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FIFTY YEARS OF THE ARCHIVES OF MECHANICS

On effecting averages and changes of scale via weighting functions

Dedicated to Prof. Henryk Zorski
on the occasion of his 70-th birthday

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WEIGHTING FUNCTIONS can be used to derive continuum equations of balance from molecular considerations, and to obtain equations governing fluid flow through porous media. The methodology of such (scale-dependent) averaging is outlined, and physical implications of specific choices of weighting function are discussed.

1. Introduction

IT IS THE PURPOSE of this note to indicate a procedure by which concepts and governing equations of one description of material behaviour can be related to those of a "coarser" description of this behaviour. The methodology employs weighting functions, and is here exemplified in two contexts. The first concerns the precise derivation of continuum equations of balance for a material system from a microscopic description in which molecules are modelled as interacting point masses. The second involves fluid flow through a porous body. Starting from a small-scale description in which pores are manifest, and flows therein are governed by the Navier–Stokes equation, a corresponding equation is determined for a large-scale description (wherein all fluid-related fields are defined throughout the region occupied by fluid *and* porous body: it is at this scale that Darcy's "law" may apply).

The transition from the discrete viewpoint to its continuum counterpart is treated in Sec. 2. A discussion of the basic physics associated with different choices of weighting function is presented in Sec. 3. Porous body considerations are addressed in Sec. 4. Some applications of the results of Secs. 2 and 4 are outlined in Sec. 6.

2. Continuum relations from a discrete model

Consider a material system $\mathcal{M}$ of distinguishable molecules, modelled as a system of interacting point masses labelled P_i $(i = 1, 2, \ldots, N)$, whose masses, locations, and velocities at time t are denoted by m_i, $\mathbf{x}_i(t)$, and $\mathbf{v}_i(t)$, respectively.

The mass density distribution appropriate to choice w of weighting function is ϱ_w, where

$$\varrho_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i w(\mathbf{x}_i(t) - \mathbf{x}). \tag{2.1}$$

Here w assigns greater contributions to the sum from particles near the geometrical point $\mathbf{x}$ than those far from $\mathbf{x}$: more details will be discussed later. Holding $\mathbf{x}$ fixed,

$$\begin{aligned} \frac{\partial \varrho_w}{\partial t} = \sum_{i=1}^{N} m_i \nabla w.\mathbf{v}_i &= -\sum_{i=1}^{N} m_i \nabla_{\mathbf{x}} w.\mathbf{v}_i \\ &= -\sum_{i=1}^{N} m_i \operatorname{div}_{\mathbf{x}}\{\mathbf{v}_i w\} = -\operatorname{div} \mathbf{p}_w\,, \end{aligned} \tag{2.2}$$

where

$$\mathbf{p}_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i \mathbf{v}_i(t) w(\mathbf{x}_i(t) - \mathbf{x}). \tag{2.3}$$

Defining the corresponding velocity field $\mathbf{v}_w$ (wherever $\varrho_w \neq 0$) by

$$\mathbf{v}_w := \mathbf{p}_w / \varrho_w \tag{2.4}$$

yields, from (2.2) and (2.3), the continuity equation

$$\partial \varrho_w / \partial t + \operatorname{div} \varrho_w \mathbf{v}_w = 0. \tag{2.5}$$

In the foregoing the only restriction upon w is that it be differentiable: to ensure spatial smoothness of ϱ_w and $\mathbf{v}_w$ it should be of class C^1. To make physical sense it is necessary that

$$\int_{\text{all space}} \varrho_w = \text{total mass} = \sum_{i=1}^{N} m_i\,. \tag{2.6}$$

This requirement, in the case of $\mathcal{M}$ consisting of a single particle, mandates

$$\int_{\text{all displacements}} w = 1. \tag{2.7}$$

The normalisation condition (2.7) suffices to deliver (2.6) in general.

