An RVE-based mutiscale theory of solids with micro-scale inertia and body force effects

E.A. de Souza Neto[♮], P.J. Blanco[§♭], P.J. Sánchez[‡♯], R.A. Feijóo[§♭]

[♮]Zienkiewicz Centre for Computational Engineering
Swansea University, Singleton Park, Swansea SA2 8PP, UK
[§]LNCC/MCTI, Av. Getúlio Vargas 333, Petrópolis, RJ, CEP: 25651-075, Brasil
[♭]INCT-MACC, Instituto Nacional de Ciência e Tecnologia
em Medicina Assistida por Computação Científica, Brasil
[‡]CIMEC-UNL-CONICET, Güemes 3450, CP 3000 Santa Fe, Argentina
[♯]GIMNI-UTN-FRSF, Lavaise 610, CP 3000 Santa Fe, Argentina

Keywords: multiscale, inertia, body forces, RVE, Hill-Mandel Principle, variational methods, homogenisation.

Abstract

A multiscale theory of solids based on the concept of Representative Volume Element (RVE) and accounting for micro-scale inertia and body forces is proposed. A simple extension of the classical Hill-Mandel Principle together with suitable kinematical constraints on the micro-scale displacements provide the variational framework within which the theory is devised. In this context, the micro-scale equilibrium equation and the homogenisation relations among the relevant macro- and micro-scale quantities are rigorously derived by means of straightforward variational arguments. In particular, it is shown that only the fluctuations of micro-scale inertia and body forces about their RVE volume averages may affect the micro-scale equilibrium problem and the resulting homogenised stress. The volume average themselves are mechanically relevant only to the macro-scale.

1 Introduction

Classical multiscale theories to predict the mechanical behaviour of solids with a microstructure have their origins in the pioneering works of Hill [9–12], Hashin and Shtrikman [8], Budiansky [3] and Mandel [17], among others. Over the last two decades or so, theories relying on the averaging of stresses and strains over a *representative volume element (RVE)* have become remarkably popular in the prediction of overall properties of heterogeneous solids in non-linear regimes. Their use in practical applications relies almost exclusively on techniques of computational homogenisation [14, 18, 19, 29]. These techniques have reached such a level of maturity that multiscale theories are now beginning to find their way in specialised applications with a very promising prospect of becoming a much needed tool to help the design of new materials and the prediction of constitutive behaviours resulting from the interaction of complex microstructural phenomena [22, 26].

Despite the success history of RVE-based multiscale thories, the consideration of inertia and body forces in general appears not to have been satisfactorily addressed to date. In the classical work of Hill [12] inertia and body forces are not considered. In the more recent literature, body forces are often removed from the theory on the basis of questionable arguments. Inertia forces, in turn, have rarely been considered in this context. In the few reported attempts to incorporate inertia effects, the theory appears to be unclear and suffers from significant inconsistencies.

At present, the increasing interest in so-called metamaterials – microsctructured materials displaying useful exotic macroscopic behaviour – puts pressure on the development of robust multiscale theories capable of predicting the overall response by accounting for the interaction of (possibly complex) phenomena at the micro-scale [7]. In this context, the consideration of inertia and body forces may become crucial. The macroscopic mechanical response of acoustic metamaterials, for example, is dictated by dynamic phenomena at the micro-scale. Any attempt to model such materials by means of RVE-based multiscale theories must properly address the consideration of micro-scale inertia effects.

Our purpose in the present paper is to show in a clear manner how inertia effects and body forces in general can be rigorously accounted for in such theories. To this end we cast the theory within a framework relying entirely on the two fundamental principles of *kinematical admissibility* and *Multiscale Virtual Power* – the latter expressed as a variational statement of an extended version of the Hill-Mandel Principle of Macrohomogeneity [12, 17]. These provide the essential link between the macro- and micro-scale kinematics and virtual power, respectively. Within this framework, once the macro- and micro-scale kinematical variables are defined and appropriate kinematical constraints are postulated to link them in a consistent manner, *all* equations of the resulting multiscale theory – including RVE equilibrium and the homogenisation relations for force- and stress-like variables – are *derived* (rather than postulated) exclusively by means of straightforward variational arguments. Here we should point out that the recent literature provides examples where extended versions of the Hill-Mandel Principle have been used for this purpose, but a deeper look into the resulting models reveals significant inconsistencies. Such inconsistencies stem either from insufficient kinematical constraints being imposed to ensure a meaningful link between the macro- and micro-scale kinematics or from the variationally inconsistent manner in which kinematical constraints have been taken into account in the treatment of the corresponding model. We begin by introducing the proposed framework in Section 2, against the background provided by the well-known classical theory (in the absence of inertia and body forces). Our main result is presented in Section 3 where we extend these ideas to the case of non-zero inertia and body forces. In this context, the role of inertia and body forces naturally emerges very clearly, allowing one to easily see how they can be taken into account in a consistent manner. A discussion of our findings follows in Section 4 and the paper closes with some concluding remarks made in Section 5.

2 Classical theory. Review

Consider a solid continuum that occupies a region Ω of the three-dimensional Euclidean space in its reference configuration. A wide family of so-called multiscale constitutive theories are derived based on the idea that any point $\mathbf{x}$ of Ω is associated with a *representative volume element* (RVE), occupying a reference domain Ω_μ of characteristic length ℓ_μ much smaller than the characteristic length ℓ of Ω. The domains Ω and Ω_μ are referred to as the macro- and micro-scale, respectively.

Classical multiscale theories [4–6, 23] that predict the macro-scale mechanical behaviour from the constitutive properties of the corresponding micro-scale can be entirely derived from two fundamental principles: (i) *kinematical admissibility*; and (ii) *multiscale virtual power*, that govern the transition between the two scales. Although by no means absolutely necessary, the derivation of all equations of the theory as a consequence of these two principles alone provides, in our view, a robust framework to treat the problem. In particular, it allows extensions of the classical theory (such as the one that is the subject matter of the present paper) to be devised in very clear steps on solid theoretical grounds. We remark that this approach has been recently employed with success by Sánchez *et al.* [27] in the derivation of a multiscale theory accounting for material failure associated with micro-scale strain localisation phenomena. We begin by illustrating in the following the use of this idea in the case of the classical theory, where inertia and body forces are asumed absent.

