Received: 9 March 2022 | Revised: 20 May 2022 | Accepted: 23 May 2022

DOI: 10.1002/zamm.202200091

ZAMM

EDITOR'S CHOICE

Stress average rule derived through the principle of virtual power

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Funding information
H2020 Marie Skłodowska-Curie Actions, Grant/Award Number: 764691

Stress and strain average rules are the key conceptual pillars of the wide field of continuum micromechanics of materials. The aforementioned rules express that the spatial average of (micro-)stress and (micro-)strain fields throughout a microscopically finite representative volume element (RVE) are equal to the (macro-)stress and (macro-)strain values associated with the corresponding macroscopically infinitesimal volume element (macroscopic material point). According to the famous contribution of Hashin, stress and strain average rules are derived from equilibrium and compatibility conditions, together with (micro-)displacement and (micro-)traction boundary conditions associated with homogeneous (macro-)strains and (macro-)stresses, respectively. However, as, strictly speaking, only displacements *or* tractions can be described at the boundary, the remaining average rule turns out as a mere definition. We here suggest a way to do without such a definition, by resorting to the principle of virtual power (PVP) as a means to guarantee mechanical equilibrium: at the boundary of the RVE, we prescribe virtual (micro-)velocities, which are linked to arbitrary, but homogeneous virtual (macro-)velocities and (macro-)strain rates, while the latter are also linked, in a multilinear fashion, with the microscopic virtual strain rate fields inside the RVE. Considering, under these conditions, equivalence of the macroscopic and the microscopic expressions for the virtual power densities of the internal and the external forces yields the well-known stress average rule and, in case of microscopically uniform force fields, a volume force average rule. The same strategy applied to an RVE hosting single forces between atomistic mass points, readily yields the macroscopic "internal virial stress tensor."

1 | INTRODUCTION—MOTIVATION AND SCOPE

Composite material mechanics [1, 2], also referred to as continuum micromechanics [3], is a very successful and versatile branch of continuum mechanics. It describes the mechanical behavior of a representative volume element (RVE) of matter, coinciding with the infinitesimal volume of classical continuum mechanics, but being considered, at the same time, as a finite volume at the microscopic scale, see Figure 1a. Stresses and strains are introduced both at the microscopic and at

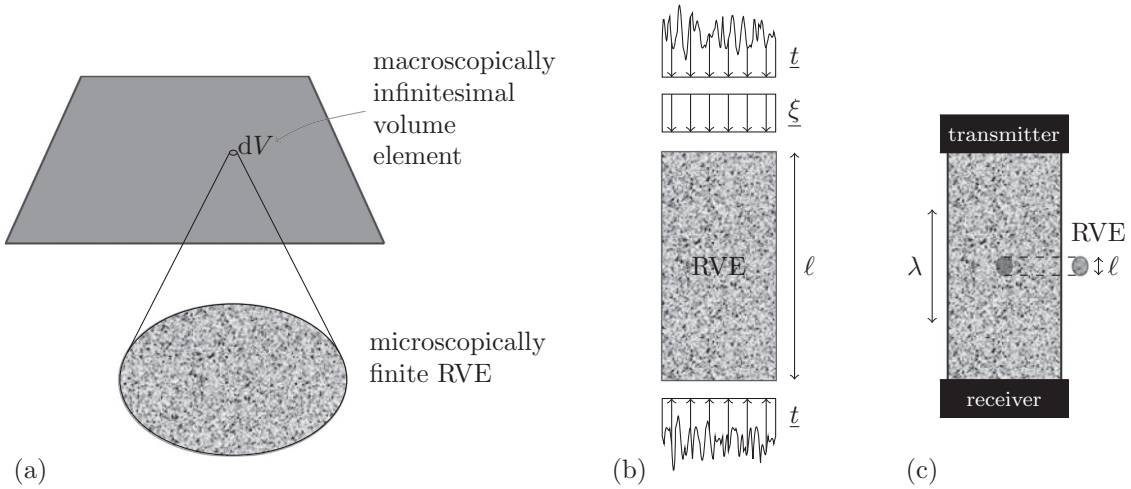

FIGURE 1 Different characteristics of the representative volume element (RVE): (a) scale separation between structural scale and material scale; (b) RVE coinciding with samples undergoing a classical mechanical test [6]; (c) RVE not coinciding with a sample undergoing an ultrasonic test with wavelength λ [3, 7, 8]

the macroscopic level, and their relation is governed by average rules. Hashin [4, 5] considered fields of microstrains and microstresses depending on a microscopic location variable $\underline{x}$, so that the strain and stress average rules read as

$$\mathbf{E} = \frac{1}{V_{\mathrm{RVE}}} \int_{V_{\mathrm{RVE}}} \boldsymbol{\varepsilon}(\underline{x}) \, \mathrm{d}V(\underline{x}) \,, \tag{1}$$

$$\boldsymbol{\Sigma} = \frac{1}{V_{\mathrm{RVE}}} \int_{V_{\mathrm{RVE}}} \boldsymbol{\sigma}(\underline{x}) \, \mathrm{d}V(\underline{x}) \,, \tag{2}$$