Linear momentum balance is obtained by considering the motion of P_i in an inertial frame. This is governed by

$$\sum_{\ell} \mathbf{f}_{i\ell} + \mathbf{b}_i = \frac{d}{dt}\{m_i \mathbf{v}_i\}\,. \tag{2.8}$$

Here $\mathbf{f}_{i\ell}$ denotes the force exerted upon P_i by P_ℓ, $\mathbf{b}_i$ the resultant force on P_i due to external agencies, and the sum is over all $\ell \neq i$. Multiplication of each term by $w(\mathbf{x}_i(t) - \mathbf{x})$ followed by summation over all i yields (see [1] for details)

$$\mathbf{f}_w + \mathbf{b}_w = \frac{\partial}{\partial t}\{\varrho_w \mathbf{v}_w\} + \operatorname{div}\{\widehat{\mathbf{D}}_w + \varrho_w \mathbf{v}_w \otimes \mathbf{v}_w\}. \tag{2.9}$$

Here

$$\mathbf{f}_w(\mathbf{x}, t) := \sum_{i=1}^{N} \sum_{\substack{\ell=1 \\ \ell \neq i}}^{N} \mathbf{f}_{i\ell}(t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.10}$$

$$\mathbf{b}_w(\mathbf{x}, t) := \sum_{i=1}^{N} \mathbf{b}_i(t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.11}$$

and

$$\widehat{\mathbf{D}}_w(\mathbf{x}, t) := \sum_{i=1}^{N} m_i \widehat{\mathbf{v}}_i(\mathbf{x}, t) \otimes \widehat{\mathbf{v}}_i(\mathbf{x}, t) w(\mathbf{x}_i(t) - \mathbf{x})\,, \tag{2.12}$$

where

$$\widehat{\mathbf{v}}_i(\mathbf{x}, t) := \mathbf{v}_i(t) - \mathbf{v}_w(\mathbf{x}, t)\,. \tag{2.13}$$

Using a theorem due to NOLL [2], the existence and explicit form of a tensor $\mathbf{T}_w^-$ such that the interaction force density

$$\mathbf{f}_w = \operatorname{div} \mathbf{T}_w^- \tag{2.14}$$

follows from very mild restriction on the decay of $\mathbf{f}_{i\ell}$ with separation of P_i, P_ℓ (satisfied quite generally by non-ionic molecules). Equations (2.9) and (2.14) yield the usual form of balance

$$\operatorname{div} \mathbf{T}_w + \mathbf{b}_w = \frac{\partial}{\partial t}\{\varrho_w \mathbf{v}_w\} + \operatorname{div}\{\varrho_w \mathbf{v}_w \otimes \mathbf{v}_w\}, \tag{2.15}$$

where the stress tensor

$$\mathbf{T}_w := \mathbf{T}_w^- - \widehat{\mathbf{D}}_w\,. \tag{2.16}$$

In particular, (2.16) demonstrates the separate contributions to stress associated with interactions ($\mathbf{T}_w^-$) and momentum transport ($-\widehat{\mathbf{D}}_w$). Further, the spatial smoothness of each of the continuum fields ϱ_w, $\mathbf{v}_w$, $\mathbf{f}_w$, $\mathbf{b}_w$, $\widehat{\mathbf{D}}_w$ and $\operatorname{div} \mathbf{T}_w^-$ is seen to be precisely the same as that of w.

Energy balance is obtained by scalar multiplication of (2.8) by $w(\mathbf{x}_i(t) - \mathbf{x})\mathbf{v}_i(t)$ followed by summation over all i. A detailed discussion is given in [1] wherein further time averaging is effected, so yielding field values in terms of local space-time averages of molecular quantities.

The foregoing may be compared with the seminal work [3] in which continuum field values were identified with space-time averages of ensemble averages (see [4] for comparison of the two approaches).

3. On the nature of the weighting function

The results obtained in Sec. 2 are only formal, since the only restrictions placed upon the weighting function were its C^1 smoothness and normalisation. Some physically sensible criteria and possible choices are now listed.

1. Defining

$$
\begin{aligned}
w(\mathbf{r}) &:= \frac{3}{4\pi r^3} \quad \text{if} \quad r := |\mathbf{r}| < \varepsilon, \\
w(\mathbf{r}) &:= 0 \qquad \text{if} \quad |\mathbf{r}| \geq \varepsilon
\end{aligned}
\tag{3.1}
$$

it is clear that w is normalised, and $\varrho_w(\mathbf{x}, t)$ represents the mass of those particles lying at time t within a sphere centred at $\mathbf{x}$ with radius ε divided by the volume of this sphere. This choice is simple, intuitive, and explicitly scale-dependent. However, wherever $|\mathbf{r}| = \varepsilon$ this function is discontinuous. It is a simple matter to "mollify" w over an interval $(\varepsilon, \varepsilon + \delta)$ in such a way that w is of arbitrary given smoothness everywhere, with $\delta(> 0)$ arbitrarily small (see [1], p. 160). Accordingly the above physical interpretation of $\varrho_w(\mathbf{x}, t)$ is essentially unchanged for small enough choice of δ.

