual power at a given point $\mathbf{x}_M$ of the macro-scale must equal the total virtual power produced at the associated micro-scale domain $\Omega_\mu$, for all kinematically admissible virtual fields. That is, the following variational equation must be satisfied,

$$|\Omega_\mu|\big(\mathbf{P}_M \cdot \hat{\mathbf{G}}_M + \mathbb{Q}_M \cdot \hat{\mathbb{G}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M\big)$$
$$= \int_{\Omega_\mu} (\mathbf{P}_\mu \cdot \nabla_\mu \hat{\mathbf{u}}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \cdot \hat{\mathbf{u}}_\mu)\, d\Omega_\mu$$
$$\forall (\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathbb{G}}_M) \text{ and } \forall \hat{\mathbf{u}}_\mu \text{ kinematically admissible.} \quad (44)$$

Or, equivalently, by introducing (24) in the above, the Principle of Multiscale Virtual Power can be expressed as

$$\begin{aligned}
&\mathbf{P}_M \cdot \hat{\mathbf{G}}_M + \mathbb{Q}_M \cdot \hat{\mathbb{G}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M \\
&= \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu \cdot (\hat{\mathbf{G}}_M + \hat{\mathbb{G}}_M \mathbf{x}_\mu + \nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu)\, d\Omega_\mu \\
&\quad - \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \\
&\quad \cdot \left(\hat{\mathbf{u}}_M + \hat{\mathbf{G}}_M \mathbf{x}_\mu + \frac{1}{2} \hat{\mathbb{G}}_M [(\mathbf{x}_\mu \otimes \mathbf{x}_\mu) - \mathbf{J}] + \hat{\tilde{\mathbf{u}}}_\mu\right) d\Omega_\mu \\
&\forall (\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathbb{G}}_M) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S,\ \forall \hat{\tilde{\mathbf{u}}}_\mu \in \tilde{\mathcal{V}}_\mu.
\end{aligned} \quad (45)$$

**Remark 8.** For further comparison with previous contributions in the field, note that PMVP (45) takes into account the effect of micro-scale body forces (including micro-scale inertia) in the physical coupling between scales. This effect was accounted for in Kouznetsova et al. (2002, 2004). In turn, although body forces were incorporated in the multi-scale formulation proposed in Luscher et al. (2010, 2012), recall that the model developed here is based on a different expansion of the micro-scale fluctuation field (kinematical insertion operation), resulting in a different expansion of the admissible variations $\hat{\tilde{\mathbf{u}}}_\mu$ that, as a consequence, characterises a different space $\tilde{\mathcal{V}}_\mu$. This affects the way in which the kinematical descriptors (displacement and deformation gradient) exert power against dual counterparts (force and stress). Therefore, the mechanical equilibrium is modified, and so are all subsequent homogenisation procedures derived from the PMVP. This will be clearly shown in the homogenised formulae derived in what follows.

### 5.2. Lagrange multiplier variational statement

The main reason for using this alternative Lagrange multiplier-based form of the PMVP is that it naturally unveils the reactive forces and stresses resulting from the kinematical constraints incorporated in the definition of the space $\tilde{\mathcal{V}}_\mu$, that takes part in (45). As we shall see later, such reactions add significant insight into the fundamental link that exists between the postulated kinematical constraints of the RVE and the homogenised force- and stress-like quantities that appear at the macro-scale.

For the present model, the Lagrange multiplier variational statement is obtained by simply removing the kinematical constraints of the space $\tilde{\mathcal{V}}_\mu$ defined by (40) or (41) and then enforcing these constraints by means of appropriate Lagrange multipliers in the PMVP. For convenience, we shall enforce these constraints explicitly in their volume integral format. i.e., we will work with (31), (33) and (36) (as in definition (41)). These constraints will be associated with the Lagrange multipliers denoted $\mathbf{c}$, $\mathbf{T}$ and $\mathbb{M}$, respectively. Accordingly, the Principle of Multiscale Virtual Power (45) is rewritten as

$$\begin{aligned}
&\mathbf{P}_M \cdot \hat{\mathbf{G}}_M + \mathbb{Q}_M \cdot \hat{\mathbb{G}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M \\
&= \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu \cdot (\hat{\mathbf{G}}_M + \hat{\mathbb{G}}_M \mathbf{x}_\mu + \nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu)\, d\Omega_\mu \\
&\quad - \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \\
&\quad \cdot \left(\hat{\mathbf{u}}_M + \hat{\mathbf{G}}_M \mathbf{x}_\mu + \frac{1}{2} \hat{\mathbb{G}}_M [(\mathbf{x}_\mu \otimes \mathbf{x}_\mu) - \mathbf{J}] + \hat{\tilde{\mathbf{u}}}_\mu\right) d\Omega_\mu \\
&\quad + \hat{\mathbf{c}} \cdot \left(\frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu\, d\Omega_\mu\right) + \mathbf{c} \cdot \left(\frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \hat{\tilde{\mathbf{u}}}_\mu\, d\Omega_\mu\right)
\end{aligned}$$

$$- \hat{\mathbf{T}} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \nabla_\mu \tilde{\mathbf{u}}_\mu \, d\Omega_\mu \right) - \mathbf{T} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu \right)$$
$$- \hat{\mathsf{M}} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} [(\nabla_\mu \tilde{\mathbf{u}}_\mu \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}]^S \, d\Omega_\mu \right)$$
$$- \mathsf{M} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} [(\nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}]^S \, d\Omega_\mu \right)$$
$$\forall (\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathsf{G}}_M) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S, \ \forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega_\mu),$$
$$\forall (\hat{\mathbf{c}}, \hat{\mathbf{T}}, \hat{\mathsf{M}}) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S, \tag{46}$$

where the signs of the terms containing the Lagrange multiplier have been chosen for convenience.

It should be noted that the volume constraints (33) and (36) were used to derive boundary conditions (34) and (39) in Section 4. However, it must be observed that in order to obtain (39) the restriction (31) has been used. Thus, the boundary constraint (39) is not independent from (31). In the Primal Variational Statement this fact has no consequences because fields in $\tilde{\mathscr{V}}_\mu$ automatically satisfy (31). However, in the Lagrange Multiplier Variational Statement restriction (39) can not be used, and it requires the enforcement of the original (volume) constraint (36).

**Remark 9.** Clearly, variational formulation (46) is valid for the case of the minimally constrained space of admissible fluctuation fields, that is $\tilde{\mathscr{V}}_\mu$. If an RVE model with additional boundary constraints is considered, it is necessary to replace the terms associated to constraints (33) and (36), that is, the terms corresponding to the Lagrange multipliers $\mathbf{T}$ and $\mathsf{M}$, and their variations $\hat{\mathbf{T}}$ and $\hat{\mathsf{M}}$, by terms with the following form

$$- \int_{\partial\Omega_\mu} \hat{\mathbf{r}}_\mu \cdot \tilde{\mathbf{u}}_\mu \, d\partial\Omega_\mu - \int_{\partial\Omega_\mu} \mathbf{r}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\partial\Omega_\mu \qquad \mathbf{r}_\mu, \hat{\mathbf{r}}_\mu \in \mathbf{L}, \tag{47}$$

where $\mathbf{L}$ is an appropriate space that characterises the structure of the Lagrange multiplier $\mathbf{r}_\mu$ and its variation. In other words, this space characterises the nature of the constraint. For example, in the case of zero fluctuation $\tilde{\mathbf{u}}_\mu$ imposed over $\partial\Omega_\mu$ we have $\mathbf{L} = \mathbf{H}^{-1/2}(\partial\Omega_\mu)$. For the sake of clarity, in the forthcoming developments the minimally constrained model (variational formulation (46)) is considered, and the connection with other (more constrained) models will be made as appropriate.

## 6. RVE equilibrium problem and homogenisation formulae

Within the framework of the Method of Multiscale Virtual Power of Blanco et al. (2016), the RVE equilibrium problem as well as the homogenisation formulae for the force- and stress-like quantities are *derived* from the PMVP, by means of straightforward variational arguments. The variational Eq. (45) is perfectly suited to this end, as it includes all the ingredients needed to complete the characterisation of the multi-scale model. Here, however, we shall opt to use the equivalent Lagrange multiplier formulation (46) instead. Since our main aim in this paper is to look deeper into the second-gradient multi-scale formulation, the adoption of (46) will be very useful in providing a clear insight into the role played by the reactive forces caused by postulated RVE kinematical constraints.