2.1 Kinematical homogenisation and kinematical admissibility

Let $\mathbf{y} \in \Omega_\mu$ denote the coordinates of an arbitrary point of the RVE associated with a point $\mathbf{x} \in \Omega$. Without loss of generality we shall assume the origin of the micro-scale coordinate system to be located at the centroid of Ω_μ, i.e.

$$\int_{\Omega_\mu} \mathbf{y} \, d\Omega_\mu = 0. \tag{1}$$

A fundamental assumption in the present class of theories is that the micro-scale displacement field $\mathbf{u}_\mu$ over Ω_μ can be expanded as

$$\begin{aligned} \mathbf{u}_\mu(\mathbf{y}) &= \mathbf{u}(\mathbf{x}) + \nabla\mathbf{u}(\mathbf{x})\,\mathbf{y} + \tilde{\mathbf{u}}_\mu(\mathbf{y}) \\ &= \mathbf{u}(\mathbf{x}) + [\mathbf{F}(\mathbf{x}) - \mathbf{I}]\,\mathbf{y} + \tilde{\mathbf{u}}_\mu(\mathbf{y}), \end{aligned} \tag{2}$$

where $\mathbf{u}(\mathbf{x})$ is the displacement of the corresponding point $\mathbf{x}$ of the macro-scale, $\nabla(\cdot)$ denotes the gradient of $(\cdot)$ with respect to the macro-scale coordinates,

$$\mathbf{F} = \mathbf{I} + \nabla\mathbf{u} \tag{3}$$

is the macro-scale deformation gradient and

$$\tilde{\mathbf{u}}_\mu \equiv \mathbf{u}_\mu - \mathbf{u} - (\mathbf{F} - \mathbf{I})\mathbf{y} \tag{4}$$

is defined as the *displacement fluctuation field* of the RVE. In view of (2) and (3) the micro-scale deformation gradient field,

$$\mathbf{F}_\mu = \mathbf{I} + \nabla_\mu \mathbf{u}_\mu, \tag{5}$$

with ∇_μ denoting the gradient with respect to the micro-scale coordinates, is equivalently expressed as

$$\mathbf{F}_\mu(\mathbf{y}) = \mathbf{I} + \nabla\mathbf{u}(\mathbf{x}) + \nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{y}) = \mathbf{F}(\mathbf{x}) + \nabla_\mu\tilde{\mathbf{u}}_\mu(\mathbf{y}). \tag{6}$$

That is, the micro-scale deformation gradient field is a sum of the macro-scale deformation gradient, inserted uniformly throughout the whole domain Ω_μ, and a micro-scale displacement fluctuation gradient $\nabla_\mu\tilde{\mathbf{u}}_\mu$.

2.1.1 Kinematical admissibility

In addition to the above, the following kinematical homogenisation (averaging) relations, linking the micro-scale displacement and deformation gradient fields to their corresponding macro-scale point values at $\mathbf{x}$, are postulated:

$$\mathbf{u} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{u}_\mu \, d\Omega_\mu \tag{7}$$

and

$$\mathbf{F} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{F}_\mu \, d\Omega_\mu, \tag{8}$$

where $|\Omega_\mu|$ denotes the measure of Ω_μ. The above postulates are equivalent to a statement of *kinematical admissibility* of micro-scale displacement fields. Indeed, (7) is itself a kinematical constraint imposed on $\mathbf{u}_\mu$. Due to the split (4) and (1), it is equivalent to

$$\int_{\Omega_\mu} \tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}. \tag{9}$$

The averaging relation (8), in turn, due to (6), is equivalent to the following constraint on $\nabla_\mu \tilde{\mathbf{u}}_\mu$:

$$\int_{\Omega_\mu} \nabla_\mu \tilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \tag{10}$$

or, after a straightforward integration by parts,

$$\int_{\Gamma_\mu} \tilde{\mathbf{u}}_\mu \otimes \mathbf{n} \, d\Gamma_\mu = \mathbf{0}, \tag{11}$$

where Γ_μ denotes the boundary of the RVE and $\mathbf{n}$ is the outward unit normal to Γ_μ. That is, only displacement fluctuation fields that satisfy the kinematical constraints (9) and (11) can be regarded as *kinematically admissible*, i.e. compatible with the kinematical averaging postulates (8) and (7). Hence, we can define a functional space of *kinematically admissible displacement fluctuations*, denoted $\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$, as

$$\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} \equiv \left\{ \mathbf{v} \in [\mathrm{H}^1(\Omega_\mu)]^3 : \textstyle\int_{\Omega_\mu} \mathbf{v} \, d\Omega_\mu = \mathbf{0}; \int_{\Gamma_\mu} \mathbf{v} \otimes \mathbf{n} \, d\Gamma_\mu = \mathbf{0} \right\}. \tag{12}$$

Note that constraint (9), which follows from (7), implies that translational rigid displacement fluctuations are excluded from $\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$. Rotational rigid displacement fluctuations, in turn, are excluded from $\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$ due to constraint (11) that follows from the deformation gradient averaging postulate (8). The corresponding space of *virtual* kinematically admissible fluctuation fields, denoted $\mathrm{Var}^*_{\tilde{\mathbf{u}}_\mu}$, coincides with $\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$ itself,

$$\mathrm{Var}^*_{\tilde{\mathbf{u}}_\mu} \equiv \left\{ \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2 : \mathbf{v}_1, \mathbf{v}_2 \in \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} \right\} = \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}. \tag{13}$$