2. The spherical averaging region associated with choice (3.1) can be generalised to that of a "cell" whose geometry is appropriate to the system of interest. For example, near planar interfaces and boundaries it is useful to consider rectangular box-shaped regions with one pair of faces parallel to the interface or boundary in question. More precisely, in such case w is a mollified version of a multiple of the characteristic function for the region: the factor approximates the reciprocal of the volume of the region, is mandated by normalisation, and depends on the thickness of the mollifying envelope.

3. Values of fields ϱ_w, $\mathbf{p}_w$, $\mathbf{f}_w$ and $\mathbf{b}_w$ are biased local volume averages of molecular quantities, and may be compared with appropriate measurement values. Since actual *local* measurements reflect local space-*time* averages (no measurement is either instantaneous or localised in a region of zero volume measure), it

is time-averaged versions of these fields that are relevant. Further, different measuring devices associated with the same physical quantity are to be expected to deliver different "sampling" of molecular behaviour and as such may be identified with different weighting functions (both in space *and* time). Such considerations accord with the practical problem of calibrating different instruments which purport to measure the same quantity.

4. Averaging via weighting functions may be repeated, by defining the w-average, f_w, of a spatial field f *via*

$$f_w(\mathbf{x}) := \int_{\text{all space}} f(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y} . \tag{3.2}$$

This accords with microscopic averages computed in Sec. 2 upon writing discrete (that is, purely microscopic) quantities in terms of distributions. For example, the microscopic mass density (at any given instant: time-dependence is suppressed)

$$\varrho_{\text{mic}}(\mathbf{x}) := \sum_{i=1}^{N} m_i \delta(\mathbf{x}_i - \mathbf{x}) , \tag{3.3}$$

where δ denotes the three-dimensional Dirac distribution. Clearly, from (3.2), (3.3) and (2.1),

$$(\varrho_{\text{mic}})_w = \varrho_w . \tag{3.4}$$

Upon repeating a w-average it is natural to compare $(f_w)_w$ with f_w. If one requires that repeated averaging yields nothing new, that is if

$$(f_w)_w = f_w , \tag{3.5}$$

then the form of w may be determined (see [1], p. 161). In unbounded domains the convolution format of (3.2) implies that the Fourier transform $\overline{w}(\mathbf{k})$ of w should satisfy

$$\overline{w}(\mathbf{k})^2 = \overline{w}(\mathbf{k}) . \tag{3.6}$$

Thus $\overline{w}(\mathbf{k}) = 0$ or 1 and the simplest (and most physical) choice is for a wave-vector "cut-off", say at $|\mathbf{k}| = \varepsilon^{-1}$ for some choice of length scale ε. That is,

$$\overline{w}(\mathbf{k}) = 1 \quad \text{if} \quad |\mathbf{k}| < \varepsilon^{-1}, \qquad \overline{w}(\mathbf{k}) = 0 \quad \text{if} \quad |\mathbf{k}| \geq \varepsilon^{-1}. \tag{3.7}$$

In such case it follows that

$$w(d) = \frac{1}{2\pi^2 d^3} \left\{ \sin\left(\frac{d}{\varepsilon}\right) - \left(\frac{d}{\varepsilon}\right) \cos\left(\frac{d}{\varepsilon}\right) \right\} , \tag{3.8}$$

where

$$d := |\mathbf{d}|\,. \tag{3.9}$$

The analogue for a bounded rectangular region of dimensions $2L_1 \times 2L_2 \times 2L_2$ yields truncated (at wavelength ε) multiple Fourier series which are delivered by

$$w(\mathbf{d}) := \frac{1}{8L_1L_2L_3} \prod_{i=1}^{3} \frac{\sin\left(\left(N_i + \frac{1}{2}\right) d_i\right)}{\sin(d_i/2)}\,, \tag{3.10}$$

where N_i is the integral part of $2L_i/\varepsilon$ and $\mathbf{d} = (d_1, d_2, d_3)$. A consequence of using (scale-dependent) weighting functions of form (3.8) or (3.10) is that averaging at scale ε_1 followed by a further averaging at scale ε_2 yields the same result as merely averaging once at the larger of the two scales.

