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LECTURE NOTES 7

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Foundations of Continuum Modelling: a Microscopic Perspective with Applications

Centre of Excellence for
Advanced Materials and Structures

WARSAW 2003

AMAS LECTURE NOTES

Production of this volume has been partially supported by the European Commission

Published and distributed by
Institute of Fundamental Technological Research
Świętokrzyska 21, 00-049 Warszawa, Poland

ISSN 1642-0578

Papier offset. kl. III, 70 g, B1
Ark. wyd.: 8,9; ark. druk.: 7,5
Skład w systemie LaTeX: T.G. Zieliński
Oddano do druku: VII 2003; druk ukończono: VIII 2003
Druk i oprawa: Drukarnia Braci Grodzickich, Piaseczno, ul. Geodetów 47a

Contents

Preface

This book contains Lectures on Continuum Mechanics with emphasis on its physical and mathematical foundations.

The lectures are directed towards anyone who wishes to understand fundamental assumptions implicit in the continuum modelling of physical phenomena, and are intended to be of interest to mathematicians, physicists, and engineers.

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Chapter 1

The continuum viewpoint: an introduction

Everyday experience leads us to regard 'matter' as smeared continuously through well-defined spatial regions. For example, looking at a stationary glass of water we sense that both the glass and the water it contains 'occupy' distinct and well-defined regions. Continuum Mechanics is that branch of the physical sciences which adopts *ab initio* such a viewpoint. Specifically, from such a perspective, material behaviour is modelled in terms of continuous 'fields' (that is, continuous functions of position and time) which represent its dominant physical features. Before well-defined mathematical problems can be posed in a given physical context, it is helpful to distinguish four basic and distinct ingredients in their formulation. These are as follows.

(i) The geometric description of the 'motion' of a 'body' (that is, a particular material system regarded from the continuum perspective), together with its consequent 'distortion', must be rendered precise. This aspect is termed **kinematics**.

(ii) Consistent with elementary Newtonian Dynamics, an appropriate concept of force must be developed for a deformable body, and related to its motion. It may prove helpful here to recall Newton's laws as applied to the motions of point masses. These laws can be used to motivate the basic 'principles' of rigid body dynamics. In our context matters are more complex since the bodies may deform, and account must accordingly be taken of forces *within* a body. In particular, it is necessary to postulate a relation which governs the time evolution of momentum.

This relation is described as the **balance of (linear) momentum**, and is invoked for *any* given body.

(iii) Different bodies can respond quite differently to the same distortion. This is self-evident if one thinks of extending a wire of a given length by a fixed amount: the force necessary to cause such an extension depends upon the material of which the wire is constituted. Thus the internal forces within a given body need to be related to the distortion undergone by the body. This is accomplished via so-called **constitutive relations**. Each such relation models a specific, 'ideal', material.

(iv) Ingredients (i)–(iii) provide, in general, systems of nonlinear differential equations which govern the **dynamics** of a given (ideal) body. Of course, such motion depends upon the initial situation and also upon the interaction of the body with its environment. Accordingly, in order to obtain a complete theory, capable of predicting how a given body will behave in a given set of circumstances, appropriate **initial and boundary value data** must be taken into account.

Remark 1.1. The foregoing considerations have only addressed **mechanical** aspects of material behaviour. In order fully to understand heat transfer (and thermal phenomena in general) it is necessary to extend the theory so as to encompass the notions of internal and kinetic energy, and of entropy. This involves postulating a relation which expresses the time evolution of energy (the so-called **balance of energy**) and a statement concerning the growth of entropy (termed the **entropy inequality**).

Remark 1.2. The best-known continuum theories, which have been shown to provide good models of the actual behaviour of many materials, are those of linearly-viscous (that is, Newtonian) fluids, and of classical (that is, linear and isotropic) elasticity. Historically, continuum theories were developed individually, in an *ad hoc* manner. However, in the last forty five years there has been increasing emphasis on analysing what all such theories have in common, and in delineating at what point they diverge. As indicated in the list of ingredients (i)–(iv), items (i) and (ii) are common to *all* theories. This emphasis on fundamental aspects of continuum modelling has aided the development of theories of rather complex systems and phenomena: for example, viscoelastic effects, liquid crystalline phases, solid-solid phase transitions, shape-memory alloys, crystal growth from melts, chemical reaction kinetics, and fluid-bearing porous media. In turn, considerations of such systems have deepened understanding of the key features of continuum modelling.

In the next chapter basic elements of Continuum Mechanics (ingredients (i) and (ii)) will be motivated and developed, and postulates of the common forms of balances of moment of momentum and energy will be presented. As an independent study of material behaviour this subject suffers from certain physical difficulties which are indicated in Chapter 3. These difficulties stem from the fundamentally-discrete nature in which matter is distributed, in the form of molecules or, more basically, atoms composed of nuclei and electrons. Subsequent chapters are devoted to demonstrating how continuum concepts can be related simply to molecular considerations, and to the manner in which this viewpoint deepens understanding of the continuum approach and elucidates basic aspects of the modelling of porous bodies and of so-called 'mixtures'.

Chapter 2

Some basic elements of continuum mechanics (1)

Basic concepts are outlined in a manner pertinent to what follows, using coordinate-free notation.

A material system of interest is termed a **body** and denoted by $\mathcal{B}$. At any time $t, \mathcal{B}$ is considered to 'occupy' a region B_t of three-dimensional Euclidean space $\mathcal{E}$. Suitably-smooth fields are ascribed to the **trajectory**

$$\mathcal{T} := \{(\mathbf{x}, t) : \mathbf{x} \in B_t,\ t \in I\} \tag{2.1}$$

of $\mathcal{B}$ in space-time, where I denotes the time interval of interest. In particular, the **mass density** $\rho : \mathcal{T} \to \mathbb{R}^+$ and **velocity** $\mathbf{v} : \mathcal{T} \to \mathcal{V}$ ($\mathcal{V}$ denotes the vector space modelling 'vectorial' quantities) have the interpretations that (2)

$$\int_R \rho(.,t) \qquad \text{and} \qquad \int_R \rho(.,t)\,\mathbf{v}(.,t) \tag{2.2}$$

deliver, respectively, the mass and linear momentum associated with the material of $\mathcal{B}$ within a region $R \subset B_t$ at time t. The deformation process undergone by $\mathcal{B}$ is described by the **motion** map χ_0 (relative to the situation

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(1) Cf., e.g., [1, 2, 3].

(2) Unless necessary in the interests of clarity, labelling of ('dummy') variables of integration will be omitted. It will be clear from the domain of integration what kind of integral is involved. Here, since R is a spatial region, volume integrals are intended. Specifically, if f denotes a function of position then $\int_R f$ denotes its integral over region R. Further, $\rho(.,t)$ and $\mathbf{v}(.,t)$ denote those functions of position appropriate to the density and velocity fields at time t.

at some particular time, t_0 say) defined as the (assumed unique) solution to the initial-value problem

$$\chi_0 : B_{t_0} \times I \to \mathcal{E} \tag{2.3}$$

where

$$\dot{\chi}_0(\hat{\mathbf{x}}, t) = \mathbf{v}(\mathbf{x}, t) \tag{2.4}$$

and

$$\mathbf{x} := \chi_0(\hat{\mathbf{x}}, t) \quad \text{with} \quad \hat{\mathbf{x}} = \chi_0(\hat{\mathbf{x}}, t_0). \tag{2.5}$$

Mass conservation corresponds to the relation

$$\int_{R_t} \rho(.,t) = \int_{R_0} \rho(.,t_0) \tag{2.6}$$

for any region $R_0 \subset B_{t_0}$, where

$$R_t := \chi_0(R_0, t). \tag{2.7}$$

Equivalently, changing the left-hand side of (2.6) into an integral over R_0 and re-arranging,

$$\int_{R_0} \{\rho(\chi_0(.,t),t)\, J(.,t) - \rho(.,t_0)\} = 0, \tag{2.8}$$

where J denotes the *Jacobian* associated with χ_0. Modulo continuity of the integrand, relation

$$\rho\big(\chi_0(.,t),t\big)\, J(.,t) = \rho(.,t_0) =: \rho_0 \tag{2.9}$$

holds pointwise on B_{t_0}. Differentiation of (2.9) with respect to time, on noting the non-trivial result

$$\dot{J} = (\operatorname{div} \mathbf{v}) J, \tag{2.10}$$

yields

$$\dot{\rho} + \rho \operatorname{div} \mathbf{v} = 0 \tag{2.11}$$

where, for any function f defined on $\mathcal{T}$ (cf. (2.1)),

$$\dot{f}(\mathbf{x},t) := \frac{d}{dt}\left\{f\big(\chi_0(\hat{\mathbf{x}},t),t\big)\right\} \tag{2.12}$$

(here $\mathbf{x}$ and $\hat{\mathbf{x}}$ are related as in $(2.5)_1$) denotes the so-called **material time derivative** of f. This result is written in abbreviated form as

$$\frac{d}{dt}\{f \circ \chi_0\} = \dot{f} \circ \chi_0. \tag{2.13}$$

Use of the chain rule for functions of several variables yields

$$\dot{f} = \frac{\partial f}{\partial t} + (\nabla f)\mathbf{v}, \tag{2.14}$$

where ∇f denotes the spatial gradient[3] of f. Accordingly, (2.11) is expressible in the form

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{v}) = 0 \tag{2.15}$$

or, on integration, as

$$\frac{d}{dt}\left\{\int_R \rho\right\} = -\int_{\partial R} \rho \mathbf{v} \,.\, \mathbf{n}, \tag{2.16}$$

where R denotes any fixed region with outward unit normal $\mathbf{n}$ to its boundary ∂R. Relation (2.15), often termed the **continuity equation**, is the local expression of **mass conservation**. Equivalently, time differentiation of (2.6) yields

$$\frac{d}{dt}\left\{\int_{R_t} \rho(.,t)\right\} = 0. \tag{2.17}$$

In an inertial frame the evolution of linear momentum associated with R_t (cf. (2.7)) is postulated to take the form

$$\frac{d}{dt}\left\{\int_{R_t} \rho \mathbf{v}\right\} = \int_{\partial R_t} \mathbf{t} + \int_{R_t} \mathbf{b}\,. \tag{2.18}$$

Here $\mathbf{t}$ denotes the **traction** field on ∂R_t, and is conventionally regarded as the force per unit area of ∂R_t exerted by that part of $\mathcal{B}$ outwith R_t upon that part within R_t. The term $\mathbf{b}$ is usually interpreted as the net force per unit volume exerted on $\mathcal{B}$ by external agencies. If $\mathbf{t}$ is assumed to be a continuous function of position and local orientation $\mathbf{n}$ then it is possible to show the existence of a linear transformation (on $\mathcal{V}$) field $\mathbf{T}$ such that

$$\mathbf{t} = \hat{\mathbf{t}}(\mathbf{n}) = \mathbf{T}\mathbf{n}. \tag{2.19}$$

Here $\mathbf{T}$ is independent of $\mathbf{n}$ and is termed the **(Cauchy) stress tensor**. Now (cf. (2.7), (2.9), (2.12) and (2.13))

$$\frac{d}{dt}\left\{\int_{R_t} \rho \mathbf{v}\right\} = \frac{d}{dt}\left\{\int_{R_0} ((\rho \mathbf{v}) \circ \chi_0) J\right\} = \frac{d}{dt}\left\{\int_{R_0} \rho_0 (\mathbf{v} \circ \chi_0)\right\}$$

$$= \int_{R_0} \rho_0 (\dot{\mathbf{v}} \circ \chi_0) = \int_{R_0} (\rho \mathbf{a}) \circ \chi_0 \, J = \int_{R_t} \rho \mathbf{a}, \tag{2.20}$$

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[3] If f is a scalar, ∇f is merely grad f; if f is a tensor with Cartesian components $f_{ij\ldots p}$ then ∇f is the tensor with components $(\nabla f)_{ij\ldots pq} = f_{ij\ldots p,q}$.

where the **acceleration** field

$$\mathbf{a} := \dot{\mathbf{v}}\,. \tag{2.21}$$

From (2.18), (2.19) and (2.20),

$$\int_{\partial R_t} \mathbf{T}\mathbf{n} + \int_{R_t} \mathbf{b} = \int_{R_t} \rho\mathbf{a}, \tag{2.22}$$

or, locally, [4]

$$\operatorname{div}\mathbf{T} + \mathbf{b} = \rho\mathbf{a}\,. \tag{2.23}$$

Using (2.21), (2.14) and (2.15) this may be expressed as

$$\operatorname{div}\mathbf{T} + \mathbf{b} = \frac{\partial}{\partial t}\,\{\rho\mathbf{v}\} + \operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}). \tag{2.24}$$

Relation (2.22) is termed the *balance of (linear) momentum* for region R_t and (2.24) the local form of such balance.

Two further balance relations, for moment of momentum, and energy, are commonly postulated which (when supplemented by constitutive relations: for example, those of linearly-viscous fluids, or elastic materials) lead to excellent models for the behaviour of many materials. However, these relations are not compatible with the macroscopic behaviour of *all* materials. Indeed, they do not adequately describe the behaviour of, for example, liquid crystalline phases, or highly inhomogeneous bodies. The reason for such shortcoming will be evident when a molecular perspective is adopted. For subsequent comparison the usual forms of these balance relations are now given.

Moment of momentum balance (about point $\mathbf{x}_0$):

$$\int_{\partial R_t} \mathbf{r}\times\mathbf{t} + \int_{R_t} \mathbf{r}\times\mathbf{b} = \frac{d}{dt}\left\{\int_{R_t} \mathbf{r}\times\rho\mathbf{v}\right\}. \tag{2.25}$$

Here $\mathbf{r}$ denotes the displacement of a point in R_t from $\mathbf{x}_0$: that is, if $\mathbf{x}\in R_t$ then

$$\mathbf{r}(\mathbf{x}) := \mathbf{x} - \mathbf{x}_0. \tag{2.26}$$

Energy balance:

$$\int_{\partial R_t} (\mathbf{t}\,.\,\mathbf{v} + q) + \int_{R_t} (\mathbf{b}\,.\,\mathbf{v} + r) = \frac{d}{dt}\left\{\int_{R_t} \rho(\mathbf{v}^2/2 + e)\right\}. \tag{2.27}$$

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[4] In Cartesian tensor notation, $(\operatorname{div}\mathbf{T})_i := T_{ij,j}$.

Here q denotes the rate of heat supply per unit area to matter inside R_t by conduction across its boundary ∂R_t, r represents the rate of heat supply per unit volume of R_t due to radiation, and e symbolises the specific internal energy (that is, the 'stored energy' per unit mass). Together the (macroscopic) kinetic energy density $\rho \mathbf{v}^2/2$ and internal energy density ρe yield the total energy per unit volume of the material.

Remark 2.1. If (2.25) is postulated to hold for a single point, $\mathbf{x}_0$ say, then it will hold for *all* points as a consequence of (2.22). If (2.25) is postulated to hold for *all* points then (2.22) may be deduced. [Prove these assertions!]

Remark 2.2. Using (2.19) it is possible to show that if q is a continuous function of position and $\mathbf{n}$ (cf. (2.19)) then there exists a vector field $\mathbf{q}$, independent of $\mathbf{n}$, such that

$$q = \hat{q}(\mathbf{n}) = -\mathbf{q}\,.\,\mathbf{n}. \qquad (2.28)$$

Vector field $\mathbf{q}$ is termed the **heat flux vector**: $-\mathbf{q}\,.\,\mathbf{n} = \mathbf{q}\,.(-\mathbf{n})$ represents the rate at which heat crosses an oriented surface, with unit normal field $\mathbf{n}$, in the direction of $-\mathbf{n}$ (in the present context *into* region R_t).

Remark 2.3. Using (2.19) and (2.23), the local form of (2.25) is

$$\mathbf{T} = \mathbf{T}^{\mathrm{T}}. \qquad (2.29)$$

Conversely, if (2.29) holds then so does (2.25). Thus the adoption of (2.25) is *equivalent* to the assumption that the stress tensor takes symmetric values. Accordingly the deduction of (2.29) from (2.25) cannot be regarded as a *proof* of such symmetry: the two stand or fall together.

Remark 2.4. Using (2.19), (2.28) and (2.23) the local form of (2.27) can be shown to be

$$r - \operatorname{div}\mathbf{q} + \mathbf{T}\cdot\mathbf{L} = \rho\dot{e}. \qquad (2.30)$$

Here

$$\mathbf{L} := \nabla\mathbf{v} \qquad (2.31)$$

denotes the velocity gradient and $\mathbf{T}\cdot\mathbf{L}$ the inner product of tensor fields $\mathbf{T}$ and $\mathbf{L}$. In Cartesian co-ordinates with respect to ordered orthonormal basis $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$,

$$L_{ij} := \mathbf{e}_i\,.\,\mathbf{L}\mathbf{e}_j = v_{i,j} \qquad (2.32)$$

and

$$\mathbf{T} \cdot \mathbf{L} = T_{ij}\, L_{ij}. \tag{2.33}$$

In $(2.32)_2$, $v_{i,j}$ denotes the (partial) derivative of $v_i (:= \mathbf{v} \,.\, \mathbf{e}_i)$ with respect to the 'j'th spatial argument, and in (2.33) summation over both suffices i and j from 1 to 3 is intended.

Remark 2.5. As examples of how the foregoing is related to well-established theory we cite three simple examples.

(i) Consider a compressible inviscid fluid in a gravitational field $\mathbf{g}$ and at a uniform temperature. Here

$$\mathbf{T} = -\hat{p}(\rho)\mathbf{1}, \quad \mathbf{b} = \rho\mathbf{g}, \tag{2.34}$$

and (2.23) reduces to

$$-\hat{p}'(\rho)\nabla\rho + \rho\mathbf{g} = \rho\mathbf{a}. \tag{2.35}$$

For steady flow $\partial\mathbf{v}/\partial t = \mathbf{0}$ so (see (2.14))

$$-\hat{p}'\nabla\rho + \rho\mathbf{g} = \rho(\nabla\mathbf{v})\mathbf{v}. \tag{2.36}$$

If $\mathbf{g} = -g\mathbf{e}_3$ (so $\mathbf{e}_3$ is directed vertically up and $\mathbf{g} = \nabla(-gx_3)$) and the flow is irrotational, so

$$\nabla\mathbf{v} = \nabla\mathbf{v}^{\mathrm{T}}, \tag{2.37}$$

then (2.36) may be written as

$$\rho\nabla\left\{\mathbf{v}^2/2 + gx_3 + \int \frac{\hat{p}'(\rho)}{\rho}\, d\rho\right\} = 0. \tag{2.38}$$

Thus

$$\mathbf{v}^2/2 + gx_3 + \int \frac{\hat{p}'(\rho)}{\rho}\, d\rho \quad \text{is spatially constant} \tag{2.39}$$

at any instant.

(ii) For a linearly-viscous incompressible fluid at uniform temperature

$$\mathbf{T} = -p\mathbf{1} + \mu\{\nabla\mathbf{v} + \nabla\mathbf{v}^{\mathrm{T}}\} \tag{2.40}$$

and

$$\rho = \rho_0, \quad \text{constant}. \tag{2.41}$$

Substitution of (2.40) in (2.24), noting from (2.15) and (2.41) that

$$\operatorname{div} \mathbf{v} = 0, \tag{2.42}$$

yields

$$-\nabla p + \mu \Delta \mathbf{v} - \rho_0 \, g \mathbf{e}_3 = \rho_0 \left\{ \frac{\partial \mathbf{v}}{\partial t} + (\nabla \mathbf{v}) \mathbf{v} \right\}. \tag{2.43}$$

Of course, this is the well-known Navier-Stokes equation.

(iii) For a rigid stationary heat conductor (so $\mathbf{v} = \mathbf{0}, \mathbf{L} = \mathbf{0}, \rho = \rho_0$, constant) in which heat conduction is given by the Fourier relation (with constant conductivity k_0)

$$\mathbf{q} = -k_0 \, \nabla \theta, \tag{2.44}$$

where θ denotes absolute temperature, and $e = \hat{e}(\theta)$, (2.30) becomes

$$r + k_0 \, \Delta \theta = \rho_0 \, \hat{e}'(\theta) \frac{\partial \theta}{\partial t}. \tag{2.45}$$

In the absence of radiation and denoting $\hat{e}'(\theta)$ by c (the specific heat at temperature θ), (2.44) becomes the familiar heat conduction equation

$$k_0 \, \Delta \theta = \rho_0 \, c \, \frac{\partial \theta}{\partial t}. \tag{2.46}$$

Chapter 3

Physical difficulties associated with the continuum viewpoint: questions of scale, interpretation, and reproducibility of phenomena

While the continuum viewpoint is consistent with our physical prejudices, engendered by sensory evidence, it gives rise to some conceptual and physical difficulties. Here we outline several of these, and indicate how one is forced into taking account of the fundamentally-discrete nature of matter.

3.1. Mass density

According to $(2.2)_1$, the mass at time t of that part of a body $\mathcal{B}$ lying in any region R within that occupied by the body at this time (namely, B_t) is

$$\int_R \rho(\cdot, t). \tag{3.1}$$

The continuity of $\rho(\cdot, t)$ can be used to prove that for any point $\mathbf{x} \in B_t$,

$$\rho(\mathbf{x}, t) = \lim_{r \to 0} \left\{ \int_{S_r(\mathbf{x})} \frac{\rho(\cdot, t)}{\frac{4}{3}\pi r^3} \right\}. \tag{3.2}$$

[Prove this!] Here $S_r(\mathbf{x})$ denotes that sphere of radius r which is centred at $\mathbf{x}$. That is, $\rho(\mathbf{x}, t)$ is obtained as the limit, as r tends to zero, of the mass in $S_r(\mathbf{x})$ at time t divided by the volume of this sphere. The problem here is that it is well-known that matter is distributed discretely in space, in the form of molecules. These are composed of atoms which in turn are made up of nuclei and electrons. To gain some idea of how little space is actually occupied by matter it should be noted that if a typical nucleus were scaled up to have characteristic dimensions of order 1cm then the nearest electron would be of order 50 m away. Accordingly, most of space is unoccupied by matter and if r is less than the smallest typical nucleus-electron separation then, for nearly all points $\mathbf{x}, \rho(\mathbf{x}, t))$ given by limit (3.2) would be zero. If $\mathbf{x}$ were located *within* a nucleus at time t then the ratio in (3.2) would become enormous as r tends to the characteristic dimension of the nucleus. Since this is not at all what we have in mind for ρ (for example, we think of the density of water being constant at a given temperature, of order 10^3 kgm^{-3}) it is clear that we must revise interpretation (3.1). Clearly, R cannot be too small. The key question is 'how small?' *In particular, we have encountered our first example of a problem associated with length scales.* Of course, no-one would think of applying continuum concepts at length scales at, or below, molecular dimensions. However, given that this is the case, what *are* the length scales appropriate to continuum modelling?

3.2. Velocity

An intuitive notion of the velocity field for a *solid* body may be gained by thinking of 'marking' or 'labelling' points in the region occupied by the body at some fixed time, t_0 say. If the mark at time t_0 is located at point $\hat{\mathbf{x}}$ then χ_0 (see (2.3)) delivers its position at any subsequent time t as point $\mathbf{x}$, where

$$\mathbf{x} = \chi_0(\hat{\mathbf{x}}, t). \tag{3.3}$$

The value of the velocity field $\mathbf{v}$ at the point $\mathbf{x}$ at time t is then the velocity of the mark which instantaneously is located at $\mathbf{x}$ at time t. This is the interpretation of relation (2.4):

$$\mathbf{v}(\mathbf{x}, t) = \dot{\chi}_0(\hat{\mathbf{x}}, t). \tag{3.4}$$

'Marking' can be thought of as 'doping' in some way a number of adjacent molecules in the body. Since in the solid state molecules which are near-neighbours at some time remain near-neighbours, such 'doping' persists in time and 'marks' can be traced. However, in fluid (that is, liquid or vapour) phases such marking cannot be implemented since molecules rapidly change their near-neighbours. One might return to the example of a solid and think of doping *individual* molecules. This would give a reasonable indication of **v** provided that the molecular *thermal* motions were somehow discounted (possibly by time averaging over intervals 'long' on a molecular time scale). If such a procedure were adopted for fluids then **v** would not be continuous since, as indicated above, adjacent molecules have very different velocities. Indeed, water molecules in a stationary glass of water have average *speeds* of order $10^3\,\mathrm{ms}^{-1}$: the continuum velocity everywhere in such case would, of course, be zero. In particular, the velocity field **v** at the location of an individual molecule in a fluid is in no way to be identified with the velocity of this molecule.

Remark. Textbooks on Fluid Dynamics sometimes refer to **v** as the velocity of a fluid 'particle'. This is misleading terminology, since 'particle' usually refers in Mechanics to an isolated physical entity (usually modelled as a point mass) and thus one may be misled into identifying 'particle' with 'molecule'.

Question: *Can we clarify the interpretation of* **v** *in such a way as to be meaningful both for solids and fluids?*

Answer: *In Chapter 4 the notion of velocity will be defined in a manner explicitly involving a length scale and independently of whether the material is solid or fluid.*

3.3. The boundary of a body

In Continuum Mechanics the boundary of a body (that is, the boundary of the region occupied by the body) is a *primitive* concept; that is, it is a basic concept upon which the subject is based yet which is not itself defined. Of course, the boundary of a body at instant t may be regarded as the boundary of the common domain of definition of the functions $\rho(\cdot,t)$ and $\mathbf{v}(\cdot,t)$. However, it is a matter of common experience that the perceived boundary of a body differs according to the manner in which it is observed. Indeed, the closer an observer approaches a body, the more additional surface features can be seen. Use of a microscope renders visible further surface topography. More precisely, for a given resolution of observational apparatus, and given separation s between observer and object, an image of the boundary of a body is obtained in which any features whose characteristic dimensions exceed $2s\sin(\lambda/2) \simeq \lambda s$ can become apparent, but features whose dimensions are smaller than λs cannot be resolved. Thus the smaller λ or s, the finer is the scale of possible detectable boundary topography. The foregoing remarks serve to establish the scale-dependent nature of the boundary of a body: λs may be regarded as the *limiting observational scale* associated with resolution λ and separation s. The perceived boundary depends upon this scale, which is a *continuous* variable. In view of the intimate link between the density field ρ and boundary characterisation it becomes desirable to examine the notion of mass density and to seek a scale-dependent interpretation thereof.

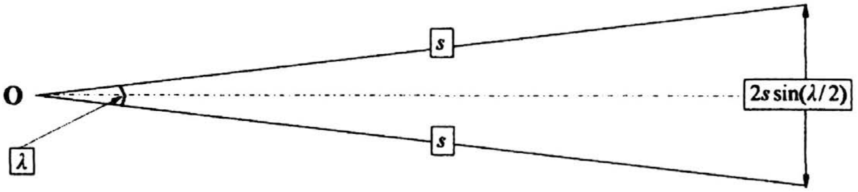

FIGURE 3.1. An observer located at **O** can distinguish features of an object which subtend an angle of λ or greater at **O**; λ is termed the (angle of) resolution for this observer. If λ is small, the smallest feature detectable at a range of s is approximately λs.

3.4. The pressure in a gas

The relationship between molecular behaviour and continuum concepts is often first studied in the context of the kinetic theory of gases. In particular, the pressure on the inner bounding surface of a closed vessel containing gas is explained in terms of gas molecules, modelled as point masses, 'bouncing' off this surface. Each 'impact' of a molecule upon the surface imparts an impulse to this surface equal to the negative of the change in its momentum due to this 'collision'. Summing contributions of those impulses experienced over a portion of the surface and during some period of time, and dividing this sum by the area of surface involved and the duration of the time interval, one obtains the average *stress* (that is, average force per unit area) exerted by the gas upon this subsurface during the time interval in question. If the subsurface is essentially plane, $\mathbf{n}$ denotes that unit normal to this plane directed into the gas, and the average stress is $-p\mathbf{n}(p > 0)$, then this stress is described as a *pressure* p. (Usual arguments consider plane walls and 'elastic' impacts; that is, collisions in which the molecular velocities have their components perpendicular to the wall reversed without change in magnitude, and tangential components unchanged. In such case the stress is always a pressure.)

Now consider linear momentum balance (2.18) for any closed region R lying strictly *within* a closed container containing gas. Here boundary ∂R encloses the geometric region R but as a hypothetical entity has no mechanical attributes. In this case the usual interpretation of

$$\int_{\partial R} \mathbf{t}(\cdot, t) \tag{3.5}$$

is of the resultant *force* (at time t) exerted by gas molecules outside R upon those within R. If the gas is moderately rarefied (this is the case for air molecules in the atmosphere, for example) then individual molecules experience forces due to the proximity of other molecules only rarely. When they do so they modify each other's trajectories and such, brief, interactions are described as 'collisions'. Thus, for a good proportion of the time a molecule is essentially force-free (if the effect of gravity is neglected) and accordingly undergoes rectilinear motion. Indeed, this gives rise to the notion of *mean free path*, which is the average distance a molecule may be expected to travel between collisions. It turns out, as a consequence of the foregoing considerations, that for any subsurface $\mathcal{S}$ of ∂R,

$$\int_{\mathcal{S}} \mathbf{t}(\cdot, t) \tag{3.6}$$

is very small. However, it is also assumed in Continuum Mechanics that, if $\mathbf{x} \in \mathcal{S}$ then in 'equilibrium' situations $\mathbf{t}(\mathbf{x}, t)$ is normal to $\mathcal{S}$ and has magnitude p, where p is the pressure on the inner boundary of the containing vessel. The latter viewpoint is borne out by measurements of pressure inside the container. There thus appears to be a paradox within the continuum viewpoint: the force represented by (3.6) is essentially negligible (on the basis of kinetic theory) yet is apparently non-negligible (on the basis of measurement).

Question: *How can this paradox be resolved?*

Answer: *In Chapters 4 and 5 continuum concepts are derived on the basis of molecular considerations. From such a perspective the interpretation* *of* **t** *is seen to be somewhat less simplistic than that given: such interpretation is the root cause of the paradox.*

3.5. Reproducibility

The understanding of natural phenomena represented by the current state of Science has come about in large measure as the consequence of patterns observed in animate and inanimate (that is, material) behaviour. Such patterns are recognised when relevant conditions are replicated. For example, bodies thrown up into the air are always observed to fall. More specifically, bodies released from rest in an evacuated enclosure fall in what appears to be exactly the same way. Such behaviour is thus *reproducible*: that is, it can be *replicated*. In posing the question of why such reproducibility occurs we are led to the notions of *cause* and *effect*. In the above example, Newtonian dynamics furnishes the cause in terms of force (in particular, the force on the falling body due to gravity) and the effect (or fall) in terms of the motion of the body (in particular, the acceleration of its centre of mass). Any model of reproducible behaviour in which precise knowledge of its cause yields exact information about this behaviour (that is, the relevant 'effect') is termed *deterministic*. Most continuum theories are deterministic.

Now consider a sequence of experiments in which a steel sphere of constant density is released from rest in a large container of stationary water at a constant temperature. If the radius of the sphere is 1cm the motions appear to be reproducible to the extent of being essentially vertical descents of the spheres. It turns out that an entirely satisfactory continuum description is possible when the water is modelled as a Newtonian incompressible liquid and the sphere as a uniform rigid body. However, if the experiments are repeated with spheres of radius 10^{-6}m the behaviour is quite different: the spheres undergo erratic, irreproducible, trajectories before reaching the bottom of the container. Accordingly the deterministic continuum theory is seen to be inappropriate at a length scale far in excess of molecular size (which in this context is $3\,\text{Å} = 3 \times 10^{-10}$m). The above erratic motions are described as *Brownian*, and derive from the inhomogeneous nature of the behaviour of water molecules at scales of 10^{-6}m and below.

Remark. Yet again the question of scale has arisen in the context of the applicability of continuum concepts.

3.6. Summary

The foregoing sections have drawn attention to certain difficulties associated with the continuum viewpoint as presented in Chapter 2. Given these difficulties, their links with molecular considerations, and the fact that matter is actually distributed discretely in space, it becomes desirable to link continuum concepts and relations to microscopic considerations. The aim of such an endeavour is to gain a deeper insight into continuum modelling: specifically, to appreciate assumptions about molecular behaviour *implicit* in the continuum approach, and to ascertain the rôle played by length scales. Further motivation is provided by the realisation that any measurement made on a material system involves sampling the system at some length scale *and* some time scale and hence in some sense must reflect a space-time average involving the molecules of the system. Since measurements are usually identified with continuum field values, it is thus helpful to relate such values to space-time averages of molecular quantities. In Chapters 4 and 5 a possible approach to the linkage of continuum quantities and molecular variables is developed.