From (12) and (2) we have that, for a given macro-scale point displacement and deformation gradient, $\mathbf{u}$ and $\mathbf{F}$, the functional set of *kinematically admissible micro-scale displacement fields* reads

$$\mathrm{Kin}^*_{\mathbf{u}_\mu} \equiv \left\{ \mathbf{v} = \mathbf{u} + [\mathbf{F} - \mathbf{I}]\mathbf{y} + \tilde{\mathbf{v}} : \tilde{\mathbf{v}} \in \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} \right\}. \tag{14}$$

The corresponding space of *virtual* kinematically admissible micro-scale displacements, in turn, is given by

$$\mathrm{Var}^*_{\mathbf{u}_\mu} \equiv \left\{ \mathbf{v} = \mathbf{v}_1 - \mathbf{v}_2 : \mathbf{v}_1, \mathbf{v}_2 \in \mathrm{Kin}^*_{\mathbf{u}_\mu} \right\} = \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}^*_{\tilde{\mathbf{u}}_\mu}. \tag{15}$$

2.1.2 Further kinematical constraints

It is worth remarking that the RVE kinematical constraints embedded in the definition of the functional space $\mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$ (or $\mathrm{Var}^*_{\mathbf{u}_\mu}$) above are the *minimal* kinematical constraints compatible with the present family of multi-scale theories of solid behaviour. That is, any relaxation of these kinematical constraints would allow for micro-scale displacement fields that fail to satisfy the fundamental kinematical averaging relations (8) or (7) and the resulting model would violate essential postulates of the theory. The enforcement of further, *more stringent*, kinematical constraints, on the other hand, is perfectly acceptable (and very sensible in many situations), provided the resulting space of kinematically admissible fluctuations is a *subspace* of its minimally constrained counterpart defined in (12). In fact, well-known multi-scale models of solid can be cast within the present framework with the simple introduction of further kinematical constraints as follows:

- *Voigt-Taylor*, *uniform strain* model or *rule of mixtures*. It assumes a uniform deformation gradient, equal to $\mathbf{F}$, over the entire RVE domain. This is equivalent to saying that the displacement fluctuations vanish over Ω_μ. Hence, within the present framework the Voigt-Taylor model is retrieved by setting the actual space $\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$, of kinematically admissible displacement fluctuations, simply as

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \{\mathbf{0}\}. \tag{16}$$

- *Linear boundary displacements* or *uniform boundary strain* model. This widely used model assumes the displacement fluctuations to vanish on Γ_μ so that the displacement field on the boundary of the RVE reads

$$\mathbf{u}_\mu(\mathbf{y}) = \mathbf{u} + [\mathbf{F} - \mathbf{I}]\mathbf{y} \qquad \forall \mathbf{y} \in \Gamma_\mu. \tag{17}$$

  The corresponding space of kinematically admissible displacement fluctuations is

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \{\mathbf{v} \in \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} : \mathbf{v}|_{\Gamma_\mu} = \mathbf{0}\}. \tag{18}$$

- *Periodic boundary fluctuations* model. This is the classical assumption adopted in the analysis of periodic media. The RVE in this case is a *unit cell* whose periodic repetition generates the macro-scale continuum. The RVE here must satisfy certain geometrical constraints so as to be compatible with the assumption of periodicity of the medium. Under such conditions, parallel RVE boundary sides (in two dimensions) or surfaces (in three dimensions) are identified in pairs. Within each side or surface a one-to-one correspondance can be identified between its points and points of the corresponding pairing side or surface. With $(\mathbf{y}^+, \mathbf{y}^-)$ denoting an arbitrary pair of boundary points related by this one-to-one correspondance, the periodicity constraint requires that displacement fluctuations at $\mathbf{y}^+$ and $\mathbf{y}^-$ be identical. The space of kinematically admissible fluctuations in this case then reads

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \{\mathbf{v} \in \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu} : \mathbf{v}(\mathbf{y}^+) = \mathbf{v}(\mathbf{y}^-) \ \ \forall \ \text{pairs} \ (\mathbf{y}^+, \mathbf{y}^-)\}. \tag{19}$$

Finally, we point out that without any kinematical constraints other than the minimal requirements of the theory, i.e. by choosing

$$\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}, \tag{20}$$

it can be shown [6] that the resulting model predicts *uniform traction on the boundary* of the RVE. In this case, with $\mathbf{P}$ denoting the First Piola-Kirchhoff stress tensor at the macro-scale point $\mathbf{x}$, $\mathbf{P}_\mu$ the corresponding micro-scale counterpart field, we have

$$\mathbf{P}_\mu(\mathbf{y})\ \mathbf{n}(\mathbf{y}) = \mathbf{P}\ \mathbf{n}(\mathbf{y}) \qquad \forall \mathbf{y} \in \Gamma_\mu. \tag{21}$$

2.2 Principle of Multiscale Virtual Power

The Hill-Mandel Principle of Macro-homogeneity [9, 12, 17] establishes the energetic consistency between the two scales. In its original form [12], it states that the volume average of the power of an equilibrium stress field over an RVE subjected to either linear boundary displacements or uniform boundary tractions equals the macro-scale stress power. Here, we rephrase the Hill-Mandel Principle as a variational statement − named the *Principle of Multiscale Virtual Power* − by requiring the stress virtual power to coincide with the volume average of its micro-scale counterpart. That is, we require that

$$\mathbf{P} : \delta\mathbf{F} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu : \delta\mathbf{F}_\mu \, d\Omega_\mu \tag{22}$$

for all virtual macro-scale deformation gradients and micro-scale deformation gradient fields, $\delta\mathbf{F}$ and $\delta\mathbf{F}_\mu$, kinematically admissible in the sense of (8). By taking (6) into account, the Hill-Mandel Principle can be expressed by the following variational equation:

$$\mathbf{P} : \delta\mathbf{F} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu : (\delta\mathbf{F} + \nabla_\mu \delta\tilde{\mathbf{u}}_\mu) \, d\Omega_\mu, \qquad \forall \delta\mathbf{F}; \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \tag{23}$$

