Novel Multiscale Models in a Multicontinuum Approach to Divide and Conquer Strategies

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Abstract

This contribution presents a comprehensive, in-depth analysis of the solution of the mechanical equilibrium problem for a generic solid with microstructure. The exact solution to this problem, referred to here as the *reference solution*, corresponds to the full-scale model of the problem that takes into account the kinematics and constitutive behavior of its entire microstructure. The analysis is carried out based on the *Principle of Multiscale Virtual Power* (PMVP) previously proposed by the authors. The PMVP provides a robust theoretical setting whereby the strong links between the reference solution and solutions of the mechanical equilibrium obtained using coarser scale models are brought to light. In this context, some fundamental properties of coarser scale solutions are identified by means of variational arguments. These findings unveil a new homogenization landscape for Representative Volume Element (RVE) multiscale theories, leading to the construction of new Minimal Kinematical Restriction (MKR)-based models where either displacements or tractions may be prescribed on the RVE boundary. A careful observation of the aforementioned landscape leads naturally to the proposal of a new, multicontinuum strategy (a generalized continuum counterpart of multigrid strategies) to approximate the reference solution at low computational cost. In the proposed strategy, the mechanical interactions among neighboring microcells are accounted for in an iterative fashion by means of suitably chosen boundary conditions enforced alternately on the new MKR-based models. The proposed developments are presented assuming a classical continuum at all scales, but the results are equally valid when different kinematical and constitutive assumptions are made at different scales.

Keywords: Multiscale Modeling, Virtual Power, Boundary Conditions, Multigrid Approach, Direct Numerical Solution

1 Introduction

The bridging between physical scales was initiated by the landmark contributions of Kirkwood and collaborators, which set the fundamental bases for the governing equations of transport phenomena in continuum media, by departing from statistical mechanics arguments [1–4]. In the field of solid mechanics, the major developments were motivated by the estimation of emergent (macroscopic) properties of heterogeneous materials [5–12]. In parallel, the use of asymptotic analysis of partial differential equations with periodic coefficients enabled the modeling of continua with periodic microstructure [13–15]. Notably, an aspect shared by all these theories is the fact that variables at the macroscopic level, usually called homogenized variables, are invariably related to some kind of averaging process of the fields defined at the microscopic level.

In more recent times, research on multiscale modeling approaches have bloomed in the context of computational mechanics, triggered by the availability of increasing computational power. Most of these approaches rely on the concept of Representative Volume Element (RVE) to model the microscale phenomena. Thus, stresses and strains at the macroscale level are characterized through volumetric averages of the corresponding fields at the RVE scale. Importantly, the mechanical model adopted to describe the physical phenomena at micro level may be different from that adopted at macro level. The conventional approach taken in the literature exploits computational homogenization techniques and finite element strategies to find the approximate solution to the problem [16–29]. Current applications in the field of solid mechanics include plasticity, thermomechanical coupling, dynamics and vibrations and problems involving material damage and failure [30]. Moreover, multiscale models have also addressed the construction of high order constitutive models [18, 19, 31–33]. These are examples where the multiscale approach can properly handle the interaction between scales even when scale separation does not hold.

A comprehensive review of the multiscale modeling approach and its applications is beyond the scope of the present work. The interested reader is referred to [34–50]. In these contributions, specific reference is made to the different areas of application of multiscale modeling.

The ever-increasing popularity of RVE-based multiscale strategies has been driven by the need to address increasingly complex problems featuring smaller scale phenomena whose full scale characterization remains beyond the reach of available computing power. Even though the solution of full-scale problems has remained elusive, multiscale models managed to deliver essential insight into the underlying mechanisms taking place at the microscopic realm, and the way in which these phenomena emerge at the macroscale (observable) level [51, 52]. Multiscale solutions have been crucial to optimize the use of existing materials, as well as to design new materials in a rational and scientific manner.

The overwhelming presence of RVE-based multiscale models in mechanical applications is historically related to the study of constitutive behavior of materials that featured a certain microstructural arquitecture at smaller scales. Currently, extensions and modifications of the multiscale theories have enabled the incorporation of more ellaborate small scale interactions. Therefore, purely constitutive multiscale modeling was transformed into an all-embracing framework capable of accounting for all sorts of physical effects, and whose impact on the observable scale of the object of study is accounted for by bridging hypotheses and homogenization rules.

In performing such homogenization, naturally, the full-scale problem is being described as a loose interconnection of different scales, typically a micro and a macro scale. The segregation of these scales is due to the fact that tackling the full-scale problem is unfeasible given the computational resources that would be required for a proper characterization of the fine scale mechanical interactions in a monolithic manner. Thus, through the segregation of microscopic physical domains (the RVEs) it is possible to set up a loosely coupled full-scale problem, where the RVEs weakly interact through the homogenization process integrated with the mechanical equilibrium configured at the macroscopic scale. Although the transfer of information between the scales provides a sense of locality at each RVEs, which is important to keep the problem decoupled, at the same time it precludes the RVEs from proper interaction with neighboring physical domains through their boundaries.

Consequently, despite the wide range of situations addressed in the current literature, there is still a gap concerning the non-local interactions among neighboring RVEs for the simple reason that they are obtained using a microcell (RVE) that is considered to be completely decoupled (isolated) from the rest of the body domain. Therefore, the finer interactions between the microcell (formerly called RVE) and its neighbors are neglected, or inadequately incorporated, due to the incorrect prescription of boundary conditions enforced at the RVE level in the formulation of these multiscale models. For example, in the traditional Taylor multiscale model, an affine displacement is prescribed all over the entire RVE, which generally is far from the actual behavior of the microcell. In the Linear Boundary Multiscale Model, a linear displacement is prescribed on the microcell boundary, something which is also generally far from the actual behavior of the microcell. A conventional multiscale model with periodic boundary conditions has little meaning in the case of arbitrarily heterogeneous material (for example, including voids), or in problems with evolving interfaces and discontinuities. In turn, the so-called Minimal Kinematical Restriction Multiscale (MKR) model, which includes only the minimum set of kinematic constraints required to satisfy the Principle of Multiscale Kinematic Admissibility [37, 38, 47], induces a piecewise uniform traction field on the solid part of the microcell boundary – something that, again, does not generally reflect the true mechanical state of the material at the micro level. We can see that isolating microcells from the rest of the body generally brings inconsistencies between neighboring domains, and this is one of the main challenges addressed in this work: how to bring neighboring information into the formulation of the microscale equilibrium problem of each microcell so as to reduce or eliminate such inconsistencies.

A proper characterization, not only of the homogenized mechanics at the coarse scale, but also of the micromechanics, requires the correct characterization of the mechanical environment in each microcell. This goal is attained only if the exact solution of the full-scale equilibrium problem is known. The solution of the single- full-scale problem that accounts for all the fine scale interactions in the entire domain shall be referred to here as the *reference solution*. By zooming into the reference solution within a certain microcell, we will see that its physical fields are the result of its interactions with neighboring microcells. Nevertheless, the characterization of this solution is not generally attainable, even with the use of high performance computers.

At this point, it is important to mention two adjoining fields of research whose main goal is to find such a reference solution by creating, or accelerating, a sequence of iterates that eventually converge to the sought solution. In this manner, these methods propose a divide and conquer approach to circumvent solving the full problem all at once.

On one hand, we have domain decomposition techniques, whose aim is to partition the domain of analysis into (overlapping or non-overlapping) subdomains for which local problems are formulated. Local problems receive local boundary conditions according to certain criteria that are responsible for defining boundary data at neighboring subdomains. Through the iterative process, the lack of continuity of the solution at the boundaries between adjacent subdomains is expected to be progressively reduced until a certain convergence threshold is achieved. Domain decomposition approaches can be formulated either at the algebraic level [53], or at the continuum level [54]. In the former case, the resulting algebraic structure of the problem is manipulated so the full algebraic problem is broken into subproblems that interchange information. In the latter approach, the formulation of boundary value problems (including Dirichlet, Neumann, or even Robin boundary data), the Stéklov-Poincaré operators plays a fundamental role to understand the theoretical concepts and ensure mathematical/energetic consistency. Domain decomposition methods are typically proposed for a set of partial differential equations, and the local problems represent such an original set of equations. Alternatively, domain decomposition formulations were proposed to work with heterogeneous models occupying non-overlapping regions within a certain domain of analysis. Examples are the coupling of surface and groundwater flows [55], the coupling of Darcy and Stokes models [56], the coupling of Biot and Navier-Stokes models [57], the classical fluid-structure interaction problem [58], and even models of different dimensions [59, 60].

On the other hand, we have multigrid methods (a class of multiresolution method) as a way to resolve the different scales featured by the problem through a family of problem discretizations performed hierarchically [61, 62]. This family of methods lies closer to the multiscale paradigm, as the fundamental idea is to coarsen the original problem, solve it and then go back to the finer model with coarse scale information, and iterate this procedure until a convergence criterion is achieved. The goal in this case is to progressively reduce the error in the finer model through the coarse-fine iterations. To achieve this, proper restriction and prolongation (also known as interpolation) operators are required, so information can be transferred between two hierarchically connected approximations. Connection between multigrid solvers and homogenization techniques is not new, and can be found in [63], where variational upscaling was applied to porous media flow simulations, and in [64] for solid mechanics. Alternative numerical strategies were also proposed using mixed approaches. For instance, in [65, 66] a multigrid approach was employed at the continuum level, which enforced the coupling conditions between beighboring subdomains in a weak manner.

It is worth noting that, except for the problems where heterogeneous models are considered spanning non-overlapping spatial regions, all the previous apporoaches address a certain problem defined by a set of partial differential equations and stick to these equations in the application of the methodology. That is, model equations are the same in the different subdomains in domain decomposition techniques, and are the same in the different discretizations in multigrid techniques. This is an example of a limitation which can be circumvented by exploiting the framework of the Method of Multiscale Virtual Power (MMVP).

In the present work, we place the problem of characterizing the reference solution for a mechanical system at the continuum level, that is, as a continuum mechanics problem, before any discretization is introduced. More specifically, we regard the RVE-based multiscale strategy as an excellent candidate to tackle the problem. The proposed developments rely on the Principle of Multiscale Virtual Power [37, 38, 47], which allows us to construct bridging rules between the mechanical phenomena at the small scale and the corresponding phenomena at any larger scale (including the macroscale), regardless of the governing equations, which may well differ at different scales. In this context, the theoretical variational basis of RVE-based methodologies is discussed in detail and the foundations are laid for the development of a new strategy to obtain the reference solution without the direct solution of the full-scale problem. By exploiting this variational basis, a novel insight emerges. In particular, it becomes clear that variational formulations of new multiscale models can be developed in which either generalized displacements or tractions may be prescribed on the boundary of the microcell, making the incorporation of the interactions with neighboring domains feasible. With the incorporation of the interactions between the microcell and its surroundings, a strategy based on the new multiscale models can be proposed as a multicontinuum approach (a generalized continuum counterpart of multigrid strategies) for the determination of the reference solution at a lower computational cost than by solving the full-scale problem monolithically.

The paper is structured as follows. In Section 2 we present the ingredients that characterize the full-scale problem and the corresponding *reference solution*. In Section 3 we show the connection between the *reference solution* and solutions obtained at coarser scales. In Sections 4 we present the properties of the *reference solution* when restricted to an arbitrary isolated microcell. Then, novel multiscale models where displacements or tractions may be prescribed on the boundary of the microcell, and which are capable of capturing important properties of the *reference solution*, are proposed in Section 5. The use of the new multiscale models in a multicontinuum approach to determine the *reference solution* is proposed in Section 6. Concluding remarks are then presented in Section 7. In addition, to make this contribution self-contained, in Appendix A and Appendix B we present the fundamental aspects of the MKR multiscale model and the Principle of Multiscale Virtual Power [37, 38, 47].

2 Full-scale problem

In this section we define the full-scale problem under consideration, and characterize its solution – the *reference solution*. The full-scale problem comprises a single scale where all heterogeneities and details of the continuum (at all length scales) are accounted for.

In what follows, we denote by Ω_μ the material configuration of the body $\mathcal{B}_\mu$ whose kinematics and constitutive behaviour may generally depend on the chosen scale μ where the model is defined. For the sake of simplicity, we limit the presentation here to the case of a classical continuum at scale μ, corresponding to a body with microstructure which may include voids randomly distributed in Ω_μ that may or may not reach its boundary $\partial\Omega_\mu$.

Remark 1 Despite the limitation of this presentation to classical continuum mechanics and specifically to solid mechanics, extensions of the fundamental concepts exposed in this paper to different kinematical models (see for example [40]) can be pursued.

For convenience, we list below some of the most important definitions and notations adopted (refer to Figure 1):

- Ω_μ: the entire domain including voids and solid material.
- $\mathbf{y}$: coordinates in Ω_μ.
- $\partial\Omega_\mu$: boundary of Ω_μ.
- Ω_μ^s: solid part of Ω_μ.
- Ω_μ^v: space occupied by voids in Ω_μ.
- $\Omega_\mu^{v_i}$: space occupied by fully internal voids in Ω_μ.
- $\Omega_\mu^{v_b}$: space occupied by voids which reach the boundary of Ω_μ.
- $\partial\Omega_\mu^{s,b}$: boundary of Ω_μ^s shared with $\partial\Omega_\mu$.
- $\partial\Omega_\mu^{v,b}$: boundary of Ω_μ^v shared with $\partial\Omega_\mu$.
- $\partial\Omega_\mu^{s,v_i}$: boundary of Ω_μ^s shared with the boundary of $\Omega_\mu^{v_i}$.
- $\partial\Omega_\mu^{s,v_b}$: boundary of Ω_μ^s shared with $\Omega_\mu^{v_b}$.

Similar notations are applied to any part $\mathcal{P}_\mu$ of Ω_μ (see Figure 1).

Let $\partial\Omega_{\mu,D}^{s,b}$ be the part of $\partial\Omega_\mu^{s,b}$ where the displacement is prescribed as a given field $\overline{\mathbf{u}}_\mu(\mathbf{y})$, $\mathbf{y} \in \partial\Omega_{\mu,D}^{s,b}$. Also, we assume that the constraints imposed on the displacement field are such that if two displacement fields satisfy $\nabla\mathbf{u}_\mu^1(\mathbf{y}) = \nabla\mathbf{u}_\mu^2(\mathbf{y}), \mathbf{y} \in \Omega_\mu^s$ then $\mathbf{u}_\mu^1(\mathbf{y}) = \mathbf{u}_\mu^2(\mathbf{y}), \mathbf{y} \in \Omega_\mu^s$.

Let $\mathcal{V}_\mu$ be a function space of vector-valued elements that are sufficiently regular so that all mathematical operations they are involved in make sense. In classical continuum mechanics in the three-dimensional space, $\mathcal{V}_\mu = [H^1(\Omega_\mu^s)]^3$. In what follows, to simplify the presentation, we assume $\mathcal{B}_\mu$ to be subject only to body forces in its interior and prescribed displacements on its boundary. Then, let Kin_μ^* be the linear manifold of kinematically admissible displacements of $\mathcal{B}_\mu$, defined by

$$Kin_\mu^* = \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathbf{u}_\mu|_{\partial\Omega_{\mu,D}^{s,b}} = \overline{\mathbf{u}}_\mu\} = \mathbf{u}_\mu^o + Var_\mu^*, \tag{1}$$

where $\mathbf{u}_\mu^o$ is an arbitrary element of Kin_μ^*, and Var_μ^* is the associated subspace of kinematically admissible virtual actions of $\mathcal{B}_\mu$:

$$Var_\mu^* = \{\mathbf{v} \in \mathcal{V}_\mu;\ \mathbf{v}|_{\partial\Omega_{\mu,D}^{s,b}} = \mathbf{0}\}. \tag{2}$$

The mechanical equilibrium of the body $\mathcal{B}_\mu$ is established by the following variational problem: *For a given load system defined by* $\{\mathbf{b}_\mu\} \in \mathcal{V}_\mu'$ *(*$\mathcal{V}_\mu'$ *is the*

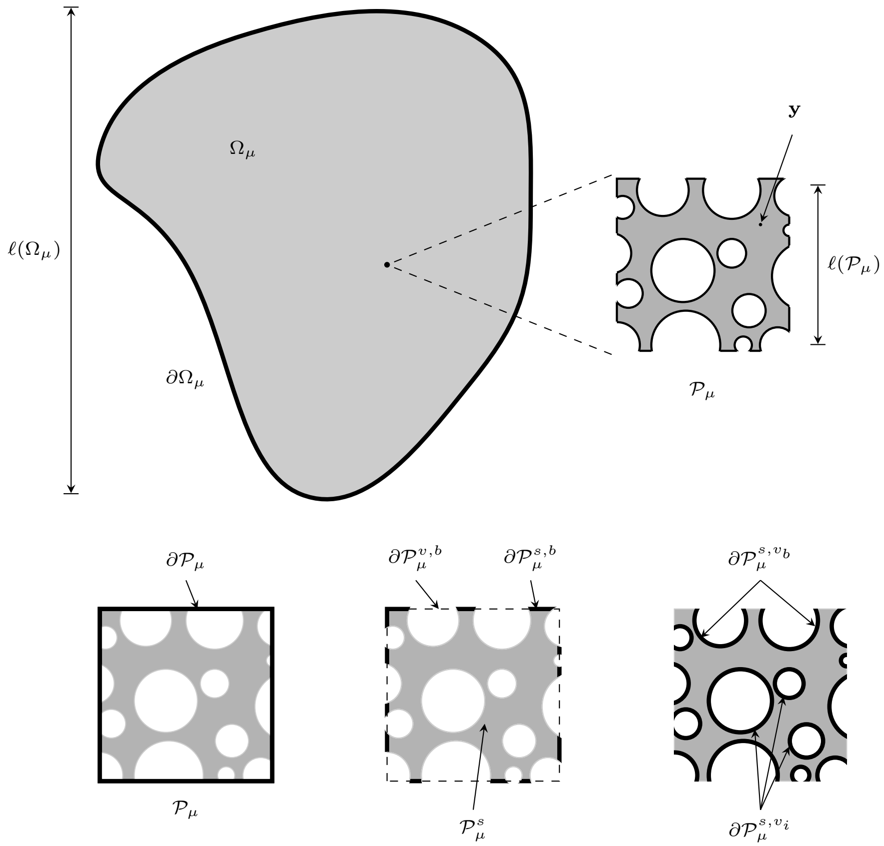

Fig. 1 Domain Ω_μ taking into account its microstructure in an arbitrary part $\mathcal{P}_\mu$.