with $\boldsymbol{\varepsilon}$ standing for the linearized microscopic strain tensor, $\boldsymbol{\sigma}$ standing for the microscopic Cauchy stress tensor, $\mathbf{E}$ denoting for the microscopic linearized strain tensor, $\boldsymbol{\Sigma}$ denoting the macroscopic Cauchy stress tensor, and V_{RVE} denoting the volume of the RVE. All the mathematical symbols and abbreviations used in the present paper are summarized in Table 1. Hashin [4, 5] showed that—in case of kinematically compatible microstrains, and of equilibrated microstresses in the absence of body forces, respectively—the relations (1) and (2) imply the following boundary conditions for the RVE:

$$\underline{\xi}(\underline{x}) = \mathbf{E} \cdot \underline{x} \,, \qquad \forall \underline{x} \in S_{\mathrm{RVE}} \,, \tag{3}$$

$$\underline{t}(\underline{x}) = \boldsymbol{\Sigma} \cdot \underline{n}(\underline{x}) \,, \qquad \forall \underline{x} \in S_{\mathrm{RVE}} \,, \tag{4}$$

with $\underline{\xi}$ as microdisplacements, $\underline{t}$ as micro-tractions, $\underline{n}$ as outward-oriented unit normal vector, and S_{RVE} as the surface of the RVE. Accordingly, Equations (3) and (4) are standardly referred to as the "Hashin boundary conditions" [2]. It should be noted that the rules (1) and (2) are normally applied simultaneously, and since the boundary conditions (3) and (4) cannot be applied simultaneously to one and the same RVE, the "Hashin boundary conditions" are less convincing than they might appear on first sight. In other words, one of the rules (1) and (2) needs to remain a definition, whenever the other one has been formulated on the basis of equilibrium or compatibility considerations. A very pragmatic way out of this somewhat unsatisfactory solution was proposed by Hori and Nemat-Nasser [6] by considering the RVE as a (presumably cuboidal or cylindrical) macroscopic sample undergoing a mechanical test, see Figure 1b. Hori and Nemat-Nasser consider the surface integrals over micro-tractions and micro-displacements as "natural quantities" arising from such a

TABLE 1 Mathematical symbols and abbreviations

$\mathbb{A}_d$	=	virtual-strain-rate-related concentration tensor
d	=	size of microheterogeneity
$\mathbf{d}$	=	microscopic actual Eulerian strain rate tensor
$\check{\mathbf{d}}$	=	microscopic virtual Eulerian strain rate tensor
$\mathbf{D}$	=	macroscopic actual Eulerian strain rate tensor
$\check{\mathbf{D}}$	=	macroscopic virtual Eulerian strain rate tensor
$\mathbf{E}$	=	macroscopic strain acting on the RVE
$\underline{e}_i$	=	orthonormal base vector
$\underline{f}$	=	microscopic volume force
$\underline{f}_i^{int}$	=	internal force acting on mass point i
$\underline{F}$	=	macroscopic volume force
$\underline{g}$	=	gravitational acceleration field
G_ρ	=	microscopic Gibbs potential per unit mass
$\mathbb{I}$	=	symmetric fourth-order identity tensor
ℓ	=	characteristic length of the RVE
$\mathcal{L}$	=	structural length
$\underline{n}$	=	outward-oriented unit normal vector on the surface of the RVE
$\mathcal{P}$	=	virtual power
$\mathcal{P}^{[ext,int]}$	=	virtual power of external and internal forces, respectively
PVP	=	principle of virtual power
RVE	=	representative volume element
S	=	surface of a (macroscopic) volume V
S_{RVE}	=	surface of the RVE
$\underline{t}$	=	microscopic surface force (traction vector)
$\underline{T}$	=	macroscopic surface force (traction vector)
V	=	macroscopic volume
$\underline{\check{v}}$	=	microscopic virtual velocity
$\underline{\check{V}}$	=	macroscopic virtual velocity
V_{RVE}	=	volume of the RVE
$\underline{x}$	=	microscopic position vector with origin at the center of gravity of the RVE
$\underline{\tilde{x}}$	=	microscopic position vector measured from an arbitrary origin
$\underline{\tilde{x}}_{CG}$	=	position of the center of gravity of the RVE from an arbitrary origin
$\underline{X}$	=	macroscopic position vector
x_i	=	ith component of microscopic position vector
$\underline{x}_i$	=	microscopic position vector of mass point i
λ	=	wavelength of ultrasonic test
$\pi^{[ext,int]}$	=	virtual power of the external and internal forces, respectively
ρ	=	microscopic mass density
$\boldsymbol{\sigma}$	=	microscopic stress tensor
$\dot{\boldsymbol{\sigma}}$	=	partial temporal derivative of microscopic stress tensor
$\boldsymbol{\Sigma}$	=	macroscopic stress acting on the RVE
$\underline{\xi}$	=	microscopic displacement vector
$\boldsymbol{\omega}$	=	spin tensor
div_x	=	microscopic divergence with respect to variable $\underline{x}$
grad_x	=	microscopic gradient with respect to variable $\underline{x}$
GRAD_X	=	macroscopic gradient with respect to variable $\underline{X}$

(Continues)

TABLE 1 (Continued)

grad_x^S	=	symmetrized microsopic gradient with respect to variable $\underline{x}$
$\bullet^T$	=	transpose operator, acting on second-order tensor as $\bullet_{ij}^T = \bullet_{ji}$
$\cdot$	=	dot product or contraction product
:	=	double contraction product
$\times$	=	cross product
$\|\| \bullet \|\|$	=	Euclidean norm
$\|\|\| \bullet \|\|\|$	=	third-order norm
$\otimes$	=	dyadic product

mechanical test. By means of micro-stress equilibrium and micro-strain compatibility, respectively, the aforementioned surface integrals are then transformed into volume integrals over stress and strain, giving way to the average rules (1) and (2). However, there are cases where the tested sample does not coincide with the RVE: in the context of ultrasonic test with different frequencies [7, 8], the size ℓ of the RVE is governed by the wavelength λ, that is, [3]: $\ell \ll \lambda$, see Figure 1c. This situation goes beyond the reasoning of Hori and Nemat-Nasser [6].