2.2.1 Stress homogenisation and micro-scale equilibrium

The variational statement of the Hill-Mandel Principle plays a fundamental role in the definition of the transition between the micro- and macro-scales. As direct consequences of (23) we have:

- The *stress homogenisation* relation,

$$\mathbf{P} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{P}_\mu \, d\Omega_\mu, \tag{24}$$

  obtained from (23) by choosing $\delta\tilde{\mathbf{u}}_\mu = \mathbf{0}$ and allowing arbitrary variations $\delta\mathbf{F}$, and;

- The *micro-scale equilibrium equation*,

$$\int_{\Omega_\mu} \mathbf{P}_\mu : \nabla_\mu \delta\tilde{\mathbf{u}}_\mu \, d\Omega_\mu = 0, \qquad \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}, \tag{25}$$

  obtained by setting $\delta\mathbf{F} = \mathbf{0}$ and allowing any kinematically admissible virtual displacement fluctuations in (23).

In the conventional approach to homogenisation problems under the assumptions of periodic displacement fluctuations or minimal kinematical constraint, translational rigid body displacement fluctuations are prevented by fixing an arbitrary point of the RVE. Here, translational rigid modes are dealt with by imposing (9) (embedded in the definition of $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$). We remark, however, that both approaches are mechanically equivalent in the absence of body forces.

Remark 2.1 *In contrast with the usual way in which multi-scale theories are presented, within the present framework the stress homogenisation expression (24) and the micro-scale equilibrium equation (25) are* not *a priori assumptions.*[1] *Rather, they are* derived *here as direct consequences of the variational statement (22) of the Hill-Mandel Principle – the Principle of Multiscale Virtual Power.*

Remark 2.2 *In the above derivation, following the usual assumption in the treatment of the classical theory (see for instance [12]), inertia and body forces have been assumed zero. It should be noted, however, that any inertia or body force field orthogonal to the space* $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$ *is consistent with the variational equilibrium equation* (25) *[4, 23]. As we shall see, the extended theory presented in Section 3 provides the natural framework to fully address the consideration of inertia and body forces.*

2.3 Summary. Macro-scale constitutive response

The complete classical multiscale theory can be summarised by the deformation gradient averaging and stress homogenisation relations, given respectively by (8) and (24), and the micro-scale equilibrium equation (25). With these at hand, together with the choice of an appropriate space $\mathrm{Kin}_{\tilde{\mathbf{u}}_\mu} = \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$, the macro-scale constitutive response at a point $\mathbf{x}$ of the macroscopic continuum with a given associated RVE, is obtained as follows:

- Given the history of deformation gradient ${}^t\mathbf{F}(\mathbf{x})$ at point $\mathbf{x}$ up to time t, find a corresponding history ${}^t\tilde{\mathbf{u}}_\mu$ of kinematically admissible micro-scale displacement fluctuation fields $\tilde{\mathbf{u}}_\mu \in \mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$, such that the RVE equilibrium equation is satisfied:

$$\int_{\Omega_\mu} \mathcal{P}_\mu(\mathbf{y}, {}^\tau\mathbf{F}_\mu) : \nabla_\mu \delta\mathbf{v}\, d\Omega_\mu = 0 \qquad \forall \delta\mathbf{v} \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}, \forall \tau \in [0, t], \tag{26}$$

  where the histories of $\mathbf{F}_\mu$ and $\tilde{\mathbf{u}}_\mu$ are related by:

$${}^\tau\mathbf{F}_\mu(\mathbf{y}) = {}^\tau\mathbf{F}(\mathbf{x}) + \nabla_\mu {}^\tau\tilde{\mathbf{u}}_\mu(\mathbf{y}) \tag{27}$$

  and $\mathcal{P}_\mu(\mathbf{y}, \cdot)$ is a given constitutive response functional that maps histories of deformation gradient into the First Piola Kirchhoff stress tensor at point $\mathbf{y}$ of the RVE:

$$\mathbf{P}_\mu(\mathbf{y}, \tau) = \mathcal{P}_\mu(\mathbf{y}, {}^\tau\mathbf{F}_\mu). \tag{28}$$

- With the solution of the above RVE equilibrium problem at hand, obtain for all $\tau \in [0, t]$ the macro-scale First Piola-Kirchhoff stress tensor according to the averaging relation (24).

3 Consideration of inertia and body forces

We shall now consider the situation where inertia and body forces may be present. Then, let $\mathbf{f}_\mu^{\mathrm{b}}$ denote the reference micro-scale body force field. That is, the body force per unit volume of the reference configuration of the RVE. In addition, let ρ_μ be the micro-scale reference mass density field.

Rather than assuming a particular format for the homogenisation of the inertia and body forces, or for the corresponding RVE equilibrium equation, we shall proceed here to *derive* them from an extended version of the Hill-Mandel Principle, which enforces energy consistency between the two scales in the present case. Note that this approach is entirely in line with the methodology adopted above in the formulation of the classical theory (in the absence of inertia and body forces) where both the homogenisation of the stress and the RVE equilibrium were derived from the variational statement of the Hill-Mandel Principle.

[1] In Hill's original work [12], equilibrium and homogenisation of stress are *a priori* assumptions which, combined, have the classical Hill-Mandel Principle as a consequence.