dual space of $\mathcal{V}_\mu$), find the reference solution $\mathbf{u}_\mu^* \in Kin_\mu^*$ such that

$$\int_{\Omega_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \qquad \forall \mathbf{v} \in Var_\mu^*, \tag{3}$$

where $\mathbf{P}_\mu$ is the first Piola-Kirchhoff stress tensor – assumed a function of the deformation gradient $\mathbf{F}_\mu = \mathbf{I} + \nabla \mathbf{u}_\mu^*$. We assume the constitutive stress-strain relation satisfying

$$\int_{\mathcal{P}_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^1) - \mathbf{P}_\mu(\mathbf{u}_\mu^2)] \cdot [\nabla(\mathbf{u}_\mu^1 - \mathbf{u}_\mu^2)] d\Omega_\mu \geq 0 \qquad \forall \mathbf{u}_\mu^1, \mathbf{u}_\mu^2 \in Kin_\mu^*, \tag{4}$$

$$\int_{\mathcal{P}_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^1) - \mathbf{P}_\mu(\mathbf{u}_\mu^2)] \cdot [\nabla(\mathbf{u}_\mu^1 - \mathbf{u}_\mu^2)] d\Omega_\mu = 0 \qquad \Leftrightarrow \nabla \mathbf{u}_\mu^1 = \nabla \mathbf{u}_\mu^2, \tag{5}$$

for any part $\mathcal{P}_\mu^s$ of Ω_μ^s. Moreover, the above requirement implies that equality in (5) is satisfied if and only if the stresses also coincide, i.e. $\mathbf{P}_\mu(\mathbf{u}_\mu^1) = \mathbf{P}_\mu(\mathbf{u}_\mu^2)$.

From (4)-(5) and the constraints prescribed over the displacement field, we have that if the solution $\mathbf{u}_\mu^*$ exists, it is unique. To see this, assume $\mathbf{u}_\mu^1$ and $\mathbf{u}_\mu^2$ to be two solutions of (3). Then,

$$\int_{\Omega_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^1) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_\mu^*, \tag{6}$$

$$\int_{\Omega_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^2) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_\mu^*. \tag{7}$$

From these equations we obtain

$$\int_{\Omega_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^1) - \mathbf{P}_\mu(\mathbf{u}_\mu^2)] \cdot \nabla \mathbf{v} d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_\mu^*. \tag{8}$$

Further, since $\mathbf{u}_\mu^1 - \mathbf{u}_\mu^2 \in Var_\mu^*$, the above implies that

$$\int_{\Omega_\mu^s} [\mathbf{P}_\mu(\mathbf{u}_\mu^1) - \mathbf{P}_\mu(\mathbf{u}_\mu^2)] \cdot \nabla(\mathbf{u}_\mu^1 - \mathbf{u}_\mu^2) d\Omega_\mu = 0, \tag{9}$$

and from (5) and the assumed contraints on admissible displacement fields, we conclude that

$$\mathbf{u}_\mu^1 = \mathbf{u}_\mu^2 = \mathbf{u}_\mu^*, \tag{10}$$

and the uniqueness of the solution of (3) is demonstrated.

In what follows we shall assume that the body force data per unit volume $\mathbf{b}_\mu$ is sufficiently regular so that the variational problem (3) is well posed in the sense that it has a solution.

3 Homogenized mechanical formulation

In this section we consider the problem of coarsening the full-scale model of Section 2 and devise a coarsened continuum that we shall refer to as the *macroscale model*. The coarsened model is linked to the fine, full-scale model through an appropriate power equivalence between the two continua, and kinematical constraints provide the conditions for this balance to be imposed in a consistent, physically meaningful manner, by means of the Principle of Multiscale Virtual Power.

Now, let $\{\mathcal{P}_\mu^i, i = 1, \ldots, N_\mu\}$ be an arbitrary partition of Ω_μ into N_μ microcells such that the following properties are satisfied:

- $\Omega_\mu^s = \bigcup_{i=1}^{N_\mu} \mathcal{P}_\mu^{i,s}$;
- $\mathcal{P}_\mu^{i,s} \cap \mathcal{P}_\mu^{j,s} = \emptyset$, for $i \neq j,\ i, j = 1, \ldots, N_\mu$;

- In the present context, N_μ is, in general, a very large integer such that the *characteristic length* of $\mathcal{P}^i_\mu$, denoted $l(\mathcal{P}^i_\mu)$, is large enough to be representative of the microstructures/heterogeneities present in the body $\mathcal{B}_\mu$, but small enough when compared to the characteristic length of the macro scale, or coarse scale. Let us denote n_i the number of heterogeneities of $\mathcal{P}^{i,s}_\mu$ and $\mathcal{H}^{i,k}_\mu, k = 1, \ldots, n_i$, $n_i > 1$, the part of the domain $\mathcal{P}^{i,s}_\mu$ occupied by heterogeneity k. We assume $\mathcal{P}^{i,s}_\mu = \bigcup_{k=1}^{n_i} \mathcal{H}^{i,k}_\mu$.

Also, for each part $\mathcal{P}^i_\mu$ of the body we define

$$I^i = \{j = 1, \ldots, N_\mu; \ \text{ for } j \neq i; \ \partial\mathcal{P}^{i,s,b}_\mu \cap \partial\mathcal{P}^{j,s,b}_\mu \neq \emptyset\} \tag{11}$$

as the set of indeces of the microcells that form the neighborhood of $\mathcal{P}^i_\mu$.

Using this partition, variational equation (3) can be rewritten as

$$\sum_{i=1}^{N_\mu} \int_{\mathcal{P}^{i,s}_\mu} [\mathbf{P}_\mu(\mathbf{u}^*_\mu) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] \, d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var^*_\mu. \tag{12}$$

Then, it is easy to show that the *reference solution* $\mathbf{u}^*_\mu \in Kin^*_\mu$ satisfies, in a weak sense, the following Euler-Lagrange equations

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}^*_\mu) + \mathbf{b}_\mu = \mathbf{0} \text{ in } \mathcal{H}^{i,k}_\mu \ k = 1, \ldots, n_i, \quad i = 1, \ldots, N_\mu, \tag{13}$$

$$[\![\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}^{i,k}_\mu \cap \partial\mathcal{H}^{i,m}_\mu, \ k \neq m, \ k, m = 1, \ldots, n_i, \quad i = 1, \ldots, N_\mu, \tag{14}$$

$$[\![\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{P}^{i,s,b}_\mu \cap \partial\mathcal{P}^{j,s,b}_\mu, \ i \neq j, \ i, j = 1, \ldots, N_\mu, \tag{15}$$

$$\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}^{i,s,v}_\mu, i = 1, \ldots, N_\mu, \tag{16}$$

$$\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu = \mathbf{r}^*_\mu \text{ on } \partial\Omega^{s,b}_{\mu,D}, \tag{17}$$

$$\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\Omega^{s,b}_\mu \backslash \partial\Omega^{s,b}_{\mu,D}, \tag{18}$$

where $\mathbf{r}^*_\mu \in (Var^*_\mu)^\perp$ is the *reaction* resulting from the prescribed displacement on the Dirichlet boundary $\partial\Omega^{s,b}_{\mu,D}$, and $\mathbf{n}_\mu$ is the unit normal vector to the boundary.

Remark 2 Equation (15) tells us that the traction, say $\mathbf{t}^{*,i}_\mu$, exerted on an arbitrary microcell boundary $\partial\mathcal{P}^{i,s,b}_\mu$ by its neighboring microcells, $\mathcal{P}^j_\mu$, $j \in I^i$, across their boundaries $\partial\mathcal{P}^{j,s,b}_\mu$, is, in general, a non-constant field over the intercell boundaries. This field given exactly by $\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu} = \mathbf{t}^{*,i}_\mu$.

With the *reference solution* at micro level, $\mathbf{u}_\mu^*$, by using the Principle of Multiscale Virtual Power (PMVP, see Appendix B) together with the homogenization procedures for displacements, displacement gradients, stress and body forces [37, 38, 47], expression (12) yields

$$\begin{aligned}
\forall \mathbf{v} \in Var_\mu^* \quad 0 &= \sum_{i=1}^{N_\mu} \int_{\mathcal{P}_\mu^{i,s}} \left[\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}\right] d\Omega_\mu \\
&= \sum_{i=1}^{N_\mu} |\mathcal{P}_\mu^i| \left\{ \mathbf{P}_M^*|_{\mathbf{x}_i} \cdot \nabla \mathbf{v}_M|_{\mathbf{x}_i} - \mathbf{b}_M^*|_{\mathbf{x}_i} \cdot \mathbf{v}_M|_{\mathbf{x}_i} \right\} \\
&= \int_{\Omega_M} [\mathbf{P}_M^* \cdot \nabla \mathbf{v}_M - \mathbf{b}_M^* \cdot \mathbf{v}_M] d\Omega_M \\
&= 0 \quad \forall \mathbf{v}_M \in Var_M^*, \qquad (19)
\end{aligned}$$

where $\mathbf{x}_i \in \Omega_M$ is the point at macroscale level associated to the microcell $\mathcal{P}_\mu^i$, $|\mathcal{P}_\mu^i|$ is the measure of the microcell $\mathcal{P}_\mu^i$ including the solid and the void parts, i.e. $|\mathcal{P}_\mu^i| = |\mathcal{P}_\mu^{i,s}| + |\mathcal{P}_\mu^{i,v}|$. The domain Ω_M is the *macro-scale* or *coarse-scale domain*, which is the same as Ω_μ but now understood as a coarsened continuum. That is, Ω_M is the fine-scale domain Ω_μ viewed through 'blurry glasses', where the fine-scale details/heterogeneities have been smoothed out as a result of the homogenization procedure. In turn, the space Var_M^* is defined as

$$Var_M^* = \{\mathbf{v}_M \in \mathcal{V}_M;\ \mathbf{v}_M|_{\partial\Omega_M^D} = \mathbf{0}\}, \qquad (20)$$

where $\partial\Omega_M^D$ is the boundary of Ω_M where Dirichlet boundary conditions are prescribed.

Finally, note that in (19), the same kinematics has been assumed for both macro- and micro-scales. However, the use of different kinematics in Ω_μ and in Ω_M is possible. See [36, 40] for two examples of problems with mixed kinematics.

Let us now look at some important conceptual details relevant as we move through the different lines of equation (19):

- The second line of (19) is obtained from its first line by exploring the Method of Multiscale Virtual Power (MMVP), proposed in [37, 38]. In particular, we have made use of the Principle of Multiscale Virtual Power (PMVP) presented in Appendix B, which postulates that the energetic consistency between the macro- and micro-scale is established when the total virtual powers at both scales coincide: *"The total macroscale virtual power at a point* $\mathbf{x}_i$ *must be equal to the total microscale virtual power of the corresponding microcell for all kinematically admissible macro- and micro-scale virtual actions"*. Hence, no approximation is introduced at this step. The identity between the first and second lines of (19) follows simply from an arbitrary partitioning of the full-scale continuum, and there is no requirement that $\mathcal{P}_\mu^i$ be a *representative volume element*. In fact, this domain must be large enough in order to adequately describe the heterogeneities (materials and topological architecture) at that level.

- Further, according to the PMVP, $\mathbf{P}^*_M|_{\mathbf{x}_i}$ and $\mathbf{b}^*_M|_{\mathbf{x}_i}$ in the second line of (19) are, respectively, the values of the macro-scale stress tensor field, $\mathbf{P}^*_M$, and the body force vector field per unit volume, $\mathbf{b}^*_M$, at point $\mathbf{x}_i$ of the macroscale, linked to the microcell $\mathcal{P}^i_\mu$. Similarly, $\mathbf{v}_M|_{\mathbf{x}_i}$ and $\nabla\mathbf{v}_M|_{\mathbf{x}_i}$ denote, respectively, the value of (coarsened) macroscale virtual action fields, $\mathbf{v}_M$, and its gradient, $\nabla\mathbf{v}_M$, at $\mathbf{x}_i$. It should also be stressed here that, as established by the PMVP, the equality between the first and second line of (19) must hold for all kinematically admissible virtual actions $\mathbf{v}_M \in Var^*_M = \{\mathbf{v}_M \in \mathcal{V}_M;\ \mathbf{v}_M|_{\partial\Omega_D} = \mathbf{0}\}$ over Ω_M – the blurry version of Ω_μ – where the solid constitutive behavior and body force depend on the mechanical interactions at the microcell level through the corresponding homogenization operators.
- The second line of (19) can be interpreted as a *midpoint quadrature formula* for the integral of the third line. Since N_μ is typically very large, we assume the numerical error introduced by the quadrature to be negligible. For this reason, we maintain the *equal sign* instead of the *the approximation symbol* between lines two and three.
- The third line of (19) implies that with the exact solution $\mathbf{u}^*_\mu$ of the full-scale equilibrium problem – the *reference solution* – at hand, the PMVP (with the associated homogenization operators) enables us to obtain the coarse-scale fields $\mathbf{P}^*_M$ and $\mathbf{b}^*_M$ over Ω_M (as well as any other homogenized field, such as, for example the homogenized constitutive tangent operator), that satisfy the macroscale equilibrium in the sense of (19).
- Finally, since the first line is zero for any $\mathbf{v} \in Var^*_\mu$, the third line must also be zero for any $\mathbf{v}_M \in Var^*_M$.

Remark 3 The above framework is not limited to only two scales (micro and macro). Any number of scales can be considered with the above reasoning applied recursively.

Remark 4 In the above, we stated that the energetic consistency was satisfied using the PMVP. The reader will notice that the balance of power between macro and micro-scales was originally proposed in [9, 11], and became known as the Hill-Mandel principle of Macrohomogeneity. While this well-known principle was originally formulated for the true power exerted at both scales, the PMVP cast the Hill-Mandel principle in a variational setting.

The tractions $\mathbf{t}^{*,i}_\mu$, as should be expected, play no role in the PMVP. Intercell tractions do not contribute to the external microscale virtual power because they are reactions, associated by duality, to the constraint of kinematical compatibility between $\mathcal{P}^i_\mu$ and its neighboring microcells. This observation allows us to see the intercell tractions $\mathbf{t}^{*,i}_\mu$ as the Lagrange multipliers needed to enforce intercell compatibility in the local equilibrium problem where $\mathcal{P}^i_\mu$

is considered isolated (decoupled) from the rest of the body, with the corresponding kinematical constraint relaxed in the sets of kinematically admissible displacements and virtual actions. This fact will be explored in Section 4, where the equilibrium of individual, isolated microcells is considered in isolation.

We stress that the solution $\mathbf{u}_\mu^*$ of the full-scale equilibrium problem that takes into account all fine details of the solid can be regarded as the *reference solution* in general multiscale modeling. In fact, its knowledge enables the *exact* determination of all macro scale fields necessary for the equilibrium and representation of the macro-scale behavior taking into account the fine mechanical interactions of the micro-scale level. However, obtaining this solution by means of numerical approximation is, in general, not feasible at present, given the prohibitive computing costs associated with the full-scale solution of more realistic problems. One approach to overcome this challenge is the use of classical, RVE-based multiscale models. This approach aims to formulate a similar, generally representative problem that will deliver a (hopefully) good approximation for $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}}$ at significantly lower computing costs. The better the multiscale model, the better the approximation will be. The classical multiscale paradigm relies on the assumption that only homogenized information is transferred between scales, and that each microcell $\mathcal{P}_\mu^i$ is considered isolated from its surroundings. The local microcell mechanical problem is then formulated in each multiscale model by assuming a particular set of microcell kinematical boundary conditions that, in some sense, tries to mimic the actual interactions of the microcell with its surroundings in the full-scale problem. These *assumed* kinematical constraints may or may not be good approximations of the real boundary interactions, and the ability to capture them with good accuracy, to be as close as possible to the reference solution, is the most crucial aim of any multiscale model.

Remark 5 As discussed in the introduction, isolation from the rest of the body generally brings inconsistencies between neighboring microcells, and this is one of the main challenges addressed in this work: how to bring neighboring information into the formulation of the microscale equilibrium problem for each microcell to reduce or eliminate such inconsistencies.

