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From clusters of moving molecules to continua: Material elements as open systems

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ABSTRACT

We discuss the discrete-to-continuum transition in the description of matter, starting from a cluster of flowing molecules with equal mass and ending up with a non-simple fluid. We account for the fluctuations beyond a local affine approximation of the velocity distribution of molecules within a space window adopted to compute some prominent statistics. The resulting continuum picture accounts for local mass variation in each space window corresponding to a point in the continuum scale. From a statistical viewpoint, every material element is thus considered as a grand-canonical ensemble. So-called C-derivatives account for macroscopic-to-mesoscopic relative motion. When considered for second-rank tensors, they extend Truesdell's derivative and reduce to Oldroyd's one when the macroscopic-to-mesoscopic relative motion vanishes. Fluctuations beyond an affine component best approximating the kinetic energy are summarized into a second-rank symmetric tensor whose time variation enters a balance equation governing transfer from velocity fluctuations to heat. Eventually, we discuss essential elements of thermodynamics in the present setting. What emerges is the possibility of a non-Fourier type heat transfer. The results address computational schemes for field representations of sparse phase dynamics, such as granular materials, and the one of bodies with transport of scattered molecules, such as pollutants in fluids or proteins in biological tissues.

1. Introduction

1.1. Discrete-to-continuum representations: a first view on a scenario

Discrete-to-continuum analyses have their roots in the work by Augustin Luis Cauchy and his contemporaries, which dates back the first half of the nineteenth century. These analyses have different aims: from the original idea of reconciling early molecular and continuum views on the description of matter (see historical remarks in Stackgold (1950), Ericksen (1977), and the treatise (Todhunter, 2014)), to analytical questions raised by Hilbert in his sixth problem (Yandell, 2001), up to the awareness that, although condensed matter appears discrete at very small spatial scales, modeling its behavior through continuous fields reduces the computational cost that could be otherwise prohibitive from various viewpoints (we may estimate by the Avogadro's number, $\sim 10^{23}$, the degrees of freedom for cm^3 of a solid at atomistic scale).

Besides analyses aiming at statistical information on a population of individual material entities – be then atoms, molecules, or else – Kalikmanov (2001), Presutti (2009), the construction of deterministic continuum models (which can be even perturbed by stochastic fluctuations) commonly rest on the analysis of phenomena into a space window (named also a *cell* or a *loculus*, or else, depending on author's choice), taken as a representative volume element of the material structure, otherwise considered homogeneous above the window scale. In the case of periodic crystals, such a window is commonly chosen to be only in energetic contact with its neighbors, a canonical ensemble in terms of statistical mechanics. Thus, the window considered is the lattice characteristic cell; we can look at it considering atoms as mass points at rest, connected with each other by springs, a scheme that we can homogenize at continuum scale, the one of (say) long wavelength approximation. Cauchy followed this view (see Stackgold, 1950). His approach re-emerged in Max Born's work on periodic crystals (Born and Huang, 1954). "Cauchy assumed that macroscopic and atomic movements are the same, where both are defined. Born modified this by assuming that applying the macroscopic deformation gradient as a linear transformation to a reference set of lattice vectors gives a possible set of lattice vectors in the deformed crystals: how atoms in a unit window are arranged is determined by solving certain equilibrium equations" (Ericksen, 2008, p. 200). This is what we call the *Cauchy–Born rule*: the deformation is assumed to be homogeneous when restricted to a single crystal ideally collapsed at a point when a body much larger than the crystal itself is under analysis at continuum scale. This view allows one to homogenize properties of the lattice, provided an identification of the local homogeneous strain with a value of the macroscopic deformation gradient at the mass center

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of the considered window. The Cauchy–Born rule has been proven rigorously for two-dimensional mass–spring lattices, an open set of model parameters (equilibrium lengths and spring constants) and all boundary data close to the identity, while it fails for another open set of parameters (Friesecke and Theil, 2002) and (in crystals) when slips occur (Zanzotto, 1992). Since elastically deformed states are in general just local energy minimizers, Cauchy–Born's rule is always valid in the elastic setting, provided appropriate choices of the unit window defining the lattice (E and Ming, 2007b), E and Ming (2007a).