Chapter 4

Continuum concepts and relations based upon discrete considerations: mass conservation, motion, body location, linear momentum balance, and the stress tensor

4.1. Introduction

Continuum mechanical modelling provides the theoretic framework within which the results of observations/measurements associated with actual macroscopic behaviour can be interpreted. In this context the following should be noted.

(i) In relating theory to behaviour, observation/measurement values have to be linked with theoretical quantities.

(ii) No 'local' measurement/observation can be either instantaneous or localised at a geometrical point. Indeed, there are associated scales of length and time associated with any such monitoring of a system.[5]

(iii) Local measurement/observation values derive from the behaviour of the fundamental discrete entities (molecules and/or ions) of which the system is constituted.

The foregoing observations motivate a study of the relationship between microscopic behaviour and continuum quantities. More specifically, since the

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[5] **For example, a photographic 'snapshot' reveals information limited by both exposure time and spatial resolution.**

values of local observations/measurements are linked to local space-time averages of ionic/molecular quantities, it is of interest to develop a model in which such linkage is *explicit.* To this end it is necessary to model ions and molecules. Here these are regarded as interacting point masses located at the relevant mass centres. The pairwise interactions are, of course, the result of interactions between systems of atomic nuclei and electrons of which the ions/molecules are constituted.[6] However, no explicit account will here be taken of such fine microstructure.

Remark 4.1. Ions and molecules are distinguished by the nature of the relevant pairwise interactions. Below the scale of average nearest-neighbour atomic separations *all* such interactions are repulsive in character. For separations above the scale of average nearest-neighbour ionic/molecular separations, ion-ion interactions are repulsive or attractive according to whether the ions have the same or opposite polarity, respectively, and the associated magnitudes are proportional to the inverse square of separations. In contrast, interactions between molecules at such scales are always attractive, and decay much more rapidly with separation. A standard model is the so-called Lennard–Jones 6–12 potential in which the force between two molecules contains two contributions: a repulsion proportional to r^{-13} and attraction proportional to r^{-7}, where r denotes the separation of mass centres. (Both contributions are directed along the line joining the mass centres.) Molecule-ion interactions have essentially the same character as intermolecular forces and decay with large separation faster than an inverse square relation. Such considerations are important in deciding whether a relevant stress *tensor* exists.

Any system of interest will, at any given time, consist of a collection of molecules and/or ions. This is formalised by defining a **material system** $\mathcal{M}$ to be an instant-by-instant identifiable set of fundamental discrete entities (ions and/or molecules). Explicit in this definition is the possibility of $\mathcal{M}$ losing or gaining ions and/or molecules as time evolves. (For example, $\mathcal{M}$ might be the set of molecules/ions in liquid phase in an 'open' container. Inevitable evaporation and condensation require that $\mathcal{M}$ be time-dependent

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[6] Interactions (in the sense employed in the following remark) at the scale of ions and molecules are essentially time averages of the resultant electromagnetic forces between the constituent nuclei and electrons of the ions/molecules in question. The time averaging duration is long on any atomic/electronic time scale. Gravitational contributions are negligible.

in this context.) However, for simplicity, in this and the following chapter, balance relations will be derived for time-*independent*[7] systems. Further, only *spatial* averaging will be implemented at this stage. This allows the fundamental spatial averaging procedure to be developed before introducing the additional complexity associated with local averaging jointly in space *and* time.

Summarising, here and in the next chapter, spatial averaging (at an explicit length scale) will be implemented to derive macroscopic continuum balance relations for fixed sets of ions and molecules modelled as interacting point masses.

4.2. Weighted averages and mass conservation

Material system (or 'body') $\mathcal{M}$ is considered to be composed of a fixed, identifiable, set of (N, say) interacting point masses. Labelling these as P_i ($i = 1, 2, \ldots, N$), the mass, location, and velocity of P_i at instant t are denoted by m_i, $\mathbf{x}_i(t)$, and $\mathbf{v}_i(t)$, respectively.

Let the value of an additive molecular[8] quantity (for example, mass, momentum, or kinetic energy) for P_i at instant t be $g_i(t)$. For any geometrical point $\mathbf{x}$ we may define

$$g_w(\mathbf{x}, t) := \sum_{i=1}^{N} g_i(t) w(\mathbf{x}_i(t) - \mathbf{x}), \tag{4.1}$$

where w denotes a function defined on the space $\mathcal{V}$ of all displacements in Euclidean space $\mathcal{E}$. Thus g_w is a *weighted average* of the molecular quantity in question with respect to the **weighting function** w. If w takes positive values with physical dimension $(\text{length})^{-3}$, satisfies

$$\int_{\mathcal{V}} w = 1, \tag{4.2}$$

and takes much larger values for small displacements than for large displacements, then $g_w(\mathbf{x}, t)$ represents a local spatial density of the molecular quantity concerned in which contributions from molecules near $\mathbf{x}$ are accorded greater 'weight' than those far from $\mathbf{x}$. The normalisation condition (4.2) ensures that the integral of $g_w(\mathbf{x}, t)$ over all space $\mathcal{E}$ yields the total quantity

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[7] That is, systems which are composed of a *fixed* set of molecules and/or ions.

[8] Here and hereafter 'molecular' will be employed whether ions or molecules are involved.

$\sum_{i=1}^{N} g_i(t)$ associated with the body. (Prove this!) Of course, integrability of $g_w(.,t)$ requires that w be integrable. More generally, any spatial continuity or smoothness possessed by w will, from (4.1), be inherited by g_w. If a Cartesian co-ordinate system is selected in which $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_3$ are the distinguished orthonormal basis vectors, then for any $\mathbf{u} \in \mathcal{V}$ we define $\hat{w} : \mathbf{R}^3 \to \mathbf{R}$ by

$$w(\mathbf{u}) = w(u_1\,\mathbf{e}_1 + u_2\,\mathbf{e}_2 + u_3\,\mathbf{e}_3) =: \hat{w}(u_1, u_2, u_3). \tag{4.3}$$

The spatial derivative, or gradient, ∇w of w is defined by

$$\nabla w := \hat{w}_{,k}\,\mathbf{e}_k = \operatorname{grad}\hat{w}. \tag{4.4}$$

Setting $g_i = m_i$ and $g_i = m_i\,\mathbf{v}_i$ we obtain local **spatial densities** ρ_w of **mass** and $\mathbf{p}_w$ of **momentum**, respectively:

$$\begin{aligned} \rho_w(\mathbf{x},t) &:= \sum_{i=1}^{N} m_i\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \\ \text{and} \quad \mathbf{p}_w(\mathbf{x},t) &:= \sum_{i=1}^{N} m_i\,\mathbf{v}_i(t) w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \end{aligned} \tag{4.5}$$

Wherever and whenever $\rho_w(\mathbf{x},t) \neq 0$, the corresponding **velocity field**

$$\mathbf{v}_w := (\rho_w)^{-1}\,\mathbf{p}_w\,. \tag{4.6}$$

Differentiating $(4.5)_1$ with respect to t, holding $\mathbf{x}$ fixed, we have

$$\frac{\partial\rho_w}{\partial t} = \sum_{i=1}^{N} m_i\,\frac{\partial w}{\partial t} = \sum_{i=1}^{N} m_i\,\nabla w\,.\,\dot{\mathbf{x}}_i = \sum_{i=1}^{N} m_i\,\nabla w\,.\,\mathbf{v}_i\,. \tag{4.7}$$

(The second equality follows by the Chain Rule.) However,

$$\begin{aligned} \operatorname{div}\mathbf{p}_w &= \sum_{i=1}^{N} m_i \operatorname{div}(w\mathbf{v}_i) = \sum_{i=1}^{N} m_i\{w \operatorname{div}\mathbf{v}_i - \nabla w\,.\,\mathbf{v}_i\} \\ &= -\sum_{i=1}^{N} m_i\,\nabla w\,.\,\mathbf{v}_i, \end{aligned} \tag{4.8}$$

since m_i and $\mathbf{v}_i$ are independent of the field variable $\mathbf{x}$. (The minus sign occurs because differentiation throughout is with respect to $\mathbf{x}$. Specifically, noting that with $\mathbf{u} := \mathbf{x}_i - \mathbf{x}$, $\nabla w := \nabla_{\mathbf{u}} w = \operatorname{grad} \hat{w} = -\nabla_{\mathbf{x}} \hat{w} = -\nabla_{\mathbf{x}} w$.) Accordingly (4.7), (4.8) and (4.6) yield

$$\frac{\partial \rho_w}{\partial t} + \operatorname{div}\{\rho_w \mathbf{v}_w\} = 0. \tag{4.9}$$

Relation (4.9) is formally identical with the mass conservation relation (2.15) and has been established without invoking either the positivity[9] of w or its normalisation (4.2). However, the *latter* condition is essential if ρ_w and $\mathbf{p}_w$ are to have physical interpretations in accord with conventional notions of mass and momentum densities. Of course, there is still a great freedom of choice concerning the weighting function w. Since our modelling ignores molecular *structure* it is natural to consider only directionally-insensitive functions: that is, functions of the form

$$w(\mathbf{u}) = \tilde{w}(u) \tag{4.10}$$

where $u := |\mathbf{u}|$. The simplest function of all is $\tilde{w}_\varepsilon(s)$, defined by

$$\left.\begin{aligned} &\tilde{w}_\varepsilon(u) = V_\varepsilon^{-1} \quad \text{if} \quad u \leqslant \varepsilon, \\ \text{and} \quad &\tilde{w}_\varepsilon(u) = 0 \qquad \text{if} \quad u > \varepsilon, \end{aligned}\right\} \tag{4.11}$$

where

$$V_\varepsilon := \frac{4}{3}\pi\varepsilon^3. \tag{4.12}$$

In such case $g_w(\mathbf{x}, t)$ involves only contributions from molecules lying within, or at, a distance ε from $\mathbf{x}$ at instant t, and all such contributions carry the same weighting factor. Of note here is the manifest length scale ε (and that *a priori* ε is arbitrary). Unfortunately, however, w_ε fails to be continuous at $u = \varepsilon$, and hence is inadmissible since the corresponding mass density, momentum, and velocity fields would likewise have discontinuities, and could not be shown to satisfy (4.9) by classical analysis. However, w_ε can be modified by smoothing the jump at $u = \varepsilon$ over an arbitrarily small interval as follows. Let ϕ denote any smooth, real-valued, monotonic function defined on [0, 1] for which $\phi(0) = 1$, $\phi(1) = 0$, $\phi'(0) = 0$, and $\phi'(1) = 0$. (The derivative

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[9] While it may prove conceptually helpful to think of w taking only non-negative values, it is later shown that this is not necessary, and that in individual contexts the explicit form of w is mandated. One such form, associated with lengthscale ε, is $w(\mathbf{u}) := \frac{1}{2\pi u^3}\left\{\sin\left(\frac{u}{\varepsilon}\right) - \frac{u}{\varepsilon}\cos\left(\frac{u}{\varepsilon}\right)\right\}$ where $u := \|\mathbf{u}\|$. This function takes both positive and negative values.

values are intended in the one-sided sense.) Define

$$\left.\begin{aligned} &\tilde{w}_{\varepsilon,h}(u) = \frac{1}{\alpha} && \text{if} \quad u \leqslant \varepsilon, \\ &\tilde{w}_{\varepsilon,h}(u) = \frac{\phi(\lambda)}{\alpha} && \text{if} \quad u = \varepsilon + \lambda h \quad (\lambda \in [0,1]), \\ \text{and} \quad &\tilde{w}_{\varepsilon,h}(u) = 0 && \text{if} \quad u \geqslant \varepsilon + h, \end{aligned}\right\} \tag{4.13}$$

where $h > 0$ and α is a constant determined by the normalisation condition (4.2). Here this takes the form

$$4\pi \int_0^\infty \tilde{w}_{\varepsilon,h}(u) u^2 \, du = 1. \tag{4.14}$$

Since $0 \leqslant \phi(\lambda) \leqslant 1$, it follows from (4.13) and (4.14) that

$$\frac{\alpha}{V_\varepsilon} = 1 + O\left(\frac{h}{\varepsilon}\right) \quad \text{as} \quad h \to 0. \tag{4.15}$$

Accordingly, by making h arbitrarily small, it is possible to approximate $\tilde{w}_\varepsilon$ for our purposes (namely, choosing $w = \tilde{w}_\varepsilon$ in equations (4.5)) by $\tilde{w}_{\varepsilon,h}$ to within as high an accuracy as is desired. Said differently, for a given choice of length scale ε, the field values for ρ_w, $\mathbf{p}_w$ and $\mathbf{v}_w$ obtained by choosing $w = \tilde{w}_\varepsilon$ in relations (4.5) and (4.6) may be approximated to any desired degree of accuracy by selecting a mollifying function ϕ (which may have any degree of smoothness up to class C^∞), choosing h suitably small, and setting $w = \tilde{w}_{\varepsilon,h}$ in (4.5) and (4.6). The resulting fields $\rho_{\varepsilon,h}$, $\mathbf{p}_{\varepsilon,h}$ and $\mathbf{v}_{\varepsilon,h}$ will inherit the degree of (spatial) smoothness possessed by ϕ. Motivated by the foregoing remarks, in what follows dependence upon h will be suppressed.

4.3. The region occupied by a body at any given scale ε

The mass density field at scale ε is, from the considerations of Section 4.2, given by (see $(4.5)_1$ and (4.11)

$$\rho_\varepsilon(\mathbf{x}, t) = \left(\sum_i^- m_i\right) V_\varepsilon^{-1}, \tag{4.16}$$

where the sum is taken over all particles distant less than or equal to ε from $\mathbf{x}$ at instant t. (This is the significance of the superposed '$-$' in the summation sign.) The **region occupied by the body at scale ε and time t** is the region $R_\varepsilon(t)$ in which 'matter' associated with the body is manifest at scale ε and time t. Such matter is detected by the mass density field ρ_ε at scale ε. Accordingly

$$R_\varepsilon(t) := \{\mathbf{x} \in \mathcal{E} : \rho_\varepsilon(\mathbf{x}, t) > 0\}. \tag{4.17}$$

It follows from (4.16) and (4.17) that

$$R_\varepsilon(t) = \bigcup_{i=1}^{N} S_\varepsilon(\mathbf{x}_i(t)), \tag{4.18}$$

where, for any point $\mathbf{y} \in \mathcal{E}$, $S_\varepsilon(\mathbf{y})$ denotes that closed ball of radius ε centred at $\mathbf{y}$: that is,

$$S_\varepsilon(\mathbf{y}) := \{\mathbf{z} \in \mathcal{E} : |\mathbf{z} - \mathbf{y}| \leqslant \varepsilon\}. \tag{4.19}$$

The **boundary of the body at scale ε and time t is $\partial R_\varepsilon(t)$**. Accordingly, from (4.18) and (4.19), a point $\mathbf{x}$ lies on $\partial R_\varepsilon(t)$ if and only if

(i) there is a molecule of the body distant ε from $\mathbf{x}$, and

(ii) all molecules of the body are distant at least ε from $\mathbf{x}$.

Remark 4.2. If ε is less than the order of nearest-neighbour molecular separations then the body will appear to be riddled with holes or even to be a disjoint collection of spheres, each one centred at a molecular mass centre. For example, in an infinite cubic lattice with nearest-neighbour separation ε_0, then $\varepsilon = \varepsilon_0$ yields no boundary, $\varepsilon = 4\varepsilon_0/5$ results in an infinite number of unconnected holes, each one of which contains the mid-point of a lattice cell, and $\varepsilon = \varepsilon_0/3$ results in a disjoint collection of isolated spheres. (Convince yourself of these situations!) Of course, selecting scales smaller than ε_0 is physically inappropriate, since quantum considerations become relevant: that is, the corpuscular modelling here adopted becomes inappropriate at such scales.

Remark 4.3. Figures 4.1 illustrate the manner in which surface features depend upon ε. A crack whose characteristic dimensions are only marginally above the scale ε_0 of nearest neighbour molecular separations is manifest at scale $\varepsilon = \varepsilon_0$ but cannot be distinguished at scale $2\varepsilon_0$.

Remark 4.4. Figures 4.2(i), (ii) indicate, in the context of a perfect semi-infinite lattice, how the boundary at scale ε differs from the bounding lattice plane. Such consideration motivates the definition of the **geometric boundary** of a body at scale ε and time t as the boundary $\partial R^g_\varepsilon(t)$ of region

$$R^g_\varepsilon(t) := \{\mathbf{x} \in R_\varepsilon(t) : d(\mathbf{x}, \partial R_\varepsilon(t)) \geqslant \varepsilon\}. \tag{4.20}$$

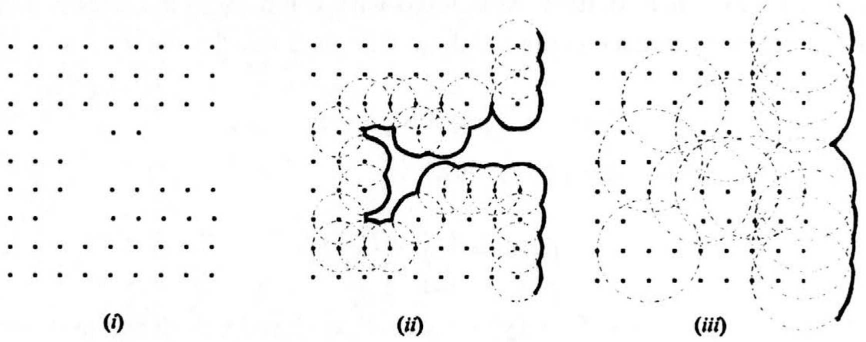

FIGURE 4.1. (*i*) represents a crack in a crystal lattice, (*ii*) depicts the boundary ∂R_ε at a scale $\varepsilon = \varepsilon_0$ where ε_0 is the nearest-neighbour separation, and (*iii*) shows the boundary at a scale $\varepsilon = 2\varepsilon_0$.

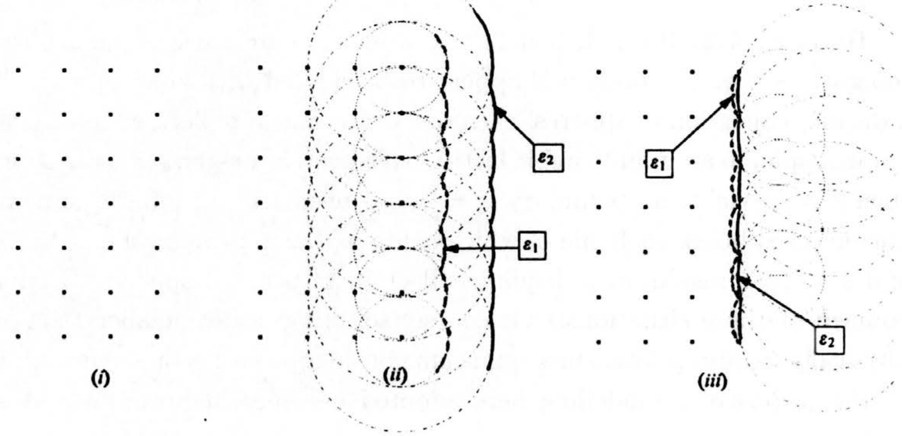

FIGURE 4.2. *(i)* represents a perfect plane lattice boundary, *(ii)* depicts the boundary ∂R_ε at two different scales ε_1 and ε_2, and *(iii)* shows the corresponding geometric boundaries at these scales.

Figures 4.2(iii) and 4.3 indicate the geometric boundaries corresponding to the semi-infinite lattice and to the crack considered in Remark 4.3. Another way of characterising $R^g_\varepsilon(t)$ is to consider the set of all closed spheres S^α_ε say ($\alpha \in \mathcal{A}$, an indexing set) of radius ε, each of which has no molecules in its interior. Then the geometrical region $R^g_\varepsilon(t)$ occupied by the body at

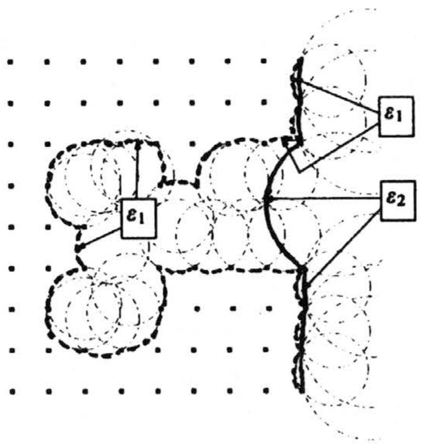

FIGURE 4.3. Geometric boundaries ∂R^g_ε of the crack shown in Figures 4.1 at the two scales ε_1 and ε_2.

instant t is

$$R^g_\varepsilon(t) = \overline{\bigcap_{\alpha\in\mathcal{A}} (S^\alpha_\varepsilon)_{\text{ext}}}, \tag{4.21}$$

where $(S^\alpha_\varepsilon)_{\text{ext}}$ denotes all space *exterior* to S^α_ε, and the superposed bar denotes closure.

Remark 4.5. An immediate consequence of (4.18) is that

$$\varepsilon_2 > \varepsilon_1 \ \text{ implies } \ R_{\varepsilon_1}(t) \subset R_{\varepsilon_2}(t), \tag{4.22}$$

where strict inclusion is intended. Further, $R_\varepsilon(t)$ grows without bound as ε increases. However, although

$$\varepsilon_2 > \varepsilon_1 \ \text{ implies } \ R^g_\varepsilon(t) \subset R^g_{\varepsilon_2}(t), \tag{4.23}$$

$R^g_\varepsilon(t)$ will be bounded at any instant t, no matter how large ε. This follows from characterisation (4.21): at instant t the set of molecular locations will be bounded, and $R^g_\varepsilon(t)$ will, for any $\varepsilon > 0$ be strictly contained within a region bounded by a system of planes. Each plane of the system is characterised as containing three non-collinear molecular locations and separating $\mathcal{E}$ into two half-spaces, one of which contains no molecules. Of course, this corresponds to the limiting case, as ε tends to infinity, of relation (4.21).

Remark 4.6. Boundaries ∂R_ε and ∂R^g_ε are defined uniquely in terms of molecular locations, but *neither* is to be identified precisely with the boundary *perceived* by an observer whose limiting observational scale is ε. Indeed, such an observer is incapable of detecting the cusps in these surfaces, and will have the impression of a surface, smoother than either, each point of which lies within ε of ∂R^g_ε.

4.4. The motion map

At scale ε the mass density and velocity fields ρ_ε and $\mathbf{v}_\varepsilon$, delivered by $(4.5)_1$ and (4.6) with $w = \tilde{w}_\varepsilon$, are defined at time t in region $R_\varepsilon(t)$ given by (4.17). For a given time t_0, and any point $\hat{\mathbf{x}} \in R_\varepsilon(t_0)$, we can consider the following initial value problem for the map $\chi^\varepsilon_0(\hat{\mathbf{x}}, .)$:

$$\begin{aligned} \dot{\chi}^\varepsilon_0(\hat{\mathbf{x}}, t) &= \mathbf{v}_\varepsilon\big(\chi^\varepsilon_0(\hat{\mathbf{x}}, t), t\big) \\ \text{with} \qquad \chi^\varepsilon_0(\hat{\mathbf{x}}, t_0) &= \hat{\mathbf{x}}. \end{aligned} \tag{4.24}$$

The function χ^ε_0 is termed the **motion appropriate to scale ε and situation at time t_0.**

Remark 4.7. Relations (4.24) are formally equivalent to equations (2.4) and (2.5). Here, however, a scale sensitivity is manifest, and the motion is seen to be a *derived* quantity (in contrast to the viewpoint of section 2 wherein the motion is a *primitive* concept). Further, the notion of *material point* (at scale ε) enters naturally at this point as an *artefact* which helps visualisation of the macroscopic motion at scale ε. To this end, each $\hat{\mathbf{x}} \in R_\varepsilon(t_0)$ is identified with a material point, $X = X(\hat{\mathbf{x}})$ say. The location of X at time t in motion $\boldsymbol{\chi}^\varepsilon_0$ is defined to be $\boldsymbol{\chi}^\varepsilon_0(\hat{\mathbf{x}}, t)$. Of course, the location of X at instant t_0 is $\hat{\mathbf{x}}$. The choice of instant t_0 is arbitrary: the essence of the matter is tracing the trajectories of solutions $\mathbf{x}(t)$ to

$$\dot{\mathbf{x}}(t) = \mathbf{v}_\varepsilon\big(\mathbf{x}(t), t\big).$$

Each such trajectory is that of a single material point. In particular, the foregoing viewpoint renders clear the following observations:

(i) The trajectory of a material point should not be confused with that of any individual molecule modelled as a particle. Molecular mass centres exhibit erratic behaviour in all condensed phases, and in fluids rapid molecular diffusion means the near-neighbours of any given molecule are continually changing very rapidly. In a solid, however, near-neighbours remain such, and a region of scale ε marked or 'doped' in some way will, roughly speaking, move to a good approximation as an ε-scale material point associated with a location within this region.

(ii) Given two molecular species which are mixed at the molecular level, there are three ε-scale velocity fields which may be considered. Each species gives rise to such a field, and the system taken as a whole yields a third field. The motions of each of the three systems, at scale ε, may be treated in terms of three categories of material point—one for each system in question. Accordingly, at a given geometrical point occupied by the whole system, there will be located simultaneously three material points. Interpreting the latter as other than mathematical artefacts can lead to conceptual difficulties.

4.5. Linear momentum balance

The motion of P_i is assumed to be governed, in an inertial frame, by

$$\sum_{j\neq i} \mathbf{f}_{ij} + \mathbf{b}_i = \frac{d}{dt}\{m_i\,\mathbf{v}_i\}. \tag{4.25}$$

Here $\mathbf{f}_{ij}$ denotes the force exerted on P_i by P_j and the sum is taken over all particles except P_i; $\mathbf{b}_i$ represents the resultant force on P_i from the material universe outwith $\mathcal{M}$. Clearly (4.25) yields, on summing over *all* particles and multiplying throughout by $w(\mathbf{x}_i - \mathbf{x})$,

$$\begin{aligned}\sum_i \sum_{j\neq i} \mathbf{f}_{ij}\, w(\mathbf{x}_i - \mathbf{x}) + \sum_i \mathbf{b}_i\, w(\mathbf{x}_i - \mathbf{x}) &= \sum_i \frac{d}{dt}\{m_i\,\mathbf{v}_i\}\, w(\mathbf{x}_i - \mathbf{x})\\ &= \frac{\partial}{\partial t}\left\{\sum_i m_i\,\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})\right\} - \sum_i m_i\,\mathbf{v}_i(\nabla w\,.\,\mathbf{v}_i). \end{aligned} \tag{4.26}$$

Here $\mathbf{x}$ denotes an arbitrary point and the 'i' sum is over all particles. Thus [10] (here and in what follows suffix 'w' will be suppressed in expressions for weighted averages)

$$\mathbf{f} + \mathbf{b} = \frac{\partial}{\partial t}\{\rho\mathbf{v}\} + \operatorname{div}\mathbf{D}, \tag{4.27}$$

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[10] In deriving term div $\mathbf{D}$ it has been noted that $m_i\,\mathbf{v}_i(\nabla\mathbf{w}\,.\,\mathbf{v}_i) = (m_i\,\mathbf{v}_i \otimes \mathbf{v}_i)\nabla w$ and $m_i\,\mathbf{v}_i \otimes \mathbf{v}_i$ is independent of spatial variable $\mathbf{x}$. Thus div $(m_i(\mathbf{v}_i \otimes \mathbf{v}_i)w) = m_i(\mathbf{v}_i \otimes \mathbf{v}_i)\nabla w$.

where

$$\mathbf{f}(\mathbf{x},t) := \sum_i \sum_{j\neq i} \mathbf{f}_{ij}(t)\, w\big(\mathbf{x}_i(t)-\mathbf{x}\big), \tag{4.28}$$

$$\mathbf{b}(\mathbf{x},t) := \sum_i \mathbf{b}_i(t)\, w\big(\mathbf{x}_i(t)-\mathbf{x}\big), \tag{4.29}$$

and

$$\mathbf{D}(\mathbf{x},t) := \sum_i m_i\, \mathbf{v}_i(t)\otimes\mathbf{v}_i(t)\, w\big(\mathbf{x}_i(t)-\mathbf{x}\big). \tag{4.30}$$

Fields **f** and **b** are termed densities of **interaction force** and **external body force**, respectively.

Remark 4.8. The sum in the definition of **f** may be written, on suppressing time dependence and noting that, for choice of suitably-small h in (4.13), w is essentially given by (4.11), as

$$\sum_i \sum_{j\neq i} \mathbf{f}_{ij}\, w(\mathbf{x}_i-\mathbf{x}) = \sum_{\substack{P_i \text{ in}\\ S_\varepsilon(\mathbf{x})}} \left\{ \sum_{\substack{P_j \text{ in}\\ S_\varepsilon(\mathbf{x}),\, j\neq i}} \mathbf{f}_{ij} + \sum_{\substack{P_j \text{ outside}\\ S_\varepsilon(\mathbf{x})}} \mathbf{f}_{ij} \right\} V_\varepsilon^{-1},$$

where $S_\varepsilon(\mathbf{x})$ denotes that sphere centred at $\mathbf{x}$ with radius ε. [Contributions from P_j which lie on the boundary of $S_\varepsilon(\mathbf{x})$ may either be considered negligible or half attributed to each term.] Now

$$\sum\sum_{\substack{P_i,P_j \text{ in } S_\varepsilon(\mathbf{x})\\ j\neq i}} \mathbf{f}_{ij} = \frac{1}{2}\left\{ \sum\sum_{\substack{P_i,P_j \text{ in } S_\varepsilon(\mathbf{x})\\ j\neq i}} (\mathbf{f}_{ij}+\mathbf{f}_{ji}) \right\} = \mathbf{0}$$

if we make the assumption (this will appear later as (4.42))

$$\mathbf{f}_{ij}+\mathbf{f}_{ji} = \mathbf{0}.$$

It follows that *force density* $\mathbf{f}(\mathbf{x})$ *is the resultant force exerted by particles outside* $S_\varepsilon(\mathbf{x})$ *upon particles inside* $S_\varepsilon(\mathbf{x})$, *divided by the volume of* $S_\varepsilon(\mathbf{x})$.

Defining the **notional**[11] **thermal velocity of P_i at x** (which depends upon the choice of w) by

$$\hat{\mathbf{v}}_i(\mathbf{x},t) := \mathbf{v}_i(t) - \mathbf{v}(\mathbf{x},t) \tag{4.31}$$

---

[11] The notional thermal velocity $\hat{\mathbf{v}}_i(\mathbf{x},t)$ of a molecule at $\mathbf{x}$ (at time t) approximates its actual thermal velocity $\tilde{\mathbf{v}}_i(t) := \mathbf{v}_i(t) - \mathbf{v}(\mathbf{x}_i(t))$. The distinction will be discussed in Section 6.1.

we have, using $(4.5)_{1,2}$ and (4.6),

$$\sum_i m_i\, \hat{\mathbf{v}}_i(\mathbf{x},t)\, w(\mathbf{x}_i(t)-\mathbf{x}) = \mathbf{p}(\mathbf{x},t) - \rho(\mathbf{x},t)\,\mathbf{v}(\mathbf{x},t) = \mathbf{0}. \tag{4.32}$$

Accordingly, from (4.30), (4.31), (4.32) and $(4.5)_1$,

$$\mathbf{D} = \boldsymbol{\mathcal{D}} + \mathbf{0}\otimes\mathbf{v} + \mathbf{v}\otimes\mathbf{0} + \rho\mathbf{v}\otimes\mathbf{v}, \tag{4.33}$$

where the **notional thermal stress tensor** [12] field $\boldsymbol{\mathcal{D}}$ takes values given by

$$\boldsymbol{\mathcal{D}}(\mathbf{x},t) := \sum_i m_i\, \hat{\mathbf{v}}_i(\mathbf{x},t)\otimes\hat{\mathbf{v}}_i(\mathbf{x},t)\, w\big(\mathbf{x}_i(t)-\mathbf{x}\big). \tag{4.34}$$

Hence (4.27) may be expressed in the form [13]

$$-\operatorname{div}\boldsymbol{\mathcal{D}} + \mathbf{f} + \mathbf{b} \;=\; \frac{\partial}{\partial t}\{\rho\mathbf{v}\} + \operatorname{div}\{\rho\mathbf{v}\otimes\mathbf{v}\} \tag{4.35}$$

$$=\; \rho\left[\frac{\partial\mathbf{v}}{\partial t} + (\nabla\mathbf{v})\mathbf{v}\right], \tag{4.36}$$

on invoking (4.9). Thus, defining the (w-dependent) acceleration field **a** by

$$\mathbf{a} := \dot{\mathbf{v}} := \frac{\partial\mathbf{v}}{\partial t} + (\nabla\mathbf{v})\mathbf{v}, \tag{4.37}$$

linear momentum balance has been established in the form

$$-\operatorname{div}\boldsymbol{\mathcal{D}} + \mathbf{f} + \mathbf{b} = \rho\mathbf{a}. \tag{4.38}$$

Modulo a certain property of interactions, delineated below, **f** may be expressed as the divergence of a tensor-valued field $\mathbf{T}^-$ as follows. As a consequence of (4.2),

$$\int_{\mathcal{E}} w(\mathbf{y}-\mathbf{x}_0)d\mathbf{y} = 1 \tag{4.39}$$

for any given point $\mathbf{x}_0$. Accordingly we may write

$$\mathbf{f}(\mathbf{x},t) = \int_{\mathcal{E}} \mathbf{g}(\mathbf{x},\mathbf{y},t)d\mathbf{y}, \tag{4.40}$$

---

[12] Justification of this terminology is given in Remark 4.13.