### 6.1. Micro-scale equilibrium problem

We start by deriving the RVE equilibrium equation. To this end, we simply set $\hat{\mathbf{u}}_M = \mathbf{0}$, $\hat{\mathbf{G}}_M = \mathbf{0}$ and $\hat{\mathsf{G}}_M = \mathbf{0}$ in (46), which leads to the following RVE variational equilibrium problem: find $\tilde{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu)$ and the triad $(\mathbf{c}, \mathbf{T}, \mathsf{M}) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S$ such that

$$\frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \Big[ (\mathbf{P}_\mu - (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))) \cdot \nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu$$
$$- ((\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c}) \cdot \hat{\tilde{\mathbf{u}}}_\mu \Big] \, d\Omega_\mu$$
$$+ \hat{\mathbf{c}} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu \right) - \hat{\mathbf{T}} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \nabla_\mu \tilde{\mathbf{u}}_\mu \, d\Omega_\mu \right)$$
$$- \hat{\mathsf{M}} \cdot \left( \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} [(\nabla_\mu \tilde{\mathbf{u}}_\mu \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}]^S \, d\Omega_\mu \right) = 0$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega_\mu), \ \forall (\hat{\mathbf{c}}, \hat{\mathbf{T}}, \hat{\mathsf{M}}) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S. \tag{48}$$

Next, we set $\hat{\mathbf{c}} = \mathbf{0}$, $\hat{\mathbf{T}} = \mathbf{0}$ and $\hat{\mathsf{M}} = \mathbf{0}$ in (48) to obtain

$$\int_{\Omega_\mu} \Big[ (\mathbf{P}_\mu - (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))) \cdot \nabla_\mu \hat{\tilde{\mathbf{u}}}_\mu$$
$$- ((\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c}) \cdot \hat{\tilde{\mathbf{u}}}_\mu \Big] \, d\Omega_\mu = 0$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega_\mu). \tag{49}$$

Integrating by parts the first term in (49) gives

$$- \int_{\Omega_\mu} [\mathrm{div}_\mu (\mathbf{P}_\mu - (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))) + (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c}] \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$$
$$+ \int_{\partial\Omega_\mu} (\mathbf{P}_\mu - (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu)))\mathbf{n}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\partial\Omega_\mu = 0$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega_\mu). \tag{50}$$

Since $\mathbf{T}$ and $\mathsf{M}$ are constant tensors, the previous expression is equivalent to

$$- \int_{\Omega_\mu} [\mathrm{div}_\mu \mathbf{P}_\mu - \mathsf{M}\mathbf{J}^{-1} + (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c}] \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\Omega_\mu$$
$$+ \int_{\partial\Omega_\mu} (\mathbf{P}_\mu - (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu)))\mathbf{n}_\mu \cdot \hat{\tilde{\mathbf{u}}}_\mu \, d\partial\Omega_\mu = 0$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega_\mu), \tag{51}$$

which, by means of a trivial variational argument, leads to the strong form of the RVE equilibrium:

$$\rho_\mu \ddot{\mathbf{u}}_\mu - \mathrm{div}_\mu \mathbf{P}_\mu = \mathbf{f}_\mu - (\mathbf{c} + \mathsf{M}\mathbf{J}^{-1}) \qquad \text{in } \Omega_\mu, \tag{52}$$

$$\mathbf{P}_\mu \mathbf{n}_\mu = (\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))\mathbf{n}_\mu \qquad \text{on } \partial\Omega_\mu. \tag{53}$$

**Remark 10.** If a model with more boundary constraints is considered (see Remark 9) then Eqs. (52) and (53) read

$$\rho_\mu \ddot{\mathbf{u}}_\mu - \mathrm{div}_\mu \mathbf{P}_\mu = \mathbf{f}_\mu - \mathbf{c} \qquad \text{in } \Omega_\mu, \tag{54}$$

$$\mathbf{P}_\mu \mathbf{n}_\mu = \mathbf{r}_\mu \qquad \text{on } \partial\Omega_\mu. \tag{55}$$

That is, the traction over the boundary is fully defined by the Lagrange multiplier $\mathbf{r}_\mu$.

This, together with the following equations naturally derived from (48),

$$\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \tag{56}$$

$$\int_{\Omega_\mu} \nabla_\mu \tilde{\mathbf{u}}_\mu \, d\partial\Omega_\mu = \mathbf{0}, \tag{57}$$

$$\int_{\Omega_\mu} [(\nabla_\mu \tilde{\mathbf{u}}_\mu \otimes \mathbf{x}_\mu) \circ \mathbf{J}^{-1}]^S \, d\Omega_\mu = \mathbf{0}, \tag{58}$$

comprise the subset of Euler-Lagrange equations that characterises the RVE (or micro-scale) equilibrium problem. Obviously, from previous developments we have that Eqs. (56), (57) and (58) are equivalent to (31), (34) and (39), respectively.

Finally, we remark that the micro-scale equilibrium problem is completely characterised when the micro-scale force per unit volume $\mathbf{f}_\mu$ is given, together with a constitutive relation $\mathbf{P}_\mu = \mathcal{P}_\mu(\nabla_\mu \mathbf{u}_\mu)$ for the micro-scale Piola-Kirchhoff stress.

*6.2. Body force homogenisation formula*

The homogenisation formula for the body force can be obtained by simply setting $\hat{\mathbf{c}} = \mathbf{0}$, $\hat{\mathbf{T}} = \mathbf{0}$, $\hat{\mathsf{M}} = \mathbf{0}$, $\hat{\mathbf{G}}_M = \mathbf{0}$, $\hat{\mathsf{G}}_M = \mathbf{0}$ and $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$ in (46). This gives

$$\mathbf{f}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\, d\Omega_\mu. \tag{59}$$

Moreover, we could decompose it into inertial and non-inertial contributions to the macro-scale body force $\mathbf{f}_M$, which allows us to arrive at the following expressions (see (1))

$$\mathbf{a}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{u}}_\mu\, d\Omega_\mu, \tag{60}$$

$$\mathbf{b}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{f}_\mu\, d\Omega_\mu. \tag{61}$$

**Remark 11.** While the homogenisation formula (59) has naturally derived within the present framework as the dual object that exerts power against the constant (uniform in space) component of the micro-scale displacement field, i.e. $\mathbf{u}_M$, (see (24)), no homogenisation formula of this kind was derived in Luscher et al. (2010, 2012) from the balance of virtual power between scales.

*6.3. Generalised stresses homogenisation formulae*

Seeting $\hat{\mathbf{c}} = \mathbf{0}$, $\hat{\mathbf{T}} = \mathbf{0}$, $\hat{\mathsf{M}} = \mathbf{0}$, $\hat{\mathbf{u}}_M = \mathbf{0}$, $\hat{\mathsf{G}}_M = \mathbf{0}$ and $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$ in (46) leads to the homogenisation formula for $\mathbf{P}_M$:

$$\mathbf{P}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{P}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \otimes \mathbf{x}_\mu)\, d\Omega_\mu. \tag{62}$$

As already anticipated, the tensor $\mathbf{P}_M$ possesses inertial and a non-inertial components, the former being a consequence of the inertia forces in the micro-scale. In the context of expression (1), putting $\mathbf{P}_M = \mathbf{A}_M + \mathbf{S}_M$, we could arrive here at the following identities

$$\mathbf{A}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \rho_\mu \ddot{\mathbf{u}}_\mu \otimes \mathbf{x}_\mu\, d\Omega_\mu, \tag{63}$$

$$\mathbf{S}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{P}_\mu - \mathbf{f}_\mu \otimes \mathbf{x}_\mu)\, d\Omega_\mu. \tag{64}$$

**Remark 12.** From expression (62) it is seen that $\mathbf{P}_M$ depends on $\ddot{\mathbf{u}}_\mu$ both explicit and implicitly. The explicit dependence is easily seen from the decomposition $\mathbf{P}_M = \mathbf{A}_M + \mathbf{S}_M$ introduced above, where $\mathbf{A}_M$ accounts for such explicit dependence. However, it is important to notice that there is still the implicit dependence in the tensor $\mathbf{P}_\mu$, which, through the equilibrium problem (49), also depends on $\ddot{\mathbf{u}}_\mu$. This implies that there exists an implicit dependence of $\mathbf{S}_M$ on $\ddot{\mathbf{u}}_\mu$.