Hence, we consider the derivation of strain and stress average rules governing simultaneously the behavior of an RVE as a topic of on-going interest. In this context, we here aim at preserving the conceptual beauty of Hashin's geometrical boundary conditions leading to Equation (1), while looking for a simultaneously open rigorous way to derive Equation (2) from a fundamental principle of continuum mechanics. In more detail, we employ the principle of virtual power (PVP) as stated by Germain [9] in 1973: a mechanical system is in equilibrium if the power performed by the external and internal forces on any virtual velocity field characterizing the aforementioned system, vanishes. After recalling this principle for a standard macroscopic continuum mechanical system, we employ it for a microscopically finite RVE playing the role of an infinitesimal volume element at the macroscopic level (see Section 2). Thereafter, we link the microscopic virtual velocity field to the virtual quantities governing the macroscopically infinitesimal volume element, that is, velocity and strain rate tensor (see Section 3). Next, the implications for computational homogenization in atomistic systems and continuum RVEs undergoing large deformations are discussed (see Section 4). The paper is concluded by setting our derivation in context to somehow related deliberations in the rich field of micromechanics (Section 5).

2 | PRINCIPLE OF VIRTUAL POWER APPLIED TO A CONTINUUM MECHANICS SYSTEM AND ITS MICROSTRUCTURALLY REPRESENTATIVE VOLUME ELEMENTS

The PVP states that a mechanical system is in equilibrium if, for any virtual motion $\check{\underline{V}}$ defining the type of mechanical system considered, the virtual power of forces associated with the mechanical system vanishes [9, 10],

$$\mathcal{P}(\check{\underline{V}}) = 0\,, \tag{5}$$

with the virtual power $\mathcal{P}$ being a multilinear form on $\check{\underline{V}}$. In the case of classical continuum mechanics under quasistatic conditions, the principle (5) takes the form [9, 10],

$$\mathcal{P}^{ext}[\check{\underline{V}}(\underline{X})] + \mathcal{P}^{int}[\check{\mathbf{D}}(\underline{X})] = 0\,, \tag{6}$$

with the virtual power of external forces $\mathcal{P}^{ext}$, the virtual power of internal forces $\mathcal{P}^{int}$, with $\check{\underline{V}}(\underline{X})$ being any three-dimensional continuous vector field across all (macroscopic) points $\underline{X}$ of the continuum with volume V and surface S, and with $\check{\mathbf{D}}(\underline{X})$ as the (macroscopic) virtual Eulerian strain rate tensor, mathematically reading as

$$\check{\mathbf{D}}(\underline{X}) = \frac{1}{2}\left\{\frac{\partial \check{\underline{V}}}{\partial \underline{X}}(\underline{X}) + \left[\frac{\partial \check{\underline{V}}}{\partial \underline{X}}(\underline{X})\right]^T\right\} = \frac{1}{2}\left\{\text{GRAD}_X\,\check{\underline{V}}(\underline{X}) + \left[\text{GRAD}_X\,\check{\underline{V}}(\underline{X})\right]^T\right\} = \text{GRAD}_X^S\,\check{\underline{V}}(\underline{X}), \tag{7}$$

whereby GRAD_X is the (macroscopic) gradient operator with respect to variable $\underline{X}$, and $\mathrm{GRAD}_X{}^S$ is its symmetrized counterpart.

$\mathcal{P}^{ext}$ and $\mathcal{P}^{int}$ are linear forms on $\underline{\check{V}}$ and $\check{\mathbf{D}}$, respectively

$$\mathcal{P}^{ext} = \int_V \underline{F}(\underline{X}) \cdot \underline{\check{V}}(\underline{X}) \, \mathrm{d}V(\underline{X}) + \int_S \underline{T}(\underline{X}) \cdot \underline{\check{V}}(\underline{X}) \, \mathrm{d}S(\underline{X}) \,, \tag{8}$$

$$\mathcal{P}^{int} = - \int_V \mathbf{\Sigma}(\underline{X}) : \check{\mathbf{D}}(\underline{X}) \, \mathrm{d}V(\underline{X}) \,, \tag{9}$$

with $\underline{F}$ as the (macroscopic) volume forces and $\underline{T}$ as the (macroscopic) surface forces.