4. Flow through a rigid porous body saturated with an incompressible fluid

Fluid flow through porous media is best described in terms of fields which are defined both in the region occupied by the fluid *and* that occupied by the porous body itself. Such an "immiscible mixture" approach (see [5]) derives from working at a scale ε_2 large compared with typical pore size and structural dimension. It is instructive to motivate the relevant equations by examining the actual flow in the pores, observed at a scale ε_1, say. The ε_2-scale equations may be obtained by averaging the (ε_1-scale) equations which govern pore flow, at least in principle. For incompressible fluid saturating pore space such a procedure is simple and elucidating.

For a Newtonian fluid, flow is governed by the Navier–Stokes equation

$$-\nabla P + \frac{\mu}{\varrho_0}\Delta\mathbf{p} + \varrho_0\mathbf{g} = \frac{\partial \mathbf{p}}{\partial t} + \frac{1}{\varrho_0}\operatorname{div}(\mathbf{p}\otimes\mathbf{p}). \tag{4.1}$$

Here P denotes pressure, μ viscosity, ϱ_0 mass density, $\mathbf{p}$ momentum density, and $\mathbf{g}$ gravitational acceleration. The w-average of any field f associated with the fluid is given by (3.2) where f is considered to be zero outside the region $\mathcal{E}_f$ occupied by fluid at scale ε_1 (more specifically, $\mathcal{E}_f$ is the support of the ε_1-scale mass density function ϱ_0). In averaging individual terms of (4.1) it is possible to relate averages of derivatives to derivatives of averages (see [6]). In particular, upon suppressing time-dependence and writing

$$\overline{f} := f_w \tag{4.2}$$

it turns out that

$$\overline{\nabla P}(\mathbf{x}) = (\nabla \overline{P})(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} P(\mathbf{y})\mathbf{n}(\mathbf{y})w(\mathbf{y}-\mathbf{x})\,dA_{\mathbf{y}}\,, \tag{4.3}$$

where

$$\mathcal{S}(\mathbf{x}) := \partial\mathcal{E}_f \cap \text{ support } (w(. - \mathbf{x})), \tag{4.4}$$

and $\mathbf{n}$ is that unit normal to the pore boundary $\partial\mathcal{E}_f$ directed *out* of the fluid region $\mathcal{E}_f$. If w corresponds to choice 1 of Sec. 3, then $\mathcal{S}(\mathbf{x})$ denotes that portion of the pore boundary within a sphere of radius $\varepsilon + \delta$ centred at $\mathbf{x}$. In this context averaging is often effected over so-called elementary representative volumes (see [7]) so that w corresponds to such a choice of "cell" (see choice 2 of Sec. 3). Further, noting that $\mathbf{p}$ vanishes on $\partial\mathcal{E}_f$ (this is the standard "no slip" hypothesis),

$$\overline{\Delta\mathbf{p}}(\mathbf{x}) = (\Delta\overline{\mathbf{p}})(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} \nabla\mathbf{p}(\mathbf{y})\mathbf{n}(\mathbf{y})w(\mathbf{y} - \mathbf{x})\, dA_{\mathbf{y}} \tag{4.5}$$

and

$$\overline{\operatorname{div}(\mathbf{p} \otimes \mathbf{p})} = (\operatorname{div}(\overline{\mathbf{p} \otimes \mathbf{p}})). \tag{4.6}$$

Finally,

$$\left\{\overline{\frac{\partial\mathbf{p}}{\partial t}}\right\} = \frac{\partial\overline{\mathbf{p}}}{\partial t} \qquad \text{and} \qquad \overline{\varrho}_0 = \varrho_0\nu, \tag{4.7}$$

where ν denotes the porosity field.

Multiplication of (4.1) (evaluated at point $\mathbf{y}$) by $w(\mathbf{y} - \mathbf{x})$ and integrating over all space yield, upon invoking results (4.3)–(4.7),

$$-\nabla\overline{P} + \frac{\mu}{\varrho_0}\Delta\overline{P} - \operatorname{div}\mathcal{D} + \mathbf{f}^{fp} + \varrho_0\nu\mathbf{g} = \frac{\partial\overline{\mathbf{p}}}{\partial t} + \operatorname{div}\left(\frac{1}{\varrho_0\nu}\overline{\mathbf{p}} \otimes \overline{\mathbf{p}}\right). \tag{4.8}$$