[13] Use is here made of the results

$$\operatorname{div}(\rho\mathbf{v}\otimes\mathbf{v}) \equiv \rho\operatorname{div}(\mathbf{v}\otimes\mathbf{v}) + (\mathbf{v}\otimes\mathbf{v})\nabla\rho \equiv \rho\{(\operatorname{div}\mathbf{v})\mathbf{v} + (\nabla\mathbf{v})\mathbf{v}\} + (\mathbf{v}\,.\,\nabla\rho)\mathbf{v}\,.$$

where

$$\mathbf{g}(\mathbf{x},\mathbf{y},t) := \sum_i \sum_{j\neq i} \mathbf{f}_{ij}(t)\, w\big(\mathbf{x}_i(t)-\mathbf{x}\big)\, w\big(\mathbf{x}_j(t)-\mathbf{y}\big). \tag{4.41}$$

On suppressing time-dependence for brevity, and assuming

$$\mathbf{f}_{ji} = -\mathbf{f}_{ij} \tag{4.42}$$

for all i, j, we have

$$\begin{aligned}\mathbf{g}(\mathbf{y},\mathbf{x}) &= \sum_{\substack{i \\ i\neq j}}\sum_{j} \mathbf{f}_{ij}\, w(\mathbf{x}_i-\mathbf{y})\, w(\mathbf{x}_j-\mathbf{x}) \\ &= \sum_{\substack{i \\ j\neq i}}\sum_{j} \mathbf{f}_{ji}\, w(\mathbf{x}_j-\mathbf{y})\, w(\mathbf{x}_i-\mathbf{x}) \\ &= -\sum_{\substack{j \\ j\neq i}}\sum_{i} \mathbf{f}_{ij}\, w(\mathbf{x}_j-\mathbf{y})\, w(\mathbf{x}_i-\mathbf{x}) = -\mathbf{g}(\mathbf{x},\mathbf{y}).\end{aligned}$$

The second equality is merely a re-labelling of indices and the third inequality follows from (4.42). Thus

$$\mathbf{g}(\mathbf{y},\mathbf{x}) = -\mathbf{g}(\mathbf{x},\mathbf{y}). \tag{4.43}$$

Provided that, for some positive number δ, $\mathbf{g}(\mathbf{x},\mathbf{y})\,|\mathbf{x}|^{3+\delta}|\mathbf{y}|^{3+\delta}$ remains boundec for all $\mathbf{x}$ and $\mathbf{y}$, and the same property holds for first derivatives of $\mathbf{g}$, then Noll's Theorem (see Noll [4] and Appendix) furnishes the *existence* of a tensor field $\mathbf{T}^-$ (the **interaction stress tensor** field) for which

$$\mathbf{f} = \operatorname{div}\mathbf{T}^-. \tag{4.44}$$

Further, this theorem furnishes the explicit form

$$\mathbf{T}^-(\mathbf{x}) := -\frac{1}{2}\int_{\mathcal{V}}\int_0^1 \mathbf{g}\big(\mathbf{x}+\alpha\mathbf{u},\, \mathbf{x}-(1-\alpha)\mathbf{u}\big)\otimes\mathbf{u}\, d\alpha\, d\mathbf{u}, \tag{4.45}$$

whence

$$\begin{aligned}\mathbf{T}^-(\mathbf{x}) = -\frac{1}{2}\int_{\mathcal{V}}\int_0^1 &\sum_{i\neq j}\sum \mathbf{f}_{ij} \\ &\otimes\mathbf{u}\, w(\mathbf{x}_i-\mathbf{x}-\alpha\mathbf{u})\, w\big(\mathbf{x}_j-\mathbf{x}+(1-\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \qquad (4.46) \\ = -\frac{1}{2}\, &\sum_{i\neq j}\sum \mathbf{f}_{ij} \\ &\otimes\int_{\mathcal{V}}\int_0^1 \mathbf{u}\, w(\mathbf{x}_i-\mathbf{x}-\alpha\mathbf{u})\, w\big(\mathbf{x}_j-\mathbf{x}+(1-\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \qquad (4.47)\end{aligned}$$

From (4.38) and (4.44) linear momentum balance is expressible as

$$\operatorname{div}\mathbf{T} + \mathbf{b} = \rho\mathbf{a}, \tag{4.48}$$

where the **(Cauchy) stress tensor** field[14] (cf. (4.34) and (4.45))

$$\mathbf{T} := \mathbf{T}^{-} - \boldsymbol{\mathcal{D}}. \tag{4.49}$$

Remark 4.9. The conditions upon $\mathbf{g}$ sufficient to obtain (4.44) are not restrictive. Indeed, it suffices that the derivative of w be bounded (although mollification involves large values of this derivative, such *are* bounded) and that interactions be governed by pairwise potentials which are bounded below (in such case any single interaction will be bounded by a particle-independent bound governed by the total energy of the system).

4.6. The stress tensor T

Since, for any pair of vectors $\mathbf{a}$ and $\mathbf{b}$, the *transpose* $(\mathbf{a}\otimes\mathbf{b})^{\mathrm{T}}$ of the simple tensor $\mathbf{a}\otimes\mathbf{b}$ satisfies

$$(\mathbf{a}\otimes\mathbf{b})^{\mathrm{T}} = \mathbf{b}\otimes\mathbf{a}, \tag{4.50}$$

it follows that simple tensors of the form $\mathbf{a}\otimes\mathbf{a}$ are symmetric. Since sums of such tensors are also symmetric, from (4.34) the field $\boldsymbol{\mathcal{D}}$ takes symmetric values. Thus from (4.49), the stress tensor field $\mathbf{T}$ takes symmetric values if and only if field $\mathbf{T}^{-}$, given by (4.47), takes symmetric values. Accordingly the symmetry or otherwise of $\mathbf{T}$ stems from relation (4.47), which explicitly involves molecular interactions and scale (the latter via the weighting function factors). This means that even in the context of point mass modelling of molecules,[15] symmetry of $\mathbf{T}$ values is not assured *a priori*. Such an observation is apparently at odds with discussions based upon statistical mechanical arguments. This difference stems from the scale-dependent definition of $\mathbf{T}^{-}$, inherent in the choice of weighting function. Such a scale is not present in the statistical approach, which corresponds to choosing a Dirac 'δ' distribu-

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[14] It is of importance to distinguish between a function and the values it takes. Here $\mathbf{T}$ is a function (of position and time, and accordingly termed a 'field') whose values are linear transformations.

[15] As will be discussed later, asymmetry of $\mathbf{T}$ values is usually associated with molecular *structure*, or material inhomogeneity at some sub-macroscopic scale.

tion[16] for w (roughly speaking, a limit of the current approach in the limit as $\varepsilon \to 0$). Introducing such distributions into (4.47), the contribution from particles P_i and P_j $(i \neq j)$ to the double sum is

$$-\frac{1}{2} \int_{\mathcal{V}} \int_0^1 \mathbf{f}_{ij} \otimes \mathbf{u}\, \delta(\mathbf{x}_i - \mathbf{x} - \alpha \mathbf{u})\, \delta\big(\mathbf{x}_j - \mathbf{x} + (1-\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \tag{4.51}$$

Noting that $\mathbf{x}$ is fixed, and that this contribution can be non-zero only if *both*

$$\mathbf{x}_i = \mathbf{x} + \alpha \mathbf{u} \quad \text{and} \quad \mathbf{x}_j = \mathbf{x} - (1-\alpha)\mathbf{u}, \tag{4.52}$$

it follows that for non-zero contributions it is necessary that

$$\mathbf{x}_i - \mathbf{x}_j = \mathbf{u}. \tag{4.53}$$

Accordingly, from (4.53) and (4.47),

$$\mathbf{T}^{-}(\mathbf{x}) = -\frac{1}{2} \sum_{i \neq j}\sum \mathbf{f}_{ij} \otimes (\mathbf{x}_i - \mathbf{x}_j)\, F_{ij}(\mathbf{x}), \tag{4.54}$$

where

$$F_{ij}(\mathbf{x}) := \int_{\mathcal{V}} \int_0^1 \delta(\mathbf{x}_i - \mathbf{x} - \alpha \mathbf{u})\, \delta\big(\mathbf{x}_j - \mathbf{x} + (1-\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \tag{4.55}$$

It follows that if $\mathbf{f}_{ij}$ is directed along the line joining P_i and P_j (so that $\mathbf{f}_{ij}$ is parallel to $(\mathbf{x}_i - \mathbf{x}_j)$) then each term in the double sum is symmetric, and hence $\mathbf{T}^{-}(\mathbf{x})$ is symmetric. Notice that $F_{ij}(\mathbf{x})$ has physical dimension $(\text{length})^{-3}$, and is a distribution. The following remark addresses the physical interpretation of the general form (4.47) of $\mathbf{T}^{-}(\mathbf{x})$. This is shown to simplify considerably in the case of form (4.54) for which $F_{ij}(\mathbf{x})$ restricts just which particle pairs are involved when $\mathbf{T}^{-}(\mathbf{x})$ is integrated over a surface.

In the event that $w \neq \delta$, so that a definite length scale (ε say) is associated with averaging, we cannot conclude that $\mathbf{T}^{-}$ takes symmetric values.

---

[16] Such a distribution has the property that if f is a function of position, $\mathbf{x}$ a given point, and R a spatial region, then

$$\int_R f(\mathbf{y})\delta(\mathbf{y} - \mathbf{x})d\mathbf{y} = f(\mathbf{x}) \quad \text{if} \quad \mathbf{x} \in R,$$

and the integral vanishes if $\mathbf{x} \notin R$.

Remark 4.10. Recall the interpretation of $\mathbf{t}$ in (2.18) as a traction, together with relation (2.19). If $\mathcal{S}$ denotes an oriented surface with unit normal field $\mathbf{n}$ then

$$\int_{\mathcal{S}} \mathbf{Tn} \tag{4.56}$$

is interpreted as the resultant force exerted by matter from that side of $\mathcal{S}$ into which $\mathbf{n}$ is directed upon matter on that side of $\mathcal{S}$ away from which $\mathbf{n}$ points. This interpretation is not strictly correct, since interactions contribute to $\mathbf{T}$ only through $\mathbf{T}^-$: see (4.49) and (4.34). The interpretation of $\boldsymbol{\mathcal{D}}$, which is due to rate of momentum transport rather than actual forces, will be discussed in Remark 4.16. A link between $\mathbf{T}^-$ and the usual interpretation of stress is provided by considering the following results.

Lemma 4.1: *If* $\mathbf{n} \in \mathcal{V}$ *with* $\mathbf{n}\,.\,\mathbf{n} = 1$, *and*

$$\mathcal{V}_{\mathbf{n}} := \{\mathbf{w} \in \mathcal{V} \,:\, \mathbf{w}\,.\,\mathbf{n} > 0\}, \tag{4.57}$$

then

$$\begin{aligned}\frac{1}{2}\int_{\mathcal{V}}\int_0^1 &\mathbf{g}\big(\mathbf{x} + \alpha\mathbf{u},\, \mathbf{x} - (1-\alpha)\mathbf{u}\big) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u} \\ &= \int_{\mathcal{V}_{\mathbf{n}}}\int_0^1 \mathbf{g}\big(\mathbf{x} + \alpha\mathbf{u},\, \mathbf{x} - (1-\alpha)\mathbf{u}\big) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u}. \end{aligned}\tag{4.58}$$

Proof. Setting $\mathbf{u} := -\mathbf{v}$ and $\beta := 1 - \alpha$, and noting that the associated Jacobian is $+1$,

$$\begin{aligned}\int_{\mathcal{V}_{\mathbf{n}}}\int_0^1 &\mathbf{g}\big(\mathbf{x} + \alpha\mathbf{u},\, \mathbf{x} - (1-\alpha)\mathbf{u}\big) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u} \\ &= \int_{\mathcal{V}_{-\mathbf{n}}}\int_1^0 \mathbf{g}\big(\mathbf{x} - (1-\beta)\mathbf{v}, \mathbf{x} + \beta\mathbf{v}\big) \otimes \mathbf{v}\, d\beta\, d\mathbf{v} \\ &= \int_{\mathcal{V}_{-\mathbf{n}}}\int_0^1 \mathbf{g}\big(\mathbf{x} + \beta\mathbf{v},\, \mathbf{x} - (1-\beta)\mathbf{v}\big) \otimes \mathbf{v}\, d\beta\, d\mathbf{v}, \end{aligned}\tag{4.59}$$

on involving property (4.43). Here the integration over $\mathcal{V}_{-\mathbf{n}}$ is understood to be equivalent to integrating over limits $v_1 : -\infty \to +\infty$, $v_2 : -\infty \to +\infty$, and $v_3 : -\infty \to 0$ with respect to Cartesian axes in which x_3 increases in the $\mathbf{n}$ direction. Accordingly, noting that, apart from the domains $\mathcal{V}_{\mathbf{n}}$ and $\mathcal{V}_{-\mathbf{n}}$, the first and last expressions are identical (β and $\mathbf{v}$ may be re-labelled as α and $\mathbf{u}$) and that, modulo a set of volume measure zero,

$$\mathcal{V} = \mathcal{V}_{\mathbf{n}} \cup \mathcal{V}_{-\mathbf{n}}, \tag{4.60}$$

we obtain (4.58). ■

Now suppose $S_{\mathbf{n}}(\mathbf{x}_0)$ denotes that (oriented) plane through point $\mathbf{x}_0$ with unit normal $\mathbf{n}$. Plane $S_{\mathbf{n}}(\mathbf{x}_0)$ divides Euclidean space $\mathcal{E}$ into the two open subsets

$$\begin{aligned} \mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0) &:= \{\mathbf{z} \in \mathcal{E} \,:\, (\mathbf{z} - \mathbf{x}_0).\,\mathbf{n} > 0\}, \\ \mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0) &:= \{\mathbf{y} \in \mathcal{E} \,:\, (\mathbf{y} - \mathbf{x}_0).\,\mathbf{n} < 0\}. \end{aligned} \tag{4.61}$$

More precisely,

$$\mathcal{E} = \mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0) \cup S_{\mathbf{n}}(\mathbf{x}_0) \cup \mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0) \tag{4.62}$$

and we note[17)]

$$\mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0) \cap \mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0) = \emptyset. \tag{4.63}$$

If S denotes a subdomain of $S_{\mathbf{n}}(\mathbf{x}_0)$ then the following result holds.

Lemma 4.2:

$$\begin{aligned} &\int_S \left\{ \frac{1}{2} \int_{\mathcal{V}} \int_0^1 \mathbf{g}(\mathbf{x} + \alpha\mathbf{u},\, \mathbf{x} - (1-\alpha)\mathbf{u}) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u} \right\} \mathbf{n}\, d\, S_{\mathbf{x}} \\ &\qquad = \int_{\mathcal{E}^+_{\mathbf{n}(\mathbf{x}_0)}} \int_{\mathcal{R}^-(S;\mathbf{z})} \mathbf{g}(\mathbf{y}, \mathbf{z}) d\mathbf{y}\, d\mathbf{z} = \int_{\mathcal{E}^-_{\mathbf{n}(\mathbf{x}_0)}} \int_{\mathcal{R}^+(S;\mathbf{y})} \mathbf{g}(\mathbf{y}, \mathbf{z})\, d\mathbf{z}\, d\mathbf{y}, \end{aligned} \tag{4.64}$$

where

$$\begin{aligned} \mathcal{R}^-(S;\mathbf{z}) &:= \{\mathbf{y} \in \mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0) : l(\mathbf{y}, \mathbf{z}) \textit{ passes through } S\}, \\ \mathcal{R}^+(S;\mathbf{y}) &:= \{\mathbf{z} \in \mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0) : l(\mathbf{y}, \mathbf{z}) \textit{ passes through } S\}, \end{aligned} \tag{4.65}$$

and $l(\mathbf{y}, \mathbf{z})$ *denotes that straight line through points* $\mathbf{y}$ *and* $\mathbf{z}$.

Proof. From Lemma 4.1 the left-hand side of (4.64) is equal to

$$\begin{aligned} &\frac{1}{2} \int_S \left\{ \int_{\mathcal{V}_{\mathbf{n}}} \int_0^1 \mathbf{g}(\mathbf{x} + \alpha\mathbf{u},\, \mathbf{x} - (1-\alpha)\mathbf{u}) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u} \right\} \mathbf{n}\, dS_{\mathbf{x}} \\ &\qquad = -\int_S \int_{\mathcal{V}_{\mathbf{n}}} \int_0^1 \mathbf{g}(\mathbf{x} - (1-\alpha)\mathbf{u},\, \mathbf{x} + \alpha\mathbf{u})\, (\mathbf{u}\,.\,\mathbf{n})\, d\alpha\, d\mathbf{u}\, dS_{\mathbf{x}}, \end{aligned} \tag{4.66}$$

[17)] $\emptyset$ denotes the empty set: (4.63) merely states that $\mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0)$ and $\mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0)$ are *disjoint* (that is, have no point in common).

on using (4.43) and recalling that if $\mathbf{a}, \mathbf{b}, \mathbf{c} \in \mathcal{V}$ then

$$(\mathbf{a} \otimes \mathbf{b})\mathbf{c} \ := \ (\mathbf{b} \, . \, \mathbf{c})\mathbf{a}. \tag{4.67}$$

Changing variables to

$$\mathbf{y} := \mathbf{x} - (1-\alpha)\mathbf{u}, \quad \mathbf{z} := \mathbf{x} + \alpha\mathbf{u} \tag{4.68}$$

results in the Jacobian $J = (\mathbf{u} \, . \, \mathbf{n})^{-1}$. To see this choose a Cartesian coordinate system with origin at $\mathbf{x}_0$ with $\mathbf{e}_3 = \mathbf{n}$, so that $\mathbf{e}_1$ and $\mathbf{e}_2$ are parallel to $S_{\mathbf{n}}(\mathbf{x}_0)$. Then, for $\beta = 1, 2$,

$$y_\beta = x_\beta - (1-\alpha)u_\beta, \ y_3 = -(1-\alpha)u_3, \ z_\beta = x_\beta + \alpha u_\beta, \ z_3 = \alpha u_3, \tag{4.69}$$

where $u_3 \in [0, \infty)$ as a consequence of definition (4.57). Since

$$J^{-1} \ = \ \frac{\partial(y_1, y_2, y_3, z_1, z_2, z_3)}{\partial(u_1, u_2, u_3, x_1, x_2, \alpha)}, \tag{4.70}$$

$$J^{-1} \ = \ \begin{vmatrix} -(1-\alpha) & 0 & 0 & 1 & 0 & u_1 \\ 0 & -(1-\alpha) & 0 & 0 & 1 & u_2 \\ 0 & 0 & -(1-\alpha) & 0 & 0 & u_3 \\ \alpha & 0 & 0 & 1 & 0 & u_1 \\ 0 & \alpha & 0 & 0 & 1 & u_2 \\ 0 & 0 & \alpha & 0 & 0 & u_3 \end{vmatrix} \tag{4.71}$$

$$\begin{aligned} = \begin{vmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ \alpha & 0 & 0 & 1 & 0 & u_1 \\ 0 & \alpha & 0 & 0 & 1 & u_2 \\ 0 & 0 & \alpha & 0 & 0 & u_3 \end{vmatrix} &= (-1)^3 \begin{vmatrix} 1 & 0 & u_1 \\ 0 & 1 & u_2 \\ 0 & 0 & u_3 \end{vmatrix} \\ &= -u_3 = -(\mathbf{u} \, . \, \mathbf{n}). \end{aligned} \tag{4.72}$$

Thus the right-hand side of (4.66) transforms to

$$\iint_{\mathcal{D}} \mathbf{g}(\mathbf{y}, \mathbf{z}) \, d\mathbf{y} \, d\mathbf{z}. \tag{4.73}$$

From (4.68), since $\mathbf{x} \in S$ and $u_3 > 0$ (since $\mathbf{u} \in \mathcal{V}_{\mathbf{n}}$), it follows that $\mathbf{y}$ and $\mathbf{z}$ are on opposite sides of S with $\mathbf{y} \in \mathcal{E}_{\mathbf{n}}^-(\mathbf{x}_0), \ \mathbf{z} \in \mathcal{E}_{\mathbf{n}}^+(\mathbf{x}_0)$, and are collinear with $\mathbf{x}$. Thus the domain $\mathcal{D}$ of integration in (4.73) is

$$\mathcal{D} = \big\{(\mathbf{y},\mathbf{z}) \in \mathcal{E}\times\mathcal{E} \,:\, \mathbf{y} \in \mathcal{E}^-_{\mathbf{n}}(\mathbf{x}_0),\ \mathbf{z} \in \mathcal{E}^+_{\mathbf{n}}(\mathbf{x}_0), \text{ and } l(\mathbf{y},\mathbf{z}) \text{ passes through } S\big\}. \quad (4.74)$$

Of course, to evaluate (4.73) it is necessary to undertake multiple integration which can be implemented in either of the two forms given in (4.64). ■

It follows from (4.45), (4.64), and (4.41) that

$$\int_S \mathbf{T}^-\mathbf{n}\,dS = -\frac{1}{2}\int_S\int_{\mathcal{V}}\int_0^1 \mathbf{g}(\mathbf{x}+\alpha\mathbf{u},\ \mathbf{x}-(1-\alpha)\mathbf{u})(\mathbf{u}\,.\,\mathbf{n})d\alpha\, d\mathbf{u}\, dS_{\mathbf{x}}$$
$$= \iint\limits_{\mathcal{D}} \mathbf{g}(\mathbf{y},\mathbf{z})\,d\mathbf{y}\,d\mathbf{z} = \sum_{\substack{i\\ i\neq j}}\sum_{j} \mathbf{f}_{ij} \iint\limits_{\mathcal{D}} w(\mathbf{x}_i-\mathbf{y})w(\mathbf{x}_j-\mathbf{z})d\mathbf{y}\,d\mathbf{z}. \quad (4.75)$$

Thus we have the following

Theorem: *For any planar surface S,*

$$\int_S \mathbf{T}^-\mathbf{n}\,dS = \sum_{\substack{i\\ i\neq j}}\sum_{j} \mathbf{f}_{ij}\ F_{ij}(S), \quad (4.76)$$

where the scalar factor

$$F_{ij}(S) := \iint\limits_{\mathcal{D}} w(\mathbf{x}_i-\mathbf{y})\,w(\mathbf{x}_j-\mathbf{z})d\mathbf{y}\,d\mathbf{z}. \quad (4.77)$$

Further, particle pairs P_i, P_j contribute to the sum in (4.76) if and only if $(\mathbf{x}_i-\mathbf{y})$ and $(\mathbf{x}_j-\mathbf{z})$ lie in the support of w, with $\mathbf{y}$ and $\mathbf{z}$ lying on opposite sides of S such that $(\mathbf{z}-\mathbf{y}).\mathbf{n} > 0$ and $l(\mathbf{y},\mathbf{z})$ passes through S.

Corollary. If the weighting function is *strictly local* [18] then

$$\int_S \mathbf{T}^-\mathbf{n}\,dS = \sum_{\substack{i\\ i\neq j}}\sum_{j} \mathbf{f}_{ij}\,G_{ij}(S), \quad (4.78)$$

where $G_{ij}(S) = 1$ if P_i and P_j are on opposite sides of S with $(\mathbf{x}_j-\mathbf{x}_i).\mathbf{n} > 0$, and such that the line through the locations $\mathbf{x}_i$ and $\mathbf{x}_j$ of P_i and P_j passes through S, and $G_{ij}(S) = 0$ otherwise.

---

[18] By this we mean $w = \delta$: see (4.51).

Remark 4.11. In a moderately rarefied gas, molecular interactions are infrequent, and almost always involve 'binary collisions'. Indeed, such interactions are precisely what give rise to the notion of 'collision'. Molecules undergo essentially rectilinear motion (for typical speeds and distances between collisions[19] the effect of gravitation is negligible) interrupted only when they come within interaction range of other molecules. If such an interaction involves only a pair of molecules then the mutual effect upon the molecules concerned is termed a binary collision (whose duration is the time interval in which the molecules are within interaction range of each other).

Remark 4.12. A stress tensor **T** is termed a **pressure** p if

$$\mathbf{T} = -p\mathbf{1}, \quad (p > 0), \tag{4.79}$$

and **pressure-like** if **T** is negative-definite: that is, if

$$\mathbf{T} = \mathbf{P}$$

where, for any vector $\mathbf{k} \neq \mathbf{0}$,

$$\mathbf{Pk} \,.\, \mathbf{k} < 0. \tag{4.80}$$

In the event that interactions are negligible then the Cauchy stress

$$\mathbf{T} = -\boldsymbol{\mathcal{D}}. \tag{4.81}$$

Now $-\boldsymbol{\mathcal{D}}$ is pressure-like [prove this!] so we conclude that when interactions are negligible the Cauchy stress is pressure-like.

Remark 4.13. Taking the trace of relation (4.34) yields, on suppressing time-dependence,

$$\operatorname{tr} \boldsymbol{\mathcal{D}}(\mathbf{x}) = \sum_i m_i \, \hat{\mathbf{v}}_i^2 \, w(\mathbf{x}_i - \mathbf{x}). \tag{4.82}$$

If the velocity field **v** is zero (for example, the whole body is macroscopically at rest) then

$$(\operatorname{tr} \boldsymbol{\mathcal{D}})(\mathbf{x}) = \sum_i m_i \, \mathbf{v}_i^2 \, w(\mathbf{x}_i - \mathbf{x}) = 2(\rho h)(\mathbf{x}). \tag{4.83}$$

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[19] Any molecular trajectory between collisions is termed a (force-) *free path*. An important parameter in the kinetic theory of gases is the *mean free path*. This distance clearly depends upon both mass density and interaction range.

Here ρh denotes[20] the **microscopic kinetic energy density** or **heat content density** at the scale prescribed by w. In identifying microscopic kinetic energy with heat one is adopting the basic tenet of the *kinetic theory of heat* (see Brush [5]). Typical molecular velocities in gases at room temperature and atmospheric pressure are 10^3 ms^{-1}, so that ρh (and $\boldsymbol{\mathcal{D}}$) are in no sense negligible in such cases. Similar situations prevail in liquids and solids.

Remark 4.14. An interesting observation follows from the considerations of Remark 4.13 in respect of stress-free situations for solids. (Such situations form a basic ingredient in the classical theory of elasticity wherein the so-called *reference configuration*[21] is assumed to be one throughout which $\mathbf{T} = \mathbf{0}$.) In such cases it follows from (4.49) and Remark 4.13 that neither $\mathbf{T}^-$ nor $\boldsymbol{\mathcal{D}}$ is in general negligible, but that these tensor fields are *equal.* Notice that whenever this occurs $\mathbf{T}^-$ must be positive-definite (that is, $\mathbf{T}^-\mathbf{k} \,.\, \mathbf{k} > 0$ for any non-zero vector $\mathbf{k}$). [Prove this!] Such a contribution $\mathbf{T}^-$ to stress is accordingly **tensile**, and is a consequence of interactions being attractive for molecular separations somewhat larger than nearest-neighbour separations. (See also Remark 4.1.)

Remark 4.15. Suppose that interactions are negligible and $\mathbf{T}$ is a multiple of the identity $\mathbf{1}$). Thus

$$\mathbf{T} = -\boldsymbol{\mathcal{D}} = -p\mathbf{1} \tag{4.84}$$

where $p > 0$ (why?). Accordingly

$$2\rho h = \operatorname{tr} \boldsymbol{\mathcal{D}} = 3p \tag{4.85}$$

so that

$$p = \frac{2}{3}\,\rho h. \tag{4.86}$$

Relation (4.86), a *local* result in that it links field values, leads to the ideal gas law in the event that these values are constant in a container of volume V in which the macroscopic velocity is zero. If there are N molecules, each

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[20] Definition $2\rho h := tr\,\boldsymbol{\mathcal{D}}$ is used in later chapters in the general context of (4.81). As will be shown, the *total* kinetic energy density is $\rho(\mathbf{v}^2/2 + h)$. That is, this density has two contributions: one macroscopic, $\rho\mathbf{v}^2/2$, and the other microscopic, ρh. The thermal nature of ρh justifies the terminology of $\boldsymbol{\mathcal{D}}$ as the notional thermal tensor ('notional' because it is defined in terms of the notional thermal velocity: see (4.31)).

[21] See, for example, Truesdell & Toupin [6].

of mass m, then[22]

$$\rho h = \frac{\frac{1}{2}\left(\sum_{i=1}^{N} m\mathbf{v}_i^2\right)}{V}, \tag{4.87}$$

and (4.86) becomes

$$pV = \frac{1}{3}\, m \sum_{i=1}^{N} \mathbf{v}_i^2 = \frac{1}{3}\, Nm\bar{v}^2. \tag{4.88}$$

Here

$$\bar{v}^2 := \frac{\sum_{i=1}^{N} \mathbf{v}_i^2}{N} \tag{4.89}$$

denotes the mean of the squares of molecular velocities.

Since the (absolute) temperature θ in a monotonic gas (given molecules are here modelled as structureless point masses, the analysis is only relevant to such a gas in the present context) satisfies (see, for example, Ohanian [7], §19.4)

$$\bar{v}^2 = \frac{3k\theta}{m}, \tag{4.90}$$

where k denotes Boltzmann's constant, from (4.87) the ideal gas relation

$$pV = Nk\theta \tag{4.91}$$

follows. Symbol θ has here been used to denote absolute temperature, rather than the more conventional 'T' to avoid confusion with the designation $\mathbf{T}$ of the stress tensor.