In continuum micromechanics [3], any infinitesimal volume element $\mathrm{d}V$ around any *macroscopic* material point $\underline{X}$ is represented by a *microscopically* finite RVE with a characteristic size ℓ; such an RVE carrying all features of a classical continuum mechanics system at the microscopic scale. In order to maintain the physical relevance of the infinitesimally small macroscopic volume elements $\mathrm{d}V$, the corresponding RVEs need to be much smaller than the structural length $\mathcal{L}$, that is, Refs. [3, 11]:

$$\ell \ll \mathcal{L} = \frac{||\mathbf{\Sigma}(\underline{X})||}{|||\mathrm{GRAD}_X \, \mathbf{\Sigma}(\underline{X})|||} \,. \tag{10}$$

Thereby, the $\ll$-sign typically refers to a factor [8] of 5 to 10. Applying the PVP to such an RVE yields

$$\mathcal{P}^{ext}_{\mathrm{RVE}} = \int_{V_{\mathrm{RVE}}} \underline{f}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}V(\underline{x}) + \int_{S_{\mathrm{RVE}}} \underline{t}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}S(\underline{x}) \,, \tag{11}$$

$$\mathcal{P}^{int}_{\mathrm{RVE}} = - \int_{V_{\mathrm{RVE}}} \boldsymbol{\sigma}(\underline{x}) : \check{\mathbf{d}}(\underline{x}) \, \mathrm{d}V(\underline{x}) \,, \tag{12}$$

so that

$$\int_{V_{\mathrm{RVE}}} \underline{f}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}V(\underline{x}) + \int_{S_{\mathrm{RVE}}} \underline{t}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}S(\underline{x}) - \int_{V_{\mathrm{RVE}}} \boldsymbol{\sigma}(\underline{x}) : \check{\mathbf{d}}(\underline{x}) \, \mathrm{d}V(\underline{x}) = 0 \,, \tag{13}$$

with $\underline{\check{v}}$ as the microscopic virtual velocities, $\underline{f}$ and $\underline{t}$ as the microscopic volume and surface forces, and $\check{\mathbf{d}}$ as the microscopic virtual strain rates, the latter reading as

$$\begin{aligned} \check{\mathbf{d}}(\underline{x}) &= \frac{1}{2} \left\{ \frac{\partial \underline{v}}{\partial \underline{x}}(\underline{x}) + \left[\frac{\partial \underline{v}}{\partial \underline{x}}(\underline{x}) \right]^T \right\} \\ &= \frac{1}{2} \left\{ \mathrm{grad}_x \, \underline{\check{v}}(\underline{x}) + \left[\mathrm{grad}_x \, \underline{\check{v}}(\underline{x}) \right]^T \right\} = \mathrm{grad}_x^S \, \underline{\check{v}}(\underline{x}) \,. \end{aligned} \tag{14}$$

In Equation (14), grad_x denotes the microscopic gradient operator, and $\mathrm{grad}_x{}^S$ denotes its symmetrized counterpart. This operator induces the microheterogeneity size d as

$$d = \frac{||\boldsymbol{\sigma}(\underline{X})||}{|||\mathrm{grad}_x \, \boldsymbol{\sigma}(\underline{X})|||} \ll \ell \,. \tag{15}$$

Thereby, the $\ll$-sign refers to a factor of 2 to 3 for spherical or parallel cylindrical inclusions embedded in a continuous matrix phase [12–14]. Integration by parts of the power of internal forces of the RVE according to Equation (12) yields

$$\mathcal{P}^{int}_{\mathrm{RVE}} = - \int_{V_{\mathrm{RVE}}} \mathrm{div}_x \left[\boldsymbol{\sigma}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \right] \mathrm{d}V(\underline{x}) + \int_{V_{\mathrm{RVE}}} \mathrm{div}_x \, \boldsymbol{\sigma}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}V(\underline{x}) \,. \tag{16}$$

with the divergence operator standing for

$$\mathrm{div}_x(\bullet) = \underline{\nabla}_x \cdot (\bullet) \qquad \text{with} \qquad \underline{\nabla}_x = \sum_{i=1}^{3} \frac{\partial}{\partial x_i} \underline{e}_i \,, \tag{17}$$

whereby $\underline{e}_1$, $\underline{e}_2$, and $\underline{e}_3$ are orthonormal base vectors. Application of the divergence theorem to the first term of the right-hand side in Equation (16) yields

$$-\int_{V_{\mathrm{RVE}}} \mathrm{div}_x \left[\boldsymbol{\sigma}(\underline{x}) \cdot \underline{\check{v}}(\underline{x})\right] \mathrm{d}V(\underline{x}) = -\int_{S_{\mathrm{RVE}}} \underline{n}(\underline{x}) \cdot \boldsymbol{\sigma}(\underline{x}) \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}S(\underline{x}). \tag{18}$$

Insertion of Equation (18) into Equation (16), and of the respective result into Equation (13), yields, after re-arrangement of the terms integrated over volumes and surfaces, respectively, the following expression:

$$\int_{V_{\mathrm{RVE}}} \left[\underline{f}(\underline{x}) + \mathrm{div}_x \, \boldsymbol{\sigma}(\underline{x})\right] \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}V(\underline{x}) + \int_{S_{\mathrm{RVE}}} \left[\underline{t}(\underline{x}) - \boldsymbol{\sigma}(\underline{x}) \cdot \underline{n}(\underline{x})\right] \cdot \underline{\check{v}}(\underline{x}) \, \mathrm{d}S(\underline{x}) = 0 \,. \tag{19}$$

As Equation (19) needs to hold for any virtual microscopic velocity field $\underline{\check{v}}$, it readily delivers equilibrium conditions for all microscopic points inside the RVE,

$$\mathrm{div}_x \, \boldsymbol{\sigma}(\underline{x}) + \underline{f}(\underline{x}) = 0 \,, \qquad \forall \underline{x} \in V_{\mathrm{RVE}} \,, \tag{20}$$

and Cauchy's fundamental theorem for the microscopic points at the surface of the RVE,

$$\underline{t}(\underline{x}) = \boldsymbol{\sigma}(\underline{x}) \cdot \underline{n}(\underline{x}) \,, \qquad \forall \underline{x} \in S_{\mathrm{RVE}} \,. \tag{21}$$