Here

$$\mathcal{D} := \frac{1}{\varrho_0}\overline{\mathbf{p} \otimes \mathbf{p}} - \frac{1}{\varrho_0\nu}\overline{\mathbf{p}} \otimes \overline{\mathbf{p}} \tag{4.9}$$

is the extra contribution to the pressure tensor $\overline{P}\mathbf{1}$ associated with re-scaling, and

$$\mathbf{f}^{fp} := \int_{\mathcal{S}} \left(-P\mathbf{1} + \frac{\mu}{\varrho_0}\nabla\mathbf{p}\right)\mathbf{n}w\, dA \tag{4.10}$$

denotes the force density associated with the effect of the porous body on the fluid. (It is of interest to note that if the fluid is at rest and the pressure P constant then $\mathbf{f}^{fp}$ reduces to $P\nabla\nu$.)

It is useful in this context to introduce the volume flux vector

$$\mathbf{Q} := \varrho_0^{-1}\mathbf{p}. \tag{4.11}$$

Writing

$$\widehat{\mathbf{f}}^{fp} := -\int_S P\mathbf{n}w\, dA \tag{4.12}$$

and

$$\mu\tilde{\mathbf{f}}^{fp} := \mathbf{f}^{fp} - \widehat{\mathbf{f}}^{fp}, \tag{4.13}$$

and making the constitutive assumption

$$\tilde{\mathbf{f}}^{fp} = -\nu\mathbf{K}^{-1}(\mathbf{V}^f - \mathbf{V}^p), \tag{4.14}$$

where

$$\mathbf{V}^f := \overline{\mathbf{p}}/\overline{\varrho} = \nu^{-1}\mathbf{Q}$$

denotes the ε_2-scale fluid velocity field and $\mathbf{V}^p$ the corresponding porous body velocity field, (4.8) becomes

$$\begin{aligned}\operatorname{div}(-\overline{P}\mathbf{1} + \mathcal{D}) + \mu\Delta\mathbf{Q} + \widehat{\mathbf{f}}^{fp} - \mu\mathbf{K}^{-1}\mathbf{Q} + \varrho_0\nu\mathbf{g} \\ = \varrho_0\left(\frac{\partial\mathbf{Q}}{\partial t} + \operatorname{div}\left(\frac{1}{\nu}\mathbf{Q}\otimes\mathbf{Q}\right)\right).\end{aligned} \tag{4.15}$$

Here the rigid body has been considered stationary ($\mathbf{V}^p = \mathbf{0}$) and $\mathbf{K}$ denotes the permeability tensor. For steady, uniform, uniaxial flow through an isotropic ($\mathbf{K} = k\mathbf{1}$) homogeneous (k and ν constant) body, (4.15) reduces to

$$\operatorname{div}(-\overline{P}\mathbf{1} - \mathcal{D}) + \widehat{\mathbf{f}}^{fp} - \frac{\mu}{k}\mathbf{Q} + \varrho_0\nu\mathbf{g} = \mathbf{0}. \tag{4.16}$$

If $\mathcal{D} = \widehat{P}\mathbf{1}$, and $\widehat{\mathbf{f}}^{fp}$ and $\varrho_0\nu\mathbf{g}$ are neglected, then (4.16) reduces to Darcy's "Law"

$$\boldsymbol{\Pi} = -\frac{\mu}{k}\mathbf{Q}, \tag{4.17}$$

where $\boldsymbol{\Pi}$ denotes the pressure gradient $\nabla(\overline{P} + \widehat{P})$.

5. Applications

The discussion of Sec. 2, when extended to take account of a further time averaging (at scale Δ, say: see [1], p.171) enables the notion of "reproducible macroscopic behaviour" at a specific pair of length-time scales to be made precise [8]. Further, such considerations form the basis of a Statistical Mechanics

approach [8, 9] to non-equilibrium macroscopically-reproducible behaviour via the definition of a "macroscopic state" at a given length scale, together with projection operator methodology.

The averaging procedure for a porous body outlined in Sec. 4 draws attention to the existence of a highly inhomogeneous interfacial region located at the boundary of the body, and facilitates detailed analysis of uniaxial flow over and within a rectangular slab of porous material subjected to a constant, externally applied, pressure gradient. Such a study elucidates the status of the *ad hoc* slip boundary condition employed for such flows introduced in [10]: see [6].

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