In fact, without loss of generality, the *reference solution* $\mathbf{u}_\mu^*$ restricted to the microcell $\mathcal{P}_\mu^i$ can be described exactly using a Taylor series-like expansion by introducing the (linear) homogenization operators, denoted by $\mathcal{H}_\mu^{\mathcal{V}}(\cdot)$ and $\mathcal{H}_\mu^{\mathcal{W}}(\cdot)$. These operators account for the affine characterization of the field, plus a fluctuation component included in the Taylor expansion (see (21) below). Thus, the microscale kinematics can be linked, through appropriate homogenization procedures, to the corresponding point-wise value (associated to $\mathcal{P}_\mu^i$) of the macroscale kinematics (see [37, 38, 47]). This expansion of the *reference* *solution* reads

$$\begin{aligned}\mathbf{u}^*_\mu|_{\mathcal{P}^{i,s}_\mu} &= \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^*_\mu|_{\mathcal{P}^{i,s}_\mu}) + \mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{u}^*_\mu|_{\mathcal{P}^{i,s}_\mu})(\mathbf{y}-\mathbf{y}_G) + \widetilde{\mathbf{u}}^*_\mu(\mathbf{y}) \\ &= \mathbf{u}^*_M|_{\mathbf{x}_i} + \mathbf{G}^*_M|_{\mathbf{x}_i}(\mathbf{y}-\mathbf{y}_G) + \widetilde{\mathbf{u}}^*_\mu(\mathbf{y}), \quad \mathbf{y}\in\mathcal{P}^{i,s}_\mu, \end{aligned} \tag{21}$$

where, for the material under consideration (heterogeneous with voids arbitrarily distributed in $\mathcal{P}^i_\mu$, that may or may not reach its boundary), $\mathbf{y}_G = \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\mathcal{P}^{i,s}_\mu} \mathbf{y}\, d\Omega_\mu$, $\widetilde{\mathbf{u}}^*_\mu$ represents the *displacement fluctuations*, i.e. the higher order term in $\mathbf{u}^*_\mu$, defined as

$$\widetilde{\mathbf{u}}^*_\mu(\mathbf{y}) = \mathbf{u}^*_\mu|_{\mathcal{P}^{i,s}_\mu} - \mathbf{u}^*_M|_{\mathbf{x}_i} - \mathbf{G}^*_M|_{\mathbf{x}_i}(\mathbf{y}-\mathbf{y}_G), \tag{22}$$

and $\mathbf{u}^*_M|_{\mathbf{x}_i}$ and $\mathbf{G}^*_M|_{\mathbf{x}_i}$ are, respectively, the displacement and gradient at the point $\mathbf{x}_i \in \Omega_M$ linked to the kinematics at the microscale by the multiscale kinematical admissibility homogenization linear operators

$$\begin{aligned}\mathbf{u}^*_M|_{\mathbf{x}_i} &= \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^*_\mu) = \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\mathcal{P}^{i,s}_\mu} \mathbf{u}^*_\mu\, d\Omega_\mu \\ &= \mathbf{u}^*_M|_{\mathbf{x}_i} + \mathcal{H}^{\mathcal{V}}_\mu(\widetilde{\mathbf{u}}^*_\mu) \\ &= \mathbf{u}^*_M|_{\mathbf{x}_i} + \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\mathcal{P}^{i,s}_\mu} \widetilde{\mathbf{u}}^*_\mu\, d\Omega_\mu, \end{aligned} \tag{23}$$

$$\begin{aligned}\mathbf{G}^*_M|_{\mathbf{x}_i} &= \mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{u}^*_\mu) = \\ &= \frac{1}{|\mathcal{P}^{i,s}_\mu|}\Bigg[\int_{\mathcal{P}^{i,s}_\mu} \nabla\mathbf{u}^*_\mu\, d\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,v_i}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \mathbf{n}^{v_i}_\mu\, d\partial\Omega_\mu \\ &- \int_{\partial\mathcal{P}^{i,s,v_b}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \mathbf{n}^{v_b}_\mu\, d\partial\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \overline{\mathbf{n}}_\mu\, d\partial\Omega_\mu\Bigg] \\ &= \frac{1}{|\mathcal{P}^{i,s}_\mu|}\Bigg[|\mathcal{P}^{i,s}_\mu|\,\mathbf{G}^*_M|_{\mathbf{x}_i} + \int_{\mathcal{P}^{i,s}_\mu} \nabla\widetilde{\mathbf{u}}^*_\mu\, d\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,v_i}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \mathbf{n}^{v_i}_\mu\, d\partial\Omega_\mu \\ &- \int_{\partial\mathcal{P}^{i,s,v_b}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \mathbf{n}^{v_b}_\mu\, d\partial\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes \overline{\mathbf{n}}_\mu\, d\partial\Omega_\mu\Bigg] \\ &= \mathbf{G}^*_M|_{\mathbf{x}_i} + \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}^*_\mu \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)\, d\partial\Omega_\mu \\ &= \mathbf{G}^*_M|_{\mathbf{x}_i} + \mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\widetilde{\mathbf{u}}^*_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu}). \end{aligned} \tag{24}$$

In the above, we used (21) and the definition of $\mathbf{y}_G$, and the vector $\overline{\mathbf{n}}_\mu$ is defined as

$$\overline{\mathbf{n}}_\mu = \frac{1}{|\partial\mathcal{P}^{i,s,b}_\mu|}\int_{\partial\mathcal{P}^{i,s,b}_\mu} \mathbf{n}_\mu d\partial\Omega_\mu. \tag{25}$$

Remark 6 Note that the gradient homogenization operator introduced at the beginning of (24) was proposed such that, after use of Gauss formula to take the gradient to the boundary, only microcell boundary terms are present. So, out of the three boundary terms, two of them were struck off after the Gauss formula was used. In this manner, the homogenization rule only depends on fluctuations occurring over the solid part of the microcell boundary ($\partial\mathcal{P}_\mu^{i,s,b}$). Otherwise, the kinematical model would allow for artificial dual forces to occur on the void boundaries, which is not physically justified. Moreover, this is the real concept of a physical experiment, in which we can mechanically test a piece of material by fully controling the kinematics over the solid part of the boundary, and study its response by evaluating the dual forces that emerge on that boundary.

Remark 7 Homogenization formula (24) is actually novel, and should be compared with those of [37, 38, 47]. The novelty is the appearance of the term related to $\overline{\mathbf{n}}_\mu$, as defined in (25). This term allows the homogenization formula to perform consistently even in the most arbitrary case in which voids randomly reach the microcell boundary. For the sake of completeness, let us say that this term is responsible for maintaining the kinematical consistency in such a general situation. A more in-depth analysis is out of the scope of the present work.

It is interesting to note that in the above homogenization operators, $\mathbf{u}_\mu^*$ and $\widetilde{\mathbf{u}}_\mu^*$ are defined only over $\overline{\mathcal{P}_\mu^{i,s}}$. Furthermore, $\mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}_\mu^{i,s,b}}(\widetilde{\mathbf{u}}^*_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}})$ is the boundary counterpart representation of the homogenization operator $\mathcal{H}^{\mathcal{W}}_\mu(\nabla\widetilde{\mathbf{u}}^*_\mu)$ for the gradient of the displacement fluctuations. Finally, due to the description (21) adopted for the *reference solution*, the displacement fluctuation $\widetilde{\mathbf{u}}_\mu^*$ has the following properties

$$\mathcal{H}^{\mathcal{V}}_\mu(\widetilde{\mathbf{u}}^*_\mu) = \mathbf{0}, \tag{26}$$

$$\mathcal{H}^{\mathcal{W}}_\mu(\nabla\widetilde{\mathbf{u}}^*_\mu) = \mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}_\mu^{i,s,b}}(\widetilde{\mathbf{u}}^*_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}}) = \mathbf{O}. \tag{27}$$

For microcells featuring arbitrarily distributed voids and/or material heterogeneities, from the above expressions it then follows that the so-called *Taylor Multiscale Model*, obtained by postulating $\widetilde{\mathbf{u}}_\mu = \mathbf{0}$ in $\mathcal{P}_\mu^{i,s}$, will not be able to represent the reference solution in the microcell. This is also the case for the *Linear Boundary Multiscale Model* since this model assumes $\widetilde{\mathbf{u}}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{0}$. The widely used *Periodic Boundary Multiscale Model*, on the other hand, has no meaning in the present case – heterogeneous materials including voids arbitrarily distributed in $\mathcal{P}_\mu^i$ that may or may not reach the microcell boundary. Finally, let us consider the *Minimal Kinematical Restriction Multiscale Model* (MKR Model) described in Appendix A. In this model, the linear manifold where the solution of the microcell equilibrium problem is sought is $Kin^{MKR}_{\mathbf{u}_\mu}$ (see (A3)). Note that, from (26) and (27), we have that $\mathbf{u}^*_\mu|_{\mathcal{P}_\mu^{i,s}} \in Kin^{MKR}_{\mathbf{u}_\mu}$ and $\widetilde{\mathbf{u}}^*_\mu \in Var^{MKR}_{\widetilde{\mathbf{u}}_\mu}$ (see (A4)). These are the largest functional sets that guarantee a consistent kinematical transfer between the different scales. Hence, these sets contain the solutions delivered by the aforementioned multiscale models as well as the *reference solution*. Notwithstanding that, the large size of these sets is also detrimental to the solution we can obtain at the microcell. A deeper analysis shows that the Lagrange multipliers (constant vector) $\mathbf{\Theta}_\mu^{MKR}$ and (constant second order tensor) $\mathbf{\Lambda}_\mu^{MKR}$, respectively associated by duality with the multiscale kinematical admissibility restrictions (26) and (27), in general do not represent adequately the interaction between the microcell $\mathcal{P}_\mu^i$ and its neighbors. Indeed, enforcing these integral constraints implies a constant (reaction) traction $\mathbf{t}_\mu^{MKR} = \mathbf{\Lambda}_\mu^{MKR}(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)$ over the boundary $\partial\mathcal{P}_\mu^{i,s,b}$. Clearly, this is not satisfied in general by the *reference solution* (see Remark 2).

At this point a question arises: how can we improve upon, say, the MKR model, so that it can deliver a better approximation of the reference solution in the microcell?. The answer to this question is the goal of the next section, where we explore a simple mechanical argument: to obtain the exact equilibrium solution for a part of the whole domain considered isolated from the rest, it is sufficient to find the equilibrium solution in the appropriate linear manifold in which the exact (reference) displacement field is prescribed on the boundary of that part. A second, equivalent alternative consists in relaxing the above boundary displacement prescription and prescribe the associated (reactive) traction on boundary.

4 Isolated microcell equilibrium

In this section we formulate the mechanical equilibrium of the microcell taking into account the constraints that must be satisfied by the kinematical fields.

In what follows, consider a microcell $\mathcal{P}_\mu^i$ in the interior of the domain Ω_μ. Also, let $\mathbf{u}_M^*$, and $\mathbf{G}_M^*$ be the macroscale fields associated to the *reference solution* $\mathbf{u}_\mu^*$ through the corresponding homogenization operators $\mathcal{H}_\mu^{\mathcal{V}}$ and $\mathcal{H}_\mu^{\mathcal{W}}$. Hence, they represent, respectively, the reference homogenized displacement and displacement gradient at the macroscale. Moreover, let $\mathbf{u}_M^*|_{\mathbf{x}_i}$, and $\mathbf{G}_M^*|_{\mathbf{x}_i}$ be the value of these fields at point $\mathbf{x}_i$ associated with the microcell $\mathcal{P}_\mu^i$. Also, let $\mathbf{t}_\mu^{*,i} = \mathbf{P}_\mu(\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}})\mathbf{n}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}}$, defined on the boundary $\partial\mathcal{P}_\mu^{i,s,b}$, be the (reference) traction exerted by the neighboring microcells of $\mathcal{P}_\mu^i$.

As already mentioned, the exact equilibrium solution in the microcell $\mathcal{P}_\mu^i$ when considered isolated from the rest of the domain Ω_μ can be obtained by two different strategies. The first one consists in prescribing the displacement on the boundary $\partial\mathcal{P}_\mu^{i,s,b}$ as $\mathbf{u}_\mu^*|_{\partial\mathcal{P}_\mu^{i,s,b}}$; in the second strategy this kinematical constraint is relaxed the corresponding (reactive) traction, $\mathbf{t}_\mu^{*,i}$ is imposed on $\partial\mathcal{P}_\mu^{i,s,b}$.

If the microcell reaches the macroscale boundary, the part of the microcell boundary that is also part of the boundary of the macroscale domain is subjected to either displacement (Dirichlet), or traction (Neumann) boundary condition. If displacement boundary conditions are prescribed, this must be reflected on the construction of the corresponding function sets containing admissible displacement fields of the microcell. If traction boundary conditions are considered instead, this must be added as an external power in the microscale virtual power balance.

4.1 Displacement boundary conditions in the microcell

To formalize this concept using the description (21), let us introduce the following notation

$$\mathbf{u}_\mu^{*,D}(\mathbf{y}) = \mathbf{u}_\mu^*|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_M^*|_{\mathbf{x}_i} + \mathbf{G}_M^*|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \widetilde{\mathbf{u}}_\mu^*(\mathbf{y}), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b}, \tag{28}$$

and the set (linear manifold) $Kin_{\mathbf{u}_\mu}^{*,D}$ defined by

$$Kin_{\mathbf{u}_\mu}^{*,D} = \{\mathbf{u}_\mu|_{\mathcal{P}_\mu^{i,s}} \in \mathcal{V}_\mu;\ \mathbf{u}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D}\}. \tag{29}$$

Note that, by construction, $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{*,D}$. Hence, the above linear manifold can be rewritten as

$$Kin_{\mathbf{u}_\mu}^{*,D} = \mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} + Var_{\mathbf{u}_\mu}^{*,D}, \tag{30}$$

where

$$Var_{\mathbf{u}_\mu}^{*,D} = \{\mathbf{v}|_{\mathcal{P}_\mu^{i,s}} \in \mathcal{V}_\mu;\ \mathbf{v}|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{0}\}. \tag{31}$$

Then, the equilibrium of the isolated microcell $\mathcal{P}_\mu^i$ subject to the prescribed displacement $\mathbf{u}_\mu^{*,D}$ on the boundary $\partial\mathcal{P}_\mu^{i,s,b}$ and to the external force per unit volume $\{\mathbf{b}_\mu\}$, is defined by the following variational problem: *Find* $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{*,D}$ *such that the following variational equation*

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla\mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^{*,D} \tag{32}$$

holds. The Euler-Lagrange equations associated to the above equilibrium problem are (see Appendix C)

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}_\mu^*) + \mathbf{b}_\mu = \mathbf{0} \text{ in } \mathcal{H}_\mu^{i,k}\ k = 1, \dots, n_i, \tag{33}$$

$$[\![\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_\mu^{i,k} \cap \partial\mathcal{H}_\mu^{i,m}, k \neq m, k, m = 1, \dots, n_i, \tag{34}$$

$$\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu = \mathbf{t}_\mu^{*,i} \text{ on } \partial\mathcal{P}_\mu^{i,s,b}, \tag{35}$$

$$\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}_\mu^{i,v}, \tag{36}$$

where $\mathbf{t}_\mu^{*,i}$ is the reactive force per unit area associated by duality with the kinematical restriction $\mathbf{u}_\mu^*|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D}$. The reactive traction satisfies the following equations

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} d\Omega_\mu = -\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu d\Omega_\mu, \tag{37}$$

and

$$\int_{\partial \mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \otimes (\mathbf{y} - \mathbf{y}_G)\, d\Omega_\mu = \int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)]\, d\Omega_\mu, \quad (38)$$

which are also obtained from the variational equation (32) (see Appendix C).

In addition, and since $\mathcal{N}(\nabla) = \{\mathbf{c} \in \mathbb{R}^{n_d}\}$ – a constant vector field – we have that $Var_{\mathbf{u}_\mu}^{*,D} \cap \mathcal{N}(\nabla) = \{\mathbf{0}\}$. Hence, any (sufficiently regular) external force field per unit volume $\{\mathbf{b}_\mu\}$ is admissible in the variational equilibrium problem (32).