Remark 4.16. Elementary expositions on the kinetic theory of gases explain how the pressure on the walls of a containing vessel are bombarded with molecules which bounce back into the interior of the vessel. The resultant of all impulses received by a subsurface ΔS of wall (of area ΔA say) over a time interval $t_1 \leqslant t \leqslant t_2$, when divided by the duration $(t_2 - t_1)$ of

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[22] See (4.82) which yields $(\rho h)(\mathbf{x})$ as the kinetic energy of molecules within a sphere of radius ε, centred at $\mathbf{x}$, divided by the volume of this sphere. If ρh is independent of $\mathbf{x}$ in a container of volume V and characteristic dimension larger than ε, then (4.86) is to be expected. Were averaging regions to be cubes of side ε then (4.86) could be proved rigorously.

the interval, yields the average force exerted on ΔS during the time interval, $\mathbf{f}(t_1, t_2)$ say. The average force per unit area on ΔS is thus

$$\frac{\bar{\mathbf{f}}(t_1, t_2)}{\Delta A}. \tag{4.92}$$

If ΔS is planar and molecules suffer no change of momentum parallel to ΔS, then expression (4.92) will be directed along unit normal $\mathbf{n}$ to ΔS *out* of the vessel. That is,

$$\frac{\bar{\mathbf{f}}(t_1, t_2)}{\Delta A} = P(t_1, t_2)\mathbf{n}. \tag{4.93}$$

Quantity $P(t_1, t_2)$ is the average pressure on ΔS over the time interval $t_1 \leqslant t \leqslant t_2$, and has been associated with molecular momentum change at ΔS. This explains 'pressure' as experienced by confining vessels, but does not address the concept of pressure *within* such vessels: that is, the spatial pressure field is not explained. However, a simple modification does the trick. Consider an arbitrary plane Π which intersects the interior of a containing vessel and in particular consider those molecules which cross a subsurface ΔS of Π (with ΔS lying inside the vessel) during the interval $[t_1, t_2]$. If $\mathbf{n}$ is a unit normal to Π then such crossings are distinguished by whether they correspond to molecular velocities $\mathbf{v}_i$ with $\mathbf{v}_i \,.\, \mathbf{n} > 0$ or $\mathbf{v}_i \,.\, \mathbf{n} < 0$. There is net momentum transport in the '$\mathbf{n}$' direction given by

$$\boldsymbol{\mathcal{P}}_{\mathbf{n}} := \sum_i{}^{+} m_i \mathbf{v}_i \; - \; \sum_i{}^{-} m_i \mathbf{v}_i\,, \tag{4.94}$$

where $\sum_i{}^{+}$ $(\sum_i{}^{-})$ is taken over molecular crossings for which $\mathbf{v}_i \,.\, \mathbf{n} > 0$ (< 0). Thus

$$\boldsymbol{\mathcal{P}}_{\mathbf{n}} = \sum_i{}' \frac{m_i \mathbf{v}_i(\mathbf{v}_i \,.\, \mathbf{n})}{|\mathbf{v}_i \,.\, \mathbf{n}|} = \left(\sum_i{}' \frac{m_i \mathbf{v}_i \otimes \mathbf{v}_i}{|\mathbf{v}_i \,.\, \mathbf{n}|} \right) \mathbf{n}, \tag{4.95}$$

where the sum is taken over all crossings in time interval $[t_1, t_2]$. It is this term which is to be identified with

$$\int_{\Delta S} \boldsymbol{\mathcal{D}} \mathbf{n} \, dS, \tag{4.96}$$

where $\boldsymbol{\mathcal{D}}$ is given by (4.34) with $\mathbf{v}_i = \hat{\mathbf{v}}_i$ when the gas is macroscopically at rest $(\mathbf{v} = \mathbf{0})$. The purpose of this remark has been to identify $\boldsymbol{\mathcal{D}}$ with that contribution to stress due to momentum exchange associated with molecular mass transport.

Remark 4.17. The methodology employed herein results directly in local forms of balance. This is in contrast to the usual postulates of balance relations for arbitrary 'parts' or subregions of space 'occupied' by the body in question: see (2.6), (2.16), (2.18), (2.25), and (2.27). Of course, integration (over an arbitrary region R throughout which all fields are defined) of relation (4.35), supplemented by (4.44) and noting (4.49), leads to

$$\begin{aligned}\int_{\partial R}\mathbf{Tn}+\int_R\mathbf{b}=\int_{\partial R}\left(\frac{\partial}{\partial t}\{\rho\mathbf{v}\}+\operatorname{div}\{\rho\mathbf{v}\otimes\mathbf{v}\}\right)&\\ =\int_R\rho\mathbf{a}=\frac{d}{dt}\left\{\int_{R_t}\rho\mathbf{v}\right\}.&\qquad(4.97)\end{aligned}$$

In the last equality (2.20) has been invoked.

Chapter 5

Balances of moment of momentum and moment of mass

5.1. Preamble

As background to the analysis of this chapter a few introductory comments may be helpful.

C.1 The commonly postulated form (2.25) of moment of momentum is equivalent, modulo suitable smoothness of fields, to symmetry (2.29) of the stress tensor **T**.

C.2 Balance (2.25) is not consistent with the behaviour of nematic liquid crystalline phases. The molecules in such phases are elongated, and tend to align[23] with near-neighbours. As a consequence the local effect of material on one side of any (hypothetical) surface S within such a phase, upon material on the other side of S, is not one of traction (a local force density per unit area of S) alone: additionally there is a couple per unit area of S. Further, since an externally-applied magnetic field causes the elongated molecules to align with this field (this phenomenon is exploited to great effect in liquid crystal devices), (body) couples per unit volume must be incorporated. Accordingly, the form of moment balance appropriate to such phases must include couple stress and body couples.

C.3 Moment of momentum balances which include couple stress and body couples have also been postulated in order to model the effect of *inho-*

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[23] Such alignment becomes less co-operative as temperature increases. At sufficiently elevated temperature this alignment disappears, resulting in a non-nematic isotropic phase.

mogeneity. One approach, for elastic media, is to allow the stress and couple stress to be functions of both first *and* second derivatives of deformations from a reference configuration. 24)

C.4 Generalised versions of balance (2.25) which include couple stress and body couple density give rise, upon invoking linear momentum balance (2.23), to a local form (the generalised version of (2.29)) which involves the skew part of $\mathbf{T}$. (See, for example, Truesdell & Noll [1] (98.25) and (127.16).) Thus postulated generalisations of balance (2.25) give a precise indication of the asymmetry of $\mathbf{T}$.

Here a local form of *generalised* 25) moment of momentum is derived for a system of interacting point masses. Such derivation is a direct consequence of the motion of individual particles as prescribed by (4.25). (Recall that relation (4.25) was also the starting point for derivation of linear momentum balance.) It turns out that the resulting balance does not involve the stress tensor $\mathbf{T}$ in any way. Further, use of Noll's theorem enables (modulo satisfaction of suitable decay characteristics of molecular interactions) the existence of an interaction couple stress tensor $\mathbf{C}^-$ to be exhibited in a form which explicitly involves interactions. (This is the precise analogue of the argument in Chapter 4 whereby the existence of the interactive stress tensor was demonstrated.) The entire couple stress is the combination of $\mathbf{C}^-$ with a kinematic contribution, just as the Cauchy stress $\mathbf{T}$ was shown in Chapter 4 to be the sum of an interactive stress $\mathbf{T}^-$ with a diffusive term $-\boldsymbol{\mathcal{D}}$. In the event that the weighting function w is chosen to be strictly local (that is, w is a Dirac-δ distribution) then $\mathbf{C}^-$ vanishes. While the discussion in this Chapter does not involve micro*structure*, attention is drawn to the link between couple-stress and inhomogeneity. This is accomplished by the derivation of a *moment of mass balance* which yields the time evolution of the displacement $\mathbf{d}(\mathbf{x}, t)$ from $\mathbf{x}$ at time t of the mass centre of molecules within a sphere, centre $\mathbf{x}$ and radius ε. (Here ε is the length scale associated with the weighting function.) This time evolution is shown to be the divergence of a tensor field which appears in the moment of momentum balance.

An immediate consequence of the results derived here is the issuing of a 'scientific health warning' concerning previously-postulated forms of moment

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24) Such materials are termed 'second grade' elastica.

25) 'Generalised' here means that a balance of rank two tensor fields is involved. The skew part of this relation corresponds to a balance of axial vector fields. The cited Truesdell & Noll balances are of this latter type.

of momentum balance. 'Intuitive' notions based upon purely continuum reasoning and experience can be misleading. This was already seen in the interpretation of stress in which the diffusive/momentum exchange contribution $-\mathcal{D}$ (see (4.34)) is not always appreciated.

5.2. Generalised moment of momentum balance

Recall equation (4.25) governing the motion of particle P_i in an inertial frame:

$$\sum_{j\neq i} \mathbf{f}_{ij} + \mathbf{b}_i = \frac{d}{dt}\{m_i\,\mathbf{v}_i\}. \tag{4.25}$$

Tensorial pre-multiplication of each term by $(\mathbf{x}_i - \mathbf{x})w(\mathbf{x}_i - \mathbf{x})$, followed by summation over all particles P_i, yields (here $\mathbf{x}$ is any fixed point)

$$\begin{aligned}\sum_i \sum_{\substack{j\\ j\neq i}} (\mathbf{x}_i - \mathbf{x}) \otimes \mathbf{f}_{ij}\, w(\mathbf{x}_i - \mathbf{x}) + \sum_i (\mathbf{x}_i - \mathbf{x}) \otimes \mathbf{b}_i\, w(\mathbf{x}_i - \mathbf{x})&\\ = \sum_i (\mathbf{x}_i - \mathbf{x}) \otimes \frac{d}{dt}\{m_i\,\mathbf{v}_i\}\, w(\mathbf{x}_i - \mathbf{x}).&\end{aligned} \tag{5.1}$$

Now

$$\begin{aligned}(\mathbf{x}_i - \mathbf{x}) \otimes \frac{d}{dt}\{m_i\,\mathbf{v}_i\}\, w(\mathbf{x}_i - \mathbf{x}) = \frac{d}{dt}\big\{(\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})\big\}&\\ - \mathbf{v}_i \otimes m_i\,\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) - \big((\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i\big)(\nabla w \cdot \mathbf{v}_i).&\end{aligned} \tag{5.2}$$

Further,[26]

$$\begin{aligned}&\big((\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i\big)(\nabla w \,.\, \mathbf{v}_i) = \big((\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i \otimes \mathbf{v}_i\big)\nabla w\\ &= -\big((\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i \otimes \mathbf{v}_i\big)\nabla_{\mathbf{x}}\, w = -\operatorname{div}\big\{\big((\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i \otimes \mathbf{v}_i\big)w(\mathbf{x}_i - \mathbf{x})\big\}\\ &\qquad - (\mathbf{v}_i \otimes m_i\,\mathbf{v}_i)w(\mathbf{x}_i - \mathbf{x}).\end{aligned} \tag{5.3}$$

From (5.2) and (5.3),

$$\begin{aligned}(\mathbf{x}_i - \mathbf{x}) \otimes \frac{d}{dt}\{m_i\,\mathbf{v}_i\}\, w(\mathbf{x}_i - \mathbf{x}) = \frac{d}{dt}\big\{(\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})\big\}&\\ + \operatorname{div}\big\{(\mathbf{x}_i - \mathbf{x}) \otimes m_i\,\mathbf{v}_i \otimes \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})\big\}.&\end{aligned} \tag{5.4}$$

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[26] $(\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})\mathbf{v} := (\mathbf{c}\,.\,\mathbf{v})(\mathbf{a}\otimes\mathbf{b})$ for any four vectors $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{v}$. Term $\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c}$ is the third rank tensor which has Cartesian representation $(\mathbf{a}\otimes\mathbf{b}\otimes\mathbf{c})_{ijk} = a_i\, b_j\, c_k$.

Hence, from (5.1), (5.2) and (5.4),

$$\mathbf{c} + \mathbf{J} = \frac{\partial}{\partial t}\{\rho \mathbf{B}\} + \operatorname{div} \mathbf{M}, \tag{5.5}$$

where

$$\mathbf{c}(\mathbf{x}, t) := \sum_{i} \sum_{\substack{j \\ j \neq i}} \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes \mathbf{f}_{ij}(t) w\big(\mathbf{x}_i(t) - \mathbf{x}\big), \tag{5.6}$$

$$\mathbf{J}(\mathbf{x}, t) := \sum_{i} \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes \mathbf{b}_i(t) w\big(\mathbf{x}_i(t) - \mathbf{x}\big), \tag{5.7}$$

$$\rho(\mathbf{x}, t)\mathbf{B}(\mathbf{x}, t) := \sum_{i} \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes m_i \, \mathbf{v}_i(t) w\big(\mathbf{x}_i(t) - \mathbf{x}\big), \tag{5.8}$$

and

$$\mathbf{M}(\mathbf{x}, t) := \sum_{i} \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes m_i \, \mathbf{v}_i(t) \otimes \mathbf{v}_i(t) w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \tag{5.9}$$

With the aim of writing $\mathbf{c}$ as the divergence of a rank-three tensor field via Noll's theorem (recall the analysis following (4.38)), we define[27)]

$$\mathbf{G}(\mathbf{x}, \mathbf{y}) := \sum_{i} \sum_{\substack{j \\ j \neq i}} \big\{(\mathbf{x}_i - \mathbf{x}) + (\mathbf{x}_j - \mathbf{y})\big\} \otimes \mathbf{f}_{ij} \, w(\mathbf{x}_i - \mathbf{x}) w(\mathbf{x}_j - \mathbf{y}), \tag{5.10}$$

it follows, on relabelling the dummy suffices i and j as j and i, respectively, that

$$\begin{aligned} \mathbf{G}(\mathbf{x}, \mathbf{y}) = \sum_{j} \sum_{\substack{i \\ i \neq j}} \big\{(\mathbf{x}_j - \mathbf{x}) + (\mathbf{x}_i - \mathbf{y})\big\} \otimes \mathbf{f}_{ji} \, w(\mathbf{x}_j - \mathbf{x}) w(\mathbf{x}_i - \mathbf{y}) \\ = -\mathbf{G}(\mathbf{y}, \mathbf{x}) \end{aligned} \tag{5.11}$$

provided

$$\mathbf{f}_{ji} = -\mathbf{f}_{ij}. \tag{4.42}$$

Assumption (4.42) was, of course, invoked in Chapter 4. Notice that

$$\int_{\mathcal{E}} \mathbf{G}(\mathbf{x}, \mathbf{y}) d\mathbf{y} = \mathbf{I}_1(\mathbf{x}) + \mathbf{I}_2(\mathbf{x}), \tag{5.12}$$

[27)] Here we suppress time-dependence. Of course, $\mathbf{G}$ depends upon t since for each $i, j = 1, 2, \ldots, N$, $\mathbf{x}_i$ and $\mathbf{x}_j$ are functions of time t.

where

$$\mathbf{I}_1(\mathbf{x}) := \sum_{i}\sum_{\substack{j\\ j\neq i}} (\mathbf{x}_i - \mathbf{x}) \otimes \mathbf{f}_{ij}\, w(\mathbf{x}_i - \mathbf{x}) \int_{\mathcal{E}} w(\mathbf{x}_j - \mathbf{y})d\mathbf{y} \tag{5.13}$$

and

$$\mathbf{I}_2(\mathbf{x}) := \sum_{i}\sum_{\substack{j\\ j\neq i}} \left(\int_{\mathcal{E}} (\mathbf{x}_j - \mathbf{y})\, w(\mathbf{x}_j - \mathbf{y})d\mathbf{y}\right) \otimes \mathbf{f}_{ij}\, w(\mathbf{x}_i - \mathbf{x}). \tag{5.14}$$

The normalisation property (4.2) of w implies that for each 'j' the integral factor on the right-hand side of (5.13) is equal to unity. Further, since w is spherically-symmetric, the integral factor for each j in the right-hand side of (5.14) vanishes. The foregoing two remarks imply that (see (5.6))

$$\int_{\mathcal{E}} \mathbf{G}(\mathbf{x},\mathbf{y})d\mathbf{y} = \sum_{i}\sum_{\substack{j\\ j\neq i}} (\mathbf{x}_i - \mathbf{x}) \otimes \mathbf{f}_{ij}\, w(\mathbf{x}_i - \mathbf{x}) = \mathbf{c}(\mathbf{x}). \tag{5.15}$$

Provided that $\mathbf{G}(\mathbf{x},\mathbf{y})\, |\mathbf{x}|^{3+\delta} |\mathbf{y}|^{3+\delta}$ remains bounded for some positive δ, for all $\mathbf{x},\mathbf{y}$, and the same property holds for first derivatives of $\mathbf{G}$, then Noll's Theorem ([4] and Appendix) yields the existence of the *interaction couple-stress tensor* $\mathbf{C}^{-}$, where

$$\mathbf{C}^{-}(\mathbf{x}) := -\frac{1}{2} \int_{\mathcal{V}} \int_0^1 \mathbf{G}(\mathbf{x} + \alpha\mathbf{u},\ \mathbf{x} - (1-\alpha)\mathbf{u}) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u}, \tag{5.16}$$

for which

$$\mathbf{c} = \operatorname{div} \mathbf{C}^{-}. \tag{5.17}$$

Explicitly, we have from (5.16) and (5.10),

$$\begin{aligned} \mathbf{C}^{-}(\mathbf{x}) = -\frac{1}{2} \sum_{i}\sum_{\substack{j\\ j\neq i}} \int_{\mathcal{V}} \int_0^1 & \left\{ (\mathbf{x}_i - \mathbf{x} - \alpha\mathbf{u}) + \big(\mathbf{x}_j - \mathbf{x} + (1-\alpha)\mathbf{u}\big) \right\} \\ & \otimes \mathbf{f}_{ij} \otimes \mathbf{u}\, w(\mathbf{x}_i - \mathbf{x} - \alpha\mathbf{u})\, w\big(\mathbf{x}_j - \mathbf{x} + (1+\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \end{aligned} \tag{5.18}$$

That is,

$$\begin{aligned} \mathbf{C}^{-}(\mathbf{x},t) = -\frac{1}{2} \sum_{i}\sum_{\substack{j\\ j\neq i}} \int_{\mathcal{V}} \int_0^1 & \left\{ \big(\mathbf{x}_i(t) - \mathbf{x} - \alpha\mathbf{u}\big) + \big(\mathbf{x}_j(t) - \mathbf{x} + (1-\alpha)\mathbf{u}\big) \right\} \\ & \otimes \mathbf{f}_{ij}(t) \otimes \mathbf{u}\, w\big(\mathbf{x}_i(t) - \mathbf{x} - \alpha\mathbf{u}\big) w\big(\mathbf{x}_j(t) + \mathbf{x} + (1+\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}. \end{aligned}$$

Balance (5.5) now takes the form

$$\operatorname{div}\mathbf{C}' + \mathbf{J} = \frac{\partial}{\partial t}\,(\rho\mathbf{B}), \tag{5.19}$$

where

$$\mathbf{C}' := \mathbf{C}^- - \mathbf{M}. \tag{5.20}$$

Recalling that the non-interaction contribution $\boldsymbol{\mathcal{D}}$ to stress (see (4.34)) involves notional thermal velocities and, with an eye on usual forms of balance having a right-hand side of form $\rho\dot{\phi}$ for some tensor field ϕ, we re-write (5.19). To this end we notice that since

$$\mathbf{v}_i = \hat{\mathbf{v}}_i(x) + \mathbf{v}(\mathbf{x}) \tag{5.21}$$

(this is an abbreviated version of the explicit relation (4.31)) we can write (see (5.9) and (5.8))

$$\mathbf{M} = \hat{\mathbf{M}} + \rho\mathbf{B}\otimes\mathbf{v}, \tag{5.22}$$

where

$$\hat{\mathbf{M}}(\mathbf{x}) := \sum_i (\mathbf{x}_i - \mathbf{x})\otimes m_i\,\mathbf{v}_i\otimes\hat{\mathbf{v}}_i\,w(\mathbf{x}_i - \mathbf{x}). \tag{5.23}$$

Thus[28)]

$$\operatorname{div}\mathbf{M} = \operatorname{div}\hat{\mathbf{M}} + \operatorname{div}(\mathbf{B}\otimes\rho\mathbf{v}) \tag{5.24}$$

$$= \operatorname{div}\hat{\mathbf{M}} + (\nabla\mathbf{B})\rho\mathbf{v} + \big(\operatorname{div}(\rho\mathbf{v})\big)\mathbf{B}. \tag{5.25}$$

Since

$$\dot{\mathbf{B}} := \frac{\partial\mathbf{B}}{\partial t} + (\nabla\mathbf{B})\mathbf{v}, \tag{5.26}$$

$$\begin{aligned}\frac{\partial}{\partial t}\{\rho\mathbf{B}\} = \frac{\partial\rho}{\partial t}\mathbf{B} + \rho\frac{\partial\mathbf{B}}{\partial t} &= -\operatorname{div}(\rho\mathbf{v})\mathbf{B} + \rho\big(\dot{\mathbf{B}} - (\nabla\mathbf{B})\mathbf{v}\big)\\ &= \rho\dot{\mathbf{B}} + \operatorname{div}(\hat{\mathbf{M}} - \mathbf{M})\end{aligned} \tag{5.27}$$

upon invoking relations (4.9) and (5.25). It follows from (5.19) and (5.27) that

$$\operatorname{div}\mathbf{C} + \mathbf{J} = \rho\dot{\mathbf{B}}, \tag{5.28}$$

[28)] Use is made here of the identity

$$\operatorname{div}(\mathbf{A}\otimes\mathbf{a}) = (\nabla\mathbf{A})\mathbf{a} + (\operatorname{div}\mathbf{a})\mathbf{A},$$

where $\mathbf{A}$ and $\mathbf{a}$ are linear transformation- and vector-valued fields, respectively. Of course, here we have chosen $\mathbf{A} = \mathbf{B}$ and $\mathbf{a} = \rho\mathbf{v}$.

where

$$\mathbf{C} := \mathbf{C}^- - \hat{\mathbf{M}}. \tag{5.29}$$

Relation (5.28) may be integrated over any regular region R within that occupied by the body to yield

$$\int_{\partial R} \mathbf{Cn} + \int_R \mathbf{J} = \int_R \rho\dot{\mathbf{B}} = \frac{d}{dt}\left\{\int_{R_t} \rho\mathbf{B}\right\}, \tag{5.30}$$

where R_t is that region deforming with the motion prescribed by $\mathbf{v}$ and which coincides with R at instant t.

Remark 5.1. Relation (5.30) is to be compared with generalisations of (2.25) which have been postulated. These take the form

$$\int_{\partial R}\{(\mathbf{x}-\mathbf{x}_0)\times\mathbf{Tn}+\hat{\mathbf{A}}\mathbf{n}\}+\int_R\{(\mathbf{x}-\mathbf{x}_0)\times\mathbf{b}+\hat{\mathbf{G}}\}$$
$$=\frac{d}{dt}\int_{R_t}\{(\mathbf{x}-\mathbf{x}_0)\times\rho\mathbf{v}+\rho\hat{\mathbf{S}}\}. \tag{5.31}$$

Since relation (5.31) involves axial vectors it may be re-couched in terms of skew-tensor fields as

$$\int_{\partial R}\{(\mathbf{x}-\mathbf{x}_0)\wedge\mathbf{Tn}+\mathbf{An}\}+\int_R\{(\mathbf{x}-\mathbf{x}_0)\wedge\mathbf{b}+\mathbf{G}\}$$
$$=\frac{d}{dt}\left\{\int_{R_t}\{(\mathbf{x}-\mathbf{x}_0)\wedge\rho\mathbf{v}+\rho\mathbf{S}\}\right\}. \tag{5.32}$$

Here $\mathbf{An}$, $\mathbf{G}$ and $\mathbf{S}$ are skew-tensor-valued fields whose corresponding axial vector-valued fields are $\hat{\mathbf{A}}\mathbf{n}$, $\hat{\mathbf{G}}$ and $\hat{\mathbf{S}}$, respectively. It is (5.32) which should be compared with the skew part of (5.30). At this point it is natural to consider the form of balance obtained by tensorial pre-multiplication of (4.25) by $(\mathbf{x}_i - \mathbf{x}_0)\,w(\mathbf{x}_i - \mathbf{x})$ rather than $(\mathbf{x}_i - \mathbf{x})\,w(\mathbf{x}_i - \mathbf{x})$: see (5.1). It was the latter multiplication that resulted in (5.28) and hence (5.30). The former will introduce terms involving $\mathbf{T}$ and $\mathbf{b}$ which appear in (5.32), but cannot yield anything new since, symbolically,

$$\sum_i(\mathbf{x}_i-\mathbf{x}_0)w(\mathbf{x}_i-\mathbf{x})(4.25)$$
$$=\sum_i(\mathbf{x}_i-\mathbf{x})w(\mathbf{x}_i-\mathbf{x})\otimes(4.25)+\sum_i(\mathbf{x}-\mathbf{x}_0)w(\mathbf{x}_i-\mathbf{x}_0)\otimes(4.25) \tag{5.33}$$

$$= (5.30) + (\mathbf{x} - \mathbf{x}_0) \otimes \sum_i (4.25)\, w(\mathbf{x}_i - \mathbf{x})$$

$$= (5.30) + (\mathbf{x} - \mathbf{x}_0) \otimes (2.23). \qquad (5.34)$$

This balance is accordingly

$$\operatorname{div} \mathbf{C} + \mathbf{J} + (\mathbf{x} - \mathbf{x}_0) \otimes (\operatorname{div} \mathbf{T} + \mathbf{b}) = \rho\dot{\mathbf{B}} + (\mathbf{x} - \mathbf{x}_0) \otimes \rho\mathbf{a} \qquad (5.35)$$

$$= \rho\{\overbrace{\mathbf{B} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{v}}^{\cdot}\} - \rho\mathbf{v} \otimes \mathbf{v}. \qquad (5.36)$$

Noting that [29]

$$\operatorname{div}\{(\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{T}\} = (\mathbf{x} - \mathbf{x}_0) \otimes \operatorname{div} \mathbf{T} + \mathbf{T}^{\mathrm{T}}, \qquad (5.37)$$

(5.35) may be written as

$$\operatorname{div}\{\mathbf{C} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{T}\} - \mathbf{T}^{\mathrm{T}} + \mathbf{J} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{b}$$

$$= \rho\{\overbrace{\mathbf{B} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{v}}^{\cdot}\} - \rho\mathbf{v} \otimes \mathbf{v}. \qquad (5.38)$$

Integrating (5.37) over region R (see (5.30)) yields the balance

$$\int_{\partial R} \{\mathbf{C}\mathbf{n} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{T}\mathbf{n}\} + \int_R \{\mathbf{J} - \mathbf{T}^{\mathrm{T}} + (\mathbf{x} - \mathbf{x}_0) \otimes \mathbf{b} + \rho\mathbf{v} \otimes \mathbf{v}\}$$

$$= \frac{d}{dt}\left\{\int_{R_t} \{\rho\mathbf{B} + (\mathbf{x} - \mathbf{x}_0) \otimes \rho\mathbf{v}\}\right\}. \qquad (5.39)$$

It is the skew part of (5.39) that should be compared with the commonly-postulated form (5.32). While one has the immediate identifications

$$sk\,\mathbf{J} \leftrightarrow \mathbf{G}, \qquad sk\,\mathbf{B} \leftrightarrow \mathbf{S}$$

and $\qquad (5.40)$

$$sk(\mathbf{C}\mathbf{n}) \leftrightarrow \mathbf{A}\mathbf{n},$$

the term $-\mathbf{T}^{\mathrm{T}}$ in (5.39) suggests there should have been an extra term $sk\,\mathbf{T}$ in the second integral of (5.32). It is such absence which results in relations of form (5.32) giving rise to local balances which involve $sk\,\mathbf{T}$ and hence apparently yield information on the asymmetry of $\mathbf{T}$.

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[29] Here we employ the identity (see previous footnote)

$$\operatorname{div}(\mathbf{a} \otimes \mathbf{A}) = \mathbf{a} \otimes \operatorname{div} \mathbf{A} + (\nabla\mathbf{a})\mathbf{A}^{\mathrm{T}}$$

with $\mathbf{a} = (\mathbf{x} - \mathbf{x}_0)$ and $\mathbf{A} = \mathbf{T}$.

5.3. Moment of mass considerations

Here we link field **B** with considerations of inhomogeneity. A measure of this, at the length scale ε associated with the weighting function, is the displacement **d** from field point **x** of the mass centre of those molecules within a distance ε of **x**. Specifically,

$$\rho(\mathbf{x},t)\,\mathbf{d}(\mathbf{x},t) := \sum_i m_i\big(\mathbf{x}_i(t)-\mathbf{x}\big)\,w\big(\mathbf{x}_i(t)-\mathbf{x}\big). \tag{5.41}$$

Differentiating with respect to t (with **x** fixed) yields

$$\begin{aligned}
\frac{\partial}{\partial t}\{\rho\mathbf{d}\} &= \sum_i m_i\,\mathbf{v}_i\,w(\mathbf{x}_i-\mathbf{x}) + \sum_i m_i\big((\mathbf{x}_i-\mathbf{x})\otimes\mathbf{v}_i\big)\nabla w \\
&= \rho\mathbf{v} - \sum_i m_i\big((\mathbf{x}_i-\mathbf{x})\otimes\mathbf{v}_i\big)\nabla_{\mathbf{x}}\,w \\
&= \rho\mathbf{v} + \left(\operatorname{div}_{\mathbf{x}}\left\{\sum_i m_i(\mathbf{x}_i-\mathbf{x})\otimes\mathbf{v}_i\right\}\right)w \\
&\qquad\qquad - \operatorname{div}_{\mathbf{x}}\left\{\sum_i(\mathbf{x}_i-\mathbf{x})\otimes m_i\,\mathbf{v}_i\,w\right\} \\
&= \rho\mathbf{v} - \sum_i m_i\,\mathbf{v}_i\,w(\mathbf{x}_i-\mathbf{x}) - \operatorname{div}\{\rho\mathbf{B}\}.
\end{aligned} \tag{5.42}$$

Here use has been made of identities

$$\operatorname{div}(\phi\mathbf{A}) = \phi\mathbf{A} + \mathbf{A}\nabla\phi,$$

with $\phi = w$ and $\mathbf{A} = m(\mathbf{x}_i-\mathbf{x})\otimes\mathbf{v}_i$, and

$$\operatorname{div}(\mathbf{a}\otimes\mathbf{b}) = (\nabla\mathbf{a})\mathbf{b} + (\operatorname{div}\mathbf{b})\mathbf{a}$$

with $\mathbf{a} = (\mathbf{x}_i-\mathbf{x})$, $b = m_i\,\mathbf{v}_i$, and noting $\nabla_{\mathbf{x}}\,\mathbf{a} = -\mathbf{1}$ and $\operatorname{div} m_i\,\mathbf{v}_i = 0$.

Thus from (5.42), $(4.5)_2$ and (4.6),

$$\frac{\partial}{\partial t}\{\rho\mathbf{d}\} = -\operatorname{div}\{\rho\mathbf{B}\}. \tag{5.43}$$

Using mass conservation relation (4.9), balance (5.43) may be written in the form

$$\rho\dot{\mathbf{d}} = -\operatorname{div}\{\rho(\mathbf{B}-\mathbf{d}\otimes\mathbf{v})\}. \tag{5.44}$$

This motivates the definition

$$\hat{\mathbf{B}} := \mathbf{B} - \mathbf{d} \otimes \mathbf{v}. \tag{5.45}$$

From (5.8) and (5.41)

$$\rho(\mathbf{x}, t)\hat{\mathbf{B}}(\mathbf{x}, t) := \sum_i \big(\mathbf{x}_i(t) - \mathbf{x} - \mathbf{d}(\mathbf{x}, t)\big) \otimes m_i\, \mathbf{v}_i(t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big), \tag{5.46}$$

so that (5.44) may be written as

$$\rho\dot{\mathbf{d}} = -\operatorname{div}\{\rho\hat{\mathbf{B}}\}. \tag{5.47}$$

Remark 5.2. $\rho(\mathbf{x}, t)\hat{\mathbf{B}}(\mathbf{x}, t)$ is the tensor moment of momentum about the mass centre of those molecules which lie within the sphere of radius ε centred at $\mathbf{x}$ at instant t. From (5.41) it follows that (see (4.31))

$$\begin{aligned} \rho(\mathbf{x}, t)\hat{\mathbf{B}}(\mathbf{x}, t) &= \sum_i \big(\mathbf{x}_i(t) - \mathbf{x} - \mathbf{d}(\mathbf{x}, t)\big) \otimes m_i\, \hat{\mathbf{v}}_i(\mathbf{x}, t)\, w(\mathbf{x}_i(t), t) \\ &= \sum_i \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes m_i\, \hat{\mathbf{v}}_i(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t), t\big) \end{aligned} \tag{5.48}$$

on invoking (4.32).

Chapter 6

Balance of energy

6.1. Preamble

The local form of energy balance is obtained from (4.25) by multiplying each term therein scalarly by $\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})$ and then summing over all particles. The balance obtained includes *thermal* quantities: these are quantities whose definitions involve molecular thermal velocities. Recall (see footnote 11) that the *thermal velocity* of P_i at instant t (*at the scale prescribed by* w) is[30]

$$\tilde{\mathbf{v}}_i(t) := \mathbf{v}_i(t) - \mathbf{v}\big(\mathbf{x}_i(t), t\big). \tag{6.1}$$

So far we have encountered two thermally-*related*[31] fields, namely

$$\boldsymbol{\mathcal{D}}(\mathbf{x}, t) := \sum_i m_i\, \hat{\mathbf{v}}_i(\mathbf{x}, t) \otimes \hat{\mathbf{v}}_i(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \tag{4.34}$$

and

$$\hat{\mathbf{M}}(\mathbf{x}, t) := \sum_i \big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes m_i\, \mathbf{v}_i(t) \otimes \hat{\mathbf{v}}_i(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \tag{5.23}$$

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[30] Of course, the scale-dependence enters here through the w-dependent definition (4.6) of $\mathbf{v}$.