A fundamental homogenisation formula equivalent to (62) is proved in Appendix B. It expresses the macro-scale stress tensor $\mathbf{P}_M$ as a function of RVE boundary data alone as

$$\mathbf{P}_M = \frac{1}{|\Omega_\mu|} \int_{\partial\Omega_\mu} \mathbf{t}_\mu \otimes \mathbf{x}_\mu\, d\partial\Omega_\mu, \tag{65}$$

where $\mathbf{t}_\mu = \mathbf{P}_\mu \mathbf{n}_\mu$.

While expression (62) can be seen as a weak homogenisation formula, the equivalent formula (65) is understood as a strong homogenisation formula, as its derivation requires the use of the strong form of the equilibrium equations.

**Remark 13.** For models with more boundary constraints, for which (54) and (55) hold, following the same procedure that led to (65) (see Appendix B), the same formula remains valid, and in this particular case reads

$$\mathbf{P}_M = \frac{1}{|\Omega_\mu|} \int_{\partial\Omega_\mu} \mathbf{r}_\mu \otimes \mathbf{x}_\mu\, d\partial\Omega_\mu, \tag{66}$$

with $\mathbf{r}_\mu$ the corresponding Lagrange multiplier (see Remark 9).

Finally, by setting $\hat{\mathbf{c}} = \mathbf{0}$, $\hat{\mathbf{T}} = \mathbf{0}$, $\hat{\mathsf{M}} = \mathbf{0}$, $\hat{\mathbf{u}}_M = \mathbf{0}$, $\hat{\mathbf{G}}_M = \mathbf{0}$ and $\hat{\tilde{\mathbf{u}}}_\mu = \mathbf{0}$, Eq. (46) gives

$$\mathsf{Q}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \Big( (\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S - \frac{1}{2} (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \otimes (\mathbf{x}_\mu \otimes \mathbf{x}_\mu - \mathbf{J}) \Big)\, d\Omega_\mu. \tag{67}$$

As with $\mathbf{P}_M$, we can understand the tensor $\mathsf{Q}_M$ as having inertial and a non-inertial components, that is, we can write $\mathsf{Q}_M = \mathsf{A}_M + \mathsf{R}_M$, where

$$\mathsf{A}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \frac{1}{2} \rho_\mu \ddot{\mathbf{u}}_\mu \otimes (\mathbf{x}_\mu \otimes \mathbf{x}_\mu - \mathbf{J})\, d\Omega_\mu, \tag{68}$$

$$\mathsf{R}_M = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \Big( (\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S - \frac{1}{2} \mathbf{f}_\mu \otimes (\mathbf{x}_\mu \otimes \mathbf{x}_\mu - \mathbf{J}) \Big)\, d\Omega_\mu. \tag{69}$$

**Remark 14.** Similar to Remark 12, from expression (67) it follows that $\mathsf{Q}_M$ depends explicitly and implicitly on $\ddot{\mathbf{u}}_\mu$, the latter through the relation between $\mathbf{P}_\mu$ and $\ddot{\mathbf{u}}_\mu$ established by the equilibrium problem (49).

In Appendix C it is proved that, like $\mathbf{P}_M$, $\mathsf{Q}_M$ can also be expressed as a function of RVE boundary data alone

$$\mathsf{Q}_M + \frac{1}{2} (\mathsf{Q}_M \mathbf{J}^{-1}) \otimes \mathbf{J} = \frac{1}{|\Omega_\mu|} \int_{\partial\Omega_\mu} \frac{1}{2} \mathbf{t}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu\, d\partial\Omega_\mu. \tag{70}$$

Analogously, expression (67) could be understood as a weak homogenisation formula, while formula (70) can be seen as a strong homogenisation formula.

**Remark 15.** For models with more boundary constraints (54) and (55) hold. In such case, the Lagrange multiplier $\mathsf{M}$ is not present in the formulation, and following the same procedure that led to (70) (see Appendix C), it is easy to show that instead of (70), the following formula holds

$$\mathsf{Q}_M = \frac{1}{|\Omega_\mu|} \int_{\partial\Omega_\mu} \frac{1}{2} \mathbf{r}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu\, d\partial\Omega_\mu, \tag{71}$$

with $\mathbf{r}_\mu$ the corresponding Lagrange multiplier (see Remark 9). Again, a formula depending solely on boundary data has been recovered.

**Remark 16.** In the absence of forces per unit volume ($\mathbf{f}_\mu = \mathbf{0}$) and inertia effects ($\ddot{\mathbf{u}}_\mu = 0$), the homogenisation formulae (62) and (67) coincide with those derived in Kouznetsova et al. (2002, 2004); Luscher et al. (2010, 2012). Nonetheless, the formulae (62) and (67), which have been shown to be equivalent to (65) and (70), have striking differences when compared to the results reported in Luscher et al. (2010, 2012). In contrast to the present results, the homogenised stresses in such contributions cannot be expressed as a function of boundary data alone. The present paper extends our previous findings for the first-order theory (de Souza Neto et al., 2015) to second-order models with body forces, and highlights the fact that macro-scale stresses must necessarily remain identifiable in terms of RVE boundary data alone. This is a fundamental property in the definition of macro-scale variables, pointed out by Hill in (Hill, 1972). A further difference with respect to Luscher et al. (2010, 2012) is that the contribution of the body forces $\mathbf{f}_\mu$ to the high-order macro-scale stress tensor $\mathbb{Q}_M$ is generated here by the tensorial product with $(\mathbf{x}_\mu \otimes \mathbf{x}_\mu - \mathbf{J})$.

### 6.4. Reactions to RVE constraints and homogenised forces and stresses

In kinematically-based mechanical variational settings, Lagrange multipliers typically used to enforce kinematical constraints are *reactions* to the constraints they are meant to enforce. In the context of the Principle of Multiscale Virtual Power (46), $\mathbf{c}$ is the reactive force required to enforce constraint (31), $\mathbf{T}$ is the reactive stress to constraint (33), and $\mathbb{M}$ a higher-order stress reactive to (36).

Further to the above comment, we prove in Appendix D that these reactive force- and stress-like quantities in fact satisfy

$$\mathbf{c} = \mathbf{f}_M, \tag{72}$$

$$\mathbf{T} = \mathbf{P}_M, \tag{73}$$

$$\mathbb{M} = \mathbb{Q}_M. \tag{74}$$

That is, the homogenised body force $\mathbf{f}_M$ is simply the reaction to the kinematical constraint (31). The homogenised stress $\mathbf{P}_M$ is the reaction to (33) and the homogenised higher-order stress $\mathbb{Q}_M$ is a reaction to constraint (36).

**Remark 17.** The characterisation of Lagrange multipliers given by (72)–(74) has been obtained under the assumption of minimal constraints for the RVE kinematics (see variational Eq. (46)). For models with further boundary constraints, expression (72) turns into the following

$$\mathbf{c} = \mathbf{f}_M - \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu} \mathbf{r}_\mu \, d\partial\Omega_\mu. \tag{75}$$

while the characterisation of the Lagrange multiplier $\mathbf{r}_\mu$ depends on the definition of the space $\mathbf{L}$ (see also Remark 9).

**Remark 18.** Now that the meaning of the Lagrange multipliers is fully understood, the RVE equilibrium problem (49) reveals that the virtual power exerted by the fluctuation of the stress state given by $\tilde{\mathbf{P}}_\mu = \mathbf{P}_\mu - (\mathbf{P}_M + \mathbb{Q}_M(\mathbf{J}^{-1}\mathbf{x}_\mu))$ equals the external virtual power exerted by the fluctuation of the force per unit volume $\tilde{\mathbf{f}}_M = (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{f}_M$, for all $\hat{\tilde{\mathbf{u}}}_\mu \in \mathbf{H}^1(\Omega)$.

These findings provide a very significant insight into the nature of homogenised force- and stress-like quantities in RVE-based multi-scale theories which, to our knowledge, has not been reported in the literature. Their identification as reactions required to enforce the postulated RVE kinematical constraints provide a very clear link between the kinematics of the RVE and the resulting homogenised force- and stress-like quantities "visible" at the macro-scale level. Obviously, this implies that RVE kinematical constraints and homogenisation formulae for force- and stress-like quantities cannot be postulated independently and that, if ignored, may lead to inconsistencies in the resulting theory.

