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A Mathematical Framework for Upscaling Operations

Microporomechanics is a continuum approach that allows one to scale of physical quantities from the microscale to the macroscale. This chapter presents some of the mathematical ingredients of this micro-to-macro approach that ultimately translates into upscaling rules of physical quantities. Two approaches are presented in this regard: one based on averaging techniques on a representative elementary volume, a second one based on a periodic assumption. From an application of averaging techniques to microscopic conservation laws we derive macroscopic conservation laws, and establish the link between kinematics and internal forces employed in microporomechanics: that is, from mass balance, the link between a microscopic velocity field and a macroscopic velocity vector; and from momentum balance, the link between microscopic stress field and macroscopic stress tensor.

1.1 Representative Elementary Volume (rev)

Continuum mechanics in general deals with the evolution of continuous material systems in three dimensions and time. Poromechanics in particular deals with the evolution of a porous continuum. One of the most critical elements of the continuum approach is the concept of an elementary volume. By definition, the elementary volume is an infinitesimal part of the three-dimensional material system under consideration. More precisely, if we denote by L and ℓ the characteristic lengths of respectively the structure and the elementary volume, the condition $\ell \ll L$ guarantees the relevance of the use of the tools of differential calculus offered by a continuum description. Furthermore, the elementary volume is expected to be large enough to be representative of the

constitutive material,¹ which explains its name as *representative elementary volume* (in short *rev*). It is intuitively understood that this property requires the characteristic size ℓ of the *rev* to be chosen so as to capture in a statistical sense all the information concerning the geometrical and physical properties of the physics at stake. Roughly speaking, if we denote by d the characteristic length scale of the local heterogeneities, typically the pore size in a porous medium, the condition $d \ll \ell$ is expected to ensure that the elementary volume is representative. In summary, the two conditions on the size of the *rev* are:

$$d \ll \ell \ll L \quad (1.1)$$

Relation (1.1) is often referred to as the condition for scale separation (or scale separability condition), which is a necessary condition for the concept of *rev* to be valid.

At the macroscopic scale, the *rev* is characterized by a position vector \underline{x} . The characteristic order of magnitude of the variation of \underline{x} is the size L of the studied material system. Furthermore, this material system is composed of different constituents, i.e. in the case of a porous continuum, one (possibly heterogeneous) solid phase and one or several fluid phases. These phases represent heterogeneities. The macroscopic poromechanics theory accounts for this heterogeneous nature of the porous material system by considering each phase as a macroscopic particle. All these particles are located at the same point \underline{x} . In other words, from a macroscopic point of view, the *rev* is regarded as the superposition of these particles in time and space.

By contrast, a poromechanics approach that starts at the microscopic scale explicitly considers the heterogeneous structure of the *rev*. It represents the solid and the fluid phases as individual separated domains in the *rev*. This requires a refinement of the geometrical description, i.e. a change in length scale. At the microscopic scale, the position vector is now denoted by \underline{z} ; the characteristic order of magnitude of the variation of \underline{z} is the size ℓ of the *rev* (Figure 1.1). Depending on \underline{z} , the microscopic particle located at point \underline{z} belongs to the solid phase or to a fluid phase.

The very existence of an *rev* is a key element for both micro- and macroporomechanics theories, albeit of different importance. In a pure macroscopic approach, the existence of an *rev* must be postulated so that the macroscopic constitutive laws derived experimentally or theoretically are representative of the response of the *rev* to various loadings. The principle of a micro-to-macro approach consists in replacing the real experiment that could be performed on a representative material sample by a thought experiment on the *rev* considered as a heterogeneous structure that is subjected to appropriate boundary conditions. The underlying idea of micromechanics is to derive the

¹The conditions for an elementary volume to be representative have been discussed by many authors. The interested reader is referred for instance to the work of Bear and Bachmat [6] or Torquato [50].

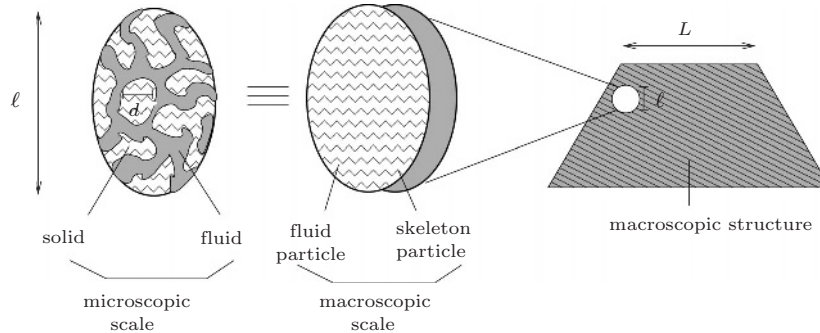


Figure 1.1 Elementary volume of porous medium in a macroscopic structure. Microscopic and macroscopic scales.

macroscopic response of the sample from the microscopic one. This requires, as a first task, clarification of the mathematical relations between the physics at each scale, the micro and the macro scales, and more particularly answers to the following two critical questions relating to the description of the kinematics and the internal forces:

- The velocity in any phase α of the porous material (e.g. $\alpha = s$ for the solid phase and $\alpha = f$ for the fluid phase) is characterized at the macroscopic scale by a vector $\underline{V}^\alpha(\underline{x})$, and by the field $\underline{v}(\underline{z})$ at the microscopic scale. What is the link between $\underline{V}^\alpha(\underline{x})$ and $\underline{v}(\underline{z})$?
- The internal forces in the α phase are characterized at the macroscopic scale by the partial stress tensor $\underline{\Sigma}^\alpha(\underline{x})$, and by the field $\underline{\sigma}(\underline{z})$ at the microscopic scale. What is the link between $\underline{\Sigma}^\alpha(\underline{x})$ and $\underline{\sigma}(\underline{z})$?

1.2 Averaging Operations

It is natural, at least for extensive physical quantities such as mass, energy, etc., to define the link between micro- and macroscales through averaging techniques defined on the *rev*; including the links between the derivative of an average (with respect to time or spatial coordinates) and the average of the derivatives. This is the focus of this section which sets out a mathematical basis for the forthcoming application of these elements in microporomechanics.