3 | EQUIVALENCE OF MACROSCOPIC AND MICROSCOPIC EXPRESSIONS FOR INTERNAL AND EXTERNAL POWER DENSITIES—STRESS AND VOLUME FORCE AVERAGING RULES

Still, the RVE-related virtual powers need to be fully governed by the virtual kinematical properties of the infinitesimal volume elements $\mathrm{d}V(\underline{X})$ at the *macroscopic* scale, that is, being proportional to the macroscopic location-dependent macroscopic virtual velocities and strain rates, $\underline{\check{V}}(\underline{X})$ and $\check{\mathbf{D}}(\underline{X})$. Accordingly, we impose the latter two macroscopic quantities onto the RVE, in terms of the following microscopic virtual velocity fields prescribed at the boundary of the RVE,

$$\forall \underline{x} \in S_{\mathrm{RVE}} : \quad \underline{\check{v}}(\underline{x}, \underline{X}) = \underline{\check{V}}(\underline{X}) + \check{\mathbf{D}}(\underline{X}) \cdot \underline{x} \,, \tag{22}$$

noting that Equation (22) can be seen as a modification and extension of the so-called "Hashin boundary conditions" [2]. Expressions (22) and (14) imply an average rule for the virtual strain rates, reading as

$$\check{\mathbf{D}}(\underline{X}) = \frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int_{V_{\mathrm{RVE}}(\underline{X})} \check{\mathbf{d}}(\underline{x}, \underline{X}) \, \mathrm{d}V(\underline{x}, \underline{X}) \,, \tag{23}$$

which appears as the rate form of the well-known strain average rule, see Equation (1). Note that $\mathrm{d}V(\underline{x}, \underline{X})$ refers to integration over the microscopic variables $\underline{x}$, at the macroscopic position $\underline{X}$. Within the RVE, the microscopic virtual strain rate needs to be proportional to the macroscopic strain rate, which we express by a multilinear concentration relation of the form

$$\check{\mathbf{d}}(\underline{x}, \underline{X}) = \mathbb{A}_d(\underline{x}, \underline{X}) : \check{\mathbf{D}}(\underline{X}) \,, \tag{24}$$

with a yet-to-be-determined continuous concentration tensor field $\mathbb{A}_d(\underline{x}, \underline{X})$.

Identification of the RVE-related and macroscopic volume element-related expressions for the power densities of internal forces, as derived from Equations (9), (12), and (24), yields

$$\pi^{int}(\underline{X}) = -\boldsymbol{\Sigma}(\underline{X}) : \check{\mathbf{D}}(\underline{X}) \overset{!}{=} \pi^{int}_{\mathrm{RVE}}(\underline{X}) = -\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \boldsymbol{\sigma}(\underline{x},\underline{X}) : \mathbb{A}_d(\underline{x},\underline{X})\, \mathrm{d}V(\underline{x},\underline{X}) : \check{\mathbf{D}}(\underline{X})\,, \tag{25}$$

where $\overset{!}{=}$ indicates the bridging of scales. Namely, the internal and external power densities remain the very same physical quantities, regardless of whether they are expressed in terms of macroscopic or microscopic virtual velocities or strain rates. An alternative expression for the internal power density as a function of the macroscopic virtual strain rate is obtained from insertion of Equation (18) into the first integral on the right-hand side of Equation (16), followed by specifying the corresponding result for the boundary conditions (22) and the equilibrium conditions (20). Accordingly, this alternative power density expression reads as

$$\begin{aligned}\pi^{int}(\underline{X}) = &-\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{S_{\mathrm{RVE}}(\underline{X})} \left[\underline{\check{V}}(\underline{X}) + \underline{x}\cdot\check{\mathbf{D}}(\underline{X})\right]\cdot\boldsymbol{\sigma}(\underline{x},\underline{X})\cdot\underline{n}(\underline{x},\underline{X})\mathrm{d}S(\underline{x},\underline{X}) \\ &-\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \left[\underline{f}(\underline{x},\underline{X})\right]\cdot\underline{\check{v}}(\underline{x},\underline{X})\,\mathrm{d}V(\underline{x},\underline{X})\,.\end{aligned} \tag{26}$$

Taking the macroscopic virtual strain rate out of the first integral of Equation (26), and applying the divergence theorem to this first integral, while considering equilibrium condition (20), yields

$$\begin{aligned}\pi^{int}(\underline{X}) = &-\left[\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \boldsymbol{\sigma}(\underline{x},\underline{X})\,\mathrm{d}V(\underline{x},\underline{X})\right] : \check{\mathbf{D}}(\underline{X}) \\ &-\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \underline{f}(\underline{x},\underline{X})\cdot\left[\underline{v}(\underline{x},\underline{X}) - \underline{\check{V}}(\underline{X}) - \check{\mathbf{D}}(\underline{X})\cdot\underline{x}\right]\mathrm{d}V(\underline{x},\underline{X})\,.\end{aligned} \tag{27}$$