Finally, we remark that for the sake of completeness, we present in Appendix E an alternative, yet equivalent, variational formulation in which the constraints (26), (27) and (28) are directly enforced, and from which the same physical interpretation of Lagrange multipliers is obtained.

### 6.5. Generalised "uniform" boundary traction formula

Under the assumption of minimal RVE kinematical constraints (31), (33) and (36), the tractions on the RVE boundary were found to be given by (53), in terms of the Lagrange multipliers $\mathbf{T}$ and $\mathbb{M}$. In light of the identities (73) and (74), the RVE boundary traction field in this case (minimal constraints) reads

$$\mathbf{P}_\mu \mathbf{n}_\mu = (\mathbf{P}_M + \mathbb{Q}_M(\mathbf{J}^{-1}\mathbf{x}_\mu))\mathbf{n}_\mu \qquad \text{on } \partial\Omega_\mu. \tag{76}$$

This identity generalises, to the present second-gradient multi-scale model, the concept of *uniform RVE boundary tractions* associated with minimal constraints in the classical (first-gradient) RVE-based mechanical theory. In the classical theory, this reads simply de Souza Neto et al. (2010)

$$\mathbf{P}_\mu \mathbf{n}_\mu = \mathbf{P}_M \mathbf{n}_\mu \qquad \text{on } \partial\Omega_\mu. \tag{77}$$

**Remark 19.** It should be noted that, if further constraints are incorporated into the RVE kinematics (e.g. properly generalised boundary periodicity, homogeneous kinematical boundary conditions), then (76) no longer holds in general. However, all other findings concerning the reactive nature of homogenised forces and stresses remain valid, regardless of the particular set of constraints chosen to describe the kinematics of the RVE.

## 7. Tangent operators

For the sake of simplicity we shall assume in the present section that the mechanical problem is quasi-static. We shall also assume that the micro-scale constitutive behavior is defined through a standard constitutive functional of the form $\mathbf{P}_\mu = \mathbf{P}_\mu(\nabla_\mu \mathbf{u}_\mu)$, which, in view of (24), can be written as

$$\mathbf{P}_\mu = \mathbf{P}_\mu(\mathbf{G}_M + \mathbb{G}_M\mathbf{x}_\mu + \nabla_\mu \tilde{\mathbf{u}}_\mu). \tag{78}$$

In addition, we have a relation $\tilde{\mathbf{u}}_\mu = \tilde{\mathbf{u}}_\mu(\mathbf{G}_M, \mathbb{G}_M)$ established through the micro-scale equilibrium problem, which is repeated here in the quasi-static case for the sake of readability

$$\int_{\Omega_\mu} [\mathbf{P}_\mu(\mathbf{G}_M + \mathbb{G}_M\mathbf{x}_\mu + \nabla_\mu\tilde{\mathbf{u}}_\mu)\cdot\nabla_\mu\hat{\tilde{\mathbf{u}}}_\mu - \mathbf{f}_\mu\cdot\hat{\tilde{\mathbf{u}}}_\mu]\, d\Omega_\mu = 0$$
$$\forall \hat{\tilde{\mathbf{u}}}_\mu \in \tilde{\mathcal{V}}_\mu. \tag{79}$$

In such case, expressions (62) and (67) state that the homogenised objects $\mathbf{P}_M$ and $\mathbb{Q}_M$ are (multi-scale) functionals of the form

$$\mathbf{P}_M = \mathbf{P}_M(\mathbf{G}_M, \mathbb{G}_M), \tag{80}$$

$$\mathbb{Q}_M = \mathbb{Q}_M(\mathbf{G}_M, \mathbb{G}_M). \tag{81}$$

Now, we are interested in calculating the following tangent operators (tensor order is also shown for clarity)

$$\text{4th order} \qquad D_{\mathbf{G}}\mathbf{P}_M[\delta\mathbf{G}_M] = \frac{d}{d\tau}\mathbf{P}_M(\mathbf{G}_M + \tau\delta\mathbf{G}_M, \mathbb{G}_M)\Big|_{\tau=0}, \tag{82}$$

$$\text{5th order} \qquad D_{\mathbb{G}}\mathbf{P}_M[\delta\mathbb{G}_M] = \frac{d}{d\tau}\mathbf{P}_M(\mathbf{G}_M, \mathbb{G}_M + \tau\delta\mathbb{G}_M)\Big|_{\tau=0}, \tag{83}$$

$$\text{5th order} \qquad D_{\mathbf{G}}\mathbb{Q}_M[\delta\mathbf{G}_M] = \frac{d}{d\tau}\mathbb{Q}_M(\mathbf{G}_M + \tau\delta\mathbf{G}_M, \mathbb{G}_M)\Big|_{\tau=0}, \tag{84}$$

$$\text{6th order} \qquad D_{\mathbb{G}}\mathbb{Q}_M[\delta\mathbb{G}_M] = \frac{d}{d\tau}\mathbb{Q}_M(\mathbf{G}_M, \mathbb{G}_M + \tau\delta\mathbb{G}_M)\Big|_{\tau=0}. \tag{85}$$

It can be readily verified that these tangent operators are composed of a Taylor-like component (explicit dependence with respect to $\mathbf{G}_M$ and $\mathbb{G}_M$, which ignores the contribution of fluctuations) and a fluctuation component (implicit dependence through the fluctuation displacement field $\tilde{\mathbf{u}}_\mu$). For example, for the tangent operator $D_{\mathbf{G}}\mathbf{P}_M$, the Taylor component, denoted by $D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M$, is easily obtained as follows

$$
\begin{aligned}
&D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{d}{d\tau}\mathbf{P}_\mu(\mathbf{G}_M+\tau\delta\mathbf{G}_M+\mathbf{G}_M\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M,\mathbf{G}_M))\Big|_{\tau=0}\,d\Omega_\mu\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu(\mathbf{G}_M+\mathbf{G}_M\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M,\mathbf{G}_M))\delta\mathbf{G}_M\,d\Omega_\mu\\
&= \left[\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\,d\Omega_\mu\right]\delta\mathbf{G}_M,
\end{aligned}
\tag{86}
$$

where $\mathbb{C}_\mu$ is the classical fourth order tangent constitutive operator of the material in the micro-scale. Therefore, we have

$$
D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\,d\Omega_\mu. \tag{87}
$$

Similarly, the fluctuation contribution to the tangent operator, denoted $\tilde{D}_{\mathbf{G}}\mathbf{P}_M$, is obtained as follows:

$$
\begin{aligned}
&\tilde{D}_{\mathbf{G}}\mathbf{P}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{d}{d\tau}\mathbf{P}_\mu(\mathbf{G}_M+\mathbf{G}_M\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M+\tau\delta\mathbf{G}_M,\mathbf{G}_M))\Big|_{\tau=0}\,d\Omega_\mu\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu[\mathbb{S}_\mu\delta\mathbf{G}_M]\,d\Omega_\mu = \left[\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\circ\mathbb{S}_\mu\,d\Omega_\mu\right]\delta\mathbf{G}_M,
\end{aligned}
\tag{88}
$$

that is (see Appendix A for the definition of operations)

$$
\tilde{D}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\circ\mathbb{S}_\mu\,d\Omega_\mu. \tag{89}
$$

In the above, the fourth order tensor $\mathbb{S}_\mu$ represents the tangent relation between $\nabla_\mu\tilde{\mathbf{u}}_\mu$ and $\mathbf{G}_M$, i.e. $\nabla_\mu\delta\tilde{\mathbf{u}}_\mu=\mathbb{S}_\mu\delta\mathbf{G}_M$, and is obtained by linearizing problem (79). That is, $\mathbb{S}_\mu$ is characterised by the following linear problem:

$$
\int_{\Omega_\mu}\mathbb{C}_\mu\nabla_\mu\delta\tilde{\mathbf{u}}_\mu\cdot\nabla_\mu\hat{\tilde{\mathbf{u}}}_\mu\,d\Omega_\mu = -\int_{\Omega_\mu}\mathbb{C}_\mu\delta\mathbf{G}_M\cdot\nabla_\mu\hat{\tilde{\mathbf{u}}}_\mu\,d\Omega_\mu \quad \forall\hat{\tilde{\mathbf{u}}}_\mu\in\tilde{\mathscr{V}}_\mu. \tag{90}
$$