1.2.1 Apparent and Intrinsic Averages

Let Ω_0 be a time-independent geometrical domain centered at the origin O of the coordinate system, which can be considered as an *rev*. For any value of \underline{x} , we assume that the elementary volume $\Omega(\underline{x})$ which is obtained from Ω_0 by a

translation² of vector \underline{x} is an *rev* for the material at the macroscopic point \underline{x} , in its current configuration. Furthermore, let $f(\underline{z})$ be a C^∞ function defined at the microscopic scale. It is equal to zero outside Ω_0 and satisfies:

$$\int f(\underline{z}) dV_z = 1 \quad (1.2)$$

The average $\bar{e}(\underline{x})$ at the macroscopic point \underline{x} of a physical quantity represented in $\Omega(\underline{x})$ by the volume density $e(\underline{z})$ is defined by:

$$\bar{e}(\underline{x}, t) = \int e(\underline{z}, t) f(\underline{z} - \underline{x}) dV_z \quad (1.3)$$

This definition depends on the choice of the function f . In practice, f can be chosen so as to tend towards the discontinuous function $\chi_0/|\Omega_0|$, where $|\Omega_0|$ is the volume of Ω_0 and χ_0 is the characteristic function of this domain defined by $\chi_0(\underline{z}) = 1$ if $\underline{z} \in \Omega_0$ and $\chi_0(\underline{z}) = 0$ if $\underline{z} \notin \Omega_0$. The definition (1.3) then asymptotically corresponds to the more familiar definition of the average:

$$\bar{e}(\underline{x}, t) \approx \frac{1}{|\Omega(\underline{x})|} \int_{\Omega(\underline{x})} e(\underline{z}, t) dV_z \quad (1.4)$$

However, it will be convenient for further calculations to take advantage of the regularity of $f(\underline{z})$ on the boundary of Ω_0 .

By way of illustration, consider the volume mass density of the porous medium $\rho_M(\underline{x})$, which at the macroscopic scale represents the total elementary mass dm contained in the *rev* $\Omega(\underline{x})$ divided by its volume:

$$\rho_M = \frac{dm}{|\Omega(\underline{x})|} \quad (1.5)$$

With the approximation $f \approx \chi_0/|\Omega_0|$, it is readily seen that:

$$\rho_M = \bar{\rho} \quad (1.6)$$

Another example is the volume fraction $\varphi(\underline{x}, t)$ of the pore space at the macroscopic point \underline{x} , which can be determined from the geometry of the microstructure from:

$$\varphi(\underline{x}, t) = \bar{\chi}^p = \int \chi^p(\underline{z}, t) f(\underline{z} - \underline{x}) dV_z \quad (1.7)$$

where $\chi^p(\underline{z}, t)$ is the characteristic function of the pore space. $\varphi(\underline{x}, t)$ is also referred to as the porosity.

From now on, \mathcal{P}^s and \mathcal{P}^f respectively denote the domains occupied by the solid and the fluid phase. In addition, \mathcal{P}^p refers to the pore space. In the saturated case, we note that $\mathcal{P}^f = \mathcal{P}^p$. All these domains a priori depend

² The image of point M by this translation is point M' such that $\underline{MM}' = \underline{x}$.

on time. We also introduce the solid, fluid and porous parts of the *rev* $\Omega(\underline{x})$, defined as $\Omega^\alpha(\underline{x}, t) = \mathcal{P}^\alpha(t) \cap \Omega(\underline{x})$ ($\alpha = s, f, p$).

For a physical quantity $e(\underline{z}, t)$ attached to the fluid, and thus defined on the fluid domain \mathcal{P}^f only, we will encounter two different averages, namely the ‘apparent’ one, $\langle e \rangle_f(\underline{x}, t)$:

$$\langle e \rangle_f(\underline{x}, t) = \overline{\chi^f e}(\underline{x}, t) = \int \chi^f(\underline{z}, t) e(\underline{z}, t) f(\underline{z} - \underline{x}) dV_z \quad (1.8)$$

and the ‘intrinsic’ one, $\bar{e}^f(\underline{x}, t)$, defined by:

$$\bar{e}^f(\underline{x}, t) = \frac{1}{\varphi} \langle e \rangle_f(\underline{x}, t) \quad (1.9)$$

where $\chi^f(\underline{z}, t)$ is the characteristic function of the fluid phase. The apparent and the intrinsic average both derive from the total amount of the physical quantity $e(\underline{z}, t)$ available in \mathcal{P}^f . However, the apparent one $\langle e \rangle_f$ refers this total amount to the total volume of the *rev*, while the intrinsic average \bar{e}^f refers the total amount to the actual domain $|\Omega^f(\underline{x}, t)|$ the fluid phase occupies in the *rev*. Analogously, it is possible to define apparent and intrinsic averages of the solid phase. It suffices indeed to replace χ^f in (1.8) by the characteristic function of the solid domain \mathcal{P}^s , $\chi^s = 1 - \chi^p$, to obtain the apparent average $\langle e \rangle_s(\underline{x}, t) = \overline{\chi^s e}(\underline{x}, t)$, and φ in (1.9) by the solid volume fraction $1 - \varphi$, to obtain the intrinsic average $\bar{e}^s(\underline{x}, t) = \langle e \rangle_s(\underline{x}, t)/(1 - \varphi)$.

By way of example, consider a component γ of the fluid phase (for instance, a solute which together with a solvent saturates the fluid domain \mathcal{P}^f). Let $\rho^\gamma(\underline{z}, t)$ be the microscopic mass density, and dm^γ the total mass of the γ component in the *rev*. The macroscopic apparent and intrinsic mass densities $\rho_a^\gamma(\underline{x}, t)$ and $\rho_M^\gamma(\underline{x}, t)$ are macroscopically defined by:

$$\rho_a^\gamma(\underline{x}, t) = \frac{dm^\gamma}{|\Omega(\underline{x})|}; \quad \rho_M^\gamma(\underline{x}, t) = \frac{dm^\gamma}{|\Omega^f(\underline{x}, t)|} \quad (1.10)$$

Using the approximation $f \approx \chi_0/|\Omega_0|$, it is readily seen that $\rho_a^\gamma(\underline{x}, t)$ and $\rho_M^\gamma(\underline{x}, t)$ are related to the field $\rho^\gamma(\underline{z}, t)$ by:

$$\rho_a^\gamma = \langle \rho^\gamma \rangle_f \quad (1.11)$$

$$\rho_M^\gamma = \rho_a^\gamma / \varphi = \overline{\rho^\gamma}^f \quad (1.12)$$

Clearly enough, it is also possible to define apparent and intrinsic averages over the pore space. This amounts to replacing χ^f in (1.8) by the characteristic function χ^p of the pore space. The case of a saturated porous medium can be defined by the condition $\chi^p(\underline{z}, t) = \chi^f(\underline{z}, t)$. In this situation, we note that the operators $\langle \cdot \rangle_p$ and $\langle \cdot \rangle_f$ are equivalent, as well as the operators $\overline{\cdot}^p$ and $\overline{\cdot}^f$.