[31] The characteristic feature of molecular thermal velocities is their erratic nature and large average magnitudes ($\sim 10^3\ \mathrm{ms}^{-1}$) at room temperature. Since $\tilde{\mathbf{v}}_i(t)$ and $\hat{\mathbf{v}}_i(\mathbf{x}, t)$ differ only by the difference in the macroscopic velocity at points $\mathbf{x}_i(t)$ and $\mathbf{x}$, $\hat{\mathbf{v}}_i(\mathbf{x}, t)$ will also be erratic, and have large average magnitudes at room temperature.

Recall

$$\hat{\mathbf{v}}_i(\mathbf{x},t) := \mathbf{v}_i(t) - \mathbf{v}(\mathbf{x},t), \tag{4.31}$$

so that

$$\check{\mathbf{v}}_i(\mathbf{x},t) := \mathbf{v}_i(t) - \mathbf{v}(\mathbf{x},t) - \big(\nabla\mathbf{v}(\mathbf{x},t)\big)\big(\mathbf{x}_i(t) - \mathbf{x}\big) \tag{6.2}$$

is a higher-order approximation (for particles near $\mathbf{x}$) to the thermal velocity than is $\hat{\mathbf{v}}_i(\mathbf{x},t)$. Specifically,

$$\hat{\mathbf{v}}_i(\mathbf{x},t) = \check{\mathbf{v}}_i(\mathbf{x},t) + \big(\mathbf{L}(\mathbf{x},t)\big)\big(\mathbf{x}_i(t) - \mathbf{x}\big), \tag{6.3}$$

where

$$\mathbf{L} := \nabla\mathbf{v}. \tag{6.4}$$

From (4.32) we note that

$$\begin{aligned} \mathbf{0} &= \sum_i m_i\,\hat{\mathbf{v}}_i(\mathbf{x},t)\,w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \\ &= \sum_i m_i\,\check{\mathbf{v}}_i(\mathbf{x},t)\,w\big(\mathbf{x}_i(t) - \mathbf{x}\big) + \mathbf{L}(\mathbf{x},t)\rho(\mathbf{x},t)\mathbf{d}(\mathbf{x},t), \end{aligned} \tag{6.5}$$

on recalling (5.41). That is, upon suppressing time dependence,

$$\sum_i m_i\,\check{\mathbf{v}}_i(\mathbf{x})w(\mathbf{x}_i - \mathbf{x}) = -(\rho\mathbf{L}\mathbf{d})(\mathbf{x}). \tag{6.6}$$

From (6.3) and the definition (4.34) of $\boldsymbol{\mathcal{D}}$,

$$\begin{aligned} \boldsymbol{\mathcal{D}} &= \sum_i m_i\big(\check{\mathbf{v}}_i + \mathbf{L}(\mathbf{x}_i - \mathbf{x})\big) \otimes \big(\check{\mathbf{v}}_i + \mathbf{L}(\mathbf{x}_i - \mathbf{x})\big)\,w(\mathbf{x}_i - \mathbf{x}) \\ &= \check{\boldsymbol{\mathcal{D}}} + \rho\big(\mathbf{L}\hat{\mathbf{B}} + (\mathbf{L}\hat{\mathbf{B}})^{\mathrm{T}}\big) - \rho\mathbf{L}\mathbf{I}\mathbf{L}^{\mathrm{T}}, \end{aligned} \tag{6.7}$$

where (see (5.46))

$$\check{\boldsymbol{\mathcal{D}}}(\mathbf{x},t) := \sum_i m_i\,\check{\mathbf{v}}_i(\mathbf{x},t) \otimes \check{\mathbf{v}}_i(\mathbf{x},t)\,w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \tag{6.8}$$

and

$$(\rho\mathbf{I})(\mathbf{x},t) := \sum_i m_i\big(\mathbf{x}_i(t) - \mathbf{x}\big) \otimes \big(\mathbf{x}_i(t) - \mathbf{x}\big)\,w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \tag{6.9}$$

In similar fashion $\hat{\mathbf{M}}$ can be expanded via (6.2) and (6.3) to yield terms involving $\check{\mathbf{v}}_i$.

6.2. Derivation of energy balance

Multiplication of each term in (4.25) scalarly by $\mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})$ and then summing over all particles yields

$$\sum_{i \neq j}\sum \mathbf{f}_{ij} \,.\, \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) + \sum_i \mathbf{b}_i \,.\, \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) \\ = \sum_i \left(\frac{d}{dt}\{m_i \mathbf{v}_i\}\right) .\, \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}). \quad (6.10)$$

From (6.10) the first term yields (on suppressing 't')

$$\sum_{i \neq j}\sum \mathbf{f}_{ij} \,.\, \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) = \sum_{i \neq j}\sum \mathbf{f}_{ij} \,.\big\{\check{\mathbf{v}}_i(\mathbf{x}) + \mathbf{v}(\mathbf{x}) + \mathbf{L}(\mathbf{x})(\mathbf{x}_i - \mathbf{x})\big\}\, w(\mathbf{x}_i - \mathbf{x}) \\ = \check{q}(\mathbf{x}) + \mathbf{f}(\mathbf{x}) \,.\, \mathbf{v}(\mathbf{x}) + \mathbf{c}(\mathbf{x}) \cdot \mathbf{L}^{\mathrm{T}}(\mathbf{x}), \quad (6.11)$$

where[32]

$$\check{q}(\mathbf{x}, t) := \sum_{i \neq j}\sum \mathbf{f}_{ij}(t) \,.\, \check{\mathbf{v}}_i(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \quad (6.12)$$

Similarly the second term in (6.10) may be written as

$$\sum_i \mathbf{b}_i \,.\, \big\{\check{\mathbf{v}}_i(\mathbf{x}) + \mathbf{v}(\mathbf{x}) + \mathbf{L}(\mathbf{x})(\mathbf{x}_i - \mathbf{x})\big\}\, w(\mathbf{x}_i - \mathbf{x}) \\ = \check{r}(\mathbf{x}) + \mathbf{b}(\mathbf{x}) \,.\, \mathbf{v}(\mathbf{x}) + \mathbf{J}(\mathbf{x}) \,.\, \mathbf{L}^{\mathrm{T}}(\mathbf{x}), \quad (6.13)$$

where

$$\check{r}(\mathbf{x}, t) := \sum_i \mathbf{b}_i(t) \,.\, \check{\mathbf{v}}_i(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \quad (6.14)$$

The right-hand side of (6.10) is

$$\sum_i \left(\frac{d}{dt}\{m_i \mathbf{v}_i\}\right) .\, \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) = \sum_i \frac{d}{dt}\left\{\frac{1}{2} m_i \mathbf{v}_i^2\right\} w(\mathbf{x}_i - \mathbf{x}) \\ = \frac{\partial}{\partial t}\left\{\sum_i \frac{1}{2} m_i \mathbf{v}_i^2\, w(\mathbf{x}_i - \mathbf{x})\right\} + \operatorname{div}\left\{\left(\sum_i \frac{1}{2} m_i \mathbf{v}_i^2\right) \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x})\right\}. \quad (6.15)$$

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[32] The inner product of two linear transformations **A** and **B** is $\mathbf{A} \cdot \mathbf{B} := \mathrm{tr}(\mathbf{A}^{\mathrm{T}}\mathbf{B}) = A_{jk}B_{jk}$ in Cartesian tensor notation. Thus $(\mathbf{a} \otimes \mathbf{b}) \cdot \mathbf{L} = \mathrm{tr}\big((\mathbf{a} \otimes \mathbf{b})^{\mathrm{T}}\, \mathbf{L}\big) = \mathrm{tr}\big((\mathbf{b} \otimes \mathbf{a})\mathbf{L}\big) = \mathrm{tr}(\mathbf{L}(\mathbf{b} \otimes \mathbf{a}) = \mathrm{tr}\big((\mathbf{L}\mathbf{b}) \otimes \mathbf{a}\big) = (\mathbf{L}\mathbf{b}) \,.\, \mathbf{a} = \mathbf{a} \,.\, \mathbf{L}\mathbf{b}$.

From (6.2) we have (recall (6.9))

$$\begin{aligned}\sum_i \frac{1}{2}\, m_i \mathbf{v}_i^2\, w(\mathbf{x}_i - \mathbf{x}) &= \sum_i \frac{1}{2}\, m_i \big(\breve{\mathbf{v}}_i + \mathbf{v} + \mathbf{L}(\mathbf{x}_i - \mathbf{x})\big)^2\, w(\mathbf{x}_i - \mathbf{x}) \\ &= \rho\breve{h} + \frac{1}{2}\,\rho\mathbf{v}^2 + \frac{1}{2}\,\rho\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\,\mathbf{L} + \left(\sum_i m_i \breve{\mathbf{v}}_i\, w\right) . \mathbf{v} \\ &\quad + \sum_i m_i \breve{\mathbf{v}}_i \,.\, \mathbf{L}(\mathbf{x}_i - \mathbf{x}) w + \mathbf{v} \,.\, \rho\mathbf{L}\mathbf{d},\end{aligned} \tag{6.16}$$

where

$$(\rho\breve{h})(\mathbf{x}, t) := \sum_i \frac{1}{2}\, m_i \breve{\mathbf{v}}_i^2(\mathbf{x}, t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big). \tag{6.17}$$

Further, from (6.6),

$$\left(\sum_i m_i \breve{\mathbf{v}}_i\, w\right) . \mathbf{v} = -\rho\mathbf{L}\mathbf{d} \,.\, \mathbf{v} \tag{6.18}$$

and, from (6.3) and (5.48),

$$\begin{aligned}\sum_i m_i \breve{\mathbf{v}}_i \,.\, \mathbf{L}(\mathbf{x}_i - \mathbf{x})\, w &= \sum_i m_i \big(\hat{\mathbf{v}}_i - \mathbf{L}(\mathbf{x}_i - \mathbf{x})\big) \,.\, \mathbf{L}(\mathbf{x}_i - \mathbf{x}) w \\ &= \rho\hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \rho\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L}.\end{aligned} \tag{6.19}$$

Thus (6.16) simplifies to

$$\sum_i \frac{1}{2}\, m_i \mathbf{v}_i^2\, w(\mathbf{x}_i - \mathbf{x}) = \rho\left(\breve{h} + \frac{1}{2}\,\mathbf{v}^2 + \hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \frac{1}{2}\,\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L}\right). \tag{6.20}$$

After considerable manipulation

$$\begin{aligned}\sum_i \left(\frac{1}{2}\, m_i \mathbf{v}_i^2\right) \mathbf{v}_i\, w(\mathbf{x}_i - \mathbf{x}) &= \rho\left\{\breve{h} + \frac{1}{2}\,\mathbf{v}^2 + \hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \frac{1}{2}\,\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L}\right\}\mathbf{v} \\ &\quad + \breve{\mathbf{k}} + \boldsymbol{\mathcal{D}}\mathbf{v} + \hat{\mathbf{M}}^{\sim} : \mathbf{L}^{\mathrm{T}} + \mathbf{L}\boldsymbol{\ell} - \boldsymbol{\mathcal{A}}^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\mathbf{v} \\ &\quad - \mathbf{R}^{\sim} : \mathbf{L}^{\mathrm{T}}\mathbf{L} - \mathbf{L}(\mathbf{L}^{\mathrm{T}}\mathbf{L} : \boldsymbol{\mathcal{S}}),\end{aligned} \tag{6.21}$$

where (suppressing time-dependence)

$$\breve{\mathbf{k}}(\mathbf{x}) := \sum_i \frac{1}{2}\,(m_i \breve{\mathbf{v}}_i^2)\breve{\mathbf{v}}_i\, w(\mathbf{x}_i - \mathbf{x}), \tag{6.22}$$

$$\boldsymbol{\ell}(\mathbf{x}) := \sum_i \frac{1}{2}\, m_i \breve{\mathbf{v}}_i^2 (\mathbf{x}_i - \mathbf{x})\, w(\mathbf{x}_i - \mathbf{x}), \tag{6.23}$$

$$\boldsymbol{\mathcal{A}}(\mathbf{x}) := \sum_i (\mathbf{x}_i - \mathbf{x}) \otimes m_i \breve{\mathbf{v}}_i\, w(\mathbf{x}_i - \mathbf{x}), \tag{6.24}$$

$$\mathbf{R}(\mathbf{x}) := \sum_i \frac{1}{2}\, m_i (\mathbf{x}_i - \mathbf{x}) \otimes (\mathbf{x}_i - \mathbf{x}) \otimes \breve{\mathbf{v}}_i\, w(\mathbf{x}_i - \mathbf{x}), \quad \text{and} \tag{6.25}$$

$$\boldsymbol{\mathcal{S}}(\mathbf{x}) := \sum_i \frac{1}{2}\, m_i (\mathbf{x}_i - \mathbf{x}) \otimes (\mathbf{x}_i - \mathbf{x}) \otimes (\mathbf{x}_i - \mathbf{x})\, w(\mathbf{x}_i - \mathbf{x}). \tag{6.26}$$

In (6.21), ':' denotes double contraction, so that for simple tensors $\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}$ and $\mathbf{p} \otimes \mathbf{q}$,

$$(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c}) : (\mathbf{p} \otimes \mathbf{q}) := (\mathbf{c} \,.\, \mathbf{p})(\mathbf{b} \,.\, \mathbf{q})\mathbf{a}, \tag{6.27}$$

and

$$(\mathbf{a} \otimes \mathbf{b} \otimes \mathbf{c})^{\sim} := \mathbf{c} \otimes \mathbf{b} \otimes \mathbf{a}. \tag{6.28}$$

Using suffix notation, for third- and second-rank Cartesian tensors P_{ijk} and C_{rs},

$$(P : C)_i := P_{ijk}\, C_{kj} \tag{6.29}$$

and

$$(P^{\sim})_{ijk} := P_{kji}. \tag{6.30}$$

From (6.11), (6.13), (6.15), (6.20) and (6.21), energy balance takes the form

$$\begin{aligned} \breve{q} + \mathbf{f} \cdot \mathbf{v} + \mathbf{c} \cdot \mathbf{L}^{\mathrm{T}} + \breve{r} + \mathbf{b} \cdot \mathbf{v} + \mathbf{J} \cdot \mathbf{L}^{\mathrm{T}} &= \frac{\partial}{\partial t}\left\{\rho\left[\breve{h} + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}} \cdot \mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I} \cdot \mathbf{L}^{\mathrm{T}}\mathbf{L}\right]\right\} \\ &\quad + \operatorname{div}\left\{\rho\left[\breve{h} + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}} \cdot \mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I} \cdot \mathbf{L}^{\mathrm{T}}\mathbf{L}\right]\mathbf{v} + \breve{\mathbf{k}} + \boldsymbol{\mathcal{D}} + \hat{\mathbf{M}}^{\sim} : \mathbf{L}^{\mathrm{T}} + \mathbf{L}\boldsymbol{\ell} \right. \\ &\qquad \left. - \boldsymbol{\mathcal{A}}^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\mathbf{v} - \mathbf{R}^{\sim} : \mathbf{L}^{\mathrm{T}}\mathbf{L} - \mathbf{L}(\mathbf{L}^{\mathrm{T}}\mathbf{L} : \boldsymbol{\mathcal{S}})\right\}. \end{aligned} \tag{6.31}$$

Now

$$\breve{q}(\mathbf{x}) = \int_{\mathcal{E}} \sum\sum_{i \neq j} \mathbf{f}_{ij} \,.\, \breve{\mathbf{v}}_i(\mathbf{x}) w(\mathbf{x}_i - \mathbf{x})\, w(\mathbf{x}_j - \mathbf{y})\, d\mathbf{y}, \tag{6.32}$$

as a consequence of (6.12) and normalisation of w:

$$\int_{\mathcal{E}} w(\mathbf{x}_j - \mathbf{y})\, d\mathbf{y} = 1.$$

Thus

$$\breve{q}(\mathbf{x}) = \int_{\mathcal{E}} \breve{g}^{+}(\mathbf{x},\mathbf{y}) + \breve{g}^{-}(\mathbf{x},\mathbf{y})\, d\mathbf{y}, \tag{6.33}$$

where

$$\breve{g}^{\pm}(\mathbf{x},\mathbf{y}) := \frac{1}{2}\sum\sum_{i\neq j} \big(\mathbf{f}_{ij} \,.\, \breve{\mathbf{v}}_i(\mathbf{x}) \pm \mathbf{f}_{ji} \,.\, \breve{\mathbf{v}}_j(\mathbf{y})\big)\, w(\mathbf{x}_i - \mathbf{x})\, w(\mathbf{x}_j - \mathbf{y}). \tag{6.34}$$

Noting that

$$\begin{aligned}\breve{g}^{-}(\mathbf{y},\mathbf{x}) := \frac{1}{2}\sum\sum_{j\neq i} \big\{\mathbf{f}_{ji} \,.\, \breve{\mathbf{v}}_j(\mathbf{x}) - \mathbf{f}_{ij} \,.\, \breve{\mathbf{v}}_i(\mathbf{x})\big\}\, w(\mathbf{x}_j - \mathbf{y})\, w(\mathbf{x}_i - \mathbf{x})& \\ = -\breve{g}^{-}(\mathbf{x},\mathbf{y}),&\end{aligned} \tag{6.35}$$

by Noll's theorem there exists a vector $\breve{\mathbf{q}}^{-}$ such that

$$(\operatorname{div} \breve{\mathbf{q}}^{-})(\mathbf{x}) = \int_{\mathcal{E}} \breve{g}^{-}(\mathbf{x},\mathbf{y})\, d\mathbf{y} =: \breve{q}^{-}(\mathbf{x}). \tag{6.36}$$

Accordingly

$$\breve{q} = \operatorname{div} \breve{\mathbf{q}}^{-} + \breve{q}^{+}, \tag{6.37}$$

where

$$\breve{q}^{+}(\mathbf{x}) := \breve{q}(\mathbf{x}) - \breve{q}^{-}(\mathbf{x}) = \int_{\mathcal{E}} \breve{g}^{+}(\mathbf{x},\mathbf{y})\, d\mathbf{y}. \tag{6.38}$$

The *heat flux vector*

$$\breve{\mathbf{q}} := -\breve{\mathbf{q}}^{-} + \breve{\mathbf{k}}, \tag{6.39}$$

so that from (6.37) and (6.39)

$$\breve{q} - \operatorname{div} \breve{\mathbf{k}} = -\operatorname{div} \breve{\mathbf{q}} + \breve{q}^{+}. \tag{6.40}$$

Invoking (4.44), (5.17) and (6.40), balance (6.31) may be expressed as

$$\begin{aligned} &-\operatorname{div} \breve{\mathbf{q}} + \breve{q}^{+} + (\operatorname{div} \mathbf{T}^{-}) \,.\, \mathbf{v} + (\operatorname{div} \mathbf{C}^{-}) \cdot \mathbf{L}^{\mathrm{T}} + \breve{r} + \mathbf{b} \,.\, \mathbf{v} + \mathbf{J} \cdot \mathbf{L}^{\mathrm{T}} \\ &\quad = \rho\Big\{\breve{h} + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}} \cdot \mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I} \cdot L^{\mathrm{T}}L\Big\}^{\boldsymbol{\cdot}} + \operatorname{div}\big\{\boldsymbol{\mathcal{D}}\mathbf{v} + \hat{\mathrm{M}}^{\sim} : \mathbf{L}^{\mathrm{T}} \\ &\qquad + \mathbf{L}\boldsymbol{\ell} - \boldsymbol{\mathcal{A}}^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\mathbf{v} - \mathbf{R}^{\sim} : \mathbf{L}^{\mathrm{T}}\mathbf{L} - \mathbf{L}(\mathbf{L}^{\mathrm{T}}\mathbf{L} : \boldsymbol{\mathcal{S}})\big\}. \end{aligned} \tag{6.41}$$

Here we have noted that, for any scalar field ϕ,

$$\frac{\partial}{\partial t}\{\rho\phi\} + \operatorname{div}\{\rho\phi\mathbf{v}\} = \rho\dot{\phi} \tag{6.42}$$

as a consequence of mass conservation (4.9), where

$$\dot{\phi} := \partial\phi/\partial t + (\nabla\phi).\,\mathbf{v} \tag{6.43}$$

denotes the material time derivative, and chosen

$$\phi := \breve{h} + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L}. \tag{6.44}$$

Relation (6.41) can be simplified in several ways. Using the identities

$$\operatorname{div}((\mathbf{T}^{-})^{\mathrm{T}}\mathbf{v}) = (\operatorname{div}\mathbf{T}^{-}).\,\mathbf{v} + \mathbf{T}^{-}\cdot\mathbf{L} \tag{6.45}$$

and

$$\operatorname{div}\big((\mathbf{C}^{-})^{\sim} : \mathbf{L}^{\mathrm{T}}\big) = (\operatorname{div}\mathbf{C}^{-})\cdot\mathbf{L}^{\mathrm{T}} + \mathbf{C}^{-}\cdot\nabla\mathbf{L}^{\mathrm{T}} \tag{6.46}$$

and the symmetry ($\boldsymbol{\mathcal{D}}^{\mathrm{T}} = \boldsymbol{\mathcal{D}}$) of $\boldsymbol{\mathcal{D}}$, (6.41) becomes

$$\begin{aligned}\breve{r} - \operatorname{div}\breve{\mathbf{q}} + \operatorname{div}(\mathbf{T}^{\mathrm{T}}\mathbf{v}) + \operatorname{div}(\mathbf{C}^{\sim} : \mathbf{L}^{\mathrm{T}}) + \mathbf{b}\,.\,\mathbf{v} + \mathbf{J}\cdot\mathbf{L}^{\mathrm{T}}& \\ = \rho\dot{\alpha} + \mathbf{T}^{-}\cdot\mathbf{L} + \mathbf{C}^{-}\cdot\nabla\mathbf{L}^{\mathrm{T}} - \breve{q}^{+} + \operatorname{div}\mathbf{j}.&\end{aligned} \tag{6.47}$$

Here

$$\alpha := \breve{h} + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L} \tag{6.48}$$

and

$$\mathbf{j} := \mathbf{L}\boldsymbol{\ell} - \boldsymbol{\mathcal{A}}^{\mathrm{T}}\mathbf{L}^{\mathrm{T}}\mathbf{v} - \mathbf{R}^{\sim} : \mathbf{L}^{\mathrm{T}}\mathbf{L} - \mathbf{L}(\mathbf{L}^{\mathrm{T}}\mathbf{L} : \boldsymbol{\mathcal{S}}). \tag{6.49}$$

Integrating (6.47) over a region R whose boundary deforms with the motion prescribed by $\mathbf{v}$ yields the integral form of energy balance as

$$\begin{aligned}\int_{\partial R}\{-\breve{\mathbf{q}}\cdot\mathbf{n} + \mathbf{Tn}\cdot\mathbf{L} + \mathbf{Cn}\cdot\mathbf{L}^{\mathrm{T}}\} + \int_{R}\{\breve{r} + \mathbf{b}\cdot\mathbf{v} + \mathbf{J}\cdot\mathbf{L}^{\mathrm{T}}\}& \\ = \frac{d}{dt}\left\{\int_{R_t}\rho\Big\{e + \frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}}\cdot\mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I}\cdot\mathbf{L}^{\mathrm{T}}\mathbf{L} + \gamma\Big\}\right\}.&\end{aligned} \tag{6.50}$$

Here

$$e := \beta + \breve{h}, \tag{6.51}$$

where

$$\dot{\beta} := \mathbf{T}^{-}\cdot\mathbf{L} + \mathbf{C}^{-}\cdot\nabla\mathbf{L}^{\mathrm{T}} - \breve{q}^{+}, \tag{6.52}$$

and

$$\dot{\gamma} := \operatorname{div} \mathbf{j}. \tag{6.53}$$

Relation (6.52) follows by defining

$$\beta(\mathbf{x}, t) := \beta\big(\hat{\mathbf{x}}(t), t\big), \tag{6.54}$$

in terms of the solution $\hat{\mathbf{x}}(\tau)$ to

$$\dot{\hat{\mathbf{x}}}(\tau) = \mathbf{v}\big(\hat{\mathbf{x}}(\tau), \tau\big) \tag{6.55}$$

which satisfies

$$\hat{\mathbf{x}}(t) = \mathbf{x}. \tag{6.56}$$

Then

$$\beta(\mathbf{x}, t) := \int_{t_0}^{t} \rho^{-1} \big[\mathbf{T}^{-} \cdot \mathbf{L} + \mathbf{C}^{-} \cdot \nabla \mathbf{L}^{\mathrm{T}} - \breve{q}^{+} + \operatorname{div} \mathbf{j}\big]\, d\tau, \tag{6.57}$$

where the integral (which involves an arbitrary constant due to the arbitrary choice of reference instant t_0) has an integrand in which fields are computed on the trajectory $\hat{\mathbf{x}}(.)$. In the same way

$$\gamma(\mathbf{x}, t) := \int_{t_0}^{t} \rho^{-1} \operatorname{div} \mathbf{j}\, d\tau. \tag{6.58}$$

Remark 6.1. Relation (6.50) is a generalisation of the usual balance, in which $\mathbf{C}$, $\mathbf{J}$, $\hat{\mathbf{B}} \cdot \mathbf{L}^{\mathrm{T}}$, $-\frac{1}{2}\mathbf{I} \cdot \mathbf{L}^{\mathrm{T}}\mathbf{L}$, and γ do not appear. Further, the decomposition of internal energy (per unit mass) given by (6.51) separates thermal ($\breve{h}$) from mechanical (β) contributions. At first sight (6.52) would seem to involve a thermal term via the presence of $\breve{q}^{+}$. This is not the case since from (6.38) and (6.34),

$$\breve{q}^{+}(\mathbf{x}) = \frac{1}{2} \sum_{i \neq j}\sum \big((\mathbf{f}_{ij} \cdot \breve{\mathbf{v}}_x) + \mathbf{f}_{ji} \cdot \breve{\mathbf{v}}_j(\mathbf{x})\big)\, w(\mathbf{x}_i - \mathbf{x}). \tag{6.59}$$

Modulo pairwise balance (4.42),

$$\mathbf{f}_{ij} \,.\, \breve{\mathbf{v}}_i(\mathbf{x}) + \mathbf{f}_{ji} \,.\, \breve{\mathbf{v}}_j(\mathbf{x}) = \mathbf{f}_{ij} \,.\, \big\{\mathbf{v}_i - \mathbf{v}_j - \mathbf{L}(\mathbf{x})(\mathbf{x}_i - \mathbf{x}_j)\big\} \tag{6.60}$$

and hence $\breve{q}^{+}(\mathbf{x})$ does not depend upon thermal velocity but is rather intimately related to the time rate of change of binding energy.

Remark 6.2. In (6.50) the expression $\rho\{\frac{1}{2}\mathbf{v}^2 + \hat{\mathbf{B}} \cdot \mathbf{L}^{\mathrm{T}} - \frac{1}{2}\mathbf{I} \cdot \mathbf{L}^{\mathrm{T}}\mathbf{L} + \gamma\}$ represents a purely *kinematic* contribution to the energy density and is essentially a macroscopic kinetic energy term.

Remark 6.3. The foregoing two Remarks relate to the deduction of a global balance of energy (6.50) from local balance (6.47), and were made to render comparison with other postulated forms of balance which incorporate couple stress. However, it is the *local* forms of balance which are used in the formulation and solution of problems. With this in mind (6.47) can be simplified using local balances (4.48) and (5.28). Specifically, we obtain from (6.41) the relation

$$\breve{r} - \operatorname{div}\breve{\mathbf{q}} + \breve{q}^{+} - \boldsymbol{\mathcal{D}} \cdot \mathbf{L} - \hat{\mathbf{M}} \cdot \nabla(\mathbf{L}^{\mathrm{T}}) - \operatorname{div}\mathbf{j} \\ = \rho\Big\{\breve{h} + \frac{1}{2}\mathbf{I} \cdot \mathbf{L}^{\mathrm{T}}\mathbf{L}\Big\}^{\boldsymbol{\cdot}} - \rho\hat{\mathbf{B}} \cdot (\mathbf{L}^{\mathrm{T}})^{\boldsymbol{\cdot}}. \quad (6.61)$$

Chapter 7

Mixture theory

7.1. Preamble

In the foregoing all molecules have been given individual status, reflected in the labelling of masses and interactions. Thus in principle all masses m_i could be different, and all pairwise interactions $\mathbf{f}_{ij}$ could be governed by distinct functions of particle separation. Of course, in practice molecules and ions may be grouped in 'species'. If only one such species is present in a material system then this system is regarded to be a 'pure substance'. More generally, a material system composed of a number of species of molecules and/or ions may be expected to behave differently according to the relative numbers in each species, and their distributions among each other. Such considerations motivate looking at each species (also termed a *constituent*) in the '*mixture*' (of species) as a material system in its own right. Naturally such a viewpoint requires that account be taken of the influence of all other constituents upon that under inspection. Here only mass conservation and linear momentum balance will be discussed. The corpuscular approach renders precise and simple such concepts as velocity and stress fields for each constituent, and resolves a paradox[33)] concerning the interpretation of such ('*partial*') stresses. For simplicity only *binary, non-reacting* mixtures are considered: that is, only two distinct species of particles are involved, and there is no mass exchange between these sets of particles.

[33)] See Gurtin, Oliver & Williams [8].

7.2. Kinematics and mass conservation

Let $\mathcal{M}$ denote a material system which consists of two time-independent material systems $\mathcal{M}_\alpha$ and $\mathcal{M}_\beta$. Thus

$$\mathcal{M} = \mathcal{M}_\alpha \cup \mathcal{M}_\beta, \tag{7.1}$$

where

$$\mathcal{M}_\alpha = \{P_{\alpha_1}, P_{\alpha_2}, \ldots, P_{\alpha_{N_\alpha}}\} \quad \text{and} \quad \mathcal{M}_\beta := \{P_{\beta_1}, P_{\beta_2}, \ldots, P_{\beta_{N_\beta}}\}. \tag{7.2}$$

If $m_{\alpha_i}, \mathbf{x}_{\alpha_i}, m_{\beta_j}$, and $\mathbf{x}_{\beta_j}$ denote the masses and locations of particles P_{α_i} and P_{β_j}, respectively, then the mass density fields ρ_α and ρ_β for $\mathcal{M}_\alpha$ and $\mathcal{M}_\beta$ are, at the scale associated with choice w of weighting function, given by (cf. $(4.5)_1$)

$$\begin{aligned} \rho_\alpha(\mathbf{x}, t) &:= \sum_{\alpha_{i=1}}^{N_\alpha} m_{\alpha_i}\, w\big(\mathbf{x}_{\alpha_i}(t) - \mathbf{x}\big) \quad \text{and} \\ \rho_\beta(\mathbf{x}, t) &:= \sum_{\beta_{j=1}}^{N_\beta} m_{\beta_j}\, w\big(\mathbf{x}_{\beta_j}(t) - \mathbf{x}\big). \end{aligned} \tag{7.3}$$

The corresponding momentum density fields are

$$\begin{aligned} \mathbf{p}_\alpha(\mathbf{x}, t) &:= \sum_{\alpha_{i=1}}^{N_\alpha} m_{\alpha_i} \mathbf{v}_{\alpha_i}(t)\, w\big(\mathbf{x}_{\alpha_i}(t) - \mathbf{x}\big) \quad \text{and} \\ \mathbf{p}_\beta(\mathbf{x}, t) &:= \sum_{\beta_{j=1}}^{N_\beta} m_{\beta_j} \mathbf{v}_{\beta_j}(t)\, w\big(\mathbf{x}_{\beta_j}(t) - \mathbf{x}\big). \end{aligned} \tag{7.4}$$

Accordingly the mass density and momentum density fields ρ and $\mathbf{p}$ for the total system $\mathcal{M}$ (see $(4.5)_{1,2}$) are given by

$$\rho(\mathbf{x}, t) = \sum_{\text{all particles}} m_i\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) = \rho_\alpha(\mathbf{x}, t) + \rho_\beta(\mathbf{x}, t) \tag{7.5}$$

and

$$\mathbf{p}(\mathbf{x}, t) = \sum_{\text{all particles}} m_i\, \mathbf{v}_i(t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) = \mathbf{p}_\alpha(\mathbf{x}, t) + \mathbf{p}_\beta(\mathbf{x}, t). \tag{7.6}$$

The velocity fields for $\mathcal{M}_\alpha, \mathcal{M}_\beta$ and $\mathcal{M}$ are defined by (cf. (4.6))

$$\mathbf{v}_\alpha := \frac{\mathbf{p}_\alpha}{\rho_\alpha}, \quad \mathbf{v}_\beta := \frac{\mathbf{p}_\beta}{\rho_\beta}, \quad \text{and} \quad \mathbf{v} := \frac{\mathbf{p}}{\rho}. \tag{7.7}$$

It follows from (7.5), (7.6) and (7.7) that

$$\rho = \rho_\alpha + \rho_\beta \tag{7.8}$$

and

$$\rho\mathbf{v} = \rho_\alpha\mathbf{v}_\alpha + \rho_\beta\mathbf{v}_\beta. \tag{7.9}$$

A binary mixture is termed 'non-diffusive' if $\mathbf{v}_\alpha = \mathbf{v}_\beta$. Such a situation would be expected if $\mathcal{M}$ were a 'solid' body. If $\mathcal{M}$ is a fluid then diffusion is possible: this is evident when a soluble dye disperses in a solvent... the dye 'moves' through the solvent, indicating that relative mass transport is taking place and hence $\mathbf{v}_{\text{dye}} \neq \mathbf{v}_{\text{solvent}}$.