Beyond the elastic setting, atomistic-to-continuum approaches are effective in the analysis of brittle behavior. They may involve Laplace and Fourier transform techniques under assumed existence of a certain steady-state limit (Slepyan, 2001a,b,c) and also, from a different viewpoint, the rigorous evaluation of the continuum limit with full nearest and next-to-nearest pair interactions (Friedrich and Schmidt, 2015). Lattice schemes offer also a schematic view on damage clustering (see, e.g., Delaplace et al. (1996), Nieves et al. (2016), Challamel et al. (2015), and, above all, the treatise (Krajcinovic, 1996)).

If we change the view and look at the quantum character of matter below the lattice scale, we can proceed towards the continuum description in terms of the Kohn–Sham density functional theory, on the basis of an approximation of the ground-state energy of an interacting inhomogeneous electron gas in a static potential. Even in this setting we find a rigorous justification of the Cauchy–Born rule under appropriate conditions (E and Lu, 2013); it has been also re-interpreted in exponential (Arroyo and Belytschko, 2004) and helical (Kumar et al., 2016) ways to account for special geometries, or even at different levels in multi-lattices, leading in this case to multi-field continuum descriptions (Mariano and Stazi, 2001, 2004).

The periodic character of the material structure plays a role. When the body is heterogeneous, we may be unable to individuate unambiguously a representative volume element to be homogenized at gross scale, rather we need to consider it in statistical sense (Krajcinovic, 1996). To this aim we may select a specific topology and consider stochastic the resulting properties; we thus homogenize by exploiting their (assumed or data-driven) statistics (Mariano et al., 2004). The stochastic approach to the representative volume element involves sophisticated analytical problems (Blanc et al., 2007c,b; Braides et al., 2018); besides their theoretical interest per se, they also sustain pertinent computational schemes (Blanc et al., 2007a).

In the common use of Cauchy–Born's rule, the spatial window is viewed as a canonical ensemble: it is in energetic contact with the environment but does not exchange mass with it.

In gases, molecules move freely one with respect to the other until they collide, restarting another path. Boltzmann's equation governs in time the probability density distribution of velocities at a given places and/or of places with a given velocity. The rigorous analysis of its continuum (hydrodynamic) limit is a hard task and implies a number of nontrivial mathematical problems (Saint-Raymond, 2006). On another side, a path leading to a continuum view rests on the analysis of moment expansion of the distribution function, as suggested by the elegant structure of Rational Extended Thermodynamics (see treatises Müller and Ruggeri, 1998; Ruggeri and Sugiyama, 2015); however, that approach does not cover solids; it is so far limited to gases that are far for being dense, gases that can even have molecules with their own internal structure.

With a perspective focused on solids, fluids, granular matter (in a sense it has intermediate behavior), and fluids with scattered solid particles, we offer here a bridge between the (static) view based on Cauchy–Born's rule and the account of statistical distribution of places and velocities.

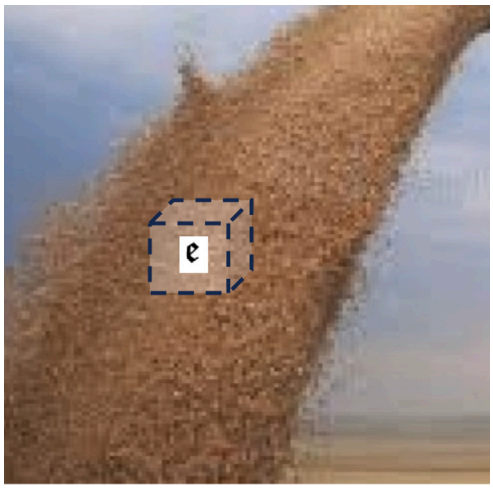

Fig. 1. A sparse phase (specifically a flow of wheat) and the space window magnified.

1.2. Structure of the setting investigated here

Consider an open, bounded, simply connected region $\mathcal{B} \subset \mathbb{R}^3$, endowed with a surface-like boundary oriented everywhere by the outward unit normal n but a finite number of corners and edges. A population of molecules flows in $\mathcal{B}$ at the instant τ; such molecules collide and may be even clustered in subgroups linked in some way with one another. We identify each molecule with a point and take a space window $\mathfrak{e}$ much smaller than $\mathcal{B}$. Fig. 1 furnishes a pictorial representation of the basic idea (the window $\mathfrak{e}$ is magnified).