1.2.2 Spatial Derivatives of an Average

Let us introduce a cartesian orthonormal frame (e_i) . The derivative of the apparent average $\langle e \rangle_f(\underline{x})$ of a physical quantity $e(\underline{z})$ defined on the fluid domain \mathcal{P}^f with respect to the spatial coordinate x_i is directly obtained from definition (1.8):

$$\frac{\partial}{\partial x_i} \langle e \rangle_f(\underline{x}, t) = - \int \chi^f(\underline{z}, t) e(\underline{z}, t) \frac{\partial f}{\partial z_i}(\underline{z} - \underline{x}) dV_z \quad (1.13)$$

where the following identity has been employed:

$$\frac{\partial}{\partial x_i} (f(\underline{z} - \underline{x})) = - \frac{\partial f}{\partial z_i}(\underline{z} - \underline{x}) \quad (1.14)$$

Integration by parts of (1.13) then yields:

$$\frac{\partial}{\partial x_i} \langle e \rangle_f(\underline{x}, t) = \int \frac{\partial(\chi^f e)}{\partial z_i}(\underline{z}, t) f(\underline{z} - \underline{x}) dV_z \quad (1.15)$$

Since $\chi^f(\underline{z}, t)$ is discontinuous across the solid–fluid interface \mathcal{I}^{sf} , relation (1.15) is to be understood in the sense of the distribution theory. More precisely, let $\delta_{\mathcal{I}^{sf}}$ be the Dirac distribution of support \mathcal{I}^{sf} . It is defined by:

$$\langle \delta_{\mathcal{I}^{sf}}, \psi \rangle = \int \delta_{\mathcal{I}^{sf}} \psi dV_z = \int_{\mathcal{I}^{sf}} \psi dS_z \quad (1.16)$$

where ψ is any function of $\mathcal{D}(\mathbb{R}^3)$.³ According to the definition of the derivative of a distribution, one obtains:

$$\left\langle \frac{\partial \chi^f}{\partial z_i}, \psi \right\rangle = - \left\langle \chi^f, \frac{\partial \psi}{\partial z_i} \right\rangle = - \int_{\mathcal{P}^f} \frac{\partial \psi}{\partial z_i} dV_z = - \int_{\mathcal{I}^{sf}} \psi n_i dS_z \quad (1.17)$$

where $\underline{n} = n_i e_i$ is the unit normal to \mathcal{I}^{sf} oriented towards the solid. Combining (1.16) and (1.17) yields:

$$\frac{\partial \chi^f}{\partial z_i} = -n_i \delta_{\mathcal{I}^{sf}} \quad (1.18)$$

The expression (1.15) can now be developed in the form:

$$\frac{\partial}{\partial x_i} \langle e \rangle_f(\underline{x}, t) = \left\langle \frac{\partial e}{\partial z_i}(\underline{z}, t) \right\rangle_f - \int_{\mathcal{I}^{sf}} e(\underline{z}, t) n_i(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.19)$$

Expression (1.19) establishes the sought link between the macroscopic spatial derivative and the microscopic one in the fluid domain \mathcal{P}^f . With the same reasoning applied to the apparent volume average of a physical quantity $e(\underline{z})$

³ $\mathcal{D}(\mathbb{R}^3)$ is the set of C^∞ functions which are equal to zero out of a bounded domain.

defined on the solid domain \mathcal{P}^s , one obtains:

$$\frac{\partial}{\partial x_i} \langle e \rangle_s(\underline{x}, t) = \left\langle \frac{\partial e}{\partial z_i}(\underline{z}, t) \right\rangle_s + \int_{\mathcal{I}^{sf}} e(\underline{z}, t) n_i(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.20)$$

where the change in sign of the second term on the right-hand side (r.h.s.) stems from the opposite direction of the outward unit normal to the solid phase.

1.2.3 Time Derivative of an Average

The time derivative of $\langle e \rangle_f$ also comprises an extra term, in addition to the volume average of the time derivative $\langle \partial e / \partial t \rangle_f$. Indeed, starting from (1.8), we obtain:

$$\frac{\partial}{\partial t} \langle e \rangle_f(\underline{x}, t) = \left\langle \frac{\partial e}{\partial t}(\underline{z}, t) \right\rangle_f + \int \frac{\partial \chi^f}{\partial t}(\underline{z}, t) e(\underline{z}, t) f(\underline{z} - \underline{x}) dV_z \quad (1.21)$$

The second term on the r.h.s. accounts for the displacement of the boundary of the fluid domain through the derivative $\partial \chi^f / \partial t$. More precisely, introducing the velocity \underline{u} of the interface \mathcal{I}^{sf} , it can be shown that:

$$\frac{\partial}{\partial t} \langle e \rangle_f(\underline{x}, t) = \left\langle \frac{\partial e}{\partial t}(\underline{z}, t) \right\rangle_f + \int_{\mathcal{I}^{sf}} e(\underline{z}, t) (\underline{u} \cdot \underline{n})(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.22)$$

where $\underline{u} \cdot \underline{n}$ represents the normal velocity of the solid–fluid interface \mathcal{I}^{sf} , oriented by unit normal \underline{n} pointing towards the solid phase.

Analogously, we obtain for the solid phase:

$$\frac{\partial}{\partial t} \langle e \rangle_s(\underline{x}, t) = \left\langle \frac{\partial e}{\partial t}(\underline{z}, t) \right\rangle_s - \int_{\mathcal{I}^{sf}} e(\underline{z}, t) (\underline{u} \cdot \underline{n})(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.23)$$

1.2.4 Spatial and Time Derivatives of \bar{e}

We finally consider the average \bar{e} in the sense of (1.3) of a physical quantity defined on the whole *rev*; that is, on both the solid and fluid phases. Using the definition (1.3), (1.14) and integrating by parts, it is readily seen that:

$$\frac{\partial}{\partial x_i} (\bar{e}) = - \int \frac{\partial f}{\partial z_i}(\underline{z} - \underline{x}) e(\underline{z}, t) dV_z = \overline{\frac{\partial e}{\partial z_i}} \quad (1.24)$$

In turn, the determination of the time derivative of \bar{e} takes advantage of the fact that the weighting function $f(\underline{z})$ does not depend on time. It follows that:

$$\frac{\partial}{\partial t} (\bar{e}) = \int f(\underline{z} - \underline{x}) \frac{\partial e}{\partial t}(\underline{z}, t) dV_z = \overline{\frac{\partial e}{\partial t}} \quad (1.25)$$

Expressions (1.24) and (1.25) could have been directly obtained from (1.19)–(1.20) and (1.22)–(1.23), provided that the physical quantity $e(\underline{z})$ defined on both the fluid and the solid domain, \mathcal{P}^f and \mathcal{P}^s , i.e. on $\Omega(\underline{x})$, is continuous over the solid–fluid interface. In the more general case, the spatial and time derivatives of \bar{e} on account of a possible discontinuity of $e(\underline{z})$ on the solid–fluid interface take the following form:

$$\frac{\partial}{\partial x_i} \bar{e}(\underline{x}, t) = \frac{\partial \bar{e}}{\partial z_i} + \int_{\mathcal{I}^{sf}} [e(\underline{z}, t)] n_i(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.26)$$

$$\frac{\partial}{\partial t} (\bar{e}) = \frac{\partial \bar{e}}{\partial t} - \int_{\mathcal{I}^{sf}} [e(\underline{z}, t)] (\underline{u} \cdot \underline{n})(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.27)$$

where $[e(\underline{z}, t)] = e^s(\underline{z}, t) - e^f(\underline{z}, t)$ denotes the jump of e over \mathcal{I}^{sf} oriented by the unit outward normal to the fluid phase.