Exactly as in Section 4.4, motion maps for $\mathcal{M}_\alpha$, $\mathcal{M}_\beta$, and $\mathcal{M}$ may be defined. Specifically, the motion χ_α of $\mathcal{M}_\alpha$ relative to the situation at instant t_0 is the solution of the initial-value problem

$$\begin{aligned} &\dot{\chi}_\alpha(\hat{\mathbf{x}}, t) = \mathbf{v}_\alpha\big(\chi_\alpha(\hat{\mathbf{x}}, t), t\big), \\ &\text{where} \quad \chi_\alpha(\hat{\mathbf{x}}, t_0) = \hat{\mathbf{x}}, \end{aligned} \tag{7.10}$$

and similarly for χ_β and χ in respect of $\mathcal{M}_\beta$ and $\mathcal{M}$, respectively. Recalling Remark 4.7., the foregoing motions may be visualised in terms of material points. Thus with each geometrical point $\hat{\mathbf{x}}$ in the region 'occupied' by $\mathcal{M}_\alpha$ at instant t_0 (that is, the region wherein $\rho_\alpha(., t_0) > 0$) may be associated a material point whose location at instant t is $\chi_\alpha(\hat{\mathbf{x}}, t)$, and similarly for $\mathcal{M}_\beta$ and $\mathcal{M}$. As emphasised in Remark 4.7., such material points are (scale-dependent) *mathematical artefacts* whose trajectories trace out the gross mass transport of $\mathcal{M}_\alpha$ particles etc. at the scale associated with w (which enters via the definition of $\mathbf{v}_\alpha$ etc.).

Remark 7.1. Mixtures of fluids inevitably involve molecules of these fluids encountering each other as near-neighbours as a consequence of molecular diffusion. However, in systems of biological or engineering interest this is not usually the case. For example, the behaviour of fluids containing cellular structures (such as blood) at scales large compared with these structures may be approached from the mixture viewpoint, but the structures will usually maintain their molecular constitution. Studies of composite bodies and fluid flow through porous media are generally concerned with properties associated with scales greater than those at which the fine structure of these systems is manifest. Such fine structure is often evident at length scales far in excess of nearest-neighbour molecular separations, and individual molecular constituents occupy distinct regions at these longer scales. For this reason, averages such as appear in (7.3) and (7.4) (computed at scales large compared with the fine structure) are said to be those appropriate to an '*immiscible*' mixture.

Mass conservation relations for $\mathcal{M}_\alpha$ and $\mathcal{M}_\beta$ may be derived precisely as delineated in (4.7) and (4.8). Thus

$$\begin{aligned} &\frac{\partial \rho_\alpha}{\partial t} + \operatorname{div}\{\rho_\alpha \mathbf{v}_\alpha\} = 0 \quad \text{and} \\ &\frac{\partial \rho_\beta}{\partial t} + \operatorname{div}\{\rho_\beta \mathbf{v}_\beta\} = 0. \end{aligned} \tag{7.11}$$

Of course, adding these relations and recalling (7.8) and (7.9) results in mass conservation for the mixture as a whole (that is, for $\mathcal{M}$): namely,

$$\frac{\partial \rho}{\partial t} + \operatorname{div}\{\rho \mathbf{v}\} = 0. \tag{7.12}$$

7.3. Linear momentum balance

In an inertial frame the motion of P_{α_i} is governed by

$$\sum_{\substack{\alpha_j \neq \alpha_i \\ \alpha_j = 1}}^{N_\alpha} \mathbf{f}_{\alpha_i \alpha_j} + \sum_{\beta_k = 1}^{N_\beta} \mathbf{f}_{\alpha_i \beta_k} + \mathbf{b}_{\alpha_i} = \frac{d}{dt}\{m_{\alpha_i} \mathbf{v}_{\alpha_i}\}. \tag{7.13}$$

Here $\mathbf{f}_{\alpha_i \alpha_j}$ and $\mathbf{f}_{\alpha_i \beta_k}$ denote the forces exerted upon P_{α_i} by P_{α_j} and P_{β_k}, respectively, and $\mathbf{b}_{\alpha_i}$ is the resultant external force on P_{α_i}. Multiplying (7.13) by $w(\mathbf{x}_{i_\alpha}(t) - \mathbf{x})$ and summing over all P_{α_i} in $\mathcal{M}_\alpha$ yields

$$\mathbf{f}_{\alpha\alpha} + \mathbf{f}_{\alpha\beta} + \mathbf{b}_\alpha = \frac{\partial}{\partial t}\{\rho_\alpha \mathbf{v}_\alpha\} + \operatorname{div}\{\rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha + \boldsymbol{\mathcal{D}}_\alpha\}, \tag{7.14}$$

where

$$\mathbf{f}_{\alpha\alpha}(\mathbf{x}, t) := \sum_{\substack{\alpha_i, \alpha_j = 1 \\ \alpha_i \neq \alpha_j}}^{N_\alpha} \sum \mathbf{f}_{\alpha_i \alpha_j}(t)\, w\big(\mathbf{x}_{\alpha_i}(t) - \mathbf{x}\big), \tag{7.15}$$

$$\mathbf{f}_{\alpha\beta}(\mathbf{x},t) := \sum_{\beta_k=1}^{N_\beta} \mathbf{f}_{\alpha_i\beta_k}(t)\, w\big(\mathbf{x}_{\alpha_i}(t)-\mathbf{x}\big), \tag{7.16}$$

$$\mathbf{v}_{\alpha}(\mathbf{x},t) := \sum_{\alpha_i=1}^{N_\alpha} \mathbf{b}_{\alpha_i}(t)\, w\big(\mathbf{x}_{\alpha_i}(t)-\mathbf{x}\big), \tag{7.17}$$

and

$$\boldsymbol{\mathcal{D}}_{\alpha}(\mathbf{x},t) := \sum_{\alpha_i=1}^{N_\alpha} m_{\alpha_i}\hat{\mathbf{v}}_{\alpha_i}(\mathbf{x},t)\otimes\hat{\mathbf{v}}_{\alpha_i}(\mathbf{x},t)\, w\big(\mathbf{x}_{\alpha_i}(t)-\mathbf{x}\big), \tag{7.18}$$

with

$$\hat{\mathbf{v}}_{\alpha_i}(\mathbf{x},t) := \mathbf{v}_{\alpha_i}(t) - \mathbf{v}_{\alpha}(\mathbf{x},t). \tag{7.19}$$

The analysis is precisely that which established (4.35): the only difference is the decomposition of the interaction force density into $\alpha-\alpha$ and $\beta-\alpha$ contributions. However, $\hat{\mathbf{v}}_{\alpha_i}$ is the notional[34] *intrinsic* thermal velocity for P_{α_i}, so-called because it is the velocity of P_{α_i} relative to the α-species velocity field (rather than the total mixture velocity field $\mathbf{v}$).

Repeating the analysis which yielded (4.36) from (4.35),

$$\frac{\partial}{\partial t}\{\rho_\alpha\mathbf{v}_\alpha\} + \operatorname{div}\{\rho_\alpha\mathbf{v}_\alpha\otimes\mathbf{v}_\alpha\} = \rho_\alpha\grave{\mathbf{a}}_\alpha \tag{7.20}$$

where the *intrinsic acceleration field* (cf. (4.37))

$$\grave{\mathbf{a}}_\alpha := \frac{\partial\mathbf{v}_\alpha}{\partial t} + (\nabla\mathbf{v}_\alpha)\mathbf{v}_\alpha. \tag{7.21}$$

At this point linear momentum balance for $\mathcal{M}_\alpha$ assumes the form (see (7.14) and (7.21) and cf. (4.38))

$$-\operatorname{div}\boldsymbol{\mathcal{D}}_\alpha + \mathbf{f}_{\alpha\alpha} + \mathbf{f}_{\alpha\beta} = \rho_\alpha\grave{\mathbf{a}}_\alpha. \tag{7.22}$$

Remark 7.2. Provided $\alpha-\alpha$ interactions are 'balanced' in the sense of (4.42), if w is given by (4.13) then (cf. Remark 4.8.) $\mathbf{f}_{\alpha\alpha}(\mathbf{x})$ is the resultant force exerted by α particles *outside* $S_\epsilon(\mathbf{x})$ upon α particles *inside* $S_\epsilon(\mathbf{x})$, divided by the volume V_ϵ of $S_\epsilon(\mathbf{x})$. Term $\mathbf{f}_{\alpha\beta}(\mathbf{x})$ represents the resultant force exerted upon α particles within $S_\epsilon(\mathbf{x})$ by β particles *anywhere* (whether inside or outside $S_\epsilon(\mathbf{x})$), divided by V_ϵ, and $\mathbf{b}_\alpha(\mathbf{x})$ denotes the resultant external force on α particles within $S_\epsilon(\mathbf{x})$ divided by V_ϵ.

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[34] The notional intrinsic thermal velocity $\mathbf{v}_{\alpha_i}(\mathbf{x},t)$ approximates, for particles near $\mathbf{x}$, the *actual* intrinsic thermal velocity $\grave{\mathbf{v}}_{\alpha_i}(t) := \mathbf{v}_{\alpha_i}(t) - \mathbf{v}_\alpha\big(\mathbf{x}_{i_\alpha}(t),t\big)$.

Remark 7.3. The notional *extrinsic*[35] thermal velocity $\tilde{\mathbf{v}}_{\alpha_i}(\mathbf{x},t)$, which approximates the *actual* extrinsic thermal velocity

$$\tilde{\mathbf{v}}_{\alpha_i}(t) := \mathbf{v}_{\alpha_i}(t) - \mathbf{v}\big(\mathbf{x}_{\alpha_i}(t),t\big) \tag{7.23}$$

if $\mathbf{x}_{\alpha_i}(t)$ is near $\mathbf{x}$, is defined by

$$\breve{\mathbf{v}}_{\alpha_i}(\mathbf{x},t) := \mathbf{v}_{\alpha_i}(t) - \mathbf{v}(\mathbf{x},t). \tag{7.24}$$

Defining (cf. (7.18))

$$\breve{\boldsymbol{\mathcal{D}}}_\alpha(\mathbf{x},t) := \sum_{\alpha_i=1}^{N_\alpha} m_{\alpha_i}\, \breve{\mathbf{v}}_{\alpha_i}(\mathbf{x},t) \otimes \breve{\mathbf{v}}_{\alpha_i}(\mathbf{x},t)\, w\big(\mathbf{x}_{\alpha_i}(t) - \mathbf{x}\big) \tag{7.25}$$

we have

$$\breve{\boldsymbol{\mathcal{D}}}_\alpha = \boldsymbol{\mathcal{D}}_\alpha + \rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha, \tag{7.26}$$

where the *diffusive velocity*

$$\mathbf{u}_\alpha := \mathbf{v}_\alpha - \mathbf{v}. \tag{7.27}$$

The extrinsic acceleration (cf. (7.21))

$$\breve{\mathbf{a}}_\alpha := \frac{\partial \mathbf{v}_\alpha}{\partial t} + (\nabla \mathbf{v}_\alpha)\mathbf{v}, \tag{7.28}$$

so that

$$\breve{\mathbf{a}}_\alpha = \grave{\mathbf{a}}_\alpha - (\nabla \mathbf{v}_\alpha)\mathbf{u}_\alpha. \tag{7.29}$$

Invoking relations between intrinsic and extrinsic fields enables linear momentum balances for $\mathcal{M}_\alpha$ and $\mathcal{M}_\beta$ to be summed to yield the corresponding balance for the combined system $\mathcal{M}$. Specifically, from (7.14) and (7.26), the balance for $\mathcal{M}_\alpha$ is

$$\mathbf{f}_{\alpha\alpha} + \mathbf{f}_{\alpha\beta} + \mathbf{b}_\alpha = \frac{\partial}{\partial t}\{\rho_\alpha \mathbf{v}_\alpha\} + \operatorname{div}\{\rho_\alpha \mathbf{v}_\alpha \otimes \mathbf{v}_\alpha - \rho_\alpha \mathbf{u}_\alpha \otimes \mathbf{u}_\alpha + \breve{\boldsymbol{\mathcal{D}}}_\alpha\}. \tag{7.30}$$

Similarly the balance for $\mathcal{M}_\beta$ is

$$\mathbf{f}_{\beta\beta} + \mathbf{f}_{\beta\alpha} + \mathbf{b}_\beta = \frac{\partial}{\partial t}\{\rho_\beta \mathbf{v}_\beta\} + \operatorname{div}\{\rho_\beta \mathbf{v}_\beta \otimes \mathbf{v}_\beta - \rho_\beta \mathbf{u}_\beta \otimes \mathbf{u}_\beta + \breve{\boldsymbol{\mathcal{D}}}_\beta\}, \tag{7.31}$$

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[35] 'Extrinsic' refers to concepts defined with respect to the mixture as a whole: that is, to system $\mathcal{M}$.

where

$$\mathbf{u}_\beta := \mathbf{v}_\beta - \mathbf{v}. \tag{7.32}$$

System $\mathcal{M}$ has balance (4.35),namely

$$\mathbf{f} + \mathbf{b} = \frac{\partial}{\partial t}\{\rho\mathbf{v}\} + \operatorname{div}\{\rho\mathbf{v}\otimes\mathbf{v} + \boldsymbol{\mathcal{D}}\}, \tag{7.33}$$

where, from basic definitions,

and

$$\begin{gathered}\mathbf{f} = \mathbf{f}_{\alpha\alpha} + \mathbf{f}_{\alpha\beta} + \mathbf{f}_{\beta\beta} + \mathbf{f}_{\beta\alpha}, \quad \mathbf{b} = \mathbf{b}_\alpha + \mathbf{b}_\beta, \\ \boldsymbol{\mathcal{D}} = \breve{\boldsymbol{\mathcal{D}}}_\alpha + \breve{\boldsymbol{\mathcal{D}}}_\beta.\end{gathered} \tag{7.34}$$

Relation (7.33) is merely the sum of relations (7.30) and (7.31), upon noting the identity

$$\rho_\alpha\mathbf{v}_\alpha\otimes\mathbf{v}_\alpha + \rho_\beta\mathbf{v}_\beta\otimes\mathbf{v}_\beta \equiv \rho_\alpha\mathbf{u}_\alpha\otimes\mathbf{u}_\alpha + \rho_\beta\mathbf{u}_\beta\otimes\mathbf{u}_\beta + \rho\mathbf{v}\otimes\mathbf{v} \tag{7.35}$$

and recalling (7.8) and (7.9).

Noll's theorem enables $\mathbf{f}_{\alpha\alpha}$ to be expressed as the divergence of a tensor field $\mathbf{T}_\alpha^-$. To this end

$$\mathbf{g}_\alpha(\mathbf{x},\mathbf{y}) := \sum_{\alpha_i\neq\alpha_j}\sum \mathbf{f}_{\alpha_i\alpha_j}\, w(\mathbf{x}_{\alpha_i} - \mathbf{x})\, w(\mathbf{x}_{\alpha_j} - \mathbf{y}), \tag{7.36}$$

where it follows exactly as in the derivation of (4.40), (4.43), (4.44) and (4.47), that

$$\mathbf{f}_{\alpha\alpha}(\mathbf{x},t) = \int_{\mathcal{E}} \mathbf{g}_\alpha(\mathbf{x},\mathbf{y})\, d\mathbf{y}, \tag{7.37}$$

$$\mathbf{g}_\alpha(\mathbf{y},\mathbf{x}) = -\mathbf{g}_\alpha(\mathbf{x},\mathbf{y}), \tag{7.38}$$

and

$$\mathbf{f}_{\alpha\alpha} = \operatorname{div}\mathbf{T}_\alpha^-, \tag{7.39}$$

where

$$\begin{aligned}\mathbf{T}_\alpha^-(\mathbf{x}) := -\frac{1}{2}\ &\sum_{\alpha_i\neq\alpha_j}\sum \mathbf{f}_{\alpha_i\alpha_j} \\ &\otimes \int_{\mathcal{V}}\int_0^1 \mathbf{u}\, w(\mathbf{x}_{\alpha_i} - \mathbf{x} - \alpha\mathbf{u})\, w\big(\mathbf{x}_{\alpha_j} - \mathbf{x} + (1-\alpha)\mathbf{u}\big)\, d\alpha\, d\mathbf{u}.\end{aligned} \tag{7.40}$$

That $\mathbf{g}_\alpha$ satisfies the conditions necessary to invoke Noll's theorem follows from the boundedness of w and its first derivatives and the bounded nature of interactions for any system with bounded total energy when such interactions are delivered by pair-potentials bounded below.

Similarly

$$\mathbf{f}_{\beta\beta} = \operatorname{div} \mathbf{T}_{\beta}^{-}, \tag{7.41}$$

where $\mathbf{T}_{\beta}^{-}$ is given by (7.40) with α replaced by β.
Balance (7.22) may now be expressed as

$$\operatorname{div} \mathbf{T}_{\alpha} + \mathbf{f}_{\alpha\beta} + \mathbf{b}_{\alpha} = \rho_{\alpha}\dot{\mathbf{a}}_{\alpha}, \tag{7.42}$$

where the *α-constituent partial stress* tensor

$$\mathbf{T}_{\alpha} := \mathbf{T}_{\alpha}^{-} - \boldsymbol{\mathcal{D}}_{\alpha}. \tag{7.43}$$

Replacing α by β yields the corresponding balance for $\mathcal{M}_{\beta}$.

Remark 7.4. It proves impossible to express $\mathbf{f}_{\alpha\beta}$ as a divergence, although this can be done for $\mathbf{f}_{\alpha\beta} + \mathbf{f}_{\beta\alpha}$. The stress tensor $\mathbf{T}$ for $\mathcal{M}$ satisfies (see $(7.34)_{1,3}$)

$$\operatorname{div} \mathbf{T} = \operatorname{div}(\mathbf{T}^{-} - \boldsymbol{\mathcal{D}}) = \operatorname{div}(\mathbf{T}_{\alpha}^{-} + \mathbf{T}_{\beta}^{-} - \breve{\boldsymbol{\mathcal{D}}}_{\alpha} - \breve{\boldsymbol{\mathcal{D}}}_{\beta}) + \mathbf{f}_{\alpha\beta} + \mathbf{f}_{\beta\alpha}. \tag{7.44}$$

Remark 7.5. The continuum theory of mixtures was introduced by Truesdell (see [6], [9]) and developed by many others including Bowen (see [10]). In this theory a balance of *form* (7.42) was *postulated*, but $\mathbf{T}_{\alpha}$ was given an erroneous physical interpretation. Specifically, if $\mathcal{S}$ is an oriented surface with unit normal field $\mathbf{n}$, $\int_{\mathcal{S}} \mathbf{T}_{\alpha}\,\mathbf{n}$ was interpreted to be the net force exerted by the *whole mixture* lying on the 'positive' side of $\mathcal{S}$ upon species α on the 'negative' side of $\mathcal{S}$. As we have seen, this quantity involves α-species diffusion across $\mathcal{S}$ (embodied in the contribution from $\boldsymbol{\mathcal{D}}_{\alpha}$) and $\alpha-\alpha$ interactions only. The Truesdell-Bowen interpretation was shown by Gurtin, Oliver & Williams [8] to lead to a paradox, but its source was not exposed. Williams [11] later arrived at an $\alpha-\alpha$ force interpretation of $\mathbf{T}_{\alpha}$ on the basis of highly complex arguments. Here it has been seen that the corpuscular viewpoint leads directly to very precise interpretations of *all* fields which appear in continuum balance relations.

Remark 7.6. Somewhat surprisingly the conditions of Noll's theorem are met by a family of ions of the same polarity. This follows from Remark 4.9. on noting that pairwise interactions in such case are Coulombic and hence bounded below. Accordingly the existence of a stress-tensor is not conditional upon any essential short-range nature of corpuscular interactions. Nevertheless, such criteria *do* apply when making *constitutive* assumptions which result in the standard theories of elastica and fluids, etc. These criteria are embodied in the 'principle of local action': see Truesdell & Noll [1], §26.

Chapter 8

Time averaging

8.1. Introduction

So far we have obtained continuum balance equations in which fields are related to local, scale-dependent, spatial averages of molecular quantities. However, to attempt to relate continuum fields values to actual observations/measurements of material behaviour, we need to appreciate that the latter involve averages both in space *and* time. Specifically, no observation/measurement can be undertaken at a single geometrical point, nor at a given instant in time. (For example, photographic 'snapshots' involve exposure times, and reveal information limited by the ultimate spatial resolution admitted by the film material.) Over and above such practical considerations, time averaging plays a central rôle in conceiving the link between microscopic behaviour and continuum modelling of its macroscopic consequences. An extreme and striking example is the case of a single molecule in a box. Consider a small part of one face of the box, of area ΔS, say, and monitor the collisions of the molecule with this part over a time interval of duration T. Each collision gives an impulse to the wall. Adding up all these impulses over the time interval and dividing by $T \times \Delta S$ gives a quantity which is the average pressure associated with this part of the box over this time interval. Such pressure 'fluctuates' with time, but if T is sufficiently large the fluctuations may be negligibly-small changes about some definite value. In such case we obtain a continuum value for the pressure: namely, the 'definite value' mentioned. Another, more general, appreciation of time averaging can be gained by considering statistical mechanical approaches to continuum mechanics. This is exemplified by examining what is meant by the 'probability density' associated with a particle system. Consider a small region of volume ΔV, so small that at most one molecule (more precisely, one molecular mass centre) can be inside this region at any given time. Observe over a time interval of duration T what proportion of this time the region actually contains a molecular mass centre. If this proportion tends to a limit as T becomes larger and larger, then this limit is regarded to be the probability of finding a particle in this 'macroscopically infinitesimal' region. The involvement of unbounded time intervals might seem here to limit physical relevance to particle systems in 'equilibrium' at the macroscopic level. However, the foregoing time-occupation proportion may 'stabilise' for time intervals of duration $T = T_0$, in the sense of merely undergoing negligible fluctuation about some fixed value. In such case we have an interpretation of the probability of finding a particle in ΔV consistent with macroscopic behaviour that evolves temporally on a scale large compared with T_0.

Remark 8.1. The foregoing remarks are not precise, but were made to draw attention to the link between time averaging and statistical mechanics. The existence of a probability density is a *modelling assumption*, which can either be interpreted as above, or via 'ensemble' averaging. We do not here discuss ensemble averages, but note that these are identified with time averages via a so-called 'ergodicity hypothesis'.

8.2. The averaging procedure

Question: *How can we average a time-dependent quantity?*

Answer: *If f is a continuous function of time then its Δ-time average at time t is*

$$f_\Delta(t) := \frac{1}{\Delta} \int_{t-\Delta}^{t} f(\tau) d\tau. \tag{8.1}$$

[Thus $f_\Delta(t)$ is the mean value of f over that time interval of duration Δ ending at time t.]

Result 8.1. If f is smooth (that is, if $\dot{f}$ is continuous) then

$$(\dot{f_\Delta}) = (\dot{f})_\Delta. \tag{8.2}$$

Proof. [36]

$$
\begin{aligned}
(\dot{f}_\Delta) &:= \frac{d}{dt}\left(f_\Delta(t)\right) = \frac{d}{dt}\left\{\frac{1}{\Delta}\int_{t-\Delta}^{t} f(\tau)\,d\tau\right\} \\
&= \frac{1}{\Delta}\left\{f(t) - f(t-\Delta)\right\} \\
&= \frac{1}{\Delta}\int_{t-\Delta}^{t} \frac{df}{d\tau}\,d\tau = (\dot{f})_\Delta .
\end{aligned}
$$

■

Result 8.2. If **A** is a vector (or higher rank tensor) field then

$$(\operatorname{div}\mathbf{A})_\Delta = \operatorname{div}(\mathbf{A}_\Delta). \tag{8.3}$$

[Proof only requires interchange of limiting processes of spatial differentiation and definite integration.]

8.3. Mass conservation

Now recall the continuity equation (4.9):

$$\frac{\partial \rho_w}{\partial t} + \operatorname{div}\{\rho_w\,\mathbf{v}_w\} = 0. \tag{4.9}$$

Time averaging, together with Results 1 and 2, yield

$$\frac{\partial}{\partial t}\left((\rho_w)_\Delta\right) + \operatorname{div}\bigl\{(\rho_w\,\mathbf{v}_w)_\Delta\bigr\} = 0. \tag{8.4}$$

Writing

$$\rho_{w,\Delta} := (\rho_w)_\Delta \tag{8.5}$$

and defining

$$\mathbf{v}_{w,\Delta} := \frac{(\rho_w\,\mathbf{v}_w)_\Delta}{\rho_{w,\Delta}}, \tag{8.6}$$

(8.4) becomes

$$\frac{\partial}{\partial t}\{\rho_{w,\Delta}\} + \operatorname{div}\{\rho_{w,\Delta}\,\mathbf{v}_{w,\Delta}\} = 0. \tag{8.7}$$

This is the continuity equation with fields interpreted in terms of space-time averages of molecular quantities.

---

[36] $\frac{d}{dt}\left\{\int_{a(t)}^{b(t)} f(t,\tau)d\tau\right\} = f(t,b(t))b'(t) - f(t,a(t))a'(t) + \int_{a(t)}^{b(t)} \frac{\partial f}{\partial t}\,d\tau.$

Caveat:

$$\mathbf{v}_{w,\Delta} \neq (\mathbf{v}_w)_\Delta \; ! \tag{8.8}$$

(Why?)

Balances of linear momentum, moment of momentum, and energy can be obtained, in more or less straightforward fashion, with field values now re-defined in terms of averages both in space *and* time. One point to note is that the notional thermal velocities now involve $\mathbf{v}_{w,\Delta}$ $(\hat{\mathbf{v}}_i(\mathbf{x}) := \mathbf{v}_i - \mathbf{v}_{w,\Delta}(\mathbf{x}))$. Details of the analysis are to be found in Murdoch & Bedeaux [12].

8.4. Points to ponder

Suppose two inertial observers, in motion with respect to each other, undertake the space time averaging discussed above. At a specific location $\mathbf{x}$ and time t the averages will involve differing molecular samples.

Point 1: Why are the molecular samples different? How does this link with measurements taken by the pair of observers?

Point 2: Can time averaging be implemented in such a way that the molecular samples are the same?

Point 3: If the molecular samples are the same in arriving at field values which are space-time averages, note that material properties/behaviour may depend on the spin of the material system relative to an (hence any) inertial frame. Why?

Point 3 has been the source of much controversy and confusion in Continuum Mechanics concerning the correct interpretation of the 'principle of material frame-indifference'.

Chapter 9

Time-dependent systems

9.1. Introduction

Consider two examples of time-dependent systems, namely radioactive decay and rocket motion. These processes are modelled by very simple differential equations. Specifically, these are

$$\dot{m} = -km \ (k > 0) \quad \text{(radioactive decay)} \tag{9.1}$$

and

$$-\dot{M}V = M\dot{v} \quad \text{(the ‘rocket’ equation).} \tag{9.2}$$

Here m denotes the mass of the radioactive body, k is a constant, M is the mass of the rocket, $\dot{v}$ its mass centre acceleration, and V the speed at which the exhaust gas leaves the rocket. Differential equations (9.1) and (9.2) are *global* descriptions of material systems which change with time. Such change actually involves discrete entities, namely ions or molecules. Other examples of such systems are evaporating or condensing bodies of liquid, or specific species of molecules or ions in chemical reactions.

Problem: *How can such systems be handled from our particle viewpoint?*

Answer/Methodology: *Adapt our procedures of space-time averaging to time-dependent systems.*

9.2. The basic approach

The key idea is to regard the time-dependent set in question as a subset of a time-*independent* material system $\mathcal{M}$. If $\mathcal{M}$ consists of particles P_i ($i = 1, 2, \ldots, N$) as in previous chapters, then, at any instant t,

$$\mathcal{M} = \mathcal{M}^+(t) \cup \mathcal{M}^-(t), \tag{9.3}$$

where $\mathcal{M}^+(t)$ denotes the system of interest at instant t and

$$\mathcal{M}^-(t) := \mathcal{M} - \mathcal{M}^+(t). \tag{9.4}$$

The particle population of $\mathcal{M}^+(t)$ at instant t is handled in terms of a '*membership function*' $e_i(t)$:

$$\begin{cases} e_i(t) := 1 & \text{if } P_i \in \mathcal{M}^+(t) \text{ at instant } t, \\ e_i(t) := 0 & \text{if } P_i \notin \mathcal{M}^+(t) \text{ at instant } t. \end{cases} \tag{9.5}$$

Here we only examine global properties and equations for system $\mathcal{M}^+$. Local balance relations which hold at specific length-time scales are derived in Murdoch [13]. It may be helpful to keep in mind some specific example, such as a rocket plus its fuel ($\mathcal{M}$:= rocket + initial fuel).

The *mass* of the system at instant τ is

$$m(\tau) := \sum_{i=1}^{N} m_i \, e_i(\tau), \tag{9.6}$$

and the total momentum is

$$\mathbf{p}(\tau) := \sum_{i=1}^{N} m_i \, \mathbf{v}_i(\tau) e_i(\tau). \tag{9.7}$$

Since we wish functions such as $m(\tau)$ and $\mathbf{p}(\tau)$ to be smooth (we shall later invoke result (8.2)), we have to modify (9.5) slightly because e_i is not continuous. Just as in spatial averaging, we *mollify* e_i. Matters are a little different, however. Suppose

$$\begin{aligned} &P_i \in \mathcal{M}^+(t) \quad \text{for} \quad t_1 < t < t_2 \quad \text{and} \\ &P_i \notin \mathcal{M}^+(t) \quad \text{for} \quad t_0 < t \leqslant t_1 \quad \text{and} \quad t_2 \leqslant t < t_3. \end{aligned}$$

Then for $t_0 < t < t_3$ definition (9.5) yields the graph depicted in Figure 9.1(i) which is mollified to that of Figure 9.7(ii). The mollifying interval for any particle arrival or departure is of duration δ, which may be fixed at a value as small as we wish in order to make the physical interpretations of (9.6) and (9.7) indistinguishable from the corresponding unmollified expressions.

Remark 9.1. In practice time-dependent material systems may not be defined as precisely as is suggested by (9.5). For example, just when is a molecule of rocket fuel to be considered as parting company with the rocket, or just when is an H_2O molecule to be considered to have 'evaporated' from a liquid phase? Such imprecision is the motivation for the theory of 'fuzzy' sets, and the foregoing formal introduction of mollification can be re-interpreted within such theory.