Any displacement field $\mathbf{u}_\mu$ that satisfies

$$\mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) = \mathbf{u}_M^*|_{\mathbf{x}_i}, \quad (39)$$

$$\mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu) = \mathbf{G}_M^*|_{\mathbf{x}_i}, \quad (40)$$

is said to satisfy the Principle of Multiscale Kinematical Admissibility (PMKA). It is crucial to highlight here that there exist elements $\mathbf{u}_\mu \in Kin_{\mathbf{u}_\mu}^{*,D}$ which do not satisfy these constraints and, therefore, do not comply with the PMKA. In fact, without loss of generality, any element $\mathbf{u}_\mu \in Kin_{\mathbf{u}_\mu}^{*,D}$ can be represented as

$$\mathbf{u}_\mu(\mathbf{y}) = \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) + \mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu)(\mathbf{y} - \mathbf{y}_G) + \widetilde{\mathbf{u}}_\mu(\mathbf{y}), \quad \mathbf{y} \in \mathcal{P}_\mu^{i,s}, \quad (41)$$

which, on the boundary, has the form

$$\begin{aligned} \mathbf{u}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} &= \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) + \mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu)(\mathbf{y} - \mathbf{y}_G)|_{\partial \mathcal{P}_\mu^{i,s,b}} \\ &+ \langle \widetilde{\mathbf{u}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle + \widetilde{\widetilde{\mathbf{u}}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}}, \end{aligned} \quad (42)$$

In the above, we made use of the following decomposition: Let $\mathbf{w}$ be a vector field on $\partial \mathcal{P}_\mu^{i,s,b}$ (in (42) it is $\widetilde{\mathbf{u}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}}$). The field $\mathbf{w}$ can be expressed as

$$\mathbf{w} = \frac{1}{|\partial \mathcal{P}_\mu^{i,s,b}|} \int_{\partial \mathcal{P}_\mu^{i,s,b}} \mathbf{w}\, d\partial\Omega_\mu + \widetilde{\mathbf{w}} = \langle \mathbf{w} \rangle + \widetilde{\mathbf{w}}, \quad (43)$$

where we have defined

$$\widetilde{\mathbf{w}} = \mathbf{w} - \langle \mathbf{w} \rangle. \quad (44)$$

Since $\mathbf{u}_\mu \in Kin_{\mathbf{u}_\mu}^{*,D}$, and using (43) for field $\widetilde{\mathbf{u}}_\mu^{*,D}|_{\partial \mathcal{P}_\mu^{i,s,b}}$, we have

$$\begin{aligned} \mathbf{u}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} - \mathbf{u}_\mu^{*,D} &= [(\mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) - \mathbf{u}_M^*|_{\mathbf{x}_i}) + (\langle \widetilde{\mathbf{u}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle - \langle \widetilde{\mathbf{u}}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle)] \\ &+ [\mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu) - \mathbf{G}_M^*|_{\mathbf{x}_i}](\mathbf{y} - \mathbf{y}_G)|_{\partial \mathcal{P}_\mu^{i,s,b}} \\ &+ \left[\widetilde{\widetilde{\mathbf{u}}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} - \widetilde{\widetilde{\mathbf{u}}}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}}\right] = \mathbf{0}, \end{aligned} \quad (45)$$

which implies

$$\mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu) - \mathbf{G}_M^*|_{\mathbf{x}_i} = \mathbf{O}, \tag{46}$$

$$(\mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) - \mathbf{u}_M^*|_{\mathbf{x}_i}) + (\langle \widetilde{\mathbf{u}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle - \langle \widetilde{\mathbf{u}}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle) = \mathbf{0}, \tag{47}$$

$$\widetilde{\widetilde{\mathbf{u}}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} - \widetilde{\widetilde{\mathbf{u}}}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}} = \mathbf{0}. \tag{48}$$

From (46), it follows that any element $\mathbf{u}_\mu \in Kin_{\mathbf{u}_\mu}^{*,D}$ is such that $\mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu) = \mathbf{G}_M^*|_{\mathbf{x}_i}$. However and from (47), $\mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) = \mathbf{u}_M^*|_{\mathbf{x}_i}$ if and only if $\langle \widetilde{\mathbf{u}}_\mu|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle = \langle \widetilde{\mathbf{u}}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}} \rangle$ (which is the case of the *reference solution* restricted to the microcell, $\mathbf{u}_\mu^*|_{\partial \mathcal{P}_\mu^{i,s,b}} \in Kin_{\mathbf{u}_\mu}^{*,D}$, among other fields in $Kin_{\mathbf{u}_\mu}^{*,D}$). As a consequence of the above considerations, it follows that the PMKA is not necessarily satisfied by all the elements of $Kin_{\mathbf{u}_\mu}^{*,D}$.

4.2 Traction boundary conditions on the microcell

The second approach to characterize the *reference solution* restricted to the isolated microcell is classical in mechanics and consists in the relaxation of the Dirichlet boundary condition given by $\mathbf{u}_\mu^{*,D}$ and replace it with the prescription of the associated (reactive) traction $\mathbf{t}_\mu^{*,i}$ as a Newmann problem. In this case, the linear manifold in which the solution is sought is $Kin_{\mathbf{u}_\mu}^{MKR}$, generated by the linear space $Var_{\widetilde{\mathbf{u}}_\mu}^{MKR}$ also satisfying $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{MKR}$ (see definitions in Appendix A). This is possible because the multiscale kinematical restrictions characterizing $Kin_{\mathbf{u}_\mu}^{MKR}$ are not of Dirichlet type and, hence, a traction field can be prescribed on the boundary. Then, the (exact) mechanical equilibrium of the isolated microcell $\mathcal{P}_\mu^i$ established by the variational equation (32) is now rewritten in the following (equivalent) form: *Find* $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{MKR}$ *such that the following variational equation holds,*

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu - \int_{\partial \mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \cdot \mathbf{v} \, d\partial\Omega_\mu = 0 \qquad \forall \mathbf{v} \in Var_{\widetilde{\mathbf{u}}_\mu}^{MKR}. \tag{49}$$

Let $\mathbf{\Theta}_\mu^*$ and $\mathbf{\Lambda}_\mu^*$ denote the Lagrange multipliers associated by duality with the two kinematical constraints included in $Kin_{\mathbf{u}_\mu}^{MKR}$. Then, the variational equilibrium equation (49) can be rewritten as

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu - \int_{\partial \mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \cdot \mathbf{v} \, d\partial\Omega_\mu - \mathbf{\Theta}_\mu^* \cdot \int_{\mathcal{P}_\mu^{i,s}} \mathbf{v} d\Omega_\mu - \mathbf{\Lambda}_\mu^* \cdot \int_{\partial \mathcal{P}_\mu^{i,s,b}} \mathbf{v} \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) d\partial\Omega_\mu = 0 \quad \forall \mathbf{v} \in \mathcal{V}_\mu. \tag{50}$$

The Euler-Lagrange equations satisfied in a weak sense by $\mathbf{u}^*_\mu$ restricted to $\mathcal{P}^{i,s}_\mu$ are then given by (see (33)-(36))

$$\underbrace{\operatorname{div}\mathbf{P}_\mu(\mathbf{u}^*_\mu)+\mathbf{b}_\mu}_{=\mathbf{0}\text{ from (33)}}+\boldsymbol{\Theta}^*_\mu=\mathbf{0}\text{ in }\mathcal{H}^{i,k}_\mu\ k=1,\dots,n_i, \tag{51}$$

$$[\![\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu]\!]=\mathbf{0}\text{ on }\partial\mathcal{H}^{i,k}_\mu\cap\partial\mathcal{H}^{i,m}_\mu, k\neq m, k,m=1,\dots,n_i, \tag{52}$$

$$\underbrace{\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu-\mathbf{t}^{*,i}_\mu}_{=\mathbf{0}\text{ from (35)}}-\boldsymbol{\Lambda}^*_\mu(\mathbf{n}_\mu-\overline{\mathbf{n}}_\mu)=\mathbf{0}\text{ on }\partial\mathcal{P}^{i,s,b}_\mu, \tag{53}$$

$$\mathbf{P}_\mu(\mathbf{u}^*_\mu)\mathbf{n}_\mu=\mathbf{0}\text{ on }\partial\mathcal{P}^{i,v}_\mu. \tag{54}$$

In addition, since the microcell is now completely unconstrained kinematically, we can take, in particular, $\mathbf{v}$ as an arbitrary constant vector field, $\mathbf{v}=\mathbf{c}\in\mathcal{V}_\mu$, $\mathbf{c}\in\mathbb{R}^{n_d}$, which yields (see (37))

$$\int_{\mathcal{P}^{i,s}_\mu}\mathbf{b}_\mu\,d\Omega_\mu+\int_{\partial\mathcal{P}^{i,s,b}_\mu}\mathbf{t}^{*,i}_\mu\,d\partial\Omega_\mu+\boldsymbol{\Lambda}^*_\mu\underbrace{\int_{\partial\mathcal{P}^{i,s,b}_\mu}(\mathbf{n}_\mu-\overline{\mathbf{n}}_\mu)\,d\partial\Omega_\mu}_{=\mathbf{0}\text{ from the definition of }\overline{\mathbf{n}}_\mu}=\mathbf{0}, \tag{55}$$

and, by taking $\mathbf{v}=\mathbf{A}(\mathbf{y}-\mathbf{y}_G)\in\mathcal{V}$, with an arbitrary constant $\mathbf{A}\in Lin$, we obtain (see (38))

$$\begin{aligned}\boldsymbol{\Lambda}^*_\mu\mathbf{B}_\mu &= \int_{\mathcal{P}^{i,s}_\mu}\mathbf{P}_\mu(\mathbf{u}^*_\mu|_{\mathcal{P}^{i,s}_\mu})d\Omega_\mu-\int_{\mathcal{P}^{i,s}_\mu}\mathbf{b}_\mu\otimes(\mathbf{y}-\mathbf{y}_G)\,d\Omega_\mu\\ &-\int_{\partial\mathcal{P}^{i,s,b}_\mu}\mathbf{t}^{*,i}_\mu\otimes(\mathbf{y}-\mathbf{y}_G)\,d\partial\Omega_\mu=\mathbf{O},\end{aligned} \tag{56}$$

where

$$\mathbf{B}_\mu=\int_{\partial\mathcal{P}^{i,s,b}_\mu}(\mathbf{n}_\mu-\overline{\mathbf{n}}_\mu)\otimes(\mathbf{y}-\mathbf{y}_G)\,d\partial\Omega_\mu, \tag{57}$$

is an invertible second order tensor.

Now, note that from (51) and (56) we obtain

$$\boldsymbol{\Theta}^*_\mu=\mathbf{0}, \tag{58}$$

$$\boldsymbol{\Lambda}^*_\mu=\mathbf{O}. \tag{59}$$

As a consequence of the above we obtain what we call the exact Minimal Kinematical Restriction Neumann Multiscale Model (MKR-N-$\mathbf{t}^*_\mu$ Model) since the reference (reaction) traction $\mathbf{t}^{*,i}_\mu$ is considered over the boundary $\partial\mathcal{P}^{i,s,b}_\mu$ as a dual counterpart to the prescription of the reference displacement field over the boundary, $\mathbf{u}^{*,D}_\mu$.

Remark 8 As expected, the MKR-N-$\mathbf{t}_\mu^*$ Multiscale Model also characterizes the *reference solution* $\mathbf{u}_\mu^*$ *restricted to the isolated microcell* $\mathcal{P}_\mu^i$. However, this is only possible if we know in advance $\mathbf{t}_\mu^{*,i}$, which is generally unknown in practice. Nevertheless, the above results give us the possibility of defining a new MKR Multiscale Model, referred to as MKR-N-$\mathbf{t}_\mu$ Model, in which the traction on the boundary is given by a traction field $\mathbf{t}_\mu$ that is generally different from $\mathbf{t}_\mu^{*,i}$, but satisfies the condition (37). Further, for this kind of traction $\mathbf{t}_\mu$ it is not difficult to show that we always have $\mathbf{\Theta}_\mu^{\mathbf{t}_\mu} = \mathbf{0}$ while, in general, $\mathbf{\Lambda}_\mu^{\mathbf{t}_\mu} \neq \mathbf{O}$. Hence, this last Lagrange multiplier can be used as an indicator of the quality of the adopted $\mathbf{t}_\mu$. The selection of an appropriate traction field $\mathbf{t}_\mu$ is an issue to be discussed and justified in the next section.

5 Novel multiscale models

In this section, we propose two novel multiscale models, named MKR-N Model and PMKA Model, that satisfy some of the properties of the *reference solution* when restricted to an isolated microcell, as shown in Section 4. The models proposed here feature, respectively, Neumann and Dirichlet boundary conditions.

To devise the new models, we will make use of the *Method of Multiscale Virtual Power* (see [37, 38, 47]). The first step here consists in defining the linear manifold Kin, of kinematically admissible displacements of the microcell satisfying the PMKA. This set together with the associated subspace of admissible virtual actions, Var, are fundamental in the definition/evaluation of the external and internal virtual powers to be used in the characterization of the equilibrium of the microcell through the PMVP (Principle of Multiscale Virtual Power).

Then, let $\mathbf{u}_M$ and $\mathbf{G}_M$ be, respectively, the displacement and displacement gradient fields in Ω_M, and let $\mathbf{u}_M|_{\mathbf{x}_i}$ and $\mathbf{G}_M|_{\mathbf{x}_i}$ be their values at the macroscale point $\mathbf{x}_i \in \Omega_M$, linked to the microcell $\mathcal{P}_\mu^i \in \Omega_\mu$.

The linear manifold $Kin_{\mathbf{u}_\mu}^D$, of kinematically admissible displacements of the microcell, is defined as

$$Kin_{\mathbf{u}_\mu}^D = \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathbf{u}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}^D\} = \mathbf{u}_\mu^0 + Var_{\mathbf{u}_\mu}^D, \tag{60}$$

where $\mathbf{u}_\mu^0$ is an arbitrary element of $Kin_{\mathbf{u}_\mu}^D$ and $\mathbf{u}^D$ is the field

$$\mathbf{u}^D(\mathbf{y}) = \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \mathbf{w}(\mathbf{y}), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b}, \tag{61}$$

with $\mathbf{w}$ such that $\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{w} \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)\, d\partial\Omega_\mu = \mathbf{O}$. Then, as shown in Section 4.1, all elements $\mathbf{u}_\mu \in Kin_{\mathbf{u}_\mu}^D$ satisfy $\mathcal{H}_\mu^{\mathcal{W}}(\nabla\mathbf{u}_\mu) = \mathbf{G}_M|_{\mathbf{x}_i}$. The subspace of virtual actions associated with $Kin_{\mathbf{u}_\mu}^D$ is

$$Var_{\mathbf{u}_\mu}^D = \{\mathbf{v} \in \mathcal{V}_\mu;\ \mathbf{v}|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{0}\}. \tag{62}$$

5.1 The MKR-N multiscale model

We start by devising the *MKR-N multiscale model* – a model for which a given traction field is prescribed on the boundary of the microcell, and whose equilibrium is defined as a Neumann problem. That is, in the MKR-N model, the microcell is subject to Neumann boundary conditions. As shown in Section 4.2, a model with prescribed microcell boundary tractions is built using the same linear manifold $Kin^{MKR}_{\mathbf{u}_\mu}$ as the classical Minimal Kinematic Restriction (MKR) Multiscale Model (refer to Appendices A and B for a detailed description of the MKR model):

$$\begin{aligned} Kin^{MKR}_{\mathbf{u}_\mu} &= \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) = \mathbf{u}_M|_{\mathbf{x}_i}, \mathcal{H}^{\mathcal{W}}_\mu(\nabla \mathbf{u}_\mu) = \mathbf{G}_M|_{\mathbf{x}_i}\} \\ &= \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathbf{u}_\mu = \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \widetilde{\mathbf{u}}_\mu, \\ &\quad \mathcal{H}^{\mathcal{V}}_\mu(\widetilde{\mathbf{u}}_\mu) = \mathbf{0}, \mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\widetilde{\mathbf{u}}_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu}) = \mathbf{O}\} \\ &= \mathbf{u}^0_\mu + Var^{MKR}_{\mathbf{u}_\mu}, \end{aligned} \tag{63}$$

where $\mathbf{u}^0_\mu$ is an arbitrary element of $Kin^{MKR}_{\mathbf{u}_\mu}$, and $Var^{MKR}_{\mathbf{u}_\mu}$ is given by

$$\begin{aligned} Var^{MKR}_{\mathbf{u}_\mu} &= \{\mathbf{v}_\mu \in \mathcal{V}_\mu;\ \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}) = \mathbf{0}, \mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\mathbf{v}|_{\partial\mathcal{P}^{i,s,b}_\mu}) = \mathbf{O}\} \\ &= Kin^{MKR}_{\widetilde{\mathbf{u}}_\mu} = Var^{MKR}_{\widetilde{\mathbf{u}}_\mu}. \end{aligned} \tag{64}$$

To take the interaction of $\mathcal{P}^i_\mu$ with its neighbors into account, let $\mathbf{t}^{MKR-N}_\mu$ be the traction prescribed on the boundary $\partial\mathcal{P}^{i,s,b}_\mu$. According to (37), the boundary traction must satisfy

$$\int_{\partial\mathcal{P}^{i,s,b}_\mu} \mathbf{t}^{MKR-N}_\mu \, d\partial\Omega_\mu = -\int_{\mathcal{P}^{i,s}_\mu} \mathbf{b}_\mu \, d\Omega_\mu. \tag{65}$$

The above property can be easily satisfied if $\mathbf{t}^{MKR-N}_\mu$ is taken as the uniform field

$$\mathbf{t}^{MKR-N}_\mu(\mathbf{y}) = -\frac{1}{|\partial\mathcal{P}^{i,s,b}_\mu|}\int_{\mathcal{P}^{i,s}_\mu} \mathbf{b}_\mu \, d\Omega_\mu, \quad \mathbf{y} \in \partial\mathcal{P}^{i,s,b}_\mu. \tag{66}$$

Alternatively, considering the property (35) satisfied by the traction $\mathbf{t}^*_\mu$ associated with the *reference solution* $\mathbf{u}^*_\mu$, we can choose a traction field distributed according to the material heterogeneities that reach the boundary. We can have, for example,

$$\mathbf{t}^{MKR-N}_\mu(\mathbf{y}) = -\frac{\alpha(\mathbf{y})}{\bar{\alpha}}\int_{\mathcal{P}^{i,s}_\mu} \mathbf{b}_\mu \, d\Omega_\mu, \quad \mathbf{y} \in \partial\mathcal{P}^{i,s,b}_\mu, \tag{67}$$

where

$$\alpha(\mathbf{y}) = |\mathbf{P}_\mu(\mathbf{G}_M|_{\mathbf{x}_i})\mathbf{n}_\mu(\mathbf{y})|, \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b}, \tag{68}$$

with $|\cdot|$ denoting the magnitude of vector $(\cdot)$, and

$$\bar{\alpha} = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \alpha(\mathbf{y})\, d\partial\Omega_\mu. \tag{69}$$

With the above at hand, we can now define the equilibrium problem of the microcell $\mathcal{P}_\mu^i$ for the MKR-N Multiscale Model.