3.1 Extended Hill-Mandel Principle

In order to account for inertia and body forces in the micro-to-macro transition, we postulate an extended version of the Hill-Mandel Principle by simply stating the *Principle of Multiscale Virtual Power* in terms of *total* virtual powers at both macro- and micro-scales [1]. The extended principle requires that the total macro-scale virtual power coincides with the volume average of its micro-scale counterpart. That is, it requires the variational equation

$$\mathbf{P} : \delta\mathbf{F} - \mathbf{f} \cdot \delta\mathbf{u} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{P}_\mu : \delta\mathbf{F}_\mu - \mathbf{f}^{\mathrm{b}}_\mu \cdot \delta\mathbf{u}_\mu + \rho_\mu \ddot{\mathbf{u}}_\mu \cdot \delta\mathbf{u}_\mu)\, d\Omega_\mu \tag{29}$$

to hold for all tensors $\delta\mathbf{F}$ and vectors $\delta\mathbf{u}$ and all virtual micro-scale deformation gradient and displacement fields, $\delta\mathbf{F}_\mu$ and $\delta\mathbf{u}_\mu$, kinematically admissible in the sense of (8) *and* (7). In (29), $\ddot{\mathbf{u}}_\mu$ is the micro-scale acceleration field. It should be noted that in stating the macro-scale total virtual power, a macro-scale force vector $\mathbf{f}$ has been introduced as the *dual* of the macro-scale displacement vector, with no reference to its specific nature (i.e. whether it results specificaly from prescribed micro-scale body forces or inertia forces). Its actual meaning – to be made clear by the homogenisation formulae linking the macro-scale force vector $\mathbf{f}$ to the micro-scale fields it originates from – will be determined as a consequence of (29) by means of simple, but rigorous, variational arguments.

By decomposing $\delta\mathbf{F}_\mu$ and $\delta\mathbf{u}_\mu$ following (2) and (6), the Principle of Multiscale Virtual Power can be re-written in the equivalent form:

$$\begin{aligned}\mathbf{P} : \delta\mathbf{F} - \mathbf{f} \cdot \delta\mathbf{u} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} & [\mathbf{P}_\mu : (\delta\mathbf{F} + \nabla_\mu \delta\tilde{\mathbf{u}}_\mu) - (\mathbf{f}^{\mathrm{b}}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \cdot (\delta\mathbf{u} \\ & + \delta\mathbf{F}\, \mathbf{y} + \delta\tilde{\mathbf{u}}_\mu)]\, d\Omega_\mu \forall \delta\mathbf{F}, \delta\mathbf{u};\ \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}.\end{aligned} \tag{30}$$

3.2 Stress, inertia and body force homogenisation and RVE equilibrium

Following the procedure of Section 2, by setting $\delta\mathbf{u} = \mathbf{0}$, $\delta\tilde{\mathbf{u}}_\mu = \mathbf{0}$, and allowing arbitrary variations $\delta\mathbf{F}$ in (30), we obtain the expression for the *stress homogenisation* in the presence of micro-scale inertia and body forces:

$$\mathbf{P} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} [\mathbf{P}_\mu - (\mathbf{f}^{\mathrm{b}}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \otimes \mathbf{y}]\, d\Omega_\mu. \tag{31}$$

Further, with $\delta\mathbf{F} = \mathbf{0}$ and $\delta\mathbf{u} = \mathbf{0}$, (30) yields the corresponding *RVE equilibrium equation*:

$$\int_{\Omega_\mu} [\mathbf{P}_\mu : \nabla_\mu \delta\tilde{\mathbf{u}}_\mu - (\mathbf{f}^{\mathrm{b}}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu) \cdot \delta\tilde{\mathbf{u}}_\mu]\, d\Omega_\mu = 0, \qquad \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \tag{32}$$

Finally, with $\delta\mathbf{F} = \mathbf{0}$ and $\delta\tilde{\mathbf{u}}_\mu = \mathbf{0}$, (30) results in the *homogenisation expression for the macro-scale force* $\mathbf{f}$:

$$\mathbf{f} = \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} (\mathbf{f}^{\mathrm{b}}_\mu - \rho_\mu \ddot{\mathbf{u}}_\mu)\, d\Omega_\mu. \tag{33}$$

Obviously, one can conveniently split $\mathbf{f}$ as

$$\mathbf{f} = \mathbf{f}^{\mathrm{b}} - \mathbf{f}^{\rho}, \tag{34}$$

with

$$\mathbf{f}^{\mathrm{b}} := \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{f}^{\mathrm{b}}_\mu\, d\Omega_\mu \tag{35}$$

identified as the *homogenised body force* and

$$\mathbf{f}^{\rho} := \frac{1}{|\Omega_\mu|} \int_{\Omega_\mu} \mathbf{f}^{\rho}_\mu\, d\Omega_\mu; \qquad \mathbf{f}^{\rho}_\mu := \rho_\mu \ddot{\mathbf{u}}_\mu, \tag{36}$$

as the *homogenised inertia force*. That is, as one might have intuitively expected, the macro-scale body force $\mathbf{f}^{\mathrm{b}}$ turns out to be the volume average of its micro-scale counterpart over the RVE, and the same applies to the macro-scale inertia force $\mathbf{f}^{\rho}$. Here, these homogenisation formulae have been naturally *derived* as consequence of the Euler-Lagrange equation of the Principle of Multiscale Virtual Power.

3.3 Inertia and body force fluctuation fields

To gain some further insight into the role of inertia and body forces in the micro-scale it is convenient to define the micro-scale *body force fluctuation field*,

$$\tilde{\mathbf{f}}^{\mathrm{b}}_\mu := \mathbf{f}^{\mathrm{b}}_\mu - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{f}^{\mathrm{b}}_\mu \, d\Omega_\mu = \mathbf{f}^{\mathrm{b}}_\mu - \mathbf{f}^{\mathrm{b}}, \tag{37}$$

and the micro-scale *inertia force fluctuation field*,

$$\tilde{\mathbf{f}}^{\rho}_\mu := \mathbf{f}^{\rho}_\mu - \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} \mathbf{f}^{\rho}_\mu \, d\Omega_\mu = \mathbf{f}^{\rho}_\mu - \mathbf{f}^{\rho}, \tag{38}$$

That is, the fields $\tilde{\mathbf{f}}^{\mathrm{b}}_\mu$ and $\tilde{\mathbf{f}}^{\rho}_\mu$ measure the *fluctuation* of $\mathbf{f}^{\mathrm{b}}_\mu$ and $\mathbf{f}^{\rho}_\mu$ about their respective volume averages, $\mathbf{f}^{\mathrm{b}}$ and $\mathbf{f}^{\rho}$.