9.3. Evolution of global momentum

The motion of point mass P_i in an inertial frame is governed by (4.25):

$$\sum_{\substack{j\neq i\\ j=1}}^{N} \mathbf{f}_{ij} + \mathbf{b}_i = m_i\,\dot{\mathbf{v}}_i. \tag{9.8}$$

Multiplication by e_i followed by summation over $i = 1, 2, \ldots, N$ yields

$$\sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_i + \sum_i \mathbf{b}_i\,e_i = \sum_i m_i\,\dot{\mathbf{v}}_i\,e_i. \tag{9.9}$$

Notice that the sum is over all particles P_i in the time-*independent* system $\mathcal{M}$: that (9.9) describes the time-*independent* system $\mathcal{M}^+$ derives from the presence of membership function factors e_i. Term

$$\sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_i = \sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_ie_j + \sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_i(1-e_j). \tag{9.10}$$

Further,

$$\begin{aligned}\sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_ie_j &= \frac{1}{2}\sum_{i\neq j}\sum (\mathbf{f}_{ij}\,e_ie_j + \mathbf{f}_{ji}\,e_je_i)\\ &= \frac{1}{2}\sum_{i\neq j}\sum (\mathbf{f}_{ij} + \mathbf{f}_{ji})\,e_ie_j. \end{aligned} \tag{9.11}$$

Hence if interactions are pairwise equilibrated (see (4.42)), from (9.10), (9.11) and (9.9),

$$\sum_{i\neq j}\sum \mathbf{f}_{ij}\,e_i(1-e_j) + \sum_i \mathbf{b}_i\,e_i = \sum_i m_i\,\dot{\mathbf{v}}_i\,e_i. \tag{9.12}$$

The first term in (9.12) represents the resultant force on $\mathcal{M}^+$ particles exerted by $\mathcal{M}^-$ particles.

Taking the Δ-time average of (9.12) at time t yields

$$\mathbf{f}_\Delta(t) + \mathbf{b}_\Delta(t) = \frac{1}{\Delta}\sum_i m_i \int_{t-\Delta}^{t} \dot{\mathbf{v}}_i(\tau) e_i(\tau)\, d\tau, \tag{9.13}$$

where

$$\mathbf{f}_\Delta(t) := \frac{1}{\Delta}\ \sum\sum_{i\neq j} \int_{t-\Delta}^{t} \mathbf{f}_{ij}(\tau) e_i(\tau)\big(1 - e_j(\tau)\big) d\tau \tag{9.14}$$

and

$$\mathbf{b}_\Delta(t) := \frac{1}{\Delta}\sum_i \int_{t-\Delta}^{t} \mathbf{b}_i(\tau) e_i(\tau)\, d\tau. \tag{9.15}$$

To understand the nature of the last term in (9.13) we consider a number of possibilities.

(i) If $P_i \in \mathcal{M}^+(t-\Delta)$ at time $t-\Delta$, stays a member of $\mathcal{M}^+$ until time $t_1 < t$, and remains in $\mathcal{M}^-$ until time t, then its contribution is

$$\frac{m_i}{\Delta}\int_{t-\Delta}^{t_1} \dot{v}_i(\tau)\, d\tau = \frac{m_i}{\Delta}\{\mathbf{v}_i(t_1) - \mathbf{v}_i(t-\Delta)\}. \tag{9.16}$$

(ii) If $P_i \in \mathcal{M}^-$ for $t - \Delta < \tau < t_2 < t$ and becomes a member of $\mathcal{M}^+$ at time t_2, staying in $\mathcal{M}^+$ for $t_2 < \tau < t$, then its contribution is

$$\frac{m_i}{\Delta}\int_{t_2}^{t} \dot{\mathbf{v}}_i(\tau) d\tau = \frac{m_i}{\Delta}\{\mathbf{v}_i(t) - \mathbf{v}_i(t_2)\}. \tag{9.17}$$

(iii) If $P_i \in \mathcal{M}^+$ for times

$$\tau \in (t_{i_1}, t_{i_2}) \cup (t_{i_3}, t_{i_4}) \cup \ldots \cup (t_{i_{2N-1}}, t_{i_{2N}})$$

where

$$t - \Delta \leqslant t_{i_1} < t_{i_2} < t_{i_3} < \cdots < t_{i_{2N}} \leqslant t$$

then its contribution is

$$\begin{aligned}\frac{m_i}{\Delta}\left\{\int_{t_{i_1}}^{t_{i_2}} \dot{v}_i(\tau) d\tau + \int_{t_{i_3}}^{t_{i_4}} \dot{\mathbf{v}}_i(\tau) d\tau + \cdots + \int_{t_{i_{2N-1}}}^{t_{i_{2N}}} \dot{\mathbf{v}}_i(\tau) d\tau\right\}& \\ = \frac{m_i}{\Delta}\big\{\mathbf{v}_i(t_{i_2}) - \mathbf{v}_i(t_{i_1}) + \mathbf{v}_i(t_{i_4}) - \mathbf{v}_i(t_{i_3}) + \cdots& \\ + \mathbf{v}_i(t_{i_{2N}}) - \mathbf{v}_i(t_{i_{2N-1}})\big\}.&\end{aligned} \tag{9.18}$$

Notice that there is a contribution $\pm m_i \mathbf{v}_i(t_{i_k})/\Delta$ at any time t_{i_k} when P_i enters or leaves $\mathcal{M}^+$ (the '+' sign corresponds to 'leaving' contributions and the '−' sign to 'entering' contributions), together with contributions from particles in $\mathcal{M}^+(t-\Delta)$ at time $t-\Delta$ (these are of form $-m_i\,\mathbf{v}_i(t-\Delta)/\Delta$) and in $\mathcal{M}^+(t)$ at time t (these are of form $+m_i \mathbf{v}_i(t)/\Delta$). Consideration of all cases yields

$$\begin{aligned}\frac{1}{\Delta}\int_{t-\Delta}^{t}\sum_i m_i\,\dot{\mathbf{v}}_i(\tau)e_i(\tau)\,d\tau &= \boldsymbol{\mathcal{F}}^{\Delta}_{\text{out}}(t)-\boldsymbol{\mathcal{F}}^{\Delta}_{\text{in}}(t)\\ &+\frac{1}{\Delta}\left\{\sum_i m_i\,\mathbf{v}_i(t)e_i(t)-\sum_i m_i\,\mathbf{v}_i(t-\Delta)e_i(t-\Delta)\right\}, \qquad (9.19)\end{aligned}$$

where

$$\boldsymbol{\mathcal{F}}^{\Delta}_{\text{out}}(t) := \frac{1}{\Delta}\sum_i\sum_{i_\ell} m_i\,\mathbf{v}_i(t_{i_\ell}) \qquad (9.20)$$

and

$$\boldsymbol{\mathcal{F}}^{\Delta}_{\text{in}}(t) := \frac{1}{\Delta}\sum_i\sum_{i_e} m_i\,\mathbf{v}_i(t_{i_e}). \qquad (9.21)$$

The sums in (9.19) and (9.20) are over all $P_i \in \mathcal{M}$ and all times $t_{i_\ell}(t_{i_e})$ at which P_i *l*eaves (*e*nters) $\mathcal{M}^+$ during the interval $(t-\Delta, t)$.

Since the last term in (9.18) is (see (9.7))

$$\begin{aligned}\frac{1}{\Delta}\{\mathbf{p}(t)-\mathbf{p}(t-\Delta)\} &= \frac{1}{\Delta}\int_{t-\Delta}^{t}\dot{\mathbf{p}}(\tau)\,d\tau\\ &= (\dot{\mathbf{p}})_\Delta = (\dot{\widehat{\mathbf{p}_\Delta}}), \qquad (9.22)\end{aligned}$$

(the last step is Result 1 (8.2)) relation (9.13) may be written as

$$\mathbf{f}_\Delta + \mathbf{b}_\Delta = \dot{\mathbf{p}}_\Delta + \boldsymbol{\mathcal{F}}^{\Delta}_{\text{out}} - \boldsymbol{\mathcal{F}}^{\Delta}_{\text{in}}, \qquad (9.23)$$

upon invoking (9.19). Here $\mathbf{f}_\Delta$ is the Δ-time averaged resultant force on $\mathcal{M}^+$ due to interactions with $\mathcal{M}^-$, $\mathbf{b}_\Delta$ the Δ-time averaged resultant external force on $\mathcal{M}^+, \dot{\mathbf{p}}_\Delta$ the time rate of change of Δ-averaged $\mathcal{M}^+$ momentum, $\boldsymbol{\mathcal{F}}^{\Delta}_{\text{out}}$ the momentum *loss* due to particles leaving $\mathcal{M}^+$, over a time interval of duration Δ, divided by Δ, and $\boldsymbol{\mathcal{F}}^{\Delta}_{\text{in}}$ is the momentum *gain* due to particles joining $\mathcal{M}^+$, over a time interval of duration Δ, divided by Δ.

It is possible to write (9.22) in an alternative (but equivalent) form. With (see (9.6) and (9.7))

$$\mathbf{v}_\Delta := \frac{\mathbf{p}_\Delta}{m_\Delta} \qquad (9.24)$$

we have

$$\dot{\mathbf{p}}_\Delta = \frac{d}{dt}\{m_\Delta\, \mathbf{v}_\Delta\} = \dot{\widehat{m_\Delta}}\, \mathbf{v}_\Delta + m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}. \tag{9.25}$$

Notice that from (8.2) and (9.6)

$$\dot{\widehat{m_\Delta}} = (\dot{m})_\Delta = \Delta^{-1}\big\{m(t) - m(t-\Delta)\big\}. \tag{9.26}$$

Writing

$$\tilde{\mathcal{F}}^{\Delta}_{\text{out}}(t) := \frac{1}{\Delta}\sum_i \sum_{t_{i_\ell}} m_i\big(\mathbf{v}_i(t_{i_\ell}) - \mathbf{v}_\Delta(t)\big) \tag{9.27}$$

and

$$\tilde{\mathcal{F}}^{\Delta}_{\text{in}}(t) := \frac{1}{\Delta}\sum_i \sum_{t_{i_e}} m_i\big(\mathbf{v}_i(t_{i_e}) - \mathbf{v}_\Delta(t)\big), \tag{9.28}$$

from (9.23), (9.25) and (9.26) we have

$$\mathbf{f}_\Delta + \mathbf{b}_\Delta = \tilde{\mathcal{F}}^{\Delta} + m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}, \tag{9.29}$$

where expression

$$\tilde{\mathcal{F}}^{\Delta} := \tilde{\mathcal{F}}^{\Delta}_{\text{in}} - \tilde{\mathcal{F}}^{\Delta}_{\text{out}} \tag{9.30}$$

represents the net momentum transfer into $\mathcal{M}^+$ from $\mathcal{M}^-$ associated with particle relative velocities $\mathbf{v}_i - \mathbf{v}_\Delta$ divided by Δ. Equivalently,

$$\mathbf{f}_\Delta + \mathbf{b}_\Delta + \tilde{\mathcal{F}}^{\Delta}_{\text{in}} - \tilde{\mathcal{F}}^{\Delta}_{\text{out}} = m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}. \tag{9.31}$$

9.4. Applications of relation (9.31)

9.4.1. Rocket propulsion

Here $\mathcal{M}$ is taken to be the molecules of the rocket together with those of the initial fuel, while $\mathcal{M}^+(\tau)$ is chosen to be the rocket molecules and the fuel molecules which remain in the rocket at instant τ. Accordingly $\mathcal{M}^-(\tau)$ denotes the fuel molecules that have left the rocket by instant τ, and $\mathbf{f}_\Delta(t)$ is here the Δ-time average at instant t of the resultant force exerted by ejected fuel upon the rocket and fuel therein. Term $\mathbf{b}_\Delta(t)$ represents the Δ-time averaged resultant external force at time t exerted by matter outwith the rocket plus initial fuel, and accordingly includes any resultant gravitational effect together with atmospheric resistance (where and when appropriate).

Quantity $\tilde{\mathcal{F}}^{\Delta}_{\text{in}}$ corresponds to ejected fuel molecules re-entering the rocket. Both $\mathbf{f}_\Delta$ and $\tilde{\mathcal{F}}^{\Delta}_{\text{in}}$ are realistically negligible, so (9.31) takes the form

$$-\tilde{\mathcal{F}}^{\Delta}_{\text{out}} + \mathbf{b}_\Delta = m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}. \tag{9.32}$$

The 'thrust', or propulsive agency, is provided by term $-\tilde{\mathcal{F}}^{\Delta}_{\text{out}}$. If all molecules ejected from the rocket do so with velocity $\mathbf{V}$ relative to the rocket then (see (9.27))

$$\begin{aligned} \tilde{\mathcal{F}}^{\Delta}_{\text{out}} &= \frac{1}{\Delta} \sum_i \sum_{i_\ell} m_i \{ (\mathbf{v}_i(t_{i_\ell}) - \mathbf{v}_\Delta(t) \} \\ &= \Big(\sum_i \sum_{i_\ell} m_i \Big) \mathbf{V}. \end{aligned} \tag{9.33}$$

Now $\sum\limits_i \sum\limits_{i_\ell} m_i$ denotes the total fuel mass ejected over the time interval $(t - \Delta, t)$. Accordingly (see (9.26))

$$\sum_i \sum_{i_\ell} m_i = m(t-\Delta) - m(t) = -\dot{\widehat{m_\Delta}}\, \Delta. \tag{9.34}$$

Thus, from (9.33) and (9.34),

$$\tilde{\mathcal{F}}^{\Delta}_{\text{out}} = -\dot{\widehat{m_\Delta}}\, \mathbf{V} \tag{9.35}$$

and (9.32) becomes

$$\dot{\widehat{m_\Delta}}\, \mathbf{V} + \mathbf{b}_\Delta = m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}. \tag{9.36}$$

In the event that gravitational forces are negligible then (9.36) becomes (see, for example, [7], p.214) the so-called 'rocket equation'

$$\dot{\widehat{m_\Delta}}\, \mathbf{V} = m_\Delta\, \dot{\widehat{\mathbf{v}_\Delta}}. \tag{9.37}$$

Notice that since $\dot{\widehat{m_\Delta}} < 0$ and $m_\Delta > 0$ vectors $\dot{\widehat{\mathbf{v}_\Delta}}$ and $\mathbf{V}$ are in opposite directions.

Remark 9.2. The assumption that all ejected molecules do so at the same velocity relative to the velocity of the rocket is, of course, highly unrealistic. However, equation (9.36) is valid quite generally provided $\mathbf{V}$ is reinterpreted via

$$\mathbf{V} := -\frac{\tilde{\mathcal{F}}^{\Delta}_{\text{out}}}{\dot{\widehat{m_\Delta}}}. \tag{9.38}$$

In such case $\mathbf{V}(t) + \mathbf{v}_\Delta(t)$ represents the sum of the momenta (computed at the instants of ejection) of all particles ejected over the time interval $(t-\Delta, t)$ divided by the total mass of these particles.

9.4.2. Jet propulsion

The difference between rocket and jet propulsion is that while a rocket must carry a combustive agent as part of its 'fuel', a jet obtains oxygen from the atmosphere. The appropriate choice of $\mathcal{M}$ is thus the molecules of the aircraft plus initial fuel plus atmosphere, and $\mathcal{M}^{+}(\tau)$ consists of the molecules of the aircraft together with remaining fuel and air within the engine(s) at time τ. Recall (9.29):

$$\mathbf{f}_{\Delta} + \mathbf{b}_{\Delta} + \tilde{\boldsymbol{\mathcal{F}}}_{\text{in}}^{\Delta} - \tilde{\boldsymbol{\mathcal{F}}}_{\text{out}}^{\Delta} = m_{\Delta}\, \dot{\widehat{\mathbf{v}_{\Delta}}}. \tag{9.29}$$

Here $\mathbf{f}_{\Delta}$ represents the time averaged resultant force exerted by atmospheric molecules ('lift' plus 'drag') and $\mathbf{b}_{\Delta}$ the effect of gravity (if $\mathbf{b}_i = m_i\,\mathbf{g}$ then $\mathbf{b}_{\Delta} = m_{\Delta}\,\mathbf{g}$, where $\mathbf{g}$ denotes gravitational acceleration). If air molecules enter the engine(s) at the same velocity $\mathbf{U}$ relative to the aircraft and never leave by an 'intake', and if air plus ejected fuel leaves exhaust(s) at the same velocity $\mathbf{V}$ relative to the aircraft, then

$$\tilde{\boldsymbol{\mathcal{F}}}_{\text{out}}^{\Delta} = \frac{M_{\text{ex}}^{\Delta}\,\mathbf{V}}{\Delta} \tag{9.39}$$

and

$$\tilde{\boldsymbol{\mathcal{F}}}_{\text{in}}^{\Delta} = \frac{M_{\text{in}}^{\Delta}\,\mathbf{U}}{\Delta}. \tag{9.40}$$

Here M_{ex}^{Δ} denotes the total mass of air plus fuel ejected over a time period of duration Δ, while M_{in}^{Δ} represents the total mass of air taken in during this period. Accordingly $M_{\text{ex}}^{\Delta} - M_{\text{in}}^{\Delta}$ denotes the net mass loss of $\mathcal{M}^{+}$ during the time period, so

$$\frac{M_{\text{ex}}^{\Delta}(t) - M_{\text{in}}^{\Delta}(t)}{\Delta} = \frac{m(t-\Delta) - m(t)}{\Delta} = -\dot{\widehat{m_{\Delta}}}(t). \tag{9.41}$$

From (9.39), (9.40) and (9.41), relation (9.29) may be written as

$$\mathbf{f}_{\Delta} + \mathbf{b}_{\Delta} + \dot{\widehat{m_{\Delta}}}\,\mathbf{V} + \frac{M_{\text{in}}^{\Delta}(\mathbf{U} - \mathbf{V})}{\Delta} = m_{\Delta}\, \dot{\widehat{\mathbf{v}_{\Delta}}}. \tag{9.42}$$

Since $\dot{\widehat{m_{\Delta}}} < 0$ and $\mathbf{V}$ is directed out of the engine exhaust, term $\dot{\widehat{m_{\Delta}}}\,\mathbf{V}$ is propulsive: that is, this term gives rise to an acceleration $\dot{\widehat{\mathbf{v}_{\Delta}}}$ in a direction opposite to the exhaust gas. Further, since $M_{\text{in}}^{\Delta} > 0$ and, realistically $\|\mathbf{U}\| \ll \|\mathbf{V}\|$ so that $\mathbf{U} - \mathbf{V}$ is also directed from engine(s) exhaust(s) to intake(s), $M_{\text{in}}^{\Delta}(\mathbf{U} - \mathbf{V})/\Delta$ is *also* propulsive.

Remark 9.3. The foregoing assumptions which led to relations (9.39) and (9.40) are, of course, unrealistic (cf. Remark 9.2.). However, using (9.39) and (9.40) to *define* **U** and **V** results in an unchanged equation (9.4) but with realistic interpretations of **U** and **V**.

9.5. Local continuum balances of mass and momentum

Defining

$$\rho_w(\mathbf{x},t) := \sum_{i=1}^{N} m_i\, e_i(t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \tag{9.43}$$

and

$$\mathbf{p}_w(x,t) := \sum_{i=1}^{N} m_i\, \mathbf{v}_i(t)\, e_i(t)\, w\big(\mathbf{x}_i(t) - \mathbf{x}\big) \tag{9.44}$$

it has been shown (see Murdoch [13], §3) that the corresponding time-averaged fields $\rho_{w,\Delta}$ and $\mathbf{p}_{w,\Delta}$ satisfy

$$\frac{\partial \rho_{w,\Delta}}{\partial t} + \operatorname{div} \mathbf{p}_{w,\Delta} = \mathcal{G}_{w,\Delta}, \tag{9.45}$$

where $\mathcal{G}_{w,\Delta}$ represents the net rate of increase of mass for $\mathcal{M}^+$ at the spatial scale associated with w and time scale Δ. Of course, the corresponding velocity field is

$$\mathbf{v}_{w,\Delta} := \frac{\mathbf{p}_{w,\Delta}}{\rho_{w,\Delta}}. \tag{9.46}$$

This velocity field can be used to construct the notion of 'material points' for $\mathcal{M}^+$ precisely as delineated in Section 4.4.

Linear momentum balance takes the form, on suppressing subscript pairs w, Δ,

$$\operatorname{div} \mathbf{T} + \mathbf{f}^{\text{ext}} + \mathbf{P}^{\text{in}} - \mathbf{P}^{\text{out}} + \mathbf{b} = \rho\dot{\mathbf{v}} + \mathcal{G}\mathbf{v}. \tag{9.47}$$

Here **T** and **b** have the same interpretation (for system $\mathcal{M}^+$) as in Chapter 4. Term $\mathbf{f}^{\text{ext}}$ represents the Δ-time averaged spatial force density associated with the effect on $\mathcal{M}^+$ particles due to $\mathcal{M}^-$ particles, and $\mathbf{P}^{\text{in}}$ ($\mathbf{P}^{\text{out}}$) denotes local rates of supply (depletion) of momentum due to $\mathcal{M}^- \to \mathcal{M}^+$ ($\mathcal{M}^+ \to \mathcal{M}^-$) transitions.

Chapter 10

Fluid flow in porous media

10.1. Introduction

A body is said to be *porous* at some length scale, ϵ_1 say, if its boundary at this scale is highly convoluted and the region it occupies at this scale (recall §4.3) is many-fold connected.[37] The *porosity* of such a body is a measure of the proportion of space 'within' the body that is 'unoccupied' by the body. As such, porosity is a concept which implicitly embodies *two* length scales: ϵ_1 as above, and the scale ϵ_2 at which the foregoing spatial proportion is computed. For most practical purposes we are interested only in the behaviour of fluid in pore space at a scale ϵ_2 large compared with characteristic pore size and porous body structural dimension. At such a scale the boundary of the body no longer contains pore boundaries. (See Figures 4.1, in which the crack can be regarded as a pore.) It is possible to gain insight into flow modelling by using averaging methodology developed in the preceding chapters. Such averaging can be implemented in two ways.

(i) Molecular behaviour can be averaged, as in the foregoing chapters, at scale ϵ_2.

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[37] That is, given any pair of points P and Q in this region, there are many classes of smooth curves which link P and Q. Within each class such a curve can be continuously deformed into any other. However, it is impossible to deform a curve in one class continuously into a curve in another class. Said more simply, if Γ_1 and Γ_2 are curves linking P to Q belonging to different classes, then a string in the form of the closed curve $\Gamma_1 \cup \Gamma_2$ cannot be shrunk (by shortening) to a point in such a way that it always remains in the region.

(ii) Behaviour at scale ϵ_1 may be modelled in a continuum manner, and then a scale ϵ_2 averaging of this continuum model may be effected.

Here we will sketch the second procedure in respect of rigid porous media saturated by incompressible fluid. Of course, in practice a porous body may undergo deformation, and may contain several fluids. In such case fluid-fluid interfaces can give rise to very significant capillarity effects, and 'common lines' (occurring, for example, where a fluid-fluid interface meets the porous body) may have an influence on fluid transport. It is in such complex situations that the (i) type averaging can be helpful. (See Murdoch & Hassanizadeh [14]. Paper [14] addressed interfaces and common lines, and treated these as time-dependent material systems in the manner of Chapter 9.)

10.2. Flow of an incompressible, linearly-viscous fluid through a rigid porous body it saturates

At scale ϵ_1 pore details are manifest, yet continuum modelling is sensible since ϵ_1 is much greater than the scale at which individual molecular behaviour is apparent or significant. Accordingly, the flow through a rigid porous body of an incompressible linearly-viscous fluid is adequately modelled by the Navier-Stokes equations

$$-\nabla P + \mu\Delta\mathbf{v} + \rho_0\,\mathbf{g} = \frac{\partial}{\partial t}\{\rho_0\,\mathbf{v}\} + \operatorname{div}\{\rho_0\,\mathbf{v}\otimes\mathbf{v}\}, \tag{10.1}$$

where

$$\operatorname{div}\mathbf{v} = 0. \tag{10.2}$$

Here P denotes the pressure, μ viscosity, $\mathbf{v}$ the (ϵ_1-scale) velocity, ρ_0 the (constant) mass density, and $\mathbf{g}$ the acceleration due to gravity. Of course, (10.2) is the consequence of mass conservation and incompressibility.

Equations (10.1) and (10.2) hold in the (fixed) region R consisting of all pore space and immediate vicinity of the porous body. These equations are supplemented by the boundary condition

$$\mathbf{v} = \mathbf{0} \quad \text{on} \quad \partial R, \tag{10.3}$$

which expresses the non-slip and non-penetration of fluid at pore 'walls'.

Question: *How can we average relation (10.1) at a scale large compared with pore size and porous body structural dimension? Here we are trying to average fields rather than discrete molecular quantities.*

Answer: *Use weighting functions! To do so we define, for a given field* f *and weighting function* w*, the* w*-average* f_w *of* f *by*

$$\langle f\rangle_w(\mathbf{x}) := \int_{\mathcal{E}} f(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y}. \tag{10.4}$$

Here $\mathcal{E}$ *denotes Euclidean space and* $\mathbf{y}$ *a typical point in* $\mathcal{E}$*. To ensure that* $\langle f\rangle_w$ *has the same physical dimensions as* f *it is necessary for the values of* w *to have dimension* L^{-3}*. Further, so that the average of any constant-valued function should yield this same function, it is necessary and sufficient that normalisation condition (4.2) should hold.*

Remark 10.1. To see the link between (10.4) and our previous weighted sums, consider the microscopic density distribution (on suppressing time-dependence)

$$\rho_{\text{mic}}(\mathbf{x}) := \sum_i m_i\, \delta(\mathbf{x}_i - \mathbf{x}), \tag{10.5}$$

where 'δ' denotes the Dirac delta distribution. Formal integration of (10.5) yields (see $(4.5)_1$)

$$\begin{aligned} \langle \rho_{\text{mic}}\rangle_w(\mathbf{x}) &:= \int_{\mathcal{E}} \rho_{\text{mic}}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \\ &= \sum_i m_i \int_{\mathcal{E}} \delta(\mathbf{x}_i - \mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \\ &= \sum_i m_i\, w(\mathbf{x}_i - \mathbf{x}) = \rho_w(\mathbf{x}). \end{aligned} \tag{10.6}$$

Remark 10.2. To obtain the averaged form of (10.1), each term is evaluated at $\mathbf{y}$, multiplied by $w(\mathbf{y}-\mathbf{x})$, and integrated over $\mathcal{E}$. However, the fields in (10.1) are defined only in the pore space and immediate vicinity of the body, denoted by R. In evaluating integrals over $\mathcal{E}$, these fields are considered to vanish outside R. The averaging of (10.1) requires that $\langle\nabla P\rangle_w, \langle\Delta\mathbf{v}\rangle_w, \langle\rho_0\,\mathbf{g}\rangle_w, \langle\frac{\partial}{\partial t}\,\{\rho_0\,\mathbf{v}\}\rangle_w$ and $\langle\operatorname{div}\{\rho_0\,\mathbf{v}\otimes\mathbf{v}\}\rangle w$ be computed.

Remark 10.3. To see that we should be clear *a priori* about the choice of w, consider the w-average of the gradient of a scalar field ϕ defined on R.

We have

$$\begin{aligned}\langle \nabla\phi\rangle_w(\mathbf{x}) &:= \int_{\mathcal{E}} \nabla\phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y}\\ &= \int_R \nabla\phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} = \int_R \nabla_{\mathbf{y}}(\phi w) - \phi\nabla_{\mathbf{y}}\, w\, d\mathbf{y}\\ &= \int_R \operatorname{div}\{\phi w \mathbf{1}\} + \phi\nabla_{\mathbf{x}}\, w\, d\mathbf{y}\\ &= \int_{\partial R} \phi w \mathbf{n}\, dA + \nabla_{\mathbf{x}} \int_R \phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y}.\end{aligned}$$

That is,

$$\langle \nabla\phi\rangle_w(\mathbf{x}) = \int_{\partial R} \phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, \mathbf{n}(\mathbf{y})\, dA_{\mathbf{y}} + \nabla\{\langle\phi\rangle_w\}(\mathbf{x}). \tag{10.7}$$

Hence the difference between the average of a gradient and the gradient of an average is the integral of $\phi w\mathbf{n}$ over the pore boundary ∂R with outward unit normal $\mathbf{n}$ to R. (Notice $\mathbf{n}$ is directed *into* the porous body.) Clearly this difference only derives from points $\mathbf{y}$ on ∂R for which $w(\mathbf{y}-\mathbf{x}) \neq 0$. For example, if w is given by (4.11) then only points on ∂R which lie within a distance of ϵ from $\mathbf{x}$ contribute to the integral term in (10.7).

Averages in the porous media literature are computed over so-called '*r*epresentative *e*lementary *v*olumes' (abbreviated to 'REV's). These are regions whose characteristic dimensions are large compared to pore and structure size. More precisely, an REV $C(\mathbf{x})$ 'centred at point $\mathbf{x}$' is defined by

$$C(\mathbf{x}) := \{\mathbf{x}+\mathbf{u} \,:\, \mathbf{u}\in\mathcal{U}\}. \tag{10.8}$$

Here $\mathcal{U}$ is a fixed set of displacements which form a neighbourhood of $\mathbf{0}\in\mathcal{V}$ (the space of all displacements between pairs of points in $\mathcal{E}$) which contains all vectors $\mathbf{u}$ with norm $\|\mathbf{u}\| \leqslant \epsilon_2$. If V denotes the volume of $C(\mathbf{x})$ (this is the same for all $\mathbf{x}$, of course... why?) then the choice of weighting function w is a mollified version of

$$\left.\begin{aligned}\hat{w}(\mathbf{u}) &:= V^{-1} &&\text{if } \mathbf{u}\in\mathcal{U},\\ \hat{w}(\mathbf{u}) &:= 0 &&\text{if } \mathbf{u}\notin\mathcal{U}.\end{aligned}\right\} \tag{10.9}$$

As in Chapter 4, mollification is effected over a physically-insignificant region, so that the values of $\int_{\mathcal{E}} f(\mathbf{y})w(\mathbf{y}-\mathbf{x})d\mathbf{y}$ and $\int_{\mathcal{E}} f(\mathbf{y})\hat{w}(\mathbf{y}-\mathbf{x})d\mathbf{y}$ are physically-indistinguishable for the fields with which we deal. Mollification is necessary in order that ∇w should exist: notice $\nabla \hat{w}$ fails to exist on the boundary of set $\mathcal{U}$. Returning to (10.7), we now note that

$$\int_{\partial R} \phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, \mathbf{n}(\mathbf{y})\, dA_{\mathbf{y}} = \int_{\mathcal{S}(\mathbf{x})} \phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, \mathbf{n}(\mathbf{y})\, dA_{\mathbf{y}} \tag{10.10}$$

where

$$\mathcal{S}(\mathbf{x}) := \partial R \cap \{\mathbf{y} \,:\, \mathbf{y}-\mathbf{x} \in \mathcal{U}\}. \tag{10.11}$$

Accordingly (10.7) becomes

$$\langle \nabla\phi \rangle_w(\mathbf{x}) = \nabla\{\langle \phi \rangle_w\}(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} \phi(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, \mathbf{n}(\mathbf{y})\, dA_{\mathbf{y}}. \tag{10.12}$$

With reference to the first term in (10.1), choice $\phi = P$ in (10.12) yields (upon suppressing explicit w-dependence for simplicity

$$\langle \nabla P \rangle(\mathbf{x}) = \nabla\{\langle P \rangle\}(\mathbf{x}) + \int_{\mathcal{S}(\mathbf{x})} P(\mathbf{y})\, \mathbf{n}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, dA_{\mathbf{y}}. \tag{10.13}$$

In abbreviated form this may be written as

$$\langle -\nabla P \rangle = -\nabla\{\langle P \rangle\} - \left(\int_{\mathcal{S}} P\, \mathbf{n}\, dA \right) / V \tag{10.14}$$

upon invoking (10.9) *et seq.* Recalling that $\mathbf{n}$ is that unit normal field on ∂R which is directed *into* the porous body, the last term in (10.14) represents an REV-volume averaged 'back pressure' exerted *on* the fluid *by* the porous body. This 'back pressure' is the reaction to the pressure exerted *on* the pore boundary *by* the fluid.