In this manner, the fluctuation component of the tangent operator results

$$
\tilde{D}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\circ\mathbb{S}_\mu\,d\Omega_\mu. \tag{91}
$$

Then, we have the complete characterisation of this tangent operator

$$
D_{\mathbf{G}}\mathbf{P}_M = D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M+\tilde{D}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbb{C}_\mu+\mathbb{C}_\mu\circ\mathbb{S}_\mu)\,d\Omega_\mu. \tag{92}
$$

In a completely analogous manner, we have that the Taylor contribution to the operator $D_{\mathbf{G}}\mathbf{P}_M$, denoted by $D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M$, is obtained as follows:

$$
\begin{aligned}
&D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{d}{d\tau}\mathbf{P}_\mu(\mathbf{G}_M+(\mathbf{G}_M+\tau\delta\mathbf{G}_M)\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M,\mathbf{G}_M))\Big|_{\tau=0}\,d\Omega_\mu\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu(\mathbf{G}_M+\mathbf{G}_M\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M,\mathbf{G}_M))(\delta\mathbf{G}_M\mathbf{x}_\mu)\,d\Omega_\mu\\
&= \left[\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\otimes\mathbf{x}_\mu\,d\Omega_\mu\right]\delta\mathbf{G}_M.
\end{aligned}
\tag{93}
$$

Hence, we obtain

$$
D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu\otimes\mathbf{x}_\mu\,d\Omega_\mu. \tag{94}
$$

The fluctuation component of this tangent operator, denoted $\tilde{D}_{\mathbf{G}}\mathbf{P}_M$, is

$$
\begin{aligned}
&\tilde{D}_{\mathbf{G}}\mathbf{P}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{d}{d\tau}\mathbf{P}_\mu(\mathbf{G}_M+\mathbf{G}_M\mathbf{x}_\mu+\nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{G}_M,\mathbf{G}_M+\tau\delta\mathbf{G}_M))\Big|_{\tau=0}\,d\Omega_\mu\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\mathbb{C}_\mu[\mathbb{S}_\mu(\delta\mathbf{G}_M\mathbf{x}_\mu)]\,d\Omega_\mu\\
&= \left[\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbb{C}_\mu\circ\mathbb{S}_\mu)\otimes\mathbf{x}_\mu\,d\Omega_\mu\right]\delta\mathbf{G}_M,
\end{aligned}
\tag{95}
$$

that is

$$
\tilde{D}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbb{C}_\mu\circ\mathbb{S}_\mu)\otimes\mathbf{x}_\mu\,d\Omega_\mu. \tag{96}
$$

Then, the complete fifth-order tangent operator reads

$$
D_{\mathbf{G}}\mathbf{P}_M = D^{\mathrm{T}}_{\mathbf{G}}\mathbf{P}_M+\tilde{D}_{\mathbf{G}}\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbb{C}_\mu+\mathbb{C}_\mu\circ\mathbb{S}_\mu)\otimes\mathbf{x}_\mu\,d\Omega_\mu. \tag{97}
$$

Following the same procedure, it is straightforward to obtain the characterisation of the fifth- and sixth-order tangent operators $D_{\mathbf{G}}\mathbf{Q}_M$ and $D_{\mathbf{G}}\mathbf{Q}_M$, given by

$$
\begin{aligned}
D_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M] &= D^{\mathrm{T}}_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M]+\tilde{D}_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}([(\mathbb{C}_\mu+\mathbb{C}_\mu\circ\mathbb{S}_\mu)\delta\mathbf{G}_M]\otimes\mathbf{x}_\mu)^{\mathrm{S}}\,d\Omega_\mu,
\end{aligned}
\tag{98}
$$

$$
\begin{aligned}
D_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M] &= D^{\mathrm{T}}_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M]+\tilde{D}_{\mathbf{G}}\mathbf{Q}_M[\delta\mathbf{G}_M]\\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}([((\mathbb{C}_\mu+\mathbb{C}_\mu\circ\mathbb{S}_\mu)\otimes\mathbf{x}_\mu)\delta\mathbf{G}_M]\otimes\mathbf{x}_\mu)^{\mathrm{S}}\,d\Omega_\mu.
\end{aligned}
\tag{99}
$$

## 8. Summary and concluding remarks

An RVE-based multi-scale model featuring a macro-scale second-gradient theory linked to a first-order classical continuum description at the micro-scale level has been derived and examined in detail within the general framework of the Method of Multiscale Virtual Power recently proposed by the authors in Blanco et al. (2016).

The MMVP has been shown here to provide a robust framework, whereby multi-scale models can be rationally derived in a kinematically-driven fashion by means of the following clear and well-defined steps:

(i) Postulation of the kinematics of the macro- and micro-scales, i.e., definition of the kinematical descriptors of each scale of the model. In the present case we have the triad $(\mathbf{u}_M,\nabla_M\mathbf{u}_M,\nabla_M\nabla_M\mathbf{u}_M)=(\mathbf{u}_M,\mathbf{G}_M,\mathbf{G}_M)$ at the generic point $\mathbf{x}_M$ of the macro-scale, and the pair $(\mathbf{u}_\mu,\ \nabla_\mu\mathbf{u}_\mu)$ of kinematical fields over the RVE domain;

(ii) Postulation of kinematical insertion and kinematical homogenisation such that kinematical quantities are preserved in the scale transition. Here, kinematical insertion is defined by (24) and kinematical homogenisation by (26)–(28). This leads to the idea of kinematical admissibility, which automatically defines the minimally constrained functional space of of kinematically admissible fluctuation fields of the RVE;

(iii) Mathematical duality then allows straightforward identification of the force- and stress-like quantities compatible with the kinematical assumptions at both scales, namely, the triad $(\mathbf{f}_M,\mathbf{P}_M,\mathbf{Q}_M)$ at $\mathbf{x}_M$, and (trivially) the pair $(\mathbf{f}_\mu-\rho_\mu\ddot{\mathbf{u}}_\mu,\mathbf{P}_\mu)$ of body force and first Piola-Kirchhoff stress fields over the RVE;

(iv) Statement of the corresponding Principle of Multiscale Virtual Power, (45) (or (46)), based on the duality pairings identified in steps (i) and (iii), whereby the total virtual power of the macro- and micro-scales are balanced. This principle leads naturally, by means of straightforward variational arguments, to the equations of equilibrium of the RVE as well as to the homogenisation formulae for the force- and stress-like quantities of the model, and completes the characterisation of the multi-scale model.

In addition, due to its variational basis, the MMVP naturally provides insight into the foundations of the model. For example, by re-writing the PMVP in the equivalent form (46), using Lagrange multipliers, the impact of the kinematical hypotheses upon the resulting model was made very clear, as the homogenised force- and stress-like quantities of the macro-scale are identified as reactions to kinematical constraints imposed upon the RVE. Also, the equivalent representation of such quantities exclusively in terms of RVE boundary data has been obtained in a straightforward manner.

Moreover, the present multi-scale model was developed in the context of transient problems, also featuring relations that describe the contribution of micro-scale inertia effects to the high-order macro-scale continuum formulation. In this regard, the MMVP allowed these inertia effects to be naturally incorporated in a straightforward manner in the analysis.

Throughout the paper, conceptual differences and similarities to existing theories have been highlighted, facilitating the analysis of the contributions made by present approach.

In summary, we believe the MMVP to be a powerful tool to address the development of new multi-scale models in a manner that avoids potential inconsistencies. This appears to be particularly true for models exhibiting distinct kinematics at the macro- and micro-scales, such as the second-gradient model presented in this paper. The method can be also very useful in analysing existing multi-scale models, as the links between kinematics, equilibrium and homogenisation rules are made clear, allowing an easy detection of possible inconsistencies. We also remark that the method is by no means restricted to classical mechanical problems. Any class of problems where a Principle of Multiscale Virtual Power makes sense can be addressed by the MMVP. This encompasses the multi-scale description of a wide range of phenomena, including the formulation of RVE-based models of multi-scale fluid mechanics, micro-scale strain localisation (Sánchez et al., 2013), micro- and macro-scale fracturing (Toro et al., 2016), multi-scale solid dynamics (de Souza Neto et al., 2015), transient heat transfer, particulate media, among others. Some of these will be addressed by the authors in forthcoming publications.