Identity of Equations (27) and (25) requires the concentration tensor $\mathbb{A}_d$ to be equal to the identity tensor

$$\mathbb{A}_d(\underline{x},\underline{X}) = \mathbb{I} \;\rightarrow\; \check{\mathbf{d}}(\underline{x},\underline{X}) = \check{\mathbf{D}}(\underline{X})\,, \qquad \forall \underline{x} \in V_{\mathrm{RVE}}(\underline{X})\,, \tag{28}$$

and the expression (22) to be not only valid at the boundary, but also throughout the entire volume of the RVE,

$$\underline{\check{v}}(\underline{x},\underline{X}) = \underline{\check{V}}(\underline{X}) + \check{\mathbf{D}}(\underline{X})\cdot\underline{x}\,, \qquad \forall \underline{x} \in V_{\mathrm{RVE}}(\underline{X})\,. \tag{29}$$

Requirement (28), together with Equation (25), yields the classical stress average rule, reading as

$$\boldsymbol{\Sigma}(\underline{X}) = \frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \boldsymbol{\sigma}(\underline{x},\underline{X})\,\mathrm{d}V(\underline{x},\underline{X})\,. \tag{30}$$

We note that the derivation of Equation (30), different from the classical derivations [2, 3], did without the requirement of vanishing volume forces $\underline{f}$.

As regards the latter, the equivalence of the macroscopic and microscopic expressions for the external power density, that is, of Equations (8) and (11), mathematically reads as

$$\pi^{ext}(\underline{X}) = \underline{F}(\underline{X})\cdot\underline{\check{V}}(\underline{X}) \overset{!}{=} \pi^{ext}_{\mathrm{RVE}}(\underline{X}) = \frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \underline{f}(\underline{x},\underline{X})\cdot\underline{\check{v}}(\underline{x},\underline{X})\,\mathrm{d}V(\underline{x},\underline{X})\,. \tag{31}$$

Inserting Equation (29) into Equation (31) results in

$$\underline{F}(\underline{X}) \cdot \underline{\check{V}}(\underline{X}) = \left[\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \underline{f}(\underline{x},\underline{X})\, \mathrm{d}V(\underline{x},\underline{X}) \right] \cdot \underline{\check{V}}(\underline{X}) + \left[\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \underline{f}(\underline{x},\underline{X}) \otimes \underline{x}\, \mathrm{d}V(\underline{x},\underline{X}) \right] : \check{\mathbf{D}}(\underline{X}) . \tag{32}$$

We will show in the following that the term in the second pair of square brackets will vanish if (i) the microscopic volume forces arise from a microscopically uniform field (such as the gravitational field), and if (ii) the microscopic location is measured from the center of gravity of the RVE. As a microscopically parallel force field, that is, as a microscopic field of uniform direction, we choose the gravitational field, which reads mathematically as

$$\underline{f}(\underline{x},\underline{X}) = \underline{g}(\underline{X})\, \rho(\underline{x},\underline{X}) , \tag{33}$$

with the gravitational acceleration $\underline{g}$ and the microscopic mass density ρ. Specifying the term in the second pair of square brackets in Equation (32), for the parallel force field (33), for yields

$$\underline{g}(\underline{X}) \otimes \left[\frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \rho(\underline{x},\underline{X})\, \underline{x}\, \mathrm{d}V(\underline{x},\underline{X}) \right] . \tag{34}$$

We are left with showing that the integral in Equation (34) vanishes if $\underline{x}$ is measured from the center of gravity of the RVE. Therefore, we adopt a location vector $\underline{\tilde{x}}$ measured from an arbitrary origin, locating the center of gravity at $\underline{\tilde{x}}_{CG}$. According to the very definition of the center of gravity, $\underline{\tilde{x}}_{CG}$ needs to fulfill

$$\int\limits_{V_{\mathrm{RVE}}(\underline{X})} \rho(\underline{\tilde{x}},\underline{X})\, \underline{\tilde{x}}\, \mathrm{d}V(\underline{\tilde{x}},\underline{X}) = \underline{\tilde{x}}_{CG} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \rho(\underline{\tilde{x}},\underline{X})\, \mathrm{d}V(\underline{\tilde{x}},\underline{X}) , \tag{35}$$

and since $\underline{x}$ is measured from the center of gravity, it is related to $\underline{\tilde{x}}$ and $\underline{\tilde{x}}_{CG}$ through

$$\underline{x} = \underline{\tilde{x}} - \underline{\tilde{x}}_{CG} . \tag{36}$$

Use of Equations (36) and (35) in Equation (34) yields

$$\int\limits_{V_{\mathrm{RVE}}} \rho(\underline{x},\underline{X})\, \underline{x}\, \mathrm{d}V(\underline{x},\underline{X}) = \int\limits_{V_{\mathrm{RVE}}} \rho(\underline{\tilde{x}},\underline{X}) \left(\underline{\tilde{x}} - \underline{\tilde{x}}_{CG} \right) \mathrm{d}V(\underline{\tilde{x}},\underline{X}) = \left(\underline{\tilde{x}}_{CG} - \underline{\tilde{x}}_{CG} \right) \int\limits_{V_{\mathrm{RVE}}} \rho(\underline{\tilde{x}},\underline{X})\, \mathrm{d}V(\underline{\tilde{x}},\underline{X}) = 0 . \tag{37}$$

Accordingly, a microscopically parallel force field (i.e., one with a uniform direction at the microscale) delivers the following volume force average rule

$$\underline{F}(\underline{X}) = \frac{1}{V_{\mathrm{RVE}}(\underline{X})} \int\limits_{V_{\mathrm{RVE}}(\underline{X})} \underline{f}(\underline{x},\underline{X})\, \mathrm{d}V(\underline{x},\underline{X}) . \tag{38}$$