Further results necessary to effect averages of all terms in (10.1) are contained in

Proposition 10.1.

$$\langle \nabla \mathbf{u} \rangle = \nabla\{\langle \mathbf{u} \rangle\} + \int_{\mathcal{S}} w \mathbf{u} \otimes \mathbf{n}\, dA, \tag{10.15}$$

$$\langle \operatorname{div} \mathbf{u} \rangle = \{\operatorname{div}\langle \mathbf{u} \rangle\} + \int_{\mathcal{S}} \mathbf{u} \,.\, \mathbf{n}\, w\, dA, \tag{10.16}$$

and

$$\langle \operatorname{div} \mathbf{B} \rangle = \operatorname{div}\{\langle \mathbf{B} \rangle\} + \int_{\mathcal{S}} \mathbf{B}\mathbf{n}\, w\, dA. \tag{10.17}$$

Here $\mathbf{u}$ and $\mathbf{B}$ are, respectively, vector and tensor-valued functions defined in the region occupied by the fluid which vanish elsewhere. Further,

$$\langle \partial \mathbf{u} / \partial t \rangle = \frac{\partial}{\partial t} \{\langle \mathbf{u} \rangle\}. \tag{10.18}$$

Proof.

$$\begin{aligned}\langle\nabla\mathbf{u}\rangle(\mathbf{x}) &:= \int_{\mathcal{E}} \nabla\mathbf{u}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \\ &= \int_R \nabla\mathbf{u}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} = \int_R \left(\nabla_{\mathbf{y}}\{w\mathbf{u}\} - \mathbf{u}\otimes\nabla_{\mathbf{y}}\, w\right) d\mathbf{y}. \qquad (10.19)\end{aligned}$$

To simplify the first term in the last integral we note that, for any fixed vector $\mathbf{k}$,

$$\begin{aligned}\left(\int_R \nabla\mathbf{u}\{w\mathbf{u}\}d\mathbf{y}\right)\mathbf{k} &= \int_R (\nabla_{\mathbf{y}}\{w\mathbf{u}\})\mathbf{k}\, d\mathbf{y} \\ &= \int_R \operatorname{div}_{\mathbf{y}}\{w\mathbf{u}\otimes\mathbf{k}\}\, d\mathbf{y} = \int_{\partial R} (w\mathbf{u}\otimes\mathbf{k})\mathbf{n}\, dA_{\mathbf{y}} \\ &= \int_{\mathcal{S}(\mathbf{x})} (w\mathbf{u}\otimes\mathbf{n})\mathbf{k}\, dA_{\mathbf{y}} = \left(\int_{\mathcal{S}(\mathbf{x})} w\mathbf{u}\otimes\mathbf{n}\, dA_{\mathbf{y}}\right)\mathbf{k}.\end{aligned}$$

Hence

$$\int_R \nabla_{\mathbf{y}}\{w\mathbf{u}\}\, d\mathbf{y} = \int_{\mathcal{S}(\mathbf{x})} w\,\mathbf{u}\otimes\mathbf{n}\, dA_{\mathbf{y}}. \qquad (10.20)$$

The last term in (10.19) is

$$-\int_R \mathbf{u}\otimes\nabla_{\mathbf{y}}\, w\, d\mathbf{y} = \int_R \mathbf{u}\otimes\nabla_{\mathbf{x}}\, w\, d\mathbf{y} = \int_R \nabla_{\mathbf{x}}\{w\mathbf{u}\}d\mathbf{y} = \nabla_{\mathbf{x}}\left\{\int_R w\mathbf{u}\, d\mathbf{y}\right\}. \qquad (10.21)$$

Relations (10.19), (10.20) and (10.21) yield (10.15).

Taking the trace of relation (10.15), recalling that $\operatorname{div}\mathbf{u} := \operatorname{tr}\{\nabla\mathbf{u}\}$, and noting $\operatorname{tr}\{\mathbf{u}\otimes\mathbf{n}\} = \mathbf{u}\cdot\mathbf{n}$, we obtain (10.16).

Similarly,

$$\begin{aligned}\langle\operatorname{div}\mathbf{B}\rangle\{\mathbf{x}\} &:= \int_{\mathcal{E}} (\operatorname{div}\mathbf{B})(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} = \int_R (\operatorname{div}\mathbf{B})(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \\ &= \int_R \operatorname{div}_{\mathbf{y}}\{w\mathbf{B}\} - \mathbf{B}(\nabla_{\mathbf{y}}\, w)dy \\ &= \int_{\partial R} w\mathbf{B}\mathbf{n}\, dA_{\mathbf{y}} + \int_R \mathbf{B}\nabla_{\mathbf{x}}\, w\, d\mathbf{y} \\ &= \int_{\mathcal{S}(\mathbf{x})} w\mathbf{B}\mathbf{n}\, dA_{\mathbf{y}} + \int_R \operatorname{div}_{\mathbf{x}}\{\mathbf{B}w\}dy \\ &= \int_{\mathcal{S}(\mathbf{x})} w\mathbf{B}\mathbf{n}\, dA_{\mathbf{y}} + \operatorname{div}_{\mathbf{x}}\left\{\int_R \mathbf{B}w\, d\mathbf{y}\right\}. \qquad (10.22)\end{aligned}$$

Thus (10.17) holds.

Finally,

$$
\begin{aligned}
\langle \partial \mathbf{u}/\partial t\rangle(\mathbf{x}) &:= \int_{\mathcal{E}} \partial \mathbf{u}/\partial t(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y} = \int_R \partial \mathbf{u}/\partial t(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y} \\
&= \int_R \frac{\partial}{\partial t}\{\mathbf{u}(\mathbf{y}) w(\mathbf{y}-\mathbf{x})\} d\mathbf{y} = \frac{\partial}{\partial t}\left\{\int_R \mathbf{u}(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y}\right\} \\
&= \frac{\partial}{\partial t}\left\{\int_{\mathcal{E}} \mathbf{u}(\mathbf{y}) w(\mathbf{y}-\mathbf{x}) d\mathbf{y}\right\}, \qquad (10.23)
\end{aligned}
$$

which establishes (10.18). Of course, here we have assumed sufficient regularity of field $\mathbf{u}$ to ensure the interchange of the limiting processes of time-differentiation and spatial integration is justified. (A similar remark is also in order in respect of relations (10.20) and (10.22) in which spatial integration and spatial differentiation are interchanged.) ■

Corollary 10.1. Consider the fluid momentum density

$$\mathbf{p} := \rho_0 \, \mathbf{v}. \qquad (10.24)$$

Then

$$\langle \nabla \mathbf{p}\rangle = \nabla\{\langle \mathbf{p}\rangle\}, \qquad (10.25)$$

$$\langle \Delta \mathbf{p}\rangle = \Delta\{\langle \mathbf{p}\rangle\} + \int_{\mathcal{S}} (\nabla \mathbf{p})\mathbf{n} w \, dA, \qquad (10.26)$$

and

$$\langle \operatorname{div}\{\mathbf{p}\otimes\mathbf{p}\}\rangle = \operatorname{div}\{\langle \mathbf{p}\otimes\mathbf{p}\rangle\}. \qquad (10.27)$$

Proof. Setting $\mathbf{u} = \mathbf{p}$ in (10.15) yields (10.25) on noting that (10.3) implies

$$\mathbf{p} = \mathbf{0} \quad \text{on} \quad \mathcal{S}, \qquad (10.28)$$

since $\mathcal{S}$ is a subset of ∂R.

Since

$$\Delta \mathbf{p} := \operatorname{div}\{\nabla \mathbf{p}\}, \qquad (10.29)$$

setting $\mathbf{B} = \nabla \mathbf{p}$ in (10.17) yields

$$\langle \Delta \mathbf{p}\rangle = \operatorname{div}\{\langle \nabla \mathbf{p}\rangle\} + \int_{\mathcal{S}} (\nabla \mathbf{p})\mathbf{n} w \, dA. \qquad (10.30)$$

However, from (10.25),

$$\operatorname{div}\{\langle\nabla\mathbf{p}\rangle\} = \operatorname{div}\{\nabla\{\langle\mathbf{p}\rangle\}\} =: \Delta\{\langle\mathbf{p}\rangle\}. \tag{10.31}$$

Result (10.26) follows from (10.30) and (10.31).

With $\mathbf{B} = \mathbf{p}\otimes\mathbf{p}$, relation (10.17) yields

$$\langle\operatorname{div}\{\mathbf{p}\otimes\mathbf{p}\}\rangle = \operatorname{div}\{\langle\mathbf{p}\otimes\mathbf{p}\rangle\} + \int_S (\mathbf{p}\otimes\mathbf{p})\mathbf{n}w\,dA. \tag{10.32}$$

Relation (10.32) yields (10.27) on noting (10.28). ■

The Navier-Stokes equation (10.1) that we wish to average may be written in the form

$$-\nabla P + (\mu/\rho_0)\Delta\mathbf{p} + \rho_0\,\mathbf{g} = \frac{\partial}{\partial t}\{\mathbf{p}\} + \left(\frac{1}{\rho_0}\right)\operatorname{div}\{\mathbf{p}\otimes\mathbf{p}\}, \tag{10.33}$$

since ρ_0 is constant. Using (10.14), (10.26), (10.27) and (10.18) with $\mathbf{u} = \mathbf{p}$, we obtain

$$\begin{aligned} &-\nabla\{\langle P\rangle\} - \left(\int_S P\mathbf{n}\right)/V + (\mu/\rho_0)[\Delta\{\langle\mathbf{p}\rangle\} + \int_S (\nabla\mathbf{p})\mathbf{n}w\,dA] \\ &\qquad + \int_R \rho_0\,\mathbf{g}\,w\,d\mathbf{y} = \frac{\partial}{\partial t}\{\langle\mathbf{p}\rangle\} + \left(\frac{1}{\rho_0}\right)\operatorname{div}\{\langle\mathbf{p}\otimes\mathbf{p}\rangle\}. \end{aligned} \tag{10.34}$$

Remark 10.4. It is tempting to note that $\rho_0\,\mathbf{g}$ is constant and invoke normalisation to write

$$\int_R \rho_0\,\mathbf{g}\,w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \rho_0\,\mathbf{g}.$$

This is not correct, however, since the domain of integration is the pore space R and not all space $\mathcal{E}$. Indeed, for a general field point $\mathbf{x}$ (notice $\mathbf{x}$ may be located in the pore space or porous body) the integration is effectively over that pore space within the REV $C(\mathbf{x})$: see (10.8). Specifically,

$$\int_R w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \left(\int_{R\cap C(\mathbf{x})} 1\ d\mathbf{y}\right)/V. \tag{10.35}$$

The value of the integral over $R\cap C(\mathbf{x})$ is the volume of the pore space within $C(\mathbf{x})$, so that the right-hand side of (10.35) represents the pore space volume within $C(\mathbf{x})$ divided by the volume of $C(\mathbf{x})$. Of course, this is the relevant measure of *porosity*, ν say. That is,

$$\nu(\mathbf{x}) := \int_R w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \langle 1-\chi_B\rangle, \tag{10.36}$$

where χ_B denotes the characteristic function for the porous body which occupies the fixed region B at scale ϵ_1. [Thus $\chi_B(\mathbf{y}) = 1$ if $\mathbf{y} \in B$, $\chi_B(\mathbf{y}) = 0$ if $\mathbf{y} \notin B$.) Accordingly,

$$\int_R \rho_0\, \mathbf{g}\, w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \rho_0\, \mathbf{g}\, \nu(\mathbf{x}). \tag{10.37}$$

As noted in the introduction, ν depends upon *two* length scales, namely ϵ_1 and ϵ_2. The former is the scale at which the pore boundary is delineated (and hence employed in the definition of R in (10.37)), while the latter is the REV scale embodied in the choice of w.

Relation (10.34) may be written as

$$-\nabla\{\langle P\rangle\} + (\mu/\rho_0)\Delta\{\langle\mathbf{p}\rangle\} + \rho_0\,\nu\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\langle\mathbf{p}\rangle\} + \operatorname{div}\{\rho_0^{-1}\langle\mathbf{p}\otimes\mathbf{p}\rangle\}, \tag{10.38}$$

where

$$\mathbf{f}^{fp} := \int_S (-P\mathbf{1} + (\mu/\rho_0)\nabla\mathbf{p})\mathbf{n}w\, dA. \tag{10.39}$$

In order to obtain a relation which resembles (10.33) as closely as possible, we re-write (10.38) as

$$-\nabla\{\langle P\rangle\} + (\mu/\rho_0)\Delta\{\langle\mathbf{p}\rangle\} + \rho_0\,\nu\mathbf{g} + \mathbf{f}^{fp} - \operatorname{div}\boldsymbol{\mathcal{D}} = \frac{\partial}{\partial t}\{\langle\mathbf{p}\rangle\} + \operatorname{div}\{\langle\rho\rangle^{-1}\langle\mathbf{p}\rangle\otimes\langle\mathbf{p}\rangle\}, \tag{10.40}$$

where

$$\boldsymbol{\mathcal{D}} := \rho_0^{-1}\langle\mathbf{p}\otimes\mathbf{p}\rangle - \langle\rho\rangle^{-1}(\langle\mathbf{p}\rangle\otimes\langle\mathbf{p}\rangle). \tag{10.41}$$

Here, using (10.36),

$$\langle\rho\rangle(\mathbf{x}) := \int_R \rho_0\, w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \rho_0\int_R w(\mathbf{y}-\mathbf{x})d\mathbf{y} = \rho_0\,\nu(\mathbf{x}). \tag{10.42}$$

Remark 10.5. Relation (10.40) may be written in several equivalent ways upon introducing two candidate velocity fields, $\mathbf{V}$ and $\mathbf{Q}$, via

$$\mathbf{V} := \frac{\langle \mathbf{p} \rangle}{\langle \rho \rangle} \tag{10.43}$$

and

$$\mathbf{Q} := \frac{\langle \mathbf{p} \rangle}{\rho_0}. \tag{10.44}$$

Of course, from (10.42), (10.43) and (10.44) we have

$$\mathbf{Q} = \nu \mathbf{V}. \tag{10.45}$$

Velocity $\mathbf{V}$ is the natural choice (cf. (4.6)) and leads from (10.40) to

$$\begin{aligned} &-\nabla\{\langle P \rangle\} + \mu\Delta\{\nu\mathbf{V}\} + \langle \rho \rangle \mathbf{g} + \mathbf{f}^{fp} - \operatorname{div} \boldsymbol{\mathcal{D}} \\ &\qquad = \frac{\partial}{\partial t}\{\langle \rho \rangle \mathbf{V}\} + \operatorname{div}\{\langle \rho \rangle \mathbf{V} \otimes \mathbf{V}\}. \end{aligned} \tag{10.46}$$

The equivalent formulation in terms of $\mathbf{Q}$ is

$$\begin{aligned} &-\nabla\{\langle P \rangle\} + \mu\Delta\mathbf{Q} + \rho_0\,\nu\mathbf{g} + \mathbf{f}^{fp} - \operatorname{div} \boldsymbol{\mathcal{D}} \\ &\qquad = \frac{\partial}{\partial t}\{\rho_0\,\mathbf{Q}\} + \operatorname{div}\{(\rho_0/\nu)(\mathbf{Q} \otimes \mathbf{Q})\}. \end{aligned} \tag{10.47}$$

Relations (10.46) and (10.47) may be compared with (10.1). To obtain the analogue of (10.2) we note that, from (10.16) and (10.3),

$$\begin{aligned} 0 = \langle \operatorname{div} \mathbf{v} \rangle &= \operatorname{div}\{\langle \mathbf{v} \rangle\} = \operatorname{div}\{\langle \rho_0\,\mathbf{v} \rangle/\rho_0\} \\ &= \operatorname{div}\{\langle \mathbf{p} \rangle/\rho_0\} = \operatorname{div}\{\langle \rho \rangle \mathbf{V}/\rho_0\} = \operatorname{div}\{\nu\mathbf{V}\}. \end{aligned} \tag{10.48}$$

Thus from (10.45)

$$\operatorname{div} \mathbf{Q} = 0, \tag{10.49}$$

while

$$\nu \operatorname{div} \mathbf{V} + \nabla\nu \,.\, \mathbf{V} = 0. \tag{10.50}$$

Clearly (10.50) indicates that

$$\textit{in general} \ \operatorname{div} \mathbf{V} \neq 0. \tag{10.51}$$

Remark 10.6. It is of passing interest to note that (10.47) may be written as

$$\operatorname{div}\mathbf{T} + \rho_0\,\nu\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\rho_0\,\mathbf{Q}\} + \operatorname{div}\{(\rho_0/\nu)\mathbf{Q}\otimes\mathbf{Q}\}, \tag{10.52}$$

where

$$\mathbf{T} := -\langle P\rangle\mathbf{1} + \mu[\nabla\mathbf{Q} + (\nabla\mathbf{Q})^{\mathrm{T}}] - \boldsymbol{\mathcal{D}}. \tag{10.53}$$

This is a consequence of the identities

$$\operatorname{div}\{(\nabla\mathbf{Q})^{\mathrm{T}}\} \equiv \nabla\{\operatorname{div}\mathbf{Q}),\quad \operatorname{div}\{\langle P\rangle\mathbf{1}\} = \nabla\{\langle P\rangle\}, \tag{10.54}$$

and relation (10.49).

In the case of *creeping flow*, (10.1) becomes

$$-\nabla P + \mu\Delta\mathbf{v} + \rho_0\,\mathbf{g} = \frac{\partial}{\partial t}\{\rho_0\,\mathbf{v}\} \tag{10.55}$$

while (10.46) and (10.47) become, respectively,

$$-\nabla\{\langle P\rangle\} + \mu\Delta\{\nu\mathbf{V}\} + \langle\rho\rangle\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\langle\rho\rangle\mathbf{V}\} \tag{10.56}$$

and

$$-\nabla\{\langle P\rangle\} + \mu\Delta\mathbf{Q} + \rho_0\,\nu\mathbf{g} + \mathbf{f}^{fp} = \frac{\partial}{\partial t}\{\rho_0\,\mathbf{Q}\}. \tag{10.57}$$

In view of (10.49) it is thus choice **Q** which results, at least for creeping flow, in the closest match between the original Navier-Stokes equations and their averaged counterparts.

Remark 10.7. The velocity field **Q** has a very important physical interpretation in the context of the foregoing, namely flow of an incompressible liquid through a rigid porous solid that it saturates. To see this it is instructive to consider mass conservation of *any* fluid which is contained within a rigid porous solid. This is given by

$$\frac{\partial\rho}{\partial t} + \operatorname{div}\mathbf{p} = 0, \tag{10.58}$$

a relation which holds throughout all pore space. (As we saw in Chapter 4, such a relation holds irrespective of whether the fluid is in liquid, vapour, or a mixture of the two separated by interfaces.) Averaging (10.58), using

(10.16) with $\mathbf{u} = \mathbf{p}$, and noting (10.18) also holds for scalar fields (and hence for ρ in particular), we obtain

$$\frac{\partial\{\langle\rho\rangle\}}{\partial t} + \operatorname{div}\{\langle\mathbf{p}\rangle\} = 0. \tag{10.59}$$

Integrating (10.59) over any fixed region $\mathcal{P}$ yields

$$\int_{\mathcal{P}} \frac{\partial\{\langle\rho\rangle\}}{\partial t}\, dV = -\int_{\partial\mathcal{P}} \langle\mathbf{p}\rangle \,.\, \mathbf{n}\, dA \tag{10.60}$$

on using the divergence theorem. Since the left-hand side of (10.60) is expressible as the rate of *increase* of mass within $\mathcal{P}$, $\langle\mathbf{p}\rangle.\,\mathbf{n}$ has the interpretation of mass flux across ∂P in the direction of $\mathbf{n}$. That is, $\langle\mathbf{p}\rangle.\,\mathbf{n}\,\Delta A$ is to be interpreted, for small areas ΔA, as delivering the mass flow per unit time, across a planar surface of area ΔA, to which $\mathbf{n}$ is a normal, in the direction of $\mathbf{n}$. From (10.44) this flow rate is $\rho_0\,\mathbf{Q}\,.\,\mathbf{n}\,\Delta A$ in the context of incompressible flow, and so the *volume* of fluid crossing 'ΔA' per unit time in the '$\mathbf{n}$' direction is $\mathbf{Q}\,.\,\mathbf{n}\,\Delta A$. For this reason (and in this context) $\mathbf{Q}$ is termed the *volumetric flux vector.*

We now examine the term $\mathbf{f}^{fp}$ which represents the force density associated with the resistance to fluid flow from the porous body. From (10.39)

$$\mathbf{f}^{fp} = \hat{\mathbf{f}}^{fp} + \mu\tilde{\mathbf{f}}^{fp}, \tag{10.61}$$

where

$$\hat{\mathbf{f}}^{fp} := -\int_{S} P\,\mathbf{n}\,w\,dA \tag{10.62}$$

and

$$\tilde{\mathbf{f}}^{fp} := \int_{S} (\nabla\mathbf{v})\,\mathbf{n}w\,dA. \tag{10.63}$$

The REV *intrinsic* average pressure $\bar{P}$ (that is, the REV-scale average pressure computed only over the pore space within an REV) is given by

$$\bar{P}(\mathbf{x}) := \frac{\displaystyle\int_R P(\mathbf{y})\,w(\mathbf{y}-\mathbf{x})\,d\mathbf{y}}{\displaystyle\int_R w(\mathbf{y}-\mathbf{x})\,d\mathbf{y}}. \tag{10.64}$$

Thus, from (10.36)

$$\bar{P} = \frac{\langle P\rangle}{\nu}. \tag{10.65}$$

Writing

$$\hat{\mathbf{f}}^{fp}(\mathbf{x}) = -\int_{\mathcal{S}(\mathbf{x})} \left(\bar{P}(\mathbf{x}) + [P(\mathbf{y}) - \bar{P}(\mathbf{x})]\right) \mathbf{n}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, dA_{\mathbf{y}} \tag{10.66}$$

yields

$$\hat{\mathbf{f}}^{fp}(\mathbf{x}) = -\bar{P}(\mathbf{x} \int_{\mathcal{S}(\mathbf{x})} \mathbf{n}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, dA_{\mathbf{y}} + \mathbf{F}^{fp}(\mathbf{x}), \tag{10.67}$$

where

$$\mathbf{F}^{fp}(\mathbf{x}) := -\int_{\mathcal{S}(\mathbf{x})} \left(P(\mathbf{y}) - \bar{P}(\mathbf{x})\right) \mathbf{n}(\mathbf{y})\, w(\mathbf{y}-\mathbf{x})\, dA_{\mathbf{y}}. \tag{10.68}$$

Now

$$\begin{aligned}\int_{\mathcal{S}(\mathbf{x})} w(\mathbf{y}-\mathbf{x})\mathbf{n}(\mathbf{y})\, dA_{\mathbf{y}} &= \int_{R} \left(\operatorname{div}(w\mathbf{1})\right)(\mathbf{y}) d\mathbf{y} = \int_{R} \nabla_{\mathbf{y}}\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} \\ &= \int_{R} -\nabla_{\mathbf{x}}\, w(\mathbf{y}-\mathbf{x})\, d\mathbf{y} = -\nabla_{\mathbf{x}} \int_{R} w(\mathbf{y}-\mathbf{x}) d\mathbf{y} = -(\nabla\nu)(\mathbf{x}).\end{aligned} \tag{10.69}$$

That is,

$$\int_{\mathcal{S}(\mathbf{x})} w(\mathbf{y}-\mathbf{x})\, n(\mathbf{y})\, dA_{\mathbf{y}} = -(\nabla\nu)(\mathbf{x}). \tag{10.70}$$

Thus (10.67) and (10.70) yield

$$\hat{\mathbf{f}}^{fp} = \bar{P}\nabla\nu + \mathbf{F}^{fp}, \tag{10.71}$$

and, using (10.65),

$$-\nabla\{\langle P\rangle\} + \hat{\mathbf{f}}^{fp} = -\nabla\{\nu\bar{P}\} + \bar{P}\nabla\nu + \mathbf{F}^{fp} = -\nu\nabla\bar{P} + \mathbf{F}^{fp}. \tag{10.72}$$

At this point (10.57) is expressible as

$$-\nu\nabla\bar{P} + \mathbf{F}^{fp} + \mu\Delta\mathbf{Q} + \rho_0\nu\mathbf{g} + \mu\tilde{\mathbf{f}}^{fp} = \frac{\partial}{\partial t}\{\rho_0\, \mathbf{Q}\}. \tag{10.73}$$

For spatially *steady* flow, the right-hand side of (10.73) vanishes. If, additionally, $\mathbf{F}^{fp}$ is negligible (see Murdoch & Hassanizadeh [14], (4.36) *et seq*), (10.73) becomes

$$-\nu\nabla\bar{P} + \mu\Delta\mathbf{Q} + \rho_0\,\nu\mathbf{g} + \mu\tilde{\mathbf{f}}^{fp} = \mathbf{0}. \tag{10.74}$$

Modelling Assumption: There exists an invertible tensor $\mathbf{K}$ (the *permeability* tensor) such that

$$\tilde{\mathbf{f}}^{fp} = -\mathbf{K}^{-1}\nu^2(\mathbf{V} - \mathbf{v}_B), \tag{10.75}$$

where $\mathbf{v}_B$ denotes the REV-scale velocity of the porous body. If the body is at rest then (10.74) becomes

$$-\nabla\bar{P} + (\mu/\nu)\Delta\mathbf{Q} + \rho_0\,\mathbf{g} - \mu\mathbf{K}^{-1}\mathbf{Q} = \mathbf{0}. \tag{10.76}$$

This is the so-called *Brinkman* equation, with gravity.

In the event that $\Delta\mathbf{Q}$ and $\rho_0\,\mathbf{g}$ are negligible, (10.76) reduces to

$$\nabla\bar{P} = -\mu\mathbf{K}^{-1}\mathbf{Q}. \tag{10.77}$$

If the porous body is isotropic at the REV scale then, for some real-valued function k,

$$\mathbf{K} = k\,\mathbf{1} \tag{10.78}$$

and (10.77) becomes Darcy's 'Law':

$$\nabla\bar{P} = -(\mu/k)\mathbf{Q}. \tag{10.79}$$

Remark 10.8. Relation (10.76), and its simplification (10.77) and (10.79), appear in the literature in alternate forms as a consequence of differing definitions of the permeability tensor. In understanding such relations it is essential that the interpretations of pressure average and velocity field be precise. Here we emphasise that $\bar{P}$ is the REV-scale intrinsic pressure average (see text before (10.64)) and $\mathbf{Q}$ is the volumetric flux vector (see (10.44) and Remark 10.7.).

Remark 10.9. The foregoing methodology has been used (see Murdoch & Soliman [15]) to investigate the widely-applied Beavers & Joseph boundary condition for liquid flow over a planar (at REV scale) boundary of a porous body. This study casts doubt on the validity of the accepted condition.

Remark 10.10. In cases when a rigid porous body is not saturated by an incompressible liquid, matters are much more complex. The Navier-Stokes equations will hold only where there is such liquid to be found. In general there will be gaseous, interfacial, and liquid phases in pore space. Nevertheless, at scale ϵ_1 linear momentum balance for the set of *all* molecules within the region occupied by the porous body at REV scale, but not those of the porous body itself, takes the form (see (4.35), (4.44) and (4.49))

$$\operatorname{div}\mathbf{T} + \rho\mathbf{g} = \frac{\partial}{\partial t}\{\rho\mathbf{v}\} + \operatorname{div}\{\rho\mathbf{v}\otimes\mathbf{v}\}, \tag{10.80}$$

in the event that the only external force is due to gravitation. Averaging (10.80) yields

$$\begin{aligned}\operatorname{div}\{\langle\mathbf{T}\rangle - \boldsymbol{\mathcal{D}}\} + \int_{\mathcal{S}}(\mathbf{Tn})\,w\,A + \langle\rho\rangle\mathbf{g}& \\ = \frac{\partial}{\partial t}\{\langle\rho\rangle\mathbf{V}\} + \operatorname{div}\{\langle\rho\rangle\mathbf{V}\otimes\mathbf{V}\rangle\},&\end{aligned} \tag{10.81}$$

where (cf. (10.41))

$$\boldsymbol{\mathcal{D}} := \langle\rho\mathbf{v}\otimes\mathbf{v}\rangle - \langle\rho\rangle\mathbf{V}\otimes\mathbf{V}. \tag{10.82}$$

At this point it is necessary to postulate constitutive relations for $\langle\mathbf{T}\rangle - \boldsymbol{\mathcal{D}}$, the integral term, and $\langle\rho\rangle$. Clearly this matter is highly context-dependent and complex.

Chapter 11

Concluding remarks

Here we summarise the foregoing results, indicate what has *not* been addressed, and draw attention to related work.

Remark 11.1. The analysis has been concerned with the derivation of balance relations based upon the simplest model of molecules (namely, interacting point masses). Within this somewhat simplistic framework, field values have been related to local spatial averages of molecular quantities computed at *any* given length scale. The *forms* of the balance relations are the same, no matter what length scale is chosen. A new balance, that of moment of mass, has been introduced (see §5.3) and linked to generalised moment of momentum balance (see (5.44) and (5.30)) More generally, it is to be hoped that the discussion has elucidated the physical interpretation of all field values. In particular, the separate contributions to the stress tensor $\mathbf{T}$ from interactions and thermal motion ($\mathbf{T}^{-}$ and $\boldsymbol{\mathcal{D}}$, respectively: see §4.6), and its interpretation for a single constituent in a mixture (see (7.43) and Remark 7.5), are not intuitive to anyone adopting an exclusively continuum/macroscopic perspective. A similar remark applies to the notion of material point (see Remark 4.7. and (7.10)).

Remark 11.2. Constitutive relations have not been considered. Here two observations are appropriate.

(i) Constitutive relations are scale-dependent. This is evident from the discussion of fluid flow through a porous body (See Chapter 10). More generally, any spatial average will fluctuate in time. Such fluctuations should be expected to increase with decrease in the choice of spatial scale.

(ii) The derivation of constitutive relations from molecular considerations is notoriously difficult, as evidenced by relations derived on the basis of the kinetic theory of moderately-rarefied gases.

Remark 11.3. Attention has been drawn to the desirability of averaging both in space *and time*, particularly if links are to be made between measurement and field values. An introduction to temporal averaging was given in Chapter 8, and utilised in Chapter 9. More detail is to be found in Murdoch & Bedeaux [12].

Remark 11.4. Spatial averaging was implemented via the use of a weighting function. The simplest choice corresponded to spherical regions (see (4.11)). However, the *forms* of balance are independent of such choice. Of course, the physical interpretation of all field values depends crucially upon the choice made. Interestingly, for point masses in a rectangular box there is a weighting function which delivers truncated Fourier series as the corresponding scale-dependent continuum fields: the scale corresponds to the wavelength cut-off selected in effecting truncation. In this context it is possible to obtain such truncated series which deliver mass and momentum density fields *equivalent* to *complete* knowledge of molecular locations and momenta. That is, a continuum description can be found which incorporates complete microscopic information, and from which full microscopic detail can be recovered. (See Murdoch & Bedeaux [16]).

Remark 11.5. The approach here adopted can be linked with modern statistical mechanics. Utilising projection operator methodology it proves possible to separate physical behaviour into reversible and irreversible parts. The key elements here are the notion of a *macroscopic state* (at given scales of length and time) and the corresponding concept of *local equilibrium*. (See Murdoch & Bedeaux [17], [18].)

Remark 11.6. Further balance relations can be obtained simply by taking higher-order tensor-valued moments of the equations governing the motions of individual point masses. Such '*multipolar*' balance relations are not easily amenable to physical interpretation. However, the moment of mass balance here introduced as (5.44) would seem to deserve further study, since it is an evolution equation for a measure of inhomogeneity. Its link with generalised moment of momentum balance (5.30), and hence with couple-stress, is interesting because theories of couple-stress have been linked with the modelling of material inhomogeneity. (See, for example, contributions to [19]).

Appendix A

Noll's theorem

In 1955 Noll [4] established that if a C^1 tensor-valued function $\mathbf{g}$ of any rank defined on $\mathcal{E} \times \mathcal{E}$ satisfies, for any pair of points $\mathbf{x}$ and $\mathbf{y}$,

$$\mathbf{g}(\mathbf{y}, \mathbf{x}) = -\mathbf{g}(\mathbf{x}, \mathbf{y}), \tag{A.1}$$

and if for some positive number δ (here we identify $\mathcal{E}$ with $\mathbb{R}^3$ by selection of a Cartesian reference frame)

$$\mathbf{g}(\mathbf{x}, \mathbf{y})|\mathbf{x}|^{3+\delta}|\mathbf{y}|^{3+\delta}$$

is bounded (and similarly for the first derivatives of $\mathbf{g}$), then

$$\begin{aligned} &\int_{\mathcal{E}} \mathbf{g}(\mathbf{x}, \mathbf{y})\, d\mathbf{y} \\ &\qquad = -\frac{1}{2}\operatorname{div}\left\{\int_{\mathcal{V}}\int_0^1 \mathbf{g}\big(\mathbf{x} + \alpha\mathbf{u}, \mathbf{x} - (1-\alpha)\mathbf{u}\big) \otimes \mathbf{u}\, d\alpha\, d\mathbf{u}\right\}. \end{aligned} \tag{A.2}$$

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