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## Appendix A. Tensor algebra

Let $\mathbf{a}, \mathbf{b}, \mathbf{c}, \ldots$ be vectors, $\mathbf{A}, \mathbf{B}, \mathbf{C}, \ldots$ second order tensors and $\mathsf{A}, \mathsf{B}, \mathsf{C}, \ldots$ third order tensors. We introduce the following operations, most of them defined in terms of the standard internal product between two vectors denoted by $\mathbf{a} \cdot \mathbf{b}$:

- given $\mathbf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2$ and $\mathbf{b}$, then $\mathbf{Ab} = (\mathbf{a}_2 \cdot \mathbf{b})\mathbf{a}_1$;
- given $\mathbf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2$, then $\mathbf{A}^T = \mathbf{a}_2 \otimes \mathbf{a}_1$;
- given $\mathbf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2$ and $\mathbf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2$, then $\mathbf{A} \cdot \mathbf{B} = (\mathbf{a}_1 \cdot \mathbf{b}_1)(\mathbf{a}_2 \cdot \mathbf{b}_2)$;
- given $\mathbf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2$ and $\mathbf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2$, then $\mathbf{AB} = (\mathbf{a}_2 \cdot \mathbf{b}_1)(\mathbf{a}_1 \otimes \mathbf{b}_2)$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$ and $\mathbf{b}$, then $\mathsf{A}\mathbf{b} = (\mathbf{a}_3 \cdot \mathbf{b})(\mathbf{a}_1 \otimes \mathbf{a}_2)$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$ and $\mathsf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2 \otimes \mathbf{b}_3$, then $\mathsf{A} \cdot \mathsf{B} = (\mathbf{a}_1 \cdot \mathbf{b}_1)(\mathbf{a}_2 \cdot \mathbf{b}_2)(\mathbf{a}_3 \cdot \mathbf{b}_3)$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$ and $\mathbf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2$, then $\mathsf{A}\mathbf{B} = (\mathbf{a}_2 \cdot \mathbf{b}_1)(\mathbf{a}_3 \cdot \mathbf{b}_2)\mathbf{a}_1$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$ and $\mathbf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2$, then $\mathsf{A} \circ \mathbf{B} = (\mathbf{a}_3 \cdot \mathbf{b}_1)(\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{b}_2)$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$, then $\mathsf{A}^\mathsf{T} = \mathbf{a}_1 \otimes \mathbf{a}_3 \otimes \mathbf{a}_2$, and $\mathsf{A}^S = \frac{1}{2}(\mathsf{A} + \mathsf{A}^\mathsf{T})$;
- given $\mathsf{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3$, then $\mathsf{A}^t = \mathbf{a}_3 \otimes \mathbf{a}_1 \otimes \mathbf{a}_2$;
- given $\mathbb{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3 \otimes \mathbf{a}_4$ and $\mathbb{B} = \mathbf{b}_1 \otimes \mathbf{b}_2 \otimes \mathbf{b}_3 \otimes \mathbf{b}_4$, then $\mathbb{A} \circ \mathbb{B} = (\mathbf{a}_3 \cdot \mathbf{b}_1)(\mathbf{a}_4 \cdot \mathbf{b}_2)(\mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{b}_3 \otimes \mathbf{b}_4)$;
- given $\mathbb{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3 \otimes \mathbf{a}_4$ and $\mathbf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2$, then $\mathbb{A}\mathbf{B} = (\mathbf{a}_3 \cdot \mathbf{b}_1)(\mathbf{a}_4 \cdot \mathbf{b}_2)(\mathbf{a}_1 \otimes \mathbf{a}_2)$;
- given $\mathfrak{A} = \mathbf{a}_1 \otimes \mathbf{a}_2 \otimes \mathbf{a}_3 \otimes \mathbf{a}_4 \otimes \mathbf{a}_5$ and $\mathsf{B} = \mathbf{b}_1 \otimes \mathbf{b}_2 \otimes \mathbf{b}_3$, then $\mathfrak{A}\mathsf{B} = (\mathbf{a}_3 \cdot \mathbf{b}_1)(\mathbf{a}_4 \cdot \mathbf{b}_2)(\mathbf{a}_5 \cdot \mathbf{b}_3)(\mathbf{a}_1 \otimes \mathbf{a}_2)$.

## Appendix B. Homogenisation of $\mathbf{P}_M$ from boundary data

Let us find a homogenisation formula equivalent to (62) that exclusively depends on boundary information. To do this we write

$$\int_{\Omega_\mu} \mathbf{P}_\mu \, d\Omega_\mu = \int_{\Omega_\mu} \mathbf{P}_\mu \nabla_\mu \mathbf{x}_\mu \, d\Omega_\mu = -\int_{\Omega_\mu} \mathrm{div}_\mu \, \mathbf{P}_\mu \otimes \mathbf{x}_\mu \, d\Omega_\mu + \int_{\partial\Omega_\mu} \mathbf{P}_\mu \mathbf{n}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \tag{B.1}$$

Using (B.1) and the equilibrium form (52) into (62) yields

$$\begin{aligned}\mathbf{P}_M &= \frac{1}{|\Omega_\mu|}\left[\int_{\Omega_\mu} (-\mathrm{div}_\mu \, \mathbf{P}_\mu \otimes \mathbf{x}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \otimes \mathbf{x}_\mu) \, d\Omega_\mu + \int_{\partial\Omega_\mu} \mathbf{P}_\mu \mathbf{n}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu\right] \\ &= \frac{1}{|\Omega_\mu|}\left[-\int_{\Omega_\mu} (\mathbf{c} + \mathsf{M}\mathbf{J}^{-1}) \otimes \mathbf{x}_\mu \, d\Omega_\mu + \int_{\partial\Omega_\mu} \mathbf{t}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu\right] \\ &= \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu} \mathbf{t}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu,\end{aligned} \tag{B.2}$$

where we denoted $\mathbf{P}_\mu \mathbf{n}_\mu = \mathbf{t}_\mu$ the traction over the boundary $\partial\Omega_\mu$, and where we have used the assumption (23) and the fact that $\mathbf{c}$, $\mathsf{M}$ and $\mathbf{J}$ are constant entities. Thus

$$\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu} \mathbf{t}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \tag{B.3}$$

## Appendix C. Homogenisation of $\mathsf{Q}_M$ from boundary data

Let us again find a homogenisation formula for $\mathsf{Q}_M$ depending exclusively upon boundary data. Firstly, in Appendix F it is proved that the following relation holds

$$\int_{\Omega_\mu} (\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S \, d\Omega_\mu = -\frac{1}{2}\int_{\Omega_\mu} \mathrm{div}_\mu \, \mathbf{P}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\Omega_\mu + \frac{1}{2}\int_{\partial\Omega_\mu} \mathbf{P}_\mu \mathbf{n}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \tag{C.1}$$

Considering (C.1) and the equilibrium (52) into (67) results

$$\begin{aligned}
\mathbf{Q}_M = &\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\Big[\frac{1}{2}(-\operatorname{div}_\mu \mathbf{P}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu))\\
&\otimes (\mathbf{x}_\mu \otimes \mathbf{x}_\mu) + \frac{1}{2}((\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\otimes \mathbf{J})\Big]\, d\Omega_\mu\\
&+ \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}\mathbf{P}_\mu \mathbf{n}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu\\
= &-\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{1}{2}(\mathbf{c} + \mathsf{M}\mathbf{J}^{-1})\otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\Omega_\mu\\
&+ \frac{1}{|\Omega_\mu|}\frac{1}{2}\Big(\int_{\Omega_\mu}(\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\, d\Omega_\mu\Big)\otimes \mathbf{J}\\
&+ \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}\mathbf{t}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu\\
= &-\frac{1}{2}\Big(\mathbf{c} + \mathsf{M}\mathbf{J}^{-1} - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\, d\Omega_\mu\Big)\otimes \mathbf{J}\\
&+ \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}\mathbf{t}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (C.2)
\end{aligned}$$

Hence, using (59), we have

$$\mathbf{Q}_M + \frac{1}{2}(\mathbf{c} + \mathsf{M}\mathbf{J}^{-1} - \mathbf{f}_M)\otimes \mathbf{J} = \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}\mathbf{t}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (C.3)$$

In view of the results given by identities (D.3) and (D.9), obtained in Appendix D, we finally arrive at the following equation

$$\mathbf{Q}_M + \frac{1}{2}(\mathbf{Q}_M\mathbf{J}^{-1})\otimes \mathbf{J} = \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}\mathbf{t}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (C.4)$$

## Appendix D. Physical meaning of the Lagrange multipliers

Let us explore the meaning of the Lagrange multipliers in the variational formulation (46), that is, for the case of minimally constrained fluctuations.