1.3 Application to Balance Laws

Upscaling rules for several physical phenomena that are present at both the microscopic and the macroscopic scale can be derived from the balance laws. Indeed, each balance law can be formulated either at the microscopic scale or at the macroscopic one. The consistency of these two approaches of the same physical principle then delivers the upscaling rule. This technique is developed in this section.⁴ The starting point is the conservation laws at the microscopic scale. Taking the average of the corresponding laws in the sense of (1.3) or the apparent average in the sense of (1.8), we obtain macroscopic formulations of the balance laws from a pure upscaling reasoning. The mass balance law is considered first; the momentum balance is addressed in Section 1.3.2.

1.3.1 Mass Balance

The mathematical formulation of mass balance classically involves the concept of velocity. For a component γ of a fluid phase, the velocity is represented at the microscopic scale by a field $\underline{v}^\gamma(\underline{z})$ defined on \mathcal{P}^f . The macroscopic counterpart is a single vector $\underline{V}^\gamma(\underline{x})$. Hence, two macroscopic mass balance equations are available: one to be derived from the average of the microscopic formulation; the second from a purely macroscopic reasoning. Since mass conservation must hold irrespective of the scale under consideration, the necessary consistency of these two approaches provides the link between the field $\underline{v}^\gamma(\underline{z})$ and the vector $\underline{V}^\gamma(\underline{x})$. This is the problem we consider here.

⁴ A review of this technique can be found in [26] and [6].

Mass Balance of a Component of a Fluid Phase

When the fluid comprises several chemical species, the macroscopic point of view describes the fluid as the superposition of several macroscopic particles, each corresponding to one of these chemical species. At the microscopic scale, the approach is similar. At each point \underline{z} of the fluid domain \mathcal{P}^f , the fluid is considered as a superposition of microscopic particles. For the γ component of the fluid, the local volume unit mass and velocity are represented by the fields $\rho^\gamma(\underline{z})$ and $\underline{v}^\gamma(\underline{z})$. The microscopic mass balance equation for this component thus reads:

$$\frac{\partial \rho^\gamma}{\partial t} + \text{div}_z(\rho^\gamma \underline{v}^\gamma) = 0 \quad (1.28)$$

where div_z is the divergence operator acting on the microscopic coordinates z_i . Note clearly that the mass balance equation (1.28) disregards any mass exchange between the γ component and any other components of the fluid.

The apparent average of (1.28) – in the sense of (1.8) – is straightforward:

$$\left\langle \frac{\partial \rho^\gamma}{\partial t} \right\rangle_f + \langle \text{div}_z \rho^\gamma \underline{v}^\gamma \rangle_f = 0 \quad (1.29)$$

We now apply (1.19) with $e = \rho^\gamma v_i^\gamma$ and (1.22) with $e = \rho^\gamma$. Taking (1.9) into account, the mass balance (1.29) takes the form:

$$\frac{\partial}{\partial t}(\overline{\varphi \rho^\gamma}) + \text{div}_x(\overline{\varphi \rho^\gamma \underline{v}^\gamma}) = \int_{\mathcal{I}^s} \rho^\gamma (\underline{u} - \underline{v}^\gamma) \cdot \underline{n} f(\underline{z} - \underline{x}) dS_z \quad (1.30)$$

where div_x is the divergence operator acting on the macroscopic coordinates x_i . The r.h.s. of (1.30) represents the mass flux of the γ component across the solid–fluid interface. This term is non-zero for dissolution, precipitation or adsorption phenomena that may take place at the solid–fluid interface. In the absence of such mass exchange between γ and the solid, the flux is zero and the following macroscopic formulation of the mass balance principle is obtained:

$$\frac{\partial}{\partial t}(\overline{\varphi \rho^\gamma}) + \text{div}_x(\overline{\varphi \rho^\gamma \underline{v}^\gamma}) = 0 \quad (1.31)$$

This macroscopic mass balance has been derived from the upscaling of its microscopic counterpart (1.28). Alternatively, a pure macroscopic approach to the mass balance principle reads:

$$\frac{\partial \rho_a^\gamma}{\partial t} + \text{div}_x \rho_a^\gamma \underline{V}^\gamma = 0 \quad (1.32)$$

where $\underline{V}^\gamma(\underline{x})$ is a macroscopic velocity vector of component γ , and ρ_a^γ has been defined in (1.11). Finally, a comparison of (1.31) and (1.32) provides the link between the microscopic and macroscopic descriptions of the kinematics.

Indeed, the compatibility between (1.28) and (1.32) requires the macroscopic momentum $\rho_a^\gamma \underline{V}^\gamma$ to be equal to the apparent average of the microscopic momentum $\overline{\varphi \rho^\gamma \underline{v}^\gamma}$; that is:

$$\underline{V}^\gamma = \frac{\overline{\rho^\gamma \underline{v}^\gamma}}{\overline{\rho^\gamma}} \quad (1.33)$$

where we made use of (1.11) and (1.12).

Homogeneous Fluid

It is instructive to consider the case of a homogeneous fluid, which by definition comprises only one single component. In this case, replacing $\rho^\gamma(\underline{z})$ in (1.33) by the fluid mass density $\rho^f(\underline{z})$, and $\underline{v}^\gamma(\underline{z})$ by the velocity field $\underline{v}(\underline{z})$, the link between the velocity of the macroscopic fluid particle $\underline{V}^f(\underline{x})$ and the microscopic velocity field is:

$$\underline{V}^f = \frac{\overline{\rho^f \underline{v}^f}}{\overline{\rho^f}} \quad (1.34)$$

It is interesting to note that the macroscopic fluid velocity is not a priori the volume average of the microscopic one. In fact, it is readily seen from (1.34) that this is only the case when the fluid phase is incompressible; that is:

$$\rho^f = \rho_0^f \Leftrightarrow \underline{V}^f = \overline{\underline{v}^f} \quad (1.35)$$

1.3.2 Momentum Balance

We now turn to a second conservation law, the momentum balance, to derive upscaling rules based on the compatibility of the micro- and macroscopic expressions of the momentum balance.