***Problem* 1** (MKR-N Multiscale Model)**:** *Find* $\mathbf{u}_\mu^{i,MKR-N} \in Kin_{\mathbf{u}_\mu}^{MKR}$ *such that the following variational equation*

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^{i,MKR-N}) \cdot \nabla\mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{MKR-N} \cdot \mathbf{v}\, d\partial\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^{MKR}, \tag{70}$$

is satisfied.

From (65) it is not difficult to show (see Appendices A and B) that the Lagrange multiplier $\mathbf{\Theta}_\mu^{i,MKR-N}$, associated with the kinematical restriction $\mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{i,MKR-N}) = \mathbf{u}_M|_{\mathbf{x}_i}$, is always zero. This is not the case, however, for the other Lagrange multiplier, $\mathbf{\Lambda}_\mu^{i,MKR-N}$, arising from the kinematical restriction $\mathcal{H}_\mu^{\mathcal{W}}(\nabla\mathbf{u}_\mu^{i,MKR-N}) = \mathbf{G}_M|_{\mathbf{x}_i}$. Very importantly, for this reason, $\mathbf{\Lambda}_\mu^{i,MKR-N}$ can be used as an indicator of the quality of the solution $\mathbf{u}_\mu^{i,MKR-N}$, with respect to the *reference solution*. That is, $\mathbf{\Lambda}_\mu^{i,MKR-N}$ can provide a measure of distance between $\mathbf{u}_\mu^{i,MKR-N}$ and the reference solution. To see this, note that (see Appendix B) it is easy to show that

$$\mathbf{\Lambda}_\mu^{i,MKR-N}\mathbf{B}_\mu = \int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^{i,MKR-N}) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{i,MKR-N} \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu, \tag{71}$$

where $\mathbf{B}_\mu$ is defined in (57).

Since $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{MKR}$, note that, if $\mathbf{t}_\mu^{i,MKR-N} = \mathbf{t}_\mu^*$, then $\mathbf{\Lambda}_\mu^{i,MKR-N} = \mathbf{O}$ and $\mathbf{u}_\mu^{i,MKR-N} = \mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}}$. That is, under specific choices of boundary data, the MKR-N Multiscale Model is able to recover the *reference solution*.

5.2 The PMKA multiscale model

This section proposes another new multiscale model, which we will refer to as the *PMKA model*. Similarly to the MKR-N model devised in Section 5.1, the solution of the microcell equilibrium problem of the PMKA model shares some important properties with the *reference solution*. To devise the new model, we start by defining the corresponding linear manifold of kinematically admissible displacement fields of the microcell:

$$Kin^{PMKA}_{\mathbf{u}_\mu} = \{\mathbf{u}^\star_\mu \in \mathcal{V}_\mu;\ \mathbf{u}^\star_\mu = \mathbf{u}_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i},\ \mathbf{u}_\mu \in Kin^D_{\mathbf{u}_\mu}\}. \quad (72)$$

From this definition, we have that all elements of $Kin^{PMKA}_{\mathbf{u}_\mu}$ satisfy the Principle of Multiscale Kinematical Admissibility (PMKA) (see (39),(40)), as $\mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^\star_\mu) = \mathbf{u}_M|_{\mathbf{x}_i}$ and $\mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{u}^\star_\mu) = \mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{u}_\mu) = \mathbf{G}_M|_{\mathbf{x}_i}$ due to the fact that $\mathbf{u}_\mu \in Kin^D_{\mathbf{u}_\mu}$. Also note that the boundary $\partial\mathcal{P}^{i,s,b}_\mu$ is partially free to move. In fact, $\mathbf{u}^\star_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu} = \mathbf{u}_\mu|_{\partial\mathcal{P}^{is,b}_\mu} - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i} = \mathbf{u}^D - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i}$, i.e. the boundary moves $\mathbf{u}^D$ plus a translation. This observation is reflected on the space of admissible displacement variations associated with the above linear manifold, which is given by

$$Var^{PMKA}_{\mathbf{u}_\mu} = \{\mathbf{v}^\star \in \mathcal{V}_\mu;\ \mathbf{v}^\star = \mathbf{v} - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}), \mathbf{v} \in Var^D_{\mathbf{u}_\mu}\}, \quad (73)$$

hence, $\mathbf{v}^\star|_{\partial\mathcal{P}^{i,s,b}_\mu} = -\mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v})$. Further, it follows from (73) that the elements $\mathbf{v}^\star \in Var^{PMKA}_{\mathbf{u}_\mu}$ can be viewed as *fluctuation displacement fields* since they satisfy $\mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}^\star) = \mathbf{0}$ and $\mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{v}^\star) = \mathbf{O}$.

The PMKA multiscale model proposed here is built on the basis of the of the above definitions of $Kin^{PMKA}_{\mathbf{u}_\mu}/Var^{PMKA}_{\mathbf{u}_\mu}$. Note that, as a first step, the model required the selection of appropriate sets, Kin/Var, satisfying the PMKA to define the internal and external virtual powers in the formulation of the Principle of Multiscale Virtual Power (PMVP) and, hence, in the characterization of the microcell equilibrium problem.

At this point it is crucial to stress that, given $\mathbf{u}^\star_\mu \in Kin^{PMKA}_{\mathbf{u}_\mu}$, there exists $\mathbf{u}_\mu \in Kin^D_{\mathbf{u}_\mu}$ such that $\mathbf{u}^\star_\mu = \mathbf{u}_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i}$. Hence, $\mathbf{u}_\mu \in Kin^D_{\mathbf{u}_\mu}$ is the variable that actually drives the problem. The same observation is valid for $\mathbf{v}^\star \in Var^{PMKA}_{\mathbf{u}_\mu}$, and the corresponding $\mathbf{v} \in Var^D_{\mathbf{u}_\mu}$. Moreover, the two sets, $Kin^{PMKA}_{\mathbf{u}_\mu}$ and $Kin^D_{\mathbf{u}_\mu}$, are isomorphic under the transformation

$$\begin{aligned} f : Kin^D_{\mathbf{u}_\mu} &\to Kin^{PMKA}_{\mathbf{u}_\mu}, \\ \mathbf{u}_\mu &\mapsto \mathbf{u}^\star_\mu = \mathbf{u}_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i}. \end{aligned} \quad (74)$$

To see this, assume that for a given $\mathbf{u}^\star_\mu \in Kin^{PMKA}_{\mathbf{u}_\mu}$ there exist two elements $\mathbf{u}^1_\mu, \mathbf{u}^2_\mu \in Kin^D_{\mathbf{u}_\mu}$ such that

$$\mathbf{u}^\star_\mu = \mathbf{u}^1_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^1_\mu) + \mathbf{u}_M|_{\mathbf{x}^i} \quad (75)$$

$$\mathbf{u}^\star_\mu = \mathbf{u}^2_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^2_\mu) + \mathbf{u}_M|_{\mathbf{x}_i}. \quad (76)$$

Then,

$$\mathbf{0} = \mathbf{v} - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}), \quad \mathbf{v} \in Var^D_{\mathbf{u}_\mu}. \tag{77}$$

The above expression is satisfied only if $\mathbf{v} = \mathbf{c}$, with $\mathbf{c}$ an arbitrary constant vector field. Since $\mathbf{v} \in Var^D_{\mathbf{u}_\mu}$, the constant field $\mathbf{c}$ must be zero, and $\mathbf{u}^1_\mu = \mathbf{u}^2_\mu$.

As a consequence of the adopted kinematics it is possible to prescribe an arbitrary traction, say $\mathbf{t}_\mu$, on the solid boundary $\partial\mathcal{P}^{i,s,b}_\mu$ of the microcell for the PMKA model. The corresponding mechanical equilibrium problem for a microcell $\mathcal{P}^i_\mu$ is defined as: *Given a traction $\mathbf{t}_\mu$ defined on $\partial\mathcal{P}^{i,s,b}_\mu$, find $\mathbf{u}^{\star,PMKA}_\mu = \mathbf{u}^{D,PMKA}_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^{D,PMKA}_\mu) + \mathbf{u}_M|_{\mathbf{x}_i} \in Kin^{PMKA}_{\mathbf{u}_\mu}$ (with $\mathbf{u}^{D,PMKA}_\mu \in Kin^D_{\mathbf{u}_\mu}$) such that the following variational equation holds:*

$$\begin{aligned}&\int_{\mathcal{P}^{i,s}_\mu} [\mathbf{P}_\mu(\mathbf{u}^{\star,PMKA}_\mu) \cdot \nabla\mathbf{v}^\star - \mathbf{b}_\mu \cdot \mathbf{v}^\star] \, d\Omega_\mu \\ &- \int_{\partial\mathcal{P}^{i,s,b}_\mu} \mathbf{t}_\mu \cdot \mathbf{v}^\star \, d\partial\Omega_\mu = 0 \quad \forall \mathbf{v}^\star \in Var^{PMKA}_{\mathbf{u}_\mu}.\end{aligned} \tag{78}$$

Before going further, we need to check if the above equilibrium problem is well defined, i.e. if $\mathbf{t}_\mu$ is admissible. The admissibility is given by the condition obtained from the above equation with virtual actions restricted to the space $Var^{PMKA}_{\mathbf{u}_\mu} \cap \mathcal{N}(\nabla)$, where $\mathcal{N}(\nabla)$ is the null space (or kernel) of the operator ∇. Then, $\mathbf{t}_\mu$ is admissible if

$$\begin{aligned}&\int_{\mathcal{P}^{i,s}_\mu} \mathbf{b}_\mu \cdot \mathbf{v}^\star \, d\Omega_\mu + \int_{\partial\mathcal{P}^{i,s,b}_\mu} \mathbf{t}_\mu \cdot \mathbf{v}^\star \, d\partial\Omega_\mu = 0 \\ &\qquad\qquad \forall \mathbf{v}^\star \in Var^{PMKA}_{\mathbf{u}_\mu} \cap \mathcal{N}(\nabla).\end{aligned} \tag{79}$$

Since $\mathcal{N}(\nabla) = \{\mathbf{c} \in \mathbb{R}^3, \mathbf{c} \text{ arbitrary constant}\}$, we have $Var^{PMKA}_{\mathbf{u}_\mu} \cap \mathcal{N}(\nabla) = \{\mathbf{0}\}$ and the above condition is satisfied for any traction field $\mathbf{t}_\mu$ prescribed on $\partial\mathcal{P}^{i,s,b}_\mu$ and problem (78) is well defined.

Now, note that the variational equation (78) must hold for all $\mathbf{v}^\star \in Var^{PMKA}_{\mathbf{u}_\mu}$, which are vector fields satisfying the restrictions $\mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}^\star) = \mathbf{0}$ and $\mathcal{H}^{\mathcal{W}}_\mu(\nabla\mathbf{v}^\star) = \mathbf{O}$. These can be equally enforced by means of Lagrange multipliers. In this case, the restrictions of $Var^{PMKA}_{\mathbf{u}_\mu}$ are relaxed and (78) is re-written in the form:

$$\begin{aligned}&\int_{\mathcal{P}^{i,s}_\mu} [\mathbf{P}_\mu(\mathbf{u}^{\star,PMKA}_\mu) \cdot \nabla\mathbf{v}^\star - (\mathbf{b}_\mu + \boldsymbol{\Theta}^{PMKA}_\mu) \cdot \mathbf{v}^\star] \, d\Omega_\mu \\ &- \int_{\partial\mathcal{P}^{i,s,b}_\mu} [\mathbf{t}_\mu + \boldsymbol{\Lambda}^{PMKA}_\mu(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)] \cdot \mathbf{v}^\star \, d\partial\Omega_\mu = 0 \quad \forall \mathbf{v}^\star \in \mathcal{V}_\mu,\end{aligned} \tag{80}$$

where $\mathbf{\Theta}_{\mu}^{PMKA}$ and $\mathbf{\Lambda}_{\mu}^{PMKA}$ are the corresponding Lagrange multipliers. Equation (80) yields the following Euler-Lagrange equations and characterization of Lagrange multipliers:

$$\operatorname{div} \underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})} + \mathbf{b}_{\mu} + \mathbf{\Theta}_{\mu} = \mathbf{0} \text{ in } \mathcal{H}_{\mu}^{i,k}\ k = 1, \ldots, n_i, \tag{81}$$

$$[\![\underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})}\mathbf{n}_{\mu}]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_{\mu}^{i,k} \cap \partial\mathcal{H}_{\mu}^{i,m}, k \neq m, k, m = 1, \ldots, n_i, \tag{82}$$

$$\underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})}\mathbf{n}_{\mu} = \mathbf{t}_{\mu} + \mathbf{\Lambda}_{\mu}^{PMKA}(\mathbf{n}_{\mu} - \overline{\mathbf{n}}_{\mu}) \text{ on } \partial\mathcal{P}_{\mu}^{i,s,b}, \tag{83}$$

$$\underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})}\mathbf{n}_{\mu} = \mathbf{0} \text{ on } \partial\mathcal{P}_{\mu}^{i,v}, \tag{84}$$

$$\mathbf{\Theta}_{\mu}^{PMKA} = -\frac{1}{|\mathcal{P}_{\mu}^{i,s}|}\left[\int_{\mathcal{P}_{\mu}^{i,s}} \mathbf{b}_{\mu} d\Omega_{\mu} + \int_{\partial\mathcal{P}_{\mu}^{i,s,b}} \mathbf{t}_{\mu} d\partial\Omega_{\mu}\right], \tag{85}$$

$$\mathbf{\Lambda}_{\mu}^{PMKA}\mathbf{B}_{\mu} = \int_{\mathcal{P}_{\mu}^{i,s}} [\underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})} - \mathbf{b}_{\mu} \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_{\mu} - \int_{\partial\mathcal{P}_{\mu}^{i,s,b}} \mathbf{t}_{\mu} \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_{\mu}, \tag{86}$$

where $\mathbf{B}_{\mu}$ is the invertible tensor defined in (57).

From the above, it follows that the solution $\mathbf{u}_{\mu}^{\star,PMKA}$ of equation (80) satisfies the properties of the *reference solution* restricted to the microcell $\mathcal{P}_{\mu}^{i,s}$ (see (33)-(38)) if the prescribed boundary traction $\mathbf{t}_{\mu}$ satisfies

$$\int_{\partial\mathcal{P}_{\mu}^{i,s,b}} \mathbf{t}_{\mu} d\partial\Omega_{\mu} = -\int_{\mathcal{P}_{\mu}^{i,s}} \mathbf{b}_{\mu} d\Omega_{\mu}, \tag{87}$$

$$\int_{\partial\mathcal{P}_{\mu}^{i,s,b}} \mathbf{t}_{\mu} \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_{\mu} = \int_{\mathcal{P}_{\mu}^{i,s}} [\underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})} - \mathbf{b}_{\mu} \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_{\mu}. \tag{88}$$

Since (87) can be easily satisfied (see (66) or (67)), let us then assume that $\mathbf{t}_{\mu}$ indeed has this property. In this case, the above Euler-Lagrange equations read

$$\operatorname{div} \underbrace{\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{\star,PMKA})}_{=\mathbf{P}_{\mu}(\mathbf{u}_{\mu}^{D,PMKA})} + \mathbf{b}_{\mu} = \mathbf{0} \text{ in } \mathcal{H}_{\mu}^{i,k}\ k = 1, \ldots, n_i, \tag{89}$$

$$[\![\underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{\star,PMKA})}_{=\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})}\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_\mu^{i,k} \cap \partial\mathcal{H}_\mu^{i,m}, k \neq m, k, m = 1, \dots, n_i, \quad (90)$$

$$\underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{\star,PMKA})}_{=\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})}\mathbf{n}_\mu = \mathbf{t}_\mu + \mathbf{\Lambda}_\mu^{PMKA}(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \text{ on } \partial\mathcal{P}_\mu^{i,s,b}, \quad (91)$$

$$\underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{\star,PMKA})}_{=\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})}\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}_\mu^{i,v}, \quad (92)$$

$$\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu d\Omega_\mu + \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu d\partial\Omega_\mu = \mathbf{0}, \quad (93)$$

$$\mathbf{\Lambda}_\mu^{PMKA}\mathbf{B}_\mu = \int_{\mathcal{P}_\mu^{i,s}} [\underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{\star,PMKA})}_{=\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})} - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)]d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu. \quad (94)$$

Now, with the above traction field $\mathbf{t}_\mu$, we return to the variational equation (78) and rewritte it in terms of the driving variables:

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) \cdot \nabla\mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] \, d\Omega_\mu + \underbrace{\left[\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu \, d\Omega_\mu + \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \, d\partial\Omega_\mu\right]}_{=\mathbf{0} \text{ from (87)}} \cdot \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{v}) = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^D. \quad (95)$$

From (87) (or (93)), the above equation allows us to define the PMKA Multiscale Model.