With the introduction of the above split of $\mathbf{f}^{\mathrm{b}}_\mu$ and $\mathbf{f}^{\rho}_\mu$ into (31) we obtain

$$\mathbf{P} = \frac{1}{|\Omega_\mu|}\left\{\int_{\Omega_\mu} [\mathbf{P}_\mu - (\tilde{\mathbf{f}}^{\mathrm{b}}_\mu - \tilde{\mathbf{f}}^{\rho}_\mu)\otimes \mathbf{y}]\, d\Omega_\mu - (\mathbf{f}^{\mathrm{b}} - \mathbf{f}^{\rho})\otimes \int_{\Omega_\mu} \mathbf{y}\, d\Omega_\mu\right\} \tag{39}$$

which, in view of (1), results in the following expression for the stress homogenisation:

$$\mathbf{P} = \frac{1}{|\Omega_\mu|}\int_{\Omega_\mu} [\mathbf{P}_\mu - (\tilde{\mathbf{f}}^{\mathrm{b}}_\mu - \tilde{\mathbf{f}}^{\rho}_\mu)\otimes \mathbf{y}]\, d\Omega_\mu. \tag{40}$$

Analogously, with the use of (37) and (38) in (32), we obtain

$$\int_{\Omega_\mu} [\mathbf{P}_\mu : \nabla_\mu \delta\tilde{\mathbf{u}}_\mu - (\tilde{\mathbf{f}}^{\mathrm{b}}_\mu - \tilde{\mathbf{f}}^{\rho}_\mu)\cdot \delta\tilde{\mathbf{u}}_\mu]\, d\Omega_\mu - (\mathbf{f}^{\mathrm{b}} - \mathbf{f}^{\rho})\cdot \int_{\Omega_\mu} \delta\tilde{\mathbf{u}}_\mu \, d\Omega_\mu = 0, \qquad \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}. \tag{41}$$

By noting that $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu} \subset \mathrm{Var}^*_{\tilde{\mathbf{u}}_\mu} = \mathrm{Kin}^*_{\tilde{\mathbf{u}}_\mu}$, the constraints of definition (12) imply that the second integral on the left hand side of (41) vanishes – the volume averages $\mathbf{f}^{\mathrm{b}}$ and $\mathbf{f}^{\rho}$ are orthogonal to $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$ – and the equilibrium of the RVE can be equivalently expressed by the variational equation

$$\int_{\Omega_\mu} [\mathbf{P}_\mu : \nabla_\mu \delta\tilde{\mathbf{u}}_\mu - (\tilde{\mathbf{f}}^{\mathrm{b}}_\mu - \tilde{\mathbf{f}}^{\rho}_\mu)\cdot \delta\tilde{\mathbf{u}}_\mu]\, d\Omega_\mu = 0, \qquad \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}, \tag{42}$$

where only the fluctuating components $\tilde{\mathbf{f}}^{\rho}_\mu$ and $\tilde{\mathbf{f}}^{\mathrm{b}}_\mu$ of the micro-scale inertia and body force take part.[2]

Finally, for the sake of completeness, by using in (40) the general tensor relation

$$\int_{\Omega_\mu} \mathbf{S}\, d\Omega_\mu = \int_{\Gamma_\mu} \mathbf{S}\mathbf{n}\otimes \mathbf{y}\, d\Gamma_\mu + \int_{\Omega_\mu} \mathrm{div}_\mu \mathbf{S}\otimes \mathbf{y}\, d\Omega_\mu, \tag{43}$$

valid for any sufficiently smooth tensor field $\mathbf{S}$, together with the strong form of (42), we obtain the alternative expression for the homogenised stress which uses only boundary information:

$$\mathbf{P} = \frac{1}{|\Omega_\mu|}\int_{\Gamma_\mu} \mathbf{P}_\mu \mathbf{n}\otimes \mathbf{y}\, d\Gamma_\mu \tag{44}$$

[2] Although not specifically relevant to the treatment of micro-scale inertia and body forces, it is worth noting that a completely analogous argument, taking into account the kinematical constraint (10) embedded in the definition of $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$, leads to a similar conclusion regarding the role of the micro-scale stress field in the RVE equilibrium equation. That is, only the micro-scale *stress fluctuation field*,

$$\tilde{\mathbf{P}}_\mu := \mathbf{P}_\mu - \mathbf{P},$$

may produce non-zero virtual power. Hence, (42) is equivalent to

$$\int_{\Omega_\mu} [\tilde{\mathbf{P}}_\mu : \nabla_\mu \delta\tilde{\mathbf{u}}_\mu - (\tilde{\mathbf{f}}^{\mathrm{b}}_\mu - \tilde{\mathbf{f}}^{\rho}_\mu)\cdot \delta\tilde{\mathbf{u}}_\mu]\, d\Omega_\mu = 0, \qquad \forall \delta\tilde{\mathbf{u}}_\mu \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu},$$

where only fluctuations of micro-scale forces *and* stresses are of relevance.

or, simply,

$$\mathbf{P} = \frac{1}{|\Omega_\mu|} \int_{\Gamma_\mu} \mathbf{t}_\mu \otimes \mathbf{y} \, d\Gamma_\mu \tag{45}$$

where $\mathbf{t}_\mu = \mathbf{P}_\mu \mathbf{n}$ is the Piola stress vector on Γ_μ. Note that $\mathbf{t}_\mu$ is a purely *reactive* boundary traction, i.e, $\mathbf{t}_\mu \perp \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$. Obviously, this expression remains valid in the absence of body forces.