4 | IMPLICATIONS FOR COMPUTATIONAL HOMOGENIZATION: INTERNAL VIRIAL STRESSES OF ATOMISTIC SYSTEMS, AND CONTINUUM RVES UNDERGOING LARGE DEFORMATIONS

Our derivation of the stress average rule also has interesting implications with respect to computational homogenization. The latter is definitely required when it comes to homogenization over discrete mechanical systems, such as atoms represented by mass points in a molecular dynamics setting [15]. In such a system, hosted within an RVE, the resultant internal

force acting on the ith atom of the assembly is the sum of all interaction forces $\underline{f}_{ij}$ between this atom and all the other atoms in the RVE. This reads mathematically as

$$\underline{f}_i^{int} = \sum_{j(\neq i)} \underline{f}_{ij}^{int}, \tag{39}$$

with the law of action and reaction (Newton's third law) requiring that [16, 17]

$$\underline{f}_{ij}^{int} = -\underline{f}_{ji}^{int}, \quad \text{with} \quad \underline{f}_{ij} \times \underline{x}_{ij} = 0, \tag{40}$$

whereby

$$\underline{x}_{ij} = \underline{x}_j - \underline{x}_i \tag{41}$$

denotes the vector pointing from position $\underline{x}_i$ to $\underline{x}_j$.

The virtual power density of internal forces acting on the atomic mass points hosted inside an RVE of volume V_{RVE} reads as

$$\pi_{\mathrm{RVE}}^{int} = \frac{1}{V_{\mathrm{RVE}}} \sum_i \underline{f}_i^{int} \cdot \check{\underline{v}}(\underline{x}_i) = \frac{1}{V_{\mathrm{RVE}}} \sum_i \left(\sum_{j(\neq i)} \underline{f}_{ij}^{int} \right) \cdot \check{\underline{v}}(\underline{x}_i). \tag{42}$$

where the virtual velocity $\check{\underline{v}}$ according to (29) appears as the mathematical tool for homogenizing, over the RVE, the discrete mechanical systems made of mass points representing single atoms. In this sense, specification of Equation (29) for specifying Equation (29) for $\underline{x} = \underline{x}_i$, and insertion of the result into Equation (42) yields

$$\pi_{\mathrm{RVE}}^{int} = \frac{1}{V_{\mathrm{RVE}}} \sum_i \left(\sum_{j(\neq i)} \underline{f}_{ij}^{int} \right) \cdot \left(\check{\underline{V}} + \check{\mathbf{D}} \cdot \underline{x}_i \right) = \frac{1}{V_{\mathrm{RVE}}} \left[\sum_i \left(\sum_{j(\neq i)} \underline{f}_{ij}^{int} \right) \otimes \underline{x}_i \right] : \check{\mathbf{D}}. \tag{43}$$

Setting equal Equation (43) with the macroscopic "homogenized" continuum mechanics expression for the power density of internal forces, see the left portion of Equation (25), yields the macroscopic Cauchy stress as

$$\boldsymbol{\Sigma} = -\frac{1}{V_{\mathrm{RVE}}} \left[\sum_i \left(\sum_{j(\neq i)} \underline{f}_{ij}^{int} \right) \otimes \underline{x}_i \right], \tag{44}$$

which is fully equivalent with the expressions, which were quite recently provided by Zhou [18] and Chen and Fish [15]. Actually, an only slight formalistic difference in the latter references arises from the use of Equation (41) in Equation (44), leading to the following alternative format for the macroscopic stresses

$$\boldsymbol{\Sigma} = \frac{1}{2\,V_{\mathrm{RVE}}} \left[\sum_i \left(\sum_{j(\neq i)} \underline{x}_{ij} \otimes \underline{f}_{ij}^{int} \right) \right], \tag{45}$$

whereby we have made use of Equation (40) and, consequently, of $\underline{f}_{ij} \otimes \underline{x}_{ij} = \underline{f}_{ji} \otimes \underline{x}_{ji}$.

We note the brevity and elegance of our approach to the homogenized stresses of Equation (45), when compared to the more expensive derivations of Zhou [18] and Chen and Fish [15]. In fact, Chen and Fish [15] applied an asymptotic expansion-based homogenization approach to a periodic discrete system of atomic mass points, while Zhou [18] started with formulating the balance of linear momentum in terms of the macroscopic spatial gradient of the homogenized stress, on the one hand, and of a discrete system of mass points, on the other hand. Subsequent Fourier transformation of the aforementioned formulation, followed by a particular inversion technique [19], yields an explicit formula for the macroscopic stress, which eventually turns out to be fully equivalent to Equation (45). In this context, Zhou [18] particularly emphasizes that the macroscopic Cauchy stresses according to Equation (45) are only related to the interaction forces

between atomic mass points, and do not depend on an additional kinetics energy term, which is often motivated by the famous 1870 paper of Clausius [20]. Zhou's reasoning is fully consistent with our derivation of Equation (45); and we may also note that, already as early as 1897, Finger [21] pointed out that mechanical stresses are only associated with the internal virial, that is, the interaction forces between point forces, and not with additional kinetic energy terms. In this sense, the macroscopic stresses Equation (45) may be appropriately called "internal virial stresses" or "interatomic virial stresses."