Average Rules for Total and Partial Stresses

We consider a porous medium saturated by a homogeneous fluid. If we denote by $\sigma(\underline{z})$ the symmetric microscopic stress field,⁵ i.e. the stress field defined at

⁵ Throughout this book, all stress quantities that are introduced, whether microscopic or macroscopic, satisfy the symmetry condition:

$$\sigma_{ij} = \sigma_{ji}$$

The basis of the continuum mechanics approach employed here can be found in classical textbooks on continuum mechanics (e.g. Salençon, [46]).

the microscopic scale on the *rev* $\Omega(\underline{x})$, the momentum balance is:

$$\frac{\partial \sigma_{ij}}{\partial z_j} + \rho f_i = 0 \quad (1.36)$$

where $\rho \underline{f}(\underline{z})$ is the density of volume forces acting at the microscopic point \underline{z} . For instance, for gravity forces the vector \underline{f} is the acceleration due to gravity \underline{g} . The mass density $\rho(\underline{z})$ depends (through \underline{z}) on the phase to which \underline{z} belongs. In the particular case of incompressible solid and fluid phases, $\rho(\underline{z})$ is equal to either the intrinsic mass density ρ^s of the solid or ρ^f of the fluid, depending on the position vector \underline{z} .

Using (1.24) with $e = \sigma_{ij}$, the average of (1.36) – in the sense of (1.3) – delivers a first macroscopic expression of the momentum balance:

$$\frac{\partial \overline{\sigma_{ij}}}{\partial x_j} + \overline{\rho f_i} = \frac{\partial}{\partial x_j}(\overline{\sigma_{ij}}) + \overline{\rho f_i} \quad (1.37)$$

In addition, a second macroscopic expression of the momentum balance is provided by the macroscopic approach:

$$\frac{\partial \Sigma_{ij}}{\partial x_j} + \rho_M F_i = 0 \quad (1.38)$$

where Σ is a macroscopic stress tensor, while $\rho_M \underline{F}(\underline{x})$ now represents the density of volume forces acting at the macroscopic scale at point \underline{x} . From the very definition of $\underline{f}(\underline{z})$ and $\underline{F}(\underline{x})$, it is readily seen that the comparison of (1.37) and (1.38) provides the following remarkable results:

- The macroscopic stress tensor Σ is the average of the microscopic stress field:

$$\Sigma = \overline{\sigma} \quad (1.39)$$

- The volume forces obey the following upscaling rule:

$$\overline{\rho F} = \overline{\rho f} \quad (1.40)$$

While readily verified for gravity forces, for which $\underline{F} = \underline{f} = \underline{g}$, the upscaling rule (1.40) is useful in some problems related, for example, to electromagnetism, allowing for the determination of $\underline{F} = \overline{\rho f} / \overline{\rho}$ from its microscopic counterpart.

In addition to the total stress Σ , a common stress quantity encountered in macroscopic approaches is known as partial stress Σ^α of the α phase ($\alpha = s$ or f). In the very same way as the total stress, this partial stress tensor is a macroscopic physical quantity. Indeed, it represents the internal forces in one of the two phases. Furthermore, in such macroscopic theories, called mixture

theories, the interaction between the solid and the fluid phase is represented, at the macroscopic scale, by a volume force $\underline{a}(\underline{x})$, such that $\underline{a}(\underline{x}) |\Omega(\underline{x})|$ represents the elementary force applied by the macroscopic fluid particle located at point \underline{x} to the macroscopic solid particle located at the same point. The principle of momentum balance applied to each phase at the macroscopic scale reads:

$$\frac{\partial \Sigma_{ij}^\alpha}{\partial x_j} + \rho_a^\alpha F_i^\alpha + \epsilon^\alpha a_i = 0 \quad (1.41)$$

where $\epsilon^s = 1$ and $\epsilon^f = -1$.

We want to give a microscopic derivation of both the partial stress and the interaction term in (1.41). To this end, we consider the partial average of (1.36):

$$\left\langle \frac{\partial \sigma_{ij}}{\partial z_j} \right\rangle_\alpha + \langle \rho^\alpha f_i^\alpha \rangle_\alpha = 0 \quad (1.42)$$

Then, applying (1.19)–(1.20) for $e = \sigma_{ij}$ yields:

$$\frac{\partial}{\partial x_j} \langle \sigma_{ij} \rangle_\alpha = \left\langle \frac{\partial}{\partial z_j} \sigma_{ij}(\underline{z}, t) \right\rangle_\alpha + \epsilon^\alpha \int_{\mathcal{I}^{sf}} \sigma_{ij}(\underline{z}, t) n_j(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.43)$$

Finally, substituting (1.43) in (1.42) yields a second macroscopic formulation of the momentum balance of phase α , in addition to (1.41), which is obtained independently from the former by means of upscaling the microscopic formulation of the same principle:

$$\text{div}_x \langle \boldsymbol{\sigma} \rangle_\alpha + \langle \rho^\alpha \underline{f}^\alpha \rangle_\alpha - \epsilon^\alpha \int_{\mathcal{I}^{sf}} \boldsymbol{\sigma}(\underline{z}, t) \cdot \underline{n}(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z = 0 \quad (1.44)$$

Finally, from a comparison of the two macroscopic momentum balance relations – the pure macroscopic one (1.41), and the one obtained by means of upscaling (1.44) – it turns out that the partial stress Σ^α is the apparent average of the microscopic stress field in the α phase:

$$\Sigma^\alpha = \langle \boldsymbol{\sigma} \rangle_\alpha \quad (1.45)$$

In turn, the volume force vector \underline{a} employed in the macroscopic approach to represent the mechanical interaction between the solid and the fluid phases is actually the integral of the interaction surface forces at the solid–fluid interface:

$$\underline{a} = - \int_{\mathcal{I}^{sf}} \boldsymbol{\sigma}(\underline{z}, t) \cdot \underline{n}(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.46)$$

It is interesting to note that the same physical phenomenon, e.g. the solid–fluid interaction, has different representations at different scales: a surface force at the microscopic scale, and a volume force at the macroscopic scale, while the link is provided by the surface integral (1.46).

Partial Stress in an Incompressible Viscous Fluid

It is instructive to study the case of an incompressible Newtonian fluid, defined by a viscosity coefficient μ^f . For simplicity, the solid phase is assumed to be rigid and the pore volume fraction φ is uniform. The microscopic stress state in the fluid is related to the strain rate tensor $\mathbf{d}(\underline{z})$, defined as the symmetric part of the microscopic velocity gradient \underline{v} , by the classical state equation of fluid mechanics:

$$\boldsymbol{\sigma} = -p(\underline{z})\mathbf{1} + 2\mu^f \mathbf{d}(\underline{z}) \quad \text{with} \quad \mathbf{d} = \frac{1}{2} (\mathbf{grad}_z \underline{v} + {}^t \mathbf{grad}_z \underline{v}) \quad (1.47)$$

where p stands for the (thermodynamic) fluid pressure. We want to determine the macroscopic partial stress $\boldsymbol{\Sigma}^f$ in the fluid. To this end, the upscaling rule (1.45) gives:

$$\boldsymbol{\Sigma}^f = \langle \boldsymbol{\sigma} \rangle_f = -\langle p \rangle_f \mathbf{1} + 2\mu^f \langle \mathbf{d} \rangle_f \quad (1.48)$$