3.4 Summary. Macro-scale response with micro-scale inertia and body forces

In the presence of inertia and micro-scale body forces or, more precisely, non-zero inertia and body force *fluctuations* at the micro-scale, the macro-scale stress response at a point $\mathbf{x}$ of the macro-continuum is obtained as follows:

- Given the history ${}^t\mathbf{F}(\mathbf{x})$ of deformation gradient at point $\mathbf{x}$ up to time t, the history ${}^t\tilde{\mathbf{f}}^{\mathrm{b}}_\mu$ of the reference micro-scale body force fluctuation field and the initial conditions $\tilde{\mathbf{u}}_\mu(t_0)$, and $\dot{\tilde{\mathbf{u}}}_\mu(t_0)$, for the displacement and velocity fluctuation fields at the initial time t_0, we solve the RVE equilibrium problem: find a corresponding history ${}^t\tilde{\mathbf{u}}_\mu$ of kinematically admissible displacement fluctuation fields $\tilde{\mathbf{u}}_\mu \in \mathrm{Kin}_{\tilde{\mathbf{u}}_\mu}$ such that

$$\int_{\Omega_\mu} \mathcal{P}_\mu(\mathbf{y}, {}^\tau\mathbf{F}_\mu) : \nabla_\mu \delta\mathbf{v} \, d\Omega_\mu - \int_{\Omega_\mu} [\tilde{\mathbf{f}}^{\mathrm{b}}_\mu(\tau) - \tilde{\mathbf{f}}^{\rho}_\mu(\tau)] \cdot \delta\mathbf{v} \, d\Omega_\mu = 0 \qquad \forall \delta\mathbf{v} \in \mathrm{Var}_{\tilde{\mathbf{u}}_\mu}, \forall \tau \in [0, t]. \tag{46}$$

- With the solution of the RVE equilibrium problem at hand, obtain for all $\tau \in [0, t]$ the macro-scale First Piola-Kirchhoff stress tensor according to the stress homogenisation relation (40) or (45). The homogenised macro-scale inertia and body forces, in turn, are obtained according to (36) and (35), respectively.

4 Discussion

In the absence of inertia and body forces, the classical procedure summarised in Section 2.3 determines the macro-scale First Piola-Kirchhoff stress tensor at a point of the macro-continuum as a function solely of the history of the macro-scale deformation gradient at that point. That is, the procedure implicitly defines a local constitutive response functional $\mathcal{P}$ for the macro-scale stress such that

$$\mathbf{P}(t) = \mathcal{P}({}^t\mathbf{F}). \tag{47}$$

In this case, the macro-scale stress response resulting from the multiscale modelling is *purely constitutive* in that it depends only on the history of the macro-scale deformation gradient.

However, if inertia or body forces are taken into account the above no longer holds true in general. Indeed, note that the stress determination procedure of Section 3.4 in fact defines the macro-scale First Piola-Kirchhoff stress as a function of the history of the macro-scale deformation gradient *and* the history of the micro-scale inertia and body force fluctuation fields. As for the history of micro-scale inertia forces, we should note that the histories ${}^t\mathbf{F}$ and ${}^t\mathbf{u}$ implicitly contain the data $\ddot{\mathbf{u}}$ and $\ddot{\mathbf{F}}$ required by the dynamic RVE equilibrium problem whose solution gives the microscale acceleration field $\ddot{\mathbf{u}}_\mu$. As the microscale inertia forces are determined from $\ddot{\mathbf{u}}_\mu$ through $(36)_2$ we have that the stress response functional, in this case denoted $\mathcal{S}_\alpha$, is such that for a given set $\alpha \equiv \{\tilde{\mathbf{u}}_\mu(t_0), \dot{\tilde{\mathbf{u}}}_\mu(t_0)\}$ of initial conditions for the micro-scale displacement and velocity flutuation fields we have

$$\mathbf{P}(t) = \mathcal{S}_\alpha({}^t\mathbf{F}, {}^t\mathbf{u}, {}^t\tilde{\mathbf{f}}^{\mathrm{b}}_\mu). \tag{48}$$

The functional $\mathcal{S}$ in this case cannot in general be classed as a *constitutive* functional in the classical sense because, in addition to the standard dependence upon the deformation gradient history, the stress here depends also on external prescribed loading – more precisely, on the micro-scale body force fluctuation fields – and on the history of the macro-scale displacement. The dependence of the stress response on the histories of displacements or external agents is non-conventional and does not fit within the classical and widely accepted framework of simple materials [20, 21].

Of course, the stress dependence upon inertia or body forces will be of practical relevance only in situations where their *fluctuations* are of sufficient intensity to have a significant effect on the solution of the RVE equilibrium problem (46) and on the stress homogenisation (40) or (45). It is worth remarking here however that, even in such cases, the macro-scale First Piola-Kirchhoff stress (as obtained in (45)) remains identifiable in terms of RVE boundary data alone – a property pointed out by Hill [12] as fundamental in the definition of macro-scale variables.