***Problem* 2** (PMKA Multiscale Model)**:** *Find* $\mathbf{u}_\mu^{D,PMKA} \in Kin_{\mathbf{u}_\mu}^D$ *such that the following variational equation*

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) \cdot \nabla\mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] \, d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^D. \quad (96)$$

is satisfied.

It is not difficult to show that the Euler-Lagrange equations associated with the above variational equation are given by

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{b}_\mu = \mathbf{0} \text{ in } \mathcal{H}_\mu^{i,k} \; k = 1, \dots, n_i, \quad (97)$$

$$[\![\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_\mu^{i,k} \cap \partial\mathcal{H}_\mu^{i,m}, k \neq m, k, m = 1, \dots, n_i, \quad (98)$$

$$\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})\mathbf{n}_\mu = \mathbf{r}_\mu^D \text{ on } \partial\mathcal{P}_\mu^{i,s,b}, \quad (99)$$

$$\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}_\mu^{i,v}, \quad (100)$$

$$\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu d\Omega_\mu + \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D d\partial\Omega_\mu = \mathbf{0}, \quad (101)$$

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu, \quad (102)$$

where $\mathbf{r}_\mu^D \in \mathcal{V}'_\mu$ is the reactive traction vector associated by duality with the (Dirichlet) kinematical restriction prescribed on $\partial\mathcal{P}_\mu^{i,s,b}$.

Now, we introduce the above properties of the field $\mathbf{u}_\mu^{D,PMKA}$ in the Euler-Lagrange equations (89)-(94). This gives

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{b}_\mu = \mathbf{0} \text{ in } \mathcal{H}_\mu^{i,k} \; k = 1, \ldots, n_i, \quad (103)$$

$$[\![\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_\mu^{i,k} \cap \partial\mathcal{H}_\mu^{i,m}, k \neq m, k, m = 1, \ldots, n_i, \quad (104)$$

$$\mathbf{r}_\mu^D - \mathbf{t}_\mu = \mathbf{\Lambda}_\mu^{PMKA}(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \text{ on } \partial\mathcal{P}_\mu^{i,s,b}, \quad (105)$$

$$\mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA})\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}_\mu^{i,v}, \quad (106)$$

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D d\partial\Omega_\mu = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu d\partial\Omega_\mu, \quad (107)$$

$$\mathbf{\Lambda}_\mu^{PMKA}\mathbf{B}_\mu = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu. \quad (108)$$

From (105) we have that, if $\mathbf{t}_\mu \to \mathbf{r}_\mu^D$ then, the reactive component associated with the Lagrange multiplier vanishes, that is $\mathbf{\Lambda}_\mu^{PMKA}(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \to \mathbf{0}$. Moreover, from (108) we obtain that, if $\int_{\partial\mathcal{P}_\mu^{i,s,b}}(\mathbf{r}_\mu^D - \mathbf{t}_\mu) \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu \to \mathbf{O}$, then $\mathbf{\Lambda}_\mu^{PMKA} \to \mathbf{O}$.

Before closing the present section, we apply the PMKA Model to a problem that, in contrast to the case studied above, does not depend exclusively on the gradient of the solution. To this end, consider the following equilibrium problem: *Find* $\mathbf{u}_\mu^{\star,PMKA} = \mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i} \in Kin_{\mathbf{u}_\mu}^{PMKA}$ *(with* $\mathbf{u}_\mu^{D,PMKA} \in Kin_{\mathbf{u}_\mu}^D$*) such that*

$$\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{K}_\mu \mathbf{u}_\mu^{\star,PMKA} \cdot \mathbf{v}^\star + \mathbf{P}_\mu(\mathbf{u}_\mu^{\star,PMKA}) \cdot \nabla\mathbf{v}^\star - \mathbf{b}_\mu \cdot \mathbf{v}^\star] \, d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \cdot \mathbf{v}^\star \, d\partial\Omega_\mu = 0 \quad \forall \mathbf{v}^\star \in Var_{\mathbf{u}_\mu}^{PMKA}, \quad (109)$$

where $\mathbf{K}_\mu$ *is a symmetric positive definite second order tensor field.*

Proceeding in a similar way as before, the above variational equation for the variable $\mathbf{u}_\mu^{D,PMKA} \in Kin_{\mathbf{u}_\mu}^D$ and its variations $\mathbf{v} \in Var_{\mathbf{u}_\mu}^D$ takes the form

$$\begin{aligned} \int_{\mathcal{P}_\mu^{i,s}} \big[\mathbf{K}_\mu(\mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}) \cdot \mathbf{v} \\ + \mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}\big] \, d\Omega_\mu \\ + \Bigg[\int_{\mathcal{P}_\mu^{i,s}} \big[\mathbf{K}_\mu(\mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}) - \mathbf{b}_\mu\big] \, d\Omega_\mu \\ - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \, d\partial\Omega_\mu \Bigg] \cdot \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{v}) = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^D, \end{aligned} \tag{110}$$

As before, by taking $\mathbf{t}_\mu = \mathbf{r}_\mu^D$ – now satisfying

$$\begin{aligned} \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \, d\partial\Omega_\mu = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D \, d\partial\Omega_\mu = \\ \int_{\mathcal{P}_\mu^{i,s}} \big[\mathbf{K}_\mu(\mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}) - \mathbf{b}_\mu\big] \, d\Omega_\mu \end{aligned} \tag{111}$$

– the variable $\mathbf{u}_\mu^{D,PMKA} \in Kin_{\mathbf{u}_\mu}^D$ is expressed as the solution of the variational equation

$$\begin{aligned} \int_{\mathcal{P}_\mu^{i,s}} \big[\mathbf{K}_\mu(\mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}) \cdot \mathbf{v} + \\ + \mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}\big] \, d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^D, \end{aligned} \tag{112}$$

and, in addition, we find that the traction vector $\mathbf{t}_\mu$ prescribed on the boundary satisfies

$$\begin{aligned} \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu \otimes (\mathbf{y} - \mathbf{y}_G) \, d\partial\Omega_\mu = \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{r}_\mu^D \otimes (\mathbf{y} - \mathbf{y}_G) \, d\partial\Omega_\mu = \\ = \int_{\mathcal{P}_\mu^{i,s}} \mathbf{P}_\mu(\mathbf{u}_\mu^{D,PMKA}) \, d\Omega_\mu + \\ + \int_{\mathcal{P}_\mu^{i,s}} \mathbf{K}_\mu(\mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}) \otimes (\mathbf{y} - \mathbf{y}_G) \, d\Omega_\mu \\ - \int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G) \, d\Omega_\mu. \end{aligned} \tag{113}$$

At this point, it is worth highlighting the following points:

- For the PMKA Multiscale Model, the solution of the mechanical equilibrium problem of the microcell subject to a prescribed traction $\mathbf{t}_\mu = \mathbf{r}_\mu^D$ on the boundary is $\mathbf{u}_\mu^{\star,PMKA} = \mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i} \in Kin_{\mathbf{u}_\mu}^{PMKA}$

where $\mathbf{u}_\mu^{D,PMKA} \in Kin_{\mathbf{u}_\mu}^D$ is the solution of an appropriate (Dirichlet) variational equation (see for example (96) or (112)). Recall that $\mathbf{r}_\mu^D$ is the reactive traction vector associated by duality with the kinematical prescription of $\mathbf{u}^D$ over the microcell boundary. Further, note that $\mathbf{u}_\mu^{\star,PMKA}$ is endowed with some properties of the *reference solution*, i.e. the Lagrange multipliers $\boldsymbol{\Theta}_\mu^{PMKA}$ and $\boldsymbol{\Lambda}_\mu^{PMKA}$ are both zero.

- The solution $\mathbf{u}_\mu^{\star,PMKA}$ is such that, when restricted to an isolated microcell $\mathcal{P}_\mu^i$, it takes the value $\mathbf{u}_\mu^{\star,PMKA}|_{\partial\mathcal{P}_\mu^{i,s.b}} = \mathbf{u}^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}$ on the boundary $\partial\mathcal{P}_\mu^{i,s.b}$. This has two major implications: (i) the mechanical equilibrium of the microcell using the MKR-N Multiscale Model with prescribed traction field $\mathbf{t}_\mu = \mathbf{r}_\mu^D$ on the boundary is exactly $\mathbf{u}_\mu^{\star,PMKA}$; (ii) if a new Dirichlet problem is defined by prescribing a displacement $\mathbf{u}^{D-New} = \mathbf{u}^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}$, then $\mathbf{u}_\mu^{\star,PMKA} \in Kin_{\mathbf{u}_\mu}^{D-New}$ and, hence, the solution of this new Dirichlet problem is exactly given by $\mathbf{u}_\mu^{\star,PMKA}$. These are important properties of the *reference solution* (see Section 4).

6 Multicontinuum approach to the full-scale problem

Following the discussion presented in the previous sections, this section proposes the use of a multiscale framework based on the MKR-N and PMKA models as a multicontinuum approach for the computation of the *reference solution*, $\mathbf{u}_\mu^*$, of the full-scale equilibrium problem. As discussed in Section 4, the equilibrium problems defined by the MKR-N and PMKA multiscale models are able to deliver, under specific conditions, the *reference solution* $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^i}$ within each microcell. In addition, as seen in Section 5, the MKR-N and PMKA models can improve the solution obtained with the MKR model when the *reference solution* is not known. The idea here is to explore these properties of the two multiscale models to devise a procedure that can approach the *reference solution* at low computational cost.

Now, let us invert the perspective and, instead of the bottom-up (micro-to-macro) approach considered so far, let us take a top-down (macro-to-micro) approach. Let $\mathbf{x}_i$ be the point at macro level associated with the microcell $\mathcal{P}_\mu^i$ and let $\mathcal{N}_{\mathbf{x}_i} = \{\mathbf{x}_j, j \in I^i\}$ be the set of points associated with the microcells $\mathcal{P}_\mu^j$ that surround $\mathcal{P}_\mu^i$ (see (11)). As a result of the homogenization inherent to the multiscale approach, for all $\mathbf{x}_j \in \mathcal{N}_{\mathbf{x}_i}$, we have

$$\mathbf{u}_M|_{\mathbf{x}_j} = \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{x}_j - \mathbf{x}_i) + o(|\mathbf{x}_j - \mathbf{x}_i|^2), \tag{114}$$

where $o(\cdot)$ denotes a term of the order of $(\cdot)$. Here we shall assume that $\mathbf{G}_M$ varies smoothly. We also assume that the points $\mathbf{x}_j$ are such that $|\mathbf{x}_j - \mathbf{x}_i| = o(l(\mathcal{P}_\mu^i))$, where $l(\mathcal{P}_\mu^i)$ denotes the characteristic length of the microcell $\mathcal{P}_\mu^i$, here assumed very small when compared to the characteristic length of the macro-scale (refer to Section 3). With $l(\mathcal{P}_\mu^i)$ sufficiently small so that terms of order $o(|\mathbf{x}_j - \mathbf{x}_i|)$ can be neglected, the previous expressions yield

$$\mathbf{u}_M|_{\mathbf{x}_j} = \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{x}_j - \mathbf{x}_i), \tag{115}$$

Let $\mathbf{u}_\mu^{i,MKR}$ be the solution of the equilibrium problem of microcell $\mathcal{P}_\mu^i$ using the MKR model (see Appendices A and B). Then, from the above considerations, it is expected that

$$\mathbf{u}_\mu^{i,MKR}(\mathbf{y}) \approx \mathbf{u}_\mu^{j,MKR}(\mathbf{y}), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b} \cap \partial\mathcal{P}_\mu^{j,s,b}, j \in I^i, \tag{116}$$

with the difference between $\mathbf{u}_\mu^{i,MKR}(\mathbf{y})$ and $\mathbf{u}_\mu^{j,MKR}(\mathbf{y})$ stemming from the discrepancy between the fluctuations $\widetilde{\mathbf{u}}_\mu^{i,MKR}(\mathbf{y})$ and $\widetilde{\mathbf{u}}_\mu^{j,MKR}(\mathbf{y})$, $\mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b} \cap \partial\mathcal{P}_\mu^{j,s,b}$, $j \in I^i$. Note that this discrepancy can be seen as a jump discontinuity in the solution on the boundaries of neighboring microcells.

To reduce this discontinuity let us first define a continuous vector-valued function over the boundary $\partial\mathcal{P}_\mu^{i,s,b}$,

$$\mathbf{d}(\mathbf{u}_\mu^{i,MKR}(\mathbf{y}), \mathbf{u}_\mu^{j,MKR}(\mathbf{y})), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b} \cap \partial\mathcal{P}_\mu^{j,s,b}, \quad j \in I^i, \tag{117}$$

satisfying the property

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{d}(\mathbf{u}_\mu^{i,MKR}(\mathbf{y}), \mathbf{u}_\mu^{j,MKR}(\mathbf{y})) \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)\, d\partial\Omega_\mu = \mathbf{O}, \tag{118}$$

and such that the following displacement on the boundary

$$\begin{aligned}\mathbf{u}^D(\mathbf{y}) &= \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \widetilde{\mathbf{u}}_\mu^{i,MKR}(\mathbf{y}) \\ &\quad + \mathbf{d}(\mathbf{u}_\mu^{i,MKR}(\mathbf{y}), \mathbf{u}_\mu^{j,MKR}(\mathbf{y})),\end{aligned} \tag{119}$$

reduces the displacement discrepancy between the microcell $\mathcal{P}_\mu^i$ and its neighbors.

Then, we use the boundary displacement field $\mathbf{u}^D$ of (119) to define the linear manifold $Kin_{\mathbf{u}_\mu}^{PMKA}$. With $Kin_{\mathbf{u}_\mu}^{PMKA}$ defined this way, the solution of the equilibrium problem of the microcell $\mathcal{P}_\mu^i$ using the PMKA model, given by $\mathbf{u}_\mu^{\star,PMKA} = \mathbf{u}_\mu^{D,PMKA} - \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu^{D,PMKA}) + \mathbf{u}_M|_{\mathbf{x}_i}$, can be obtained. This PMKA solution is such that the discontinuity of the displacement between the microcell $\mathcal{P}_\mu^i$ and its neighbors is reduced.

It should be noted, however, that the PMKA solution above does not in general lead to continuity of boundary tractions on the interface between $\mathcal{P}_\mu^i$ and its neighboring microcells. In fact, there will be generally a jump in the traction field at such interfaces. That is,

$$\underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{i,\star,PMKA})\mathbf{n}_\mu}_{\mathbf{t}_\mu^i} \neq \underbrace{\mathbf{P}_\mu(\mathbf{u}_\mu^{j,\star,PMKA})\mathbf{n}_\mu}_{-\mathbf{t}_\mu^j} \quad \text{on } \partial\mathcal{P}_\mu^{i,s,b} \cap \partial\mathcal{P}_\mu^{j,s,b}, j \in I^i. \tag{120}$$

To reduce the traction discontinuity, we shall adopt an analogous approach to that proposed above to address the displacement discontinuity – now using an appropriate MKR-N model with the traction $\mathbf{t}_\mu^N$ defined as follows. We define a vector-valued function over the microcell boundary,

$$\mathbf{j}(\mathbf{t}_\mu^i(\mathbf{y}), \mathbf{t}_\mu^j(\mathbf{y})), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b} \cap \partial\mathcal{P}_\mu^{j,s,b}, j \in I^i, \tag{121}$$

with the property

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{j}(\mathbf{t}_\mu^i(\mathbf{y}), \mathbf{t}_\mu^j(\mathbf{y})) d\partial\Omega_\mu = \mathbf{0}, \tag{122}$$

and such that the prescribed boundary traction

$$\mathbf{t}_\mu^N(\mathbf{y}) = \mathbf{t}_\mu^i(\mathbf{y}) + \mathbf{j}(\mathbf{t}_\mu^i(\mathbf{y}), \mathbf{t}_\mu^j(\mathbf{y})), \quad \mathbf{y} \in \partial\mathcal{P}_\mu^{i,s,b}, \tag{123}$$

reduces the boundary traction discrepancy between the microcell $\mathcal{P}_\mu^i$ and its neighbors.

Remark 9 Note that the operators $\mathbf{d}$ and $\mathbf{j}$ introduced in (117) and (121) have not yet been defined. These operators are at the core of the cyclic iterative procedure. If they are linear operators, then properties (119) and (123) can be trivially satisfied by construction. In such a case, linear combination of the arguments leads to sub/over relaxation approaches, and we are in the realm of Gauss-Jacobi (or Gauss-Seidel) methods. More involved situations can be envisaged if we considered Krylov methods to generate updates in the displacement and/or traction fields (see also Remark 11).

Based on the above considerations, a cyclic iterative process can be proposed where displacements and tractions are alternately enforced on the regions of the microcell boundary shared with its neighbors using, respectively, the PMKA and MKR-N models. In Figure 2 we illustrate the idea of the proposed multiscale method as a strategy to exchange boundary data between neighboring microcells within a divide and conquer paradigm.