Then, applying (1.19) with $e = v_j$, we obtain:

$$\frac{\partial}{\partial x_i} \langle v_j \rangle_f(\underline{x}, t) = \left\langle \frac{\partial v_j}{\partial z_i}(\underline{z}, t) \right\rangle_f - \int_{\mathcal{I}^{sf}} v_j(\underline{z}, t) n_i(\underline{z}, t) f(\underline{z} - \underline{x}) dS_z \quad (1.49)$$

This equation is simplified by the boundary condition $\underline{v} = 0$ at the solid–fluid interface \mathcal{I}^{sf} :

$$\frac{\partial}{\partial x_i} \langle v_j \rangle_f(\underline{x}, t) = \left\langle \frac{\partial v_j}{\partial z_i}(\underline{z}, t) \right\rangle_f \quad (1.50)$$

Finally, recalling (1.35), (1.50) reveals that the macroscopic strain rate $\mathbf{D}(\underline{V}^f)$ associated with the velocity \underline{V}^f is the intrinsic average of the microscopic strain rate:

$$\mathbf{D}(\underline{V}^f) = \frac{1}{2} (\mathbf{grad}_x \underline{V}^f + {}^t \mathbf{grad}_x \underline{V}^f) = \frac{1}{\varphi} \langle \mathbf{d} \rangle_f = \bar{\mathbf{d}}^f \quad (1.51)$$

We note that the incompressibility condition $\text{tr} \mathbf{d} = 0$ is upscaled in the form $\text{tr} \mathbf{D} = 0$. Furthermore, substitution of (1.51) in (1.48) yields:

$$\boldsymbol{\Sigma}^f = -\varphi \bar{p}^f \mathbf{1} + 2\varphi \mu^f \mathbf{D}(\underline{V}^f) \quad (1.52)$$

It therefore turns out that the partial stress $\boldsymbol{\Sigma}^f$ which represents, at the macroscopic scale, the internal forces in the fluid phase is identical to the stress in a homogeneous viscous fluid of viscosity $\varphi \mu^f$ which is subjected to the pressure $\varphi \bar{p}^f$. In what follows, we will refer to \bar{p}^f as the macroscopic pressure denoted by P :

$$P = \bar{p}^f \quad (1.53)$$

Finally, it is instructive to determine the solid–fluid interaction volume force \underline{a} for the considered case. To this end, we insert expression (1.52) for the partial

stress Σ^f into the macroscopic balance equation of the fluid (1.41). As the porosity φ is homogeneous, we obtain:

$$\varphi \left(-\underline{\text{grad}}_x P + \mu^f \Delta_x \underline{V}^f + \rho^f \underline{F}^f \right) - \underline{a} = 0 \quad (1.54)$$

where the differential operators, the Laplace operator Δ and the gradient operator $\underline{\text{grad}}$ act on the macroscopic position vector \underline{x} . We will see in Chapter 2 that $\underline{\text{grad}} P$ can be related to the macroscopic fluid velocity (Darcy's law), for which relation (1.54) will provide a means of determining \underline{a} as a function of the macroscopic velocity and its derivatives.

1.4 The Periodic Cell Assumption

1.4.1 Introduction

Natural porous media and particularly geomaterials are disordered materials. These materials are a priori best addressed through the *rev* concept introduced in Section 1.1. Nevertheless, in some situations it will prove helpful to model a microstructure in the framework of periodic media. The idea of the periodic media theory is that the fundamental information concerning the physical properties of the constituents and the morphology of the microstructure can be captured in an elementary cell. Then, a periodic model for the real material can be obtained by filling the entire space with this elementary pattern in a periodic way.

The characteristic size of the elementary cell is a priori of the order of the local inhomogeneity d (see Section 1.1). For clarity and without loss of generality, the periodic framework is hereafter presented with the assumption that the cell is a cube, the edges of which are parallel to the directions $(\underline{e}_1, \underline{e}_2, \underline{e}_3)$ of an orthonormal frame. The edge length a is of the order of d ; U denotes the cubic domain $[0, a] \times [0, a] \times [0, a]$. U_s and U_f respectively denote the solid and fluid domains in U .

As in Section 1.1, we will consider a macroscopic structure of characteristic size L . The scale separation condition still reads $d \ll L$, and means here that the macrostructure comprises a sufficient large number of elementary cells.

In the framework of the periodic assumption, the elementary cell concept is used instead of an *rev*. The elementary cell is not an *rev*, since its characteristic length is not necessarily large with respect to that of the heterogeneities.⁶

The periodic media theory is based on the premise that it is possible to represent spatial variations of a physical quantity as a combination of local

⁶ However, accurate estimates of macroscopic properties in the periodic framework require a refined description of the microstructure within the elementary cell whose size may become larger.

fluctuations at the level of the elementary cell and a drift at the level of the macroscopic structure. This separation is represented by two dimensionless spatial variables, $\underline{Z} = \underline{z}/a$ and $\underline{X} = \underline{z}/L$, which allow a representation of any physical quantity $e(\underline{z})$ in the form $e(\underline{Z}, \underline{X})$. The mathematical way by which \underline{X} is responsible for the long scale drift, and local fluctuations are taken into account through the variable \underline{Z} , is to introduce the condition that $e(\underline{Z}, \underline{X})$ is a periodic function of \underline{Z} for any prescribed value of \underline{X} :

$$(\forall n_1, n_2, n_3 \in \mathbb{N}) \quad e(\underline{Z} + n_1 \underline{e}_1 + n_2 \underline{e}_2 + n_3 \underline{e}_3, \underline{X}) = e(\underline{Z}, \underline{X}) \quad (1.55)$$

This periodicity condition actually proves that the drift δe of e on one period in the direction i is related to the derivative of e with respect to X_i :

$$\delta e = e(\underline{z} + a \underline{e}_i) - e(\underline{z}) = e\left(\underline{Z}, \underline{X} + \frac{a}{L} \underline{e}_i\right) - e(\underline{Z}, \underline{X}) = \frac{a}{L} \frac{\partial e}{\partial X_i} + o\left(\frac{a}{L}\right) \quad (1.56)$$

In fact, \underline{X} appears as the dimensionless counterpart of the macroscopic position vector \underline{x} . In particular, we note that:

$$\frac{1}{L} \frac{\partial}{\partial X_i} = \frac{\partial}{\partial x_i} \Rightarrow \delta e = a \frac{\partial e}{\partial x_i} \quad (1.57)$$

The dimensionless variables \underline{X} and \underline{Z} are now regarded as independent. Taking advantage of the periodicity of e with respect to the ‘fluctuation’ variable \underline{Z} , the average \bar{e} of the physical quantity e is defined by integration *with respect to \underline{Z}* over any elementary cell, while \underline{X} is regarded as a constant. More precisely, let U_Z denote the domain obtained by applying the transformation $Z_i = z_i/a$ to the elementary cell U . In other words, U_Z is the cubic domain $[0, 1] \times [0, 1] \times [0, 1]$. The average \bar{e} is:

$$\bar{e}(\underline{X}, t) = \int_{U_Z} e(\underline{Z}, \underline{X}, t) dV_Z \quad (1.58)$$

By construction, we thus define \bar{e} as a macroscopic quantity which depends only on the ‘drift’ variable \underline{X} .