The consideration of body forces in the multiscale modelling of solids has been recently addressed in [15, 16, 25]. In the context of a homogenisation procedure based on the Irving-Kirkwood statistical mechanical theory [13], Mandadapu *et al.* [16] arrived at an expression for the homogenised body force which reduces to that of (35) for a suitable choice of weighting function in their theory. Interestingly, following a variational approach similar to the one reported here, where macro- and micro-scale body forces are correctly accounted for, Ricker *et al.* [25] concluded that the extended Hill-Mandel approach is consistent only with self-equilibrated micro-scale body forces (and consequently zero macro-scale body force). Their analysis was conducted under the assumption of periodic RVE boundary conditions. Their conclusion is at odds with the findings of the present paper and can be explained as follows. In [25], no kinematical constraint has been imposed on the micro-scale displacement field to link it to the macro-scale displacement. That is, without a constraint of the type (7), the kinematically admissible displacements within the RVE domain are independent of the macro-displacement. As a consequence, the corresponding space of virtual RVE displacements contains rigid translations and the extended Hill-Mandel Principle can only hold if the volume average of the micro-scale body forces vanishes. Hence, the conclusion of [25] is variationally consistent with the kinematics they adopted. However, since body forces are work-conjugate to displacements, the inclusion of the virtual power of (macro- and micro-scale) body forces into the Hill-Mandel Principle must be accompanied by an appropriate kinematical constraint that, just as (6) and (10) link the macro- and micro-scale displacement gradients, links the macro- and micro-scale displacements in a physically meaningful way. This issue is fully resolved with the simple incorporation of the fundamental constraint (7). Within the present framework, where the entire theory derives from the fundamental concept of kinematical admissibility and the Principle of Multiscale Virtual Power, once the constraint (7) is in place, the homogenisation formulae and RVE equilibrium equation that correctly account for possible non-zero inertia and body forces follow naturally from straightforward variational arguments. Note that, due to the nature of constraint (7), only the fluctuating (zero volume average) components of the micro-scale inertia and body force fields contribute to the micro-scale virtual power and are relevant to the RVE equilibrium equation. Their uniform (volume average) component is *orthogonal* to the space $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$ (see Remark 2.2) and therefore "invisible" to the RVE equilibrium problem. That is, the uniform components $\mathbf{f}^\rho$ and $\mathbf{f}^{\mathrm{b}}$ of the micro-scale inertia and body forces, defined in (36) and (35), are balanced by a *purely reactive* force field generated by the kinematical constraint (7). We remark that the present findings – fluctuation and volume average force components only "visible" at the micro- and macro-scale respectively – are consistent with those reported by Sanchez-Palencia [28] in the context of asymptotic expansion treatment of rapidly varying body force fields in linear elasticity of periodic media.

These observations shed light on an issue which, in our view, appears to be quite unclear in the recent literature (see [24]). The apparent confusion surrounding this issue seems to stem partly from the non-conventional nature of the kinematical constraint (7) – a volume integral constraint – imposed upon the microscale displacement field. However, once the theory is properly cast in variational form, the consequences of this constraint (in particular, the reactive nature of the uniform component of the microscale inertia and body forces) can be rigorously dealt with in exactly the same way as the conventional kinematical constraints of solid mechanics by simply observing the orthogonality between the functional spaces of reactive forces and kinematically admissible virtual displacements. As an interesting practical consequence of these variational considerations we have the following. Note that under the assumptions of minimal kinematical constraint or periodic boundary fluctuations the domain integral constraint (7) serves only to prevent rigid translations. Hence, in these cases an RVE equilibrium problem mechanically equivalent to (46) can be defined by relaxing the constraint (7) of $\mathrm{Var}_{\tilde{\mathbf{u}}_\mu}$ and loading the RVE only with the fluctuating components $\tilde{\mathbf{f}}^\rho_\mu$ and $\tilde{\mathbf{f}}^{\mathrm{b}}_\mu$ of the inertia and body forces. Obviously, in such cases another kinematical constraint (e.g. the typical boundary point displacement constraints [23] used in RVE computations in the absence of inertia and body forces) must be imposed to prevent rigid translations in the mechanically equivalent problem. This approach is likely to be simpler in practical computations as it does not require the domain integral constraint to be considered at all. However, if the full inertia or body forces are applied to the RVE (i.e. fluctuating plus volume average components) then the constraint (7) must be imposed in the solution of the RVE equilibrium problem. Also noteworthy is the fact that, under the assumption of linear RVE boundary displacements, rigid translations are fully prevented by the boundary constraints alone and (7) is a further kinematical constraint. Hence, unlike the periodic boundary fluctuations and the minimally contrained models, in this case there is in general no mechanically equivalent RVE equilibrium problem that does not require the domain integral constraint (7) to be imposed explicitly.

5 Conclusion

An RVE-based multiscale theory of solids accounting for the effects of micro-scale inertia and body forces has been proposed and discussed in detail. The theory was cast within a framework relying entirely on the two fundamental principles of *kinematical admissibility* and *Multiscale Virtual Power*. These principles are regarded as fundamental in that they provide the essential link between the macro- and micro-scale kinematics and virtual power, respectively. In this context, it has been shown that a simple extension of the Hill-Mandel Principle that accounts for the *total* virtual power, together with a suitable set of kinematical constraints upon the RVE displacements, provide an appropriate framework to address the effects of inertia and body forces on the micro-to-macro transition. Within this framework, the RVE equilibrium equation and the homogenisation relations among the relevant macro- and micro-scale quantities are naturally derived by means of straightforward variational arguments. The following findings are of particular relevance:

- As one would intuitively expect, the macro-scale inertia and body force are obtained simply as the volume average of the micro-scale inertia and body force fields over the RVE domain, respectively;
- The contribution of the micro-scale inertia and body force fields to the homogenised stress is such that the macro-scale stress tensor remains, as in the classical theory of Hill [12], representable exclusively in terms of RVE boundary tractions;
- Only fluctuations of the micro-scale inertia and body force fields about their homogenised (volume average) values are of relevance to the RVE equilibrium equation. Uniform micro-scale inertia and body force fields are "invisible" to the RVE equilibrium problem (as they produce no virtual power in the micro-scale) and, therefore, do not contribute to the homogenised stress.

To the authors' knowledge, these findings are novel in this context and clarify the issue of inertia and body forces within this class of multiscale theories – an issue which appears to not to have been satisfactorily addressed in the literature. We finish by noting that a generalisation of the framework adopted here – where the entire theory can be derived from the principles of kinematical admissibility and Multiscale Virtual Power alone – is currently under development [1, 2] and will be the subject of a forthcoming publication. The generalised framework extends the concepts discussed here to tackle non-classical multiscale problems involving, for example, kinematical discontinuities, higher order kinematics or distinct kinematics at micro- and macro-scales.

Acknowledgment

This work was partially supported by the Brazilian agencies CNPq and FAPERJ. This support is gratefully acknowledged. P.J. Sánchez acknowledges the financial support from CONICET (grant PIP 2013-2015 631), Argentina, and from the European Research Council under the FP7 (2007-2013) programme (ERC grant agreement no. 320815 – Advanced Grant Project on *Advanced tools for computational design of engineering materials* COMP-DES-MAT).

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