Computational homogenization in the classical narrower sense relates to continuous systems undergoing large deformations; and the average rule for the Cauchy stress according to Equation (30) is indeed valid, regardless of whether the system has undergone small or large deformations leading to its current configuration. Still, for the study of actual material behavior, the stress average rule needs to be complemented by relations pertaining to geometric compatibility and (micro-)constitutive behavior. As regards the former, the virtual strain rate average rule (23) naturally motivates to introduce an actual strain rate average rule of the format [22, 23]

$$\mathbf{D}(\underline{X}) = \frac{1}{V_{\mathrm{RVE}}} \int_{V_{\mathrm{RVE}}} \mathbf{d}(\underline{x},\underline{X})\, \mathrm{d}V(\underline{x},\underline{X})\,, \tag{46}$$

and temporal integration over an arbitrary succession of such strain rates allows for the representation of any large strain deformation [22, 23]. As regards constitutive modeling, Equation (46) can be complemented by thermodynamically consistent, microscopic hypoelasticity, where microscopic strain rates arise from the action of objective micro-stress rates [22–25]

$$\mathbf{d} = \rho\, \frac{\partial^2 G_\rho}{\partial \boldsymbol{\sigma}\, \partial \boldsymbol{\sigma}} : (\dot{\boldsymbol{\sigma}} + \boldsymbol{\sigma}\cdot\boldsymbol{\omega} - \boldsymbol{\omega}\cdot\boldsymbol{\sigma})\,, \tag{47}$$

with the spin tensor $\boldsymbol{\omega}$, the microscopic Gibbs potential per unit mass, G_ρ, and the partial temporal derivative of the stress tensor, $\dot{\boldsymbol{\sigma}}$. Based on the stress average rule (30), as well as on kinematic compatibility (46) and (micro-) constitutive behavior (47), a complete formalism for up and downscaling of stresses, strain rates, and spins can be derived [22, 23, 26]. This formalism allows for rigid body motions of microstructural entities, which may evolve independently of the overall macroscopic deformation state. The latter phenomenon is called non-affine microstructural deformation, and such deformation patterns are repeatedly encountered, typically so in biological materials [27]. In the more particular case of affine deformations where the overall elastic energy is fully governed by the deformation gradient (linking the current to the reference configuration), the Cauchy stresses can be transformed into Piola–Kirchhoff stresses, along with the very popular hyperelastic formulations linking Piola–Kirchhoff stresses to Green–Lagrange strains. For this case, there exists a very rich scientific literature on stress and strain averaging rules, as collected in pertinent review papers, such as the one provided by Saeb et al. [28].

5 | DISCUSSION AND CONCLUSION

Widening the perspective on the classical stress average rule in micromechanics, beyond Hashin's idea [2–5] of an equilibrated RVE subjected to homogeneous stress boundary conditions (so that the strain average rule becomes a mere definition) and also beyond the straightforward identification of an RVE with a mechanically tested sample on which average traction forces are measured [6], we here derived the stress average rule from the PVP. In this context, we note that we applied the PVP not only to the microscopically finite RVE itself, but also to the macroscopic system consisting of infinitely many such RVEs seen as infinitesimal volume elements. This way, our derivation does without prescribing (micro-)tractions at the boundary of the RVE, be they related to homogeneous (macroscopic) stresses or to experimental measurements. The main theoretical tool enabling this independence are the relations (22) and (23), linking macroscopic and microscopic virtual velocities and their symmetric gradients. In this sense, our derivation obviously extends the application range of the stress average rule beyond the confines resulting from its classical derivation, and our new derivation also upgrades the stress average rule from a "useful definition" to a theoretically sound result arising from the most fundamental principle in continuum mechanics.

This gives further conceptual credibility concerning the use of this rule for many material systems described by classical Mori–Tanaka [29, 30] or self-consistent [3, 31] homogenization schemes. These schemes are based on the stress average rule, and they are applied all the way from construction materials, such as concrete or wood [32–34], to biological and biomedical materials, such as bone or ceramic tissue engineering scaffolds [7, 35, 36].

We are aware that both the stress average rule (30), and even the less classical volume force relation (32) have been reported in the open literature, often in the context of the so-called Hill's lemma [37], and most clearly so by Nicot et al. [38]. However, the key aspect of the present contribution is to not take the stress average rule as granted (Nicot et al. [38] introduce it as a *definition*), but to employ the PVP as a theoretical means for exploring the (micro-)equilibrium of an RVE the virtual kinematics of which is fully governed by two macroscopic quantities: the macroscopic virtual velocity and its symmetric gradient (i.e., the macroscopic virtual Eulerian strain rate tensor). Then, the stress average rule and the volume force average rule for a microscopically parallel volume force field arise as *results*.

This use of the PVP to explore equilibrium conditions (or in the dynamic case, motion rules) is the target already of the original paper of Germain [9], where he covered classical and second-order continua. This example has been followed by very many examples from different branches of the rich field of mechanics and beyond, such as second-order fluid–solid interaction or poromechanics [39, 40], structural mechanics [41–43], bio-macromolecule homogenization [44], or elastic parameter homogenization [45].

ACKNOWLEDGMENTS

The authors gratefully acknowledge financial support in the framework of the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 764691.

CONFLICT OF INTEREST

The authors have declared no conflict of interest.

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How to cite this article: Jiménez Segura, N., Pichler, B.L.A., Hellmich, C.: Stress average rule derived through the principle of virtual power. Z. Angew. Math. Mech. 102, e202200091 (2022).
https://doi.org/10.1002/zamm.202200091