In turn, the apparent average $\langle e \rangle_\alpha$ is defined by analogy with (1.8) as $\overline{\chi^\alpha e}$:

$$\langle e \rangle_\alpha(\underline{X}, t) = \int_{U_Z} (\chi^\alpha e)(\underline{Z}, \underline{X}, t) dV_Z \quad (1.59)$$

Furthermore, the intrinsic average \bar{e}^α is defined by analogy with (1.9). Hence, for the fluid:

$$\bar{e}^f(\underline{X}, t) = \frac{1}{\varphi} \int_{U_Z} (\chi^f e)(\underline{Z}, \underline{X}, t) dV_Z \quad (1.60)$$

Since the reference microstructure is itself periodic, the characteristic function χ^α in the reference state is periodic as well. However, in the case of a

deformable solid phase, χ^α becomes a function of time and can also depend on the drift variable \underline{X} if the microscopic displacement does.

The idea to define the average by integration over a period aims at capturing all the information available on the morphology of the microstructure as well as the physical properties of the constituents. The integral in (1.58), however, is performed on the period corresponding to the reference (i.e. non-deformed) state, which restricts its application to small perturbations of the geometry of the microstructure. In particular, the dependence of χ^α with respect to the drift variable is disregarded.

The following chain rule for differentiation is the starting point for the derivation of the periodic counterpart of (1.19), (1.22) and (1.24):

$$\frac{\partial e}{\partial z_i} = \frac{1}{a} \frac{\partial e}{\partial Z_i} + \frac{1}{L} \frac{\partial e}{\partial X_i} \quad (1.61)$$

Given the scale separation condition $d \ll L$, and the fact that a is on the order of d , it could be appealing to consider in the total spatial derivation the first term on the r.h.s., i.e. the fluctuation term $(1/a)(\partial e/\partial Z_i)$, as dominant over the drift term $(1/L)(\partial e/\partial X_i)$. This depends, however, on the function $e(\underline{Z}, \underline{X})$. To illustrate this purpose, consider in a one-dimensional setting the displacement $\xi(z) = u(X) + \delta^n v(Z)$, where $\delta = a/L$. Application of the chain rule (1.61) yields the linearized strain:

$$\varepsilon = \frac{\partial \xi}{\partial z} = \frac{1}{L} \left(\delta^{n-1} \frac{dv}{dZ} + \frac{du}{dX} \right) \quad (1.62)$$

Given $a \ll L$, and provided that dv/dZ and du/dX are on the same order of magnitude, we observe indeed, for $n = 0$, that the fluctuation term dominates the drift term in the total spatial derivative. On the other hand, for $n = 1$, both terms may be equally important; for higher values $n \geq 2$, the drift term dominates the fluctuation term.

1.4.2 Spatial and Time Derivative of \bar{e} in the Periodic Case

Integrating the chain rule (1.61) with respect to \underline{Z} , we obtain:

$$\int_{U_Z} \frac{\partial e}{\partial z_i} dV_Z = \frac{1}{a} \int_{U_Z} \frac{\partial e}{\partial Z_i} dV_Z + \frac{1}{L} \int_{U_Z} \frac{\partial e}{\partial X_i} dV_Z \quad (1.63)$$

The first integral on the r.h.s. is transformed into a surface integral over the cell boundary:

$$\int_{U_Z} \frac{\partial e}{\partial Z_i} dV_Z = \int_{\partial U_Z} e n_i dS_Z \quad (1.64)$$

which is equal to zero because of the periodicity condition (1.55). On the other hand, the second integral on the r.h.s. in (1.63) can be developed in the form:

$$\int_{U_Z} \frac{\partial e}{\partial X_i} dV_Z = \frac{\partial}{\partial X_i} \left(\int_{U_Z} e(\underline{Z}, \underline{X}, t) dV_Z \right) = \frac{\partial}{\partial X_i} (\bar{e}) \quad (1.65)$$

Thus, the periodic counterpart of (1.24) is:

$$\frac{\overline{\partial e}}{\partial z_i} = \frac{1}{L} \frac{\partial}{\partial X_i} (\bar{e}) = \frac{\partial}{\partial x_i} (\bar{e}) \quad (1.66)$$

As in Section 1.3.2, this equation can be used to derive the link between the microscopic stress field and the macroscopic stress tensor. Indeed, by letting $e = \sigma_{ij}$ in (1.66), identical results are obtained, namely $\Sigma = \bar{\sigma}$. Similarly, the upscaling rules (1.33), (1.34) and (1.35) concerning the fluid velocities can be extended to the periodic case.

Lastly, the average rule concerning the time derivative is straightforward:

$$\frac{\partial}{\partial t} (\bar{e}) = \int_{U_Z} \frac{\partial e}{\partial t} (\underline{Z}, \underline{X}, t) dV_Z = \overline{\frac{\partial e}{\partial t}} \quad (1.67)$$

1.4.3 Spatial and Time Derivative of $\langle e \rangle_\alpha$ in the Periodic Case

The spatial derivative $\langle e \rangle_\alpha$ is developed here for the fluid phase. We recall that the geometry changes of the solid–fluid interface are neglected. This implies that the characteristic function χ^f of the fluid domain is a periodic function. Hence, it depends only on \underline{Z} and not on the drift variable \underline{X} . Applying definition (1.59), we thus obtain:

$$\frac{\partial}{\partial X_i} (\langle e \rangle_f) = \int_{U_Z} \frac{\partial}{\partial X_i} (\chi^f e) dV_Z = \int_{U_Z} \chi^f(\underline{Z}) \frac{\partial e}{\partial X_i} dV_Z \quad (1.68)$$

The chain rule (1.61) integrated over the fluid domain in the elementary cell U_Z gives:

$$\begin{aligned} \left\langle \frac{\partial e}{\partial z_i} \right\rangle_f &= \int_{U_Z} \chi^f(\underline{Z}) \frac{\partial e}{\partial z_i} dV_Z \\ &= \frac{1}{a} \int_{U_Z} \chi^f(\underline{Z}) \frac{\partial e}{\partial Z_i} dV_Z + \frac{1}{L} \int_{U_Z} \chi^f(\underline{Z}) \frac{\partial e}{\partial X_i} dV_Z \end{aligned} \quad (1.69)$$

In order to calculate the first integral on the r.h.s., we observe that:

$$\chi^f \frac{\partial e}{\partial Z_i} = \frac{\partial}{\partial Z_i} (\chi^f e) - e \frac{\partial \chi^f}{\partial Z_i} \quad (1.70)$$