Consider that $\hat{\tilde{\mathbf{u}}}_\mu$ is the constant vector function in the variational Eq. (49). Then, we arrive at the following relation

$$\int_{\Omega_\mu}((\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c})\, d\Omega_\mu = \mathbf{0}. \qquad (D.1)$$

Since the Lagrange multiplier $\mathbf{c}$ is itself a constant, we have

$$\mathbf{c} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}(\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\, d\Omega_\mu, \qquad (D.2)$$

or, in view of (59)

$$\mathbf{c} = \mathbf{f}_M. \qquad (D.3)$$

Consider the homogenisation formula for $\mathbf{P}_M$ derived in (B.3). Now, introducing the expression for the traction $\mathbf{t}_\mu = \mathbf{P}_\mu \mathbf{n}_\mu$ obtained in (53) into (B.3), yields

$$\mathbf{P}_M = \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}(\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))\mathbf{n}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (D.4)$$

For simplicity, consider Cartesian coordinates and, recalling (23) and that $\mathbf{T}$, $\mathsf{M}$ and $\mathbf{J}$ are constant tensors, let us develop the right hand side in the expression above

$$\begin{aligned}
[\mathbf{P}_M]_{ij} = &\frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}([\mathbf{T}]_{ik} + [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}[\mathbf{x}_\mu]_n)[\mathbf{n}_\mu]_k[\mathbf{x}_\mu]_j \, d\partial\Omega_\mu\\
= &[\mathbf{T}]_{ik}\frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}[\mathbf{n}_\mu]_k[\mathbf{x}_\mu]_j \, d\partial\Omega_\mu\\
&+ [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}\frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}[\mathbf{x}_\mu]_n[\mathbf{n}_\mu]_k[\mathbf{x}_\mu]_j \, d\partial\Omega_\mu\\
= &[\mathbf{T}]_{ik}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{\partial[\mathbf{x}_\mu]_j}{\partial[\mathbf{x}_\mu]_k}\, d\Omega_\mu\\
&+ [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{\partial}{\partial[\mathbf{x}_\mu]_k}([\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_j)\, d\Omega_\mu\\
= &[\mathbf{T}]_{ik}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{I}]_{jk}\, d\Omega_\mu\\
&+ [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}([\mathbf{I}]_{nk}[\mathbf{x}_\mu]_j + [\mathbf{I}]_{jk}[\mathbf{x}_\mu]_n)\, d\Omega_\mu\\
= &[\mathbf{T}]_{ij} + [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mk}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_j \, d\Omega_\mu\\
&+ [\mathsf{M}]_{ijm}[\mathbf{J}^{-1}]_{mn}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_n \, d\Omega_\mu\\
= &[\mathbf{T}]_{ij}. \qquad (D.5)
\end{aligned}$$

Hence, we obtain

$$\mathbf{T} = \mathbf{P}_M. \qquad (D.6)$$

Consider now the homogenisation formula for $\mathbf{Q}_M$ obtained in (C.3). Using the result derived in (D.3) and the expression for the traction $\mathbf{t}_\mu = \mathbf{P}_\mu \mathbf{n}_\mu$ given by (53) into (C.3), leads to

$$\begin{aligned}
&\mathbf{Q}_M + \frac{1}{2}(\mathsf{M}\mathbf{J}^{-1})\otimes \mathbf{J}\\
&= \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}(\mathbf{T} + \mathsf{M}(\mathbf{J}^{-1}\mathbf{x}_\mu))\mathbf{n}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (D.7)
\end{aligned}$$

Analogous to the previous development, let us consider Cartesian coordinates, recall (23), take into account that $\mathbf{T}$, $\mathsf{M}$ and $\mathbf{J}$ are constant tensors and that $\mathsf{M}^{\mathrm{T}} = \mathsf{M}$ and $\mathbf{J} = \mathbf{J}^T$. Then, the development of the right hand side in expression (D.7) gives

$$\begin{aligned}
&[\mathbf{Q}_M]_{ijk} + \frac{1}{2}[\mathsf{M}]_{imn}[\mathbf{J}^{-1}]_{mn}[\mathbf{J}]_{jk}\\
&= \frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}\frac{1}{2}([\mathbf{T}]_{il} + [\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{mn}[\mathbf{x}_\mu]_n)[\mathbf{n}_\mu]_l[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\partial\Omega_\mu\\
&= [\mathbf{T}]_{il}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}[\mathbf{n}_\mu]_l[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\partial\Omega_\mu\\
&\quad + [\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{mn}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\partial\Omega_\mu}[\mathbf{x}_\mu]_n[\mathbf{n}_\mu]_l[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\partial\Omega_\mu\\
&= [\mathbf{T}]_{il}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k)\, d\Omega_\mu\\
&\quad + [\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{mn}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k)\, d\Omega_\mu\\
&= [\mathbf{T}]_{il}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}([\mathbf{I}]_{jl}[\mathbf{x}_\mu]_k + [\mathbf{I}]_{kl}[\mathbf{x}_\mu]_j)\, d\Omega_\mu\\
&\quad + [\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{mn}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}([\mathbf{I}]_{nl}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k\\
&+ [\mathbf{I}]_{jl}[\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_k + [\mathbf{I}]_{kl}[\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_j)\, d\Omega_\mu\\
&= [\mathbf{T}]_{ij}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_k \, d\Omega_\mu + [\mathbf{T}]_{ik}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_j \, d\Omega_\mu\\
&\quad + [\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{ml}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\Omega_\mu\\
&\quad + [\mathsf{M}]_{ijm}[\mathbf{J}^{-1}]_{mn}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_k \, d\Omega_\mu\\
&\quad + [\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}\frac{1}{2}\frac{1}{|\Omega_\mu|}\int_{\Omega_\mu}[\mathbf{x}_\mu]_n[\mathbf{x}_\mu]_j \, d\Omega_\mu\\
&= \frac{1}{2}[\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{ml}[\mathbf{J}]_{jk} + \frac{1}{2}[\mathsf{M}]_{ijm}[\mathbf{J}^{-1}]_{mn}[\mathbf{J}]_{nk} + \frac{1}{2}[\mathsf{M}]_{ikm}[\mathbf{J}^{-1}]_{mn}[\mathbf{J}]_{nj}\\
&= \frac{1}{2}[\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{lm}[\mathbf{J}]_{jk} + \frac{1}{2}[\mathsf{M}]_{ijm}[\mathbf{I}]_{mk} + \frac{1}{2}[\mathsf{M}]_{ikm}[\mathbf{I}]_{mj}
\end{aligned}$$

$$= \frac{1}{2}[\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{lm}[\mathbf{J}]_{jk} + \frac{1}{2}[\mathsf{M}]_{ijk} + \frac{1}{2}[\mathsf{M}]_{ikj}$$
$$= \frac{1}{2}[\mathsf{M}]_{ilm}[\mathbf{J}^{-1}]_{lm}[\mathbf{J}]_{jk} + [\mathsf{M}]_{ijk}. \tag{D.8}$$