Such iterative procedure generates a sequence of solutions which, is expected to converge to a solution where both displacements and tractions have no jumps on the microcell boundaries. For more about the convergence and alternative strategies, see Remark 9.

Let us assume now that finite element discretizations of the macro- and micro-continuum equilibrium variational problems are adopted to produce approximate solutions, and the partitions into finite elements are sufficiently fine to ensure that the approximate solutions of the corresponding variational equilibrium equations are accurate enough. These solutions will be denoted

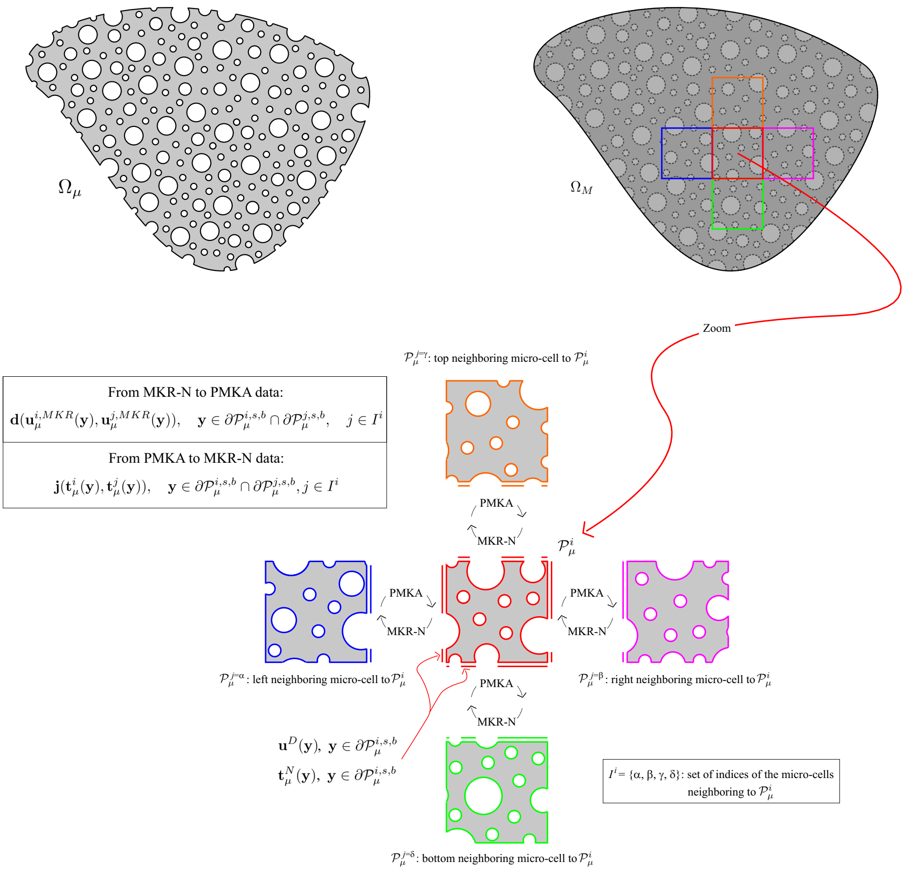

Fig. 2 Illustration of boundary data exchange between PMKA and MKR-N multiscale models for neighboring microcells.

$\mathbf{u}_M^{\star,h_M}$ and $\mathbf{u}_\mu^{\star,h_\mu}$ respectively. Note that in general, the computation of the full-scale finite element solution $\mathbf{u}_\mu^{\star,h_\mu}$ in a monolithic manner is generally not feasible for realistic problems at present, even with the help high performance computers. We also consider that the macro-continuum partition into micro-cells is performed over a finite element mesh built at micro level in such a way that the finite element domains are never crossed by the boundaries of the microcells, $\partial\mathcal{P}_\mu^i, i = 1, \ldots, N_\mu$. In other words, we are restricted to conformal finite element meshes for $\mathcal{P}_\mu^i$ and their neighbors $\mathcal{P}_\mu^j, j \in I^i$. Also, we assume that the partition of the macro domain into finite elements must be such that each integration point $\mathbf{x}_i$ of the macro-scale finite elements at macro level is associated with a microcell $\mathcal{P}_\mu^i$.

Then, we propose the following iterative algorithm based on the alternate application of the PMKA and MKR-N multiscale models to obtain $\mathbf{u}_\mu^{\star,h_\mu}$. For the sake of notation, the superscripts h_M and h_μ are suppressed in what follows.

Multiscale Algorithm
for the computation of the *reference solution* $\mathbf{u}^*_\mu$

- STEP 1. Using the MKR multiscale model find the homogenized constitutive operator, $\mathfrak{C}_M$, at each macro-scale finite element integration point $\mathbf{x}_i$.
- STEP 2. Solve the macroscale variational equilibrium (19) to get $\mathbf{u}^\star_M$ and $\mathbf{G}^\star_M$ at any point $\mathbf{x} \in \Omega_M$.
- STEP 3. For $i = 1, \dots, N_\mu$ do
  - For the microcell $\mathcal{P}^i_\mu$, solve the MKR multiscale model using $\mathbf{u}^\star_M|_{\mathbf{x}_i}$ and $\mathbf{G}^\star_M|_{\mathbf{x}_i}$ as input, which amounts to finding the solution $\mathbf{u}^i_\mu$ (and hence the fluctuation $\widetilde{\mathbf{u}}^i_\mu$) of the variational equilibrium equation (B8).
- STEP 4. Set the iteration number, $N_{\text{iter}} = 1$.
- STEP 5. **Application of the PMKA model**:
  - Set ContDispl = TRUE
  - For each microcell $\mathcal{P}^i_\mu, i = 1, \dots, N_\mu$ do
    * Evaluate $\mathbf{d}$ (see (117)).
    * Evaluate $|\mathbf{d}| = [\int_{\partial\mathcal{P}^{i,s,b}_\mu} (\mathbf{d} \cdot \mathbf{d}) \, d\partial\Omega_\mu]^{\frac{1}{2}}$.
    * Evaluate $|\mathbf{u}^i_\mu| = [\int_{\partial\mathcal{P}^{i,s,b}_\mu} (\mathbf{u}^i_\mu \cdot \mathbf{u}^i_\mu) \, d\partial\Omega_\mu]^{\frac{1}{2}}$.
    * Evaluate $e^i_D = \frac{|\mathbf{d}|}{|\mathbf{u}^i_\mu|}$.
    * Displacement continuity control: If $e^i_D > e_D$ (e_D a user defined tolerance)
      Then:
      · Set ContDispl = FALSE
      · Evaluate $\mathbf{u}^D$ (see (119)) .
      · With $\mathbf{u}^D$ define the PMKA model and find its solution $\mathbf{u}^{\star,PMKA}_\mu = \mathbf{u}^{i,S}_\mu - \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}^{i,S}_\mu) + \mathbf{u}^\star_M|_{\mathbf{x}_i}$, where $\mathbf{u}^{i,S}_\mu$ is given by Problem 2, i.e. equation (96) (or any other corresponding variational equation), and the (reactive) traction $\mathbf{t}^i_\mu$ on $\partial\mathcal{P}^{i,s,b}_\mu$.

      Else: continue.
- STEP 6. **Application of the MKR-N model**:
  - Set NullJump = TRUE
  - For each microcell $\mathcal{P}^i_\mu, i = 1, \dots, N_\mu$ do
    * Evaluate $\mathbf{j}$ (see (121)).
    * Evaluate $|\mathbf{j}| = [\int_{\partial\mathcal{P}^{i,s,b}_\mu} (\mathbf{j} \cdot \mathbf{j}) \, d\partial\Omega_\mu]^{\frac{1}{2}}$.
    * Evaluate $|\mathbf{t}^i_\mu| = [\int_{\partial\mathcal{P}^{i,s,b}_\mu} (\mathbf{t}^i_\mu \cdot \mathbf{t}^i_\mu) \, d\partial\Omega_\mu]^{\frac{1}{2}}$.
    * Evaluate $e^i_N = \frac{|\mathbf{j}|}{|\mathbf{t}^i_\mu|}$
    * Traction jump control. If $e^i_N > e_N$ (e_N a user-defined tolerance)
      Then:

· Make NullJump = FALSE
· Evaluate $\mathbf{t}_\mu^N(\mathbf{y})$ (see (123)).
· With $\mathbf{t}_\mu^N$ and using the MKR-N model find the solution $\mathbf{u}_\mu^{i,MKR-N}$ of Problem 1, i.e. the variational equilibrium equation (70).
· Set $\mathbf{u}_\mu^i = \mathbf{u}_\mu^{i,MKR-N}$.

Else : continue.

- STEP 7. If ContDispl= TRUE and NullJump = TRUE or $N_{\text{iter}} \geq$ MaxNiter Then: END
  Else: Set $N_{\text{iter}} = N_{\text{iter}} + 1$ and go to STEP 5.

Remark 10 STEP 5 mitigates the displacement discontinuity while STEP 6 mitigates the traction discontinuity on the boundary of neighboring microcells.

Now, we compare the computational cost, $\mathcal{C}_{DNS}$, of the evaluation of the *reference solution* addressing the full-scale problem (often referred to as a direct numerical simulation, or DNS solution) with the computational cost, $\mathcal{C}_{MSA}$, of the solution obtained with the proposed multicontinuum strategy based on the multiscale paradigm. To do this let us introduce the following notations

- $\mathsf{N_{el}}_M$ denotes the number of finite elements used for the solution at macroscale,
- $\mathsf{N_{eq}}_M$ denotes the number of equations associated to the solution at macroscale,
- $\mathsf{N_{el}}_\mu$ denotes the number of finite elements used for the computation of the *reference solution* using DNS (the full-scale solution),
- $\mathsf{N_{eq}}_\mu$ denotes the number of equations to be solved for the evaluation of the *reference solution* using DNS,
- $\mathsf{N_{el}}_{\mathcal{P}_\mu^i}$, $i = 1, \ldots, N_\mu$ denotes the number of finite elements used for the solution of the equilibrium corresponding to the isolated microcell $\mathcal{P}_\mu^i$ using the MKR together with the PMKA and MKR-N multiscale models,
- $\mathsf{N_{eq}}_{\mathcal{P}_\mu^i}$, $i = 1, \ldots, N_\mu$ denotes the number of equations associated to the solution of the equilibrium of the isolated microcell $\mathcal{P}_\mu^i$ using the MKR together with the PMKA and MKR-N multiscale models.

Now let $\mathcal{C}(\mathsf{N_{eq}})$ be the computational cost associated to the solution of $\mathsf{N_{eq}}$ equations which we assume here to be of the order of $o({\mathsf{N_{eq}}}^2)$ (optimistic estimate using preconditioned iterative methods for solving the corresponding algebraic systems of equations). We also assume that the number of equations to be solved at each $\mathcal{P}_\mu^i$, $\mathsf{N_{eq}}_{\mathcal{P}_\mu^i}$, is the same for all $i = 1, \ldots, N_\mu$. Hence, the number of equations $\mathsf{N_{eq}}_\mu$ associated to the DNS approach is

$$\mathsf{N_{eq}}_\mu = \sum_{i=1}^{N_\mu} \mathsf{N_{eq}}_{\mathcal{P}_\mu^i} = N_\mu \times \mathsf{N_{eq}}_{\mathcal{P}_\mu^i}. \tag{124}$$

Then, the expected computational cost $\mathcal{C}_{DNS}$ is

$$\mathcal{C}_{DNS} = o(\mathsf{N_{eq}}_\mu^2) \approx N_\mu^2 \times o(\mathsf{N_{eq}}_{\mathcal{P}_\mu^i}^2). \tag{125}$$

In turn, disregarding the computational cost of macro level solution, the computational cost associated with the proposed $\mathcal{C}_{MSA}$ algorithm is

$$\mathcal{C}_{MSA} \approx (2 \times N_{\text{iter}} + 1) \times N_\mu \times o(\mathsf{N_{eq}}_{\mathcal{P}_\mu^i}^2). \tag{126}$$

The comparison between the computational costs (125) and (126) gives the ratio

$$\frac{\mathcal{C}_{DNS}}{\mathcal{C}_{MSA}} \approx \frac{N_\mu}{(2 \times N_{\text{iter}} + 1)}, \tag{127}$$

which in is general a very large number if the number of iterations to achieve convergence remains bounded.

Remark 11 The proposed algorithm can be understood as a sort of Dirichlet (PMKA) and Neumann (MKR-N) exchange between neighboring microcells. In this regard, this is a sort of Gauss-Jacobi (or Gauss-Seidel) iterative procedure, where convergence only occurs if certain conditions are satisfied. These conditions depend on the stiffness of the neighboring microcell mechanical problems. Situations where neighboring microcell domains contain materials with substantially different mechanical properties, or neighboring microcells with significantly different sizes could harm convergence. One general strategy to mitigate this is to add sub-relaxation, as commented above, but the sub-relaxation parameter may depend on the specific problem and boundary conditions [54]. Another approach is to rely on iterative procedures which are more powerful than Gauss-Jacobi-type methods. Alternative algorithms such as Newton methods, or matrix-free versions of the GMRES approach can be very helpful in addressing more challenging scenarios [53].

7 Final Remarks

An in-depth analysis of the mechanical equilibrium problem for a solid continuum featuring small scale heterogeneities was presented, based on the Principle of Multiscale Virtual Power previously proposed by the authors. The analysis revealed important properties of the *reference solution* – the exact solution of the problem accounting for all small scale heterogeneities – leading to generalisations of the classical Minimum Kinematical Restriction multiscale model where displacement or traction boundary conditions may be enforced on the boundary of the microcell. The framework provided by the new models led naturally to the proposal of a new, multicontinuum strategy to search for the reference solution at low computational cost in an iterative fashion. The proposed new strategy consists in first solving a coarsened equilibrium problem (defining a macro- or coarse scale) weakly coupled to the microscale domains – the microcells. The material points of the coarse scale model are linked to given microcells that describe the heterogeneities of the body under consideration. Then, once the weakly coupled problem is solved, an iterative algorithm is used to reduce the discontinuities in the displacement and traction fields at the interfaces between neighboring microcells through the alternate solution of suitably formulated Dirichlet (PMKA model) and Neumann (MKR-N model) problems. The reference solution is retrieved if all such discontinuities vanish. Finally, we remark that the present work lays the foundations of a continuum counterpart of a domain decomposition approach, with all the potential generalizations brought about by the Method of Multiscale Virtual Power.

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Conflict of Interest. Not Applicable

Appendix A The MKR multiscale model

According to [37, 38, 47], a kinematically admissible displacement $\mathbf{u}_\mu \in \mathcal{V}_\mu$ is characterized by the Minimal Kinematical Restriction multiscale model (MKR model), which satisfies the Principle of Multiscale Kinematical Admissibility. This implies that the following relations are satisfied: $\mathbf{u}_M|_{\mathbf{x}_i} = \mathcal{H}^{\mathcal{V}}_\mu(\mathbf{u}_\mu)$ and $\mathbf{G}_M|_{\mathbf{x}_i} = \mathcal{H}^{\mathcal{W}}_\mu(\nabla \mathbf{u}_\mu)$, leading to the kinematical restrictions

$$\mathcal{H}^{\mathcal{V}}_\mu(\widetilde{\mathbf{u}}_\mu) = \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\mathcal{P}^{i,s}_\mu} \widetilde{\mathbf{u}}_\mu \, d\Omega_\mu = \mathbf{0}, \tag{A1}$$

$$\begin{aligned}
\mathcal{H}^{\mathcal{W}}_\mu(\nabla\widetilde{\mathbf{u}}_\mu) &= \frac{1}{|\mathcal{P}^{i,s}_\mu|}\Bigg[\int_{\mathcal{P}^{i,s}_\mu} \nabla\widetilde{\mathbf{u}}_\mu \, d\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,v_i}_\mu} \widetilde{\mathbf{u}}_\mu \otimes \mathbf{n}^{v_i}_\mu \, d\partial\Omega_\mu \\
&\quad - \int_{\partial\mathcal{P}^{i,s,v_b}_\mu} \widetilde{\mathbf{u}}_\mu \otimes \mathbf{n}^{v_b}_\mu \, d\partial\Omega_\mu - \int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}_\mu \otimes \overline{\mathbf{n}}_\mu \, d\partial\Omega_\mu\Bigg] \\
&= \frac{1}{|\mathcal{P}^{i,s}_\mu|}\int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}_\mu \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \, d\partial\Omega_\mu \\
&= \mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\widetilde{\mathbf{u}}_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu}) = \mathbf{O}.
\end{aligned} \tag{A2}$$

Then, the kinematically admissible displacements for the MKR model live in the linear manifold $Kin_{\mathbf{u}_\mu}^{MKR}$ characterized by

$$\begin{aligned} Kin_{\mathbf{u}_\mu}^{MKR} &= \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{u}_\mu) = \mathbf{u}_M|_{\mathbf{x}_i}, \mathcal{H}_\mu^{\mathcal{W}}(\nabla \mathbf{u}_\mu) = \mathbf{G}_M|_{\mathbf{x}_i}\} \\ &= \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathbf{u}_\mu = \mathbf{u}_M|_{\mathbf{x}_i} + \mathbf{G}_M|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \widetilde{\mathbf{u}}_\mu, \\ &\quad \mathcal{H}_\mu^{\mathcal{V}}(\widetilde{\mathbf{u}}_\mu) = \mathbf{0}, \mathcal{H}_{\mu,\partial\mathcal{P}_\mu^{i,s,b}}^{\mathcal{W}}(\widetilde{\mathbf{u}}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}}) = \mathbf{O}\} \\ &= \mathbf{u}_\mu^0 + Var_{\widetilde{\mathbf{u}}_\mu}^{MKR}, \end{aligned} \tag{A3}$$

where $\mathbf{u}_\mu^0$ is an arbitrary element of $Kin_{\mathbf{u}_\mu}^{MKR}$, and $Var_{\widetilde{\mathbf{u}}_\mu}^{MKR}$ is given by

$$Var_{\widetilde{\mathbf{u}}_\mu}^{MKR} = \{\mathbf{v}_\mu \in \mathcal{V}_\mu;\ \mathcal{H}_\mu^{\mathcal{V}}(\mathbf{v}) = \mathbf{0}, \mathcal{H}_{\mu,\partial\mathcal{P}_\mu^{i,s,b}}^{\mathcal{W}}(\mathbf{v}|_{\partial\mathcal{P}_\mu^{i,s,b}}) = \mathbf{O}\}. \tag{A4}$$

Appendix B Principle of Multiscale Virtual Power

The energetic consistency between scales is satisfied through the formulation of the Principle of Multiscale Virtual Power (PMVP). This balance of power between macro and micro-scales was originally proposed in [9, 11] through the so-called Hill-Mandel principle of Macrohomogeneityt, which was claimed to hold for the true powers exerted at both scales. In [37, 38, 47], the PMVP was postulated by re-casting the Hill-Mandel principle in a variational setting.