As in Section 1.2.2, the above identity must be understood in the sense of the distribution theory, since it involves the derivatives of the discontinuous function χ^f . In addition, the fact that $\chi^f e$ is a periodic function of the fluctuation

variable \underline{Z} implies that:

$$\int_{U_Z} \frac{\partial}{\partial Z_i} (\chi^f e) dV_Z = \int_{\partial U_Z} n_i^Z \chi^f e dS_Z = 0 \quad (1.71)$$

Let \mathcal{I}_Z^{sf} be the image of the solid–fluid interface \mathcal{I}^{sf} in U obtained by the transformation $Z_i = z_i/a$. Recalling that χ^f does not depend on the drift variable \underline{X} , the derivative of the discontinuous function χ^f in (1.70) can be determined as in (1.18):

$$\frac{\partial \chi^f}{\partial Z_i} = -n_i^Z \delta_{\mathcal{I}_Z^{sf}}(\underline{Z}) \quad (1.72)$$

where n_i^Z are the components of the unit normal to the interface \mathcal{I}_Z^{sf} oriented towards the solid. Substituting (1.69), (1.70), (1.71) and (1.72) into (1.68) yields the periodic counterpart of (1.19):

$$\begin{aligned} \frac{\partial}{\partial x_i} \langle (e)_f \rangle &= \frac{1}{L} \frac{\partial}{\partial X_i} \langle (e)_f \rangle = \left\langle \frac{\partial e}{\partial z_i} \right\rangle_f - \frac{1}{a} \int_{\mathcal{I}_Z^{sf}} e n_i^Z dS_Z \\ &= \left\langle \frac{\partial e}{\partial z_i} \right\rangle_f - \frac{1}{|U|} \int_{\mathcal{I}^{sf}} e n_i dS_Z \end{aligned} \quad (1.73)$$

Finally, the time derivative of an apparent average is derived as in (1.21):

$$\frac{\partial}{\partial t} \langle (e)_f \rangle(\underline{x}, t) = \left\langle \frac{\partial e}{\partial t} \right\rangle_f + \int_{U_Z} \frac{\partial \chi^f}{\partial t} e dV_Z \quad (1.74)$$

The second term on the r.h.s. of (1.74) accounts for the velocity \underline{u} of the solid–fluid interface, and reduces to \underline{u}/a in the domain of dimensionless coordinates. Hence, the periodic counterpart of (1.22) is:

$$\begin{aligned} \frac{\partial}{\partial t} \langle (e)_f \rangle(\underline{x}, t) &= \left\langle \frac{\partial e}{\partial t} \right\rangle_f + \frac{1}{a} \int_{\mathcal{I}_Z^{sf}} e (\underline{u} \cdot \underline{n}) dS_Z \\ &= \left\langle \frac{\partial e}{\partial t} \right\rangle_f + \frac{1}{|U|} \int_{\mathcal{I}^{sf}} e (\underline{u} \cdot \underline{n}) dS_Z \end{aligned} \quad (1.75)$$

The previous relations, (1.73) and (1.75), are readily employed for extending the upscaling rules of partial stresses (see Section 1.3.2) to the periodic case.

1.4.4 Application: Micro- versus Macroscopic Compatibility

One question which comes immediately to mind when micro-to-macro approaches are applied to deformable media is the question of geometrical compatibility on both scales. To address this question, we first postulate⁷ that

⁷ A detailed discussion is given in Sections 4.2.3 and 4.2.5.

the macroscopic linearized strain tensor $\mathbf{E}(\underline{x})$ is the volume average of the linearized microscopic strains $\varepsilon(\underline{z})$:

$$\mathbf{E}(\underline{x}) = \overline{\varepsilon(\underline{z})} \quad (1.76)$$

A necessary condition for the validity of an average relation of the form (1.76) is that the geometrical compatibility of the microscopic strain field $\varepsilon(\underline{z})$ entails the geometrical compatibility of the macroscopic strain tensor $\mathbf{E}(\underline{x})$. The microscopic conditions of geometrical compatibility are:

$$\frac{\partial^2}{\partial z_k \partial z_l}(\varepsilon_{ij}) + \frac{\partial^2}{\partial z_i \partial z_j}(\varepsilon_{kl}) - \frac{\partial^2}{\partial z_j \partial z_l}(\varepsilon_{ik}) - \frac{\partial^2}{\partial z_i \partial z_k}(\varepsilon_{jl}) = 0 \quad (1.77)$$

and their macroscopic counterparts are:

$$\frac{\partial^2}{\partial x_k \partial x_l}(E_{ij}) + \frac{\partial^2}{\partial x_i \partial x_j}(E_{kl}) - \frac{\partial^2}{\partial x_j \partial x_l}(E_{ik}) - \frac{\partial^2}{\partial x_i \partial x_k}(E_{jl}) = 0 \quad (1.78)$$

with $i, j, k, l = 1, 2, 3$. A proof of this result can be obtained with (1.24) (resp. (1.66)). It comprises two identical steps. First, this identity is applied to $e = \varepsilon_{ij}$ and gives:

$$\frac{\partial \overline{\varepsilon_{ij}}}{\partial z_k} = \frac{\partial}{\partial x_k}(\overline{\varepsilon_{ij}}) = \frac{\partial}{\partial x_k}(E_{ij}) \quad (1.79)$$

The second step consists of applying the same identity to $e = \partial \varepsilon_{ij} / \partial z_k$. We now obtain:

$$\frac{\partial}{\partial z_l} \left(\frac{\partial \overline{\varepsilon_{ij}}}{\partial z_k} \right) = \frac{\partial}{\partial x_l} \left(\frac{\partial \overline{\varepsilon_{ij}}}{\partial z_k} \right) \quad (1.80)$$

Finally, a combination of (1.79) and (1.80) yields:

$$\frac{\partial}{\partial z_l} \left(\frac{\partial \overline{\varepsilon_{ij}}}{\partial z_k} \right) = \frac{\partial^2}{\partial x_k \partial x_l}(E_{ij}) \quad (1.81)$$

Hence, the macroscopic compatibility (1.78) is a direct consequence of (1.81).

It is instructive to note that the previous result could have been directly obtained by application of relation (1.24) with a microscopic displacement $e = \xi_j(\underline{z})$ associated with the microscopic strain field $\varepsilon(\underline{\xi}) = \frac{1}{2}(\mathbf{grad}_{z\underline{\xi}} \xi + {}^t \mathbf{grad}_{z\underline{\xi}} \xi)$, as follows:

$$\varepsilon(\underline{\xi}) = \overline{\varepsilon(\underline{\xi})} = \mathbf{E}(\underline{x}) \quad (1.82)$$

where $\overline{\xi}(\underline{x})$ is the volume average of the microscopic displacement field. In other words, $\mathbf{E}(\underline{x})$ is the strain tensor associated with $\overline{\xi}(\underline{x})$. This immediately ensures the geometrical compatibility of $\mathbf{E}(\underline{x})$.