Now note that the second term in the left hand side is identical to the first term in the right hand side, therefore we arrive at the following result

$$\mathsf{M} = \mathsf{Q}_M. \tag{D.9}$$

## Appendix E. Alternative analysis of the Lagrange multipliers

Alternatively to the variational formulation (46), let us enforce kinematical constraints (26), (27) and (28) through Lagrange multipliers, which are denoted by $\mathbf{c}^*$, $\mathbf{T}^*$ and $\mathsf{M}^*$, respectively. The Principle of Multiscale Virtual Power (45) is then rewritten as follows

$$\begin{aligned}
&\mathbf{P}_M \cdot \hat{\mathbf{G}}_M + \mathsf{Q}_M \cdot \hat{\mathsf{G}}_M - \mathbf{f}_M \cdot \hat{\mathbf{u}}_M \\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} (\mathbf{P}_\mu \cdot \nabla_\mu \hat{\mathbf{u}}_\mu - (\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\cdot \hat{\mathbf{u}}_\mu)\, d\Omega_\mu \\
&\quad - \hat{\mathbf{c}}^* \cdot \left(\mathbf{u}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \, d\Omega_\mu\right) \\
&\quad - \mathbf{c}^* \cdot \left(\hat{\mathbf{u}}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \hat{\mathbf{u}}_\mu \, d\Omega_\mu\right) \\
&\quad + \hat{\mathbf{T}}^* \cdot \left(\mathbf{G}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_\mu \mathbf{u}_\mu \, d\Omega_\mu\right) \\
&\quad + \mathbf{T}^* \cdot \left(\hat{\mathbf{G}}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_\mu \hat{\mathbf{u}}_\mu \, d\Omega_\mu\right) \\
&\quad + \hat{\mathsf{M}}^* \cdot \left(\mathsf{G}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} [(\nabla_\mu \mathbf{u}_\mu \otimes \mathbf{x}_\mu)\circ \mathbf{J}^{-1}]^S \, d\Omega_\mu\right) \\
&\quad + \mathsf{M}^* \cdot \left(\hat{\mathsf{G}}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} [(\nabla_\mu \hat{\mathbf{u}}_\mu \otimes \mathbf{x}_\mu)\circ \mathbf{J}^{-1}]^S \, d\Omega_\mu\right) \\
&\quad \forall (\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathsf{G}}_M) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S,\ \forall \hat{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu), \\
&\quad \forall (\hat{\mathbf{c}}^*, \hat{\mathbf{T}}^*, \hat{\mathsf{M}}^*) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S.
\end{aligned} \tag{E.1}$$

Rearranging terms in (E.1) leads to

$$\begin{aligned}
&(\mathbf{P}_M - \mathbf{T}^*) \cdot \hat{\mathbf{G}}_M + (\mathsf{Q}_M - \mathsf{M}^*) \cdot \hat{\mathsf{G}}_M - (\mathbf{f}_M - \mathbf{c}^*) \cdot \hat{\mathbf{u}}_M \\
&= \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \Big[(\mathbf{P}_\mu - (\mathbf{T}^* + \mathsf{M}^*(\mathbf{J}^{-1}\mathbf{x}_\mu))) \cdot \nabla_\mu \hat{\mathbf{u}}_\mu \\
&\quad - ((\mathbf{f}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) - \mathbf{c}^*) \cdot \hat{\mathbf{u}}_\mu\Big]\, d\Omega_\mu \\
&\quad - \hat{\mathbf{c}}^* \cdot \left(\mathbf{u}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \, d\Omega_\mu\right) \\
&\quad + \hat{\mathbf{T}}^* \cdot \left(\mathbf{G}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \nabla_\mu \mathbf{u}_\mu \, d\Omega_\mu\right) \\
&\quad + \hat{\mathsf{M}}^* \cdot \left(\mathsf{G}_M - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} [(\nabla_\mu \mathbf{u}_\mu \otimes \mathbf{x}_\mu)\circ \mathbf{J}^{-1}]^S \, d\Omega_\mu\right) \\
&\quad \forall (\hat{\mathbf{u}}_M, \hat{\mathbf{G}}_M, \hat{\mathsf{G}}_M) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S,\ \forall \hat{\mathbf{u}}_\mu \in \mathbf{H}^1(\Omega_\mu), \\
&\quad \forall (\hat{\mathbf{c}}^*, \hat{\mathbf{T}}^*, \hat{\mathsf{M}}^*) \in \mathbb{R}^3 \times \mathbb{R}^{3\times 3} \times (\mathbb{R}^{3\times 3\times 3})^S.
\end{aligned} \tag{E.2}$$

Clearly, restrictions (26), (27) and (28) are now natural conditions that follow as Euler-Lagrange equations from (E.2). Moreover, note that (24) is no longer taken into consideration. Thus, we readily obtain the physical interpretation of the Lagrange multipliers

$$\mathbf{c}^* = \mathbf{f}_M, \tag{E.3}$$

$$\mathbf{T}^* = \mathbf{P}_M, \tag{E.4}$$

$$\mathsf{M}^* = \mathsf{Q}_M. \tag{E.5}$$

Comparing, respectively, (E.3), (E.4) and (E.5) to (D.3), (D.6) and (D.9), we obtain that the Lagrange multipliers from variational Eq. (46) are the same as those from variational formulation (E.2), that is $\mathbf{c}^* = \mathbf{c}$, $\mathbf{T}^* = \mathbf{T}$ and $\mathsf{M}^* = \mathsf{M}$. This implies that both variational formulations, (46) and (E.2) are equivalent. In other words, the enforcement of constraints (26), (27) and (28) leads to the same result as when the enforcement of constraints (31), (33) and (36) is considered.

## Appendix F. Auxiliary calculations

For simplicity let us consider Cartesian coordinates to see that

$$\begin{aligned}
&[(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk} \\
&= \frac{1}{2}\Big([\mathbf{P}_\mu]_{ij}[\mathbf{x}_\mu]_k + [\mathbf{P}_\mu]_{ik}[\mathbf{x}_\mu]_j\Big) \\
&= \frac{1}{2}\left([\mathbf{P}_\mu]_{il}\frac{\partial[\mathbf{x}_\mu]_j}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_k + [\mathbf{P}_\mu]_{il}\frac{\partial[\mathbf{x}_\mu]_k}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j\right) \\
&= \frac{1}{2}\left(\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \right.\\
&\qquad \left. - [\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j\frac{\partial[\mathbf{x}_\mu]_k}{\partial[\mathbf{x}_\mu]_l}\right) \\
&\quad + \frac{1}{2}\left(\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_k[\mathbf{x}_\mu]_j) - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_k[\mathbf{x}_\mu]_j \right.\\
&\qquad \left. - [\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_k\frac{\partial[\mathbf{x}_\mu]_j}{\partial[\mathbf{x}_\mu]_l}\right) \\
&= \frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \\
&\quad - \frac{1}{2}\Big([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j\delta_{kl} + [\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_k\delta_{jl}\Big) \\
&= \frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \\
&\quad - \frac{1}{2}\Big([\mathbf{P}_\mu]_{ik}[\mathbf{x}_\mu]_j + [\mathbf{P}_\mu]_{ij}[\mathbf{x}_\mu]_k\Big) \\
&= \frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) \\
&\quad - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k - [(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk}.
\end{aligned} \tag{F.1}$$

Thus, integrating over the micro-scale domain $\Omega_\mu$, it results

$$\begin{aligned}
&\int_{\Omega_\mu} [(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk}\, d\Omega_\mu \\
&= \int_{\Omega_\mu} \left[\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) \right.\\
&\quad \left. - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k - [(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk}\right] d\Omega_\mu,
\end{aligned} \tag{F.2}$$

that is

$$\begin{aligned}
&2\int_{\Omega_\mu} [(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk}\, d\Omega_\mu \\
&= \int_{\Omega_\mu} \left[\frac{\partial}{\partial[\mathbf{x}_\mu]_l}([\mathbf{P}_\mu]_{il}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k) - \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k\right] d\Omega_\mu,
\end{aligned} \tag{F.3}$$

and taking the first term in the right hand side to the boundary results

$$\begin{aligned}
&2\int_{\Omega_\mu} [(\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S]_{ijk}\, d\Omega_\mu \\
&= \int_{\partial\Omega_\mu} [\mathbf{P}_\mu]_{il}[\mathbf{n}_\mu]_l[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\partial\Omega_\mu \\
&\quad - \int_{\Omega_\mu} \frac{\partial[\mathbf{P}_\mu]_{il}}{\partial[\mathbf{x}_\mu]_l}[\mathbf{x}_\mu]_j[\mathbf{x}_\mu]_k \, d\Omega_\mu.
\end{aligned} \tag{F.4}$$

Therefore, this finally implies

$$\int_{\Omega_\mu} (\mathbf{P}_\mu \otimes \mathbf{x}_\mu)^S \, d\Omega_\mu = -\frac{1}{2}\int_{\Omega_\mu} \mathrm{div}_\mu \, \mathbf{P}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\Omega_\mu + \frac{1}{2}\int_{\partial\Omega_\mu} \mathbf{P}_\mu \mathbf{n}_\mu \otimes \mathbf{x}_\mu \otimes \mathbf{x}_\mu \, d\partial\Omega_\mu. \qquad (F.5)$$

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