The PMVP applied to the isolated microcell $\mathcal{P}_\mu^i$ within the context of the MKR Model, is given by

$$\begin{aligned} \mathbf{P}_M|_{\mathbf{x}_i} \cdot \widehat{\mathbf{G}}_M|_{\mathbf{x}_i} &- \mathbf{b}_M|_{\mathbf{x}_i} \cdot \widehat{\mathbf{u}}_M|_{\mathbf{x}_i} = \\ &= \frac{1}{|\mathcal{P}_\mu^i|}\Bigg[\int_{\mathcal{P}_\mu^{i,s}} (\mathbf{P}_\mu(\mathbf{u}_\mu) \cdot (\widehat{\mathbf{G}}_M|_{\mathbf{x}_i} + \nabla \mathbf{v}) \\ &- \mathbf{b}_\mu \cdot (\widehat{\mathbf{u}}_M|_{\mathbf{x}_i} + \widehat{\mathbf{G}}_M|_{\mathbf{x}_i}(\mathbf{y} - \mathbf{y}_G) + \mathbf{v}))\Bigg] d\Omega_\mu, \\ &\forall\ (\widehat{\mathbf{u}}_M|_{\mathbf{x}_i}, \widehat{\mathbf{G}}_M|_{\mathbf{x}_i}, \mathbf{v}) \in \mathbb{R}_{\mathcal{V}_M}^{\mathbf{x}_i} \times \mathbb{R}_{\mathcal{W}_M}^{\mathbf{x}_i} \times Var_{\widetilde{\mathbf{u}}_\mu}^{MKR}. \end{aligned} \tag{B5}$$

By using standard variational arguments, (B5) yields

- $\mathbf{P}_M|_{\mathbf{x}_i}$-Homogenization $((\mathbf{0}, \forall \widehat{\mathbf{G}}_M|_{\mathbf{x}_i}, \mathbf{0}) \in \mathbb{R}_{\mathcal{V}_M}^{\mathbf{x}_i} \times \mathbb{R}_{\mathcal{W}_M}^{\mathbf{x}_i} \times Var_{\widetilde{\mathbf{u}}_\mu}^{MKR})$

$$\mathbf{P}_M|_{\mathbf{x}_i} = \frac{1}{|\mathcal{P}_\mu^i|}\left[\int_{\mathcal{P}_\mu^{i,s}} (\mathbf{P}_\mu(\mathbf{u}_\mu) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G))\, d\Omega_\mu\right]. \tag{B6}$$

- $\mathbf{b}_M|_{\mathbf{x}_i}$-Homogenization $((\forall \widehat{\mathbf{u}}_M|_{\mathbf{x}_i}, \mathbf{O}, \mathbf{0}) \in \mathbb{R}_{\mathcal{V}_M}^{\mathbf{x}_i} \times \mathbb{R}_{\mathcal{W}_M}^{\mathbf{x}_i} \times Var_{\widetilde{\mathbf{u}}_\mu}^{MKR})$

$$\mathbf{b}_M|_{\mathbf{x}_i} = \frac{1}{|\mathcal{P}_\mu^i|}\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu\, d\Omega_\mu. \tag{B7}$$

- Equilibrium of the isolated microcell $\mathcal{P}^i_\mu$ given by the following variational problem: *Find* $\mathbf{u}^i_\mu \in Kin^{MKR}_{\mathbf{u}_\mu}$ *(or equivalent find* $\widetilde{\mathbf{u}}^i_\mu \in Var^{MKR}_{\widetilde{\mathbf{u}}_\mu}$*) such that satisfies the following variational equation*

$$\int_{\mathcal{P}^{i,s}_\mu} [\mathbf{P}_\mu(\mathbf{u}^i_\mu) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var^{MKR}_{\widetilde{\mathbf{u}}_\mu}. \tag{B8}$$

Let $\mathbf{\Theta}^{MKR}_\mu$ and $\mathbf{\Lambda}^{MKR}_\mu$ be the Lagrange multipliers corresponding to the kinematical restrictions $\mathcal{H}^{\mathcal{V}}_\mu(\mathbf{v}) = \mathbf{0}$ and $\mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\mathbf{v}|_{\partial\mathcal{P}^{i,s,b}_\mu}) = \mathbf{O}$ in $Var^{MKR}_{\widetilde{\mathbf{u}}_\mu}$, then the above variational problem can be rewritten as follows: *Given* $\mathbf{u}_M|_{\mathbf{x}_i}$ *and* $\mathbf{G}_M|_{\mathbf{x}_i}$ *find* $\widetilde{\mathbf{u}}^i_\mu \in \mathcal{V}_\mu$, $\mathbf{\Theta}^{MKR}_\mu \in \mathbb{R}^{\mathbf{x}_i}_{\mathcal{V}_M}$ *and* $\mathbf{\Lambda}^{MKR}_\mu \in \mathbb{R}^{\mathbf{x}_i}_{\mathcal{W}_M}$ *such that satisfy the following variational equation*

$$\begin{aligned}
&\int_{\mathcal{P}^{i,s}_\mu} [\mathbf{P}_\mu(\mathbf{u}^i_\mu) \cdot \nabla \mathbf{v} - (\mathbf{b}_\mu + \mathbf{\Theta}^{MKR}_\mu) \cdot \mathbf{v}] d\Omega_\mu \\
&- \mathbf{\Lambda}^{MKR}_\mu \cdot \int_{\partial\mathcal{P}^{i,s,b}_\mu} \mathbf{v} \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)\, d\partial\Omega_\mu \\
&- \widehat{\mathbf{\Theta}}^{MKR}_\mu \cdot \int_{\mathcal{P}^{i,s}_\mu} \widetilde{\mathbf{u}}^i_\mu \, d\Omega_\mu - \widehat{\mathbf{\Lambda}}^{MKR}_\mu \cdot \int_{\partial\mathcal{P}^{i,s,b}_\mu} \widetilde{\mathbf{u}}^i_\mu \otimes (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu)\, d\partial\Omega_\mu = 0, \\
&\forall (\widehat{\mathbf{\Theta}}^{MKR}_\mu, \widehat{\mathbf{\Lambda}}^{MKR}_\mu, \mathbf{v}) \in \mathbb{R}^{\mathbf{x}_i}_{\mathcal{V}_M} \times \mathbb{R}^{\mathbf{x}_i}_{\mathcal{W}_M} \times \mathcal{V}_\mu.
\end{aligned} \tag{B9}$$

The Euler-Lagrange equations associated with the above variational equilibrium problem are given by

$$\mathcal{H}^{\mathcal{V}}_\mu(\widetilde{\mathbf{u}}^i_\mu) = \mathbf{0}, \tag{B10}$$

$$\mathcal{H}^{\mathcal{W}}_{\mu,\partial\mathcal{P}^{i,s,b}_\mu}(\widetilde{\mathbf{u}}^i_\mu|_{\partial\mathcal{P}^{i,s,b}_\mu}) = \mathbf{O}, \tag{B11}$$

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}^i_\mu) + \mathbf{b}_\mu + \mathbf{\Theta}^{MKR}_\mu = \mathbf{0} \text{ in } \mathcal{H}^{i,k}_\mu \; k = 1, \ldots, n_i, \tag{B12}$$

$$[\![\mathbf{P}_\mu(\mathbf{u}^i_\mu)\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}^{i,k}_\mu \cap \partial\mathcal{H}^{i,m}_\mu, k \neq m, k, m = 1, \ldots, n_i, \tag{B13}$$

$$\mathbf{P}_\mu(\mathbf{u}^i_\mu)\mathbf{n}_\mu = \mathbf{\Lambda}^{MKR}_\mu(\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \text{ on } \partial\mathcal{P}^{i,s,b}_\mu, \tag{B14}$$

$$\mathbf{P}_\mu(\mathbf{u}^i_\mu)\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}^{i,v}_\mu. \tag{B15}$$

Since (B9) must be satisfied for all $\mathbf{v} \in \mathcal{V}_\mu$ and in particular for an arbitrary constant vector $\mathbf{v} = \mathbf{c}$, we obtain an additional Euler-Lagrange equation characterizing the Lagrange multiplier $\mathbf{\Theta}^{MKR}_\mu \in \mathbb{R}^{\mathbf{x}_i}_{\mathcal{V}_M}$

$$\mathbf{\Theta}^{MKR}_\mu = -\frac{1}{|\mathcal{P}^{i,s}_\mu|} \int_{\mathcal{P}^{i,s}_\mu} \mathbf{b}_\mu d\Omega_\mu. \tag{B16}$$

Furthermore, considering variations of the form $\mathbf{v} = \mathbf{A}(\mathbf{y} - \mathbf{y}_G)$ characterized by any constant second order tensor $\mathbf{A} \in Lin$, we also obtain

$$
\mathbf{A} \cdot \left[\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^i) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu \right.
$$

$$
\left. - \boldsymbol{\Lambda}_\mu^{MKR} \int_{\partial \mathcal{P}_\mu^{i,s,b}} (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu \right] = 0 \quad \forall \mathbf{A} \in Lin. \qquad \text{(B17)}
$$

From the above expression we obtain the Euler-Lagrange equation that characterizes the Lagrange multiplier $\boldsymbol{\Lambda}_\mu^{MKR}$

$$
\boldsymbol{\Lambda}_\mu^{MKR} \mathbf{B}_\mu = \int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^i) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu, \qquad \text{(B18)}
$$

where $\mathbf{B}_\mu$ is given by

$$
\mathbf{B}_\mu = \int_{\partial \mathcal{P}_\mu^{i,s,b}} (\mathbf{n}_\mu - \overline{\mathbf{n}}_\mu) \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu. \qquad \text{(B19)}
$$

For the previous developments, spaces $\mathbb{R}_{\mathcal{V}_M}^{\mathbf{x}_i}$ and $\mathbb{R}_{\mathcal{W}_M}^{\mathbf{x}_i}$ depend on the spatial dimension of the problem. For three dimensional problems, we have $\mathbb{R}_{\mathcal{V}_M}^{\mathbf{x}_i} \to \mathbb{R}^3$ and $\mathbb{R}_{\mathcal{W}_M}^{\mathbf{x}_i} \to \mathbb{R}^{3\times 3}$.

Appendix C Isolated microcell equilibrium

The equilibrium of the isolated microcell $\mathcal{P}_\mu^i$ submitted to the prescribed displacement $\mathbf{u}_\mu^{*,D}$ at the boundary $\partial\mathcal{P}_\mu^{i,s,b}$ and to a force system given by $\{\mathbf{b}_\mu\}$ is characterized by the following variational problem: *Find* $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in Kin_{\mathbf{u}_\mu}^{*,D}$ *such that satisfies the following variational equation*

$$
\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu = 0 \quad \forall \mathbf{v} \in Var_{\mathbf{u}_\mu}^{*,D}, \qquad \text{(C20)}
$$

where

$$
Kin_{\mathbf{u}_\mu}^{*,D} = \{\mathbf{u}_\mu \in \mathcal{V}_\mu;\ \mathbf{u}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D}\} = \mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} + Var_{\mathbf{u}_\mu}^{*,D}, \qquad \text{(C21)}
$$

and

$$
Var_{\mathbf{u}_\mu}^{*,D} = \{\mathbf{v} \in \mathcal{V}_\mu;\ \mathbf{v}|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{0}\}. \qquad \text{(C22)}
$$

The variational problem (C20) can be redefined by relaxing the kinematical restriction $\mathbf{u}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D}$. This procedure leads to the following equivalent variational problem: *Find* $\mathbf{u}_\mu^*|_{\mathcal{P}_\mu^{i,s}} \in \mathcal{V}_\mu$ *such that satisfies the following variational equation*

$$
\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) \cdot \nabla \mathbf{v} - \mathbf{b}_\mu \cdot \mathbf{v}] d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \cdot \mathbf{v} d\partial\Omega_\mu
$$

$$-\int_{\partial\mathcal{P}_\mu^{i,s,b}} \hat{\mathbf{t}}_\mu \cdot (\mathbf{u}_\mu^*|_{\partial\mathcal{P}_\mu^{i,s,b}} - \mathbf{u}_\mu^{*,D}) d\partial\Omega_\mu = 0$$
$$\forall (\mathbf{v}, \hat{\mathbf{t}}_\mu) \in \mathcal{V}_\mu \times \mathcal{V}'_\mu(\partial\mathcal{P}_\mu^{i,s,b}), \qquad \text{(C23)}$$

where $\mathbf{t}_\mu^{*,i}$ is the (Lagrange multiplier) vector traction field over $\partial\mathcal{P}_\mu^{i,s,b}$ associated by duality with the kinematical restriction $\mathbf{u}_\mu|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D}$, and $\hat{\mathbf{t}}_\mu$ is its virtual variation.

The Euler-Lagrange equations associated to the variational problem (C23) are given by

- Taking $\mathbf{v} = \mathbf{0}$ and for all $\hat{\mathbf{t}}_\mu \in \mathcal{V}'_\mu$ we have

$$\mathbf{u}_\mu^*|_{\partial\mathcal{P}_\mu^{i,s,b}} = \mathbf{u}_\mu^{*,D} \text{ on } \partial\mathcal{P}_\mu^{i,s,b}. \qquad \text{(C24)}$$

- Taking $\hat{\mathbf{t}}_\mu = \mathbf{0}$ and for all $\mathbf{v} \in \mathcal{V}_\mu$ we have

$$\operatorname{div} \mathbf{P}_\mu(\mathbf{u}_\mu^*) + \mathbf{b}_\mu = \mathbf{0} \text{ in } \mathcal{H}_\mu^{i,k} \; k = 1, \ldots, n_i, \qquad \text{(C25)}$$
$$[\![\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu]\!] = \mathbf{0} \text{ on } \partial\mathcal{H}_\mu^{i,k} \cap \partial\mathcal{H}_\mu^{i,m}, k \neq m, k, m = 1, \ldots, n_i, \qquad \text{(C26)}$$
$$\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu = \mathbf{t}_\mu^{*,i} \text{ on } \partial\mathcal{P}_\mu^{i,s,b}, \qquad \text{(C27)}$$
$$\mathbf{P}_\mu(\mathbf{u}_\mu^*)\mathbf{n}_\mu = \mathbf{0} \text{ on } \partial\mathcal{P}_\mu^{i,v}, \qquad \text{(C28)}$$

Now, since (C23) must be satisfied for all $\mathbf{v} \in \mathcal{V}_\mu$, it particularly holds for any arbitrary constant vector field $\mathbf{v} = \mathbf{c}$. Then, it results

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} d\partial\Omega_\mu = -\int_{\mathcal{P}_\mu^{i,s}} \mathbf{b}_\mu d\Omega_\mu. \qquad \text{(C29)}$$

Also, (C23) must be satisfied for all fields of the form $\mathbf{v} = \mathbf{A}(\mathbf{y} - \mathbf{y}_G)$ characterized by any constant second order tensor $\mathbf{A} \in Lin$. Then

$$\mathbf{A} \cdot \left[\int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu - \int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu \right] = 0 \quad \forall \mathbf{A} \in Lin. \qquad \text{(C30)}$$

From the above expression we obtain

$$\int_{\partial\mathcal{P}_\mu^{i,s,b}} \mathbf{t}_\mu^{*,i} \otimes (\mathbf{y} - \mathbf{y}_G) d\partial\Omega_\mu = \int_{\mathcal{P}_\mu^{i,s}} [\mathbf{P}_\mu(\mathbf{u}_\mu^*) - \mathbf{b}_\mu \otimes (\mathbf{y} - \mathbf{y}_G)] d\Omega_\mu. \qquad \text{(C31)}$$

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