The properties of events in $\mathfrak{e}$ are averaged in a sense rendered precise in the subsequent sections. Averages are then intended as values of continuous fields over $\mathcal{B}$.

So, the appropriate geometrical environment in which we act is a fiber bundle $\mathcal{Y}$ with canonical projection $\pi : \mathcal{Y} \longrightarrow \mathbb{R}^3$, a continuous surjective map. Typical fiber is an isomorphic copy of $\mathbb{R}^3$, indicated by $\tilde{\mathbb{R}}^3$. The isomorphism $\imath : \tilde{\mathbb{R}}^3 \longrightarrow \mathbb{R}^3$ is merely the identification.

For the sake of simplicity, we consider flat spaces, namely orthonormal reference frames in both $\mathbb{R}^3$ and $\tilde{\mathbb{R}}^3$. As stated above, the two spaces are identical.

The kinetic circumstances occurring within each window may be multifaceted; but, in the present theory only averages of momentum and first moments are brought on stage as continuous fields. We derive their evolution laws in Eulerian representation from a unique first principle: invariance of the *external* power alone over any generic part of the region occupied by the body (so we do not call upon the virtual power principle, which is the a priori prescription of the weak form of the balance equations). We choose to act in Eulerian representation – fields defined over the present configuration – because for a sparse phase, although we can choose any configuration as a reference one, we cannot assure always a one-to-one correspondence with current configurations due to rearrangements and transfer of matter within the body itself.

Then, we show also how in this setting fluctuations can be associated with what we commonly intend as heat at macroscopic scale.

In this sketch of the viewpoint adopted here, parallelism with schemes based on molecular dynamics can be detected because those approaches are constructed on averages pertaining to the dynamics of a molecular cluster over a cell. Related to such averages we can mention the approach by W. Noll (Noll, 1955) (see the English translation (Lehoucq and Von Lilienfeld-Toal, 2010)), who started from J. H. Irving's and J. G. Kirkwood's work (Irving and Kirkwood, 1950) developing his own original path based on a version of the divergence theorem (see related – in some sense – works like Murdoch (1985), Pitteri (1986), Di Carlo (2019), Di Carlo et al. (2023)). We also mention

M. Parrinello's and A. Rahman's proposal (Parrinello and Rahman, 1980, 1981), which opened a body of work in molecular dynamics (for pertinent remarks from the viewpoint of continuum mechanics see Podio-Guidugli (2010)).

These views generically imply a representation of the resulting homogenized body that falls within the traditional setting of continuum mechanics (see above all (Noll, 1955)) in which the average velocity v alone is entitled to describe mechanics (and forces are entities defined by the power they develop in it). All fluctuations with respect to v are considered to be sources of heat (see the explicit analysis in Noll (1955) – recall (Lehoucq and Von Lilienfeld-Toal, 2010)).

With the aim of describing the anisotropies in a sparse phase that emerge during the molecular transport, we decompose fluctuations beyond average in two terms: one of affine character, due to a version of the Cauchy–Born rule written in terms of velocity, the other described by a vector field with null average when evaluated with respect to the mass center of a molecular cluster in the prototype space window $\mathfrak{e}(x)$. We consider the first term to enter the mechanical description at continuum level, attributing heat only to fluctuations beyond an affine component selected in a specific way. The boundary between mechanics and thermodynamics depends, indeed, on the details that we include in what we model as mechanics. The resulting modeling structure is naturally multi-field; however it differs from the multiple fields reached along a different path in M. Pitteri's work (Pitteri, 1990). The approach also differs from I. Müller's and T. Ruggeri's Rational Extended Thermodynamics, already mentioned (Müller and Ruggeri, 1998), Ruggeri and Sugiyama (2015).

Specifically, the path that we follow rests on a program so far developed in Brocato and Capriz (2011), Capriz (2003, 2006, 2008, 2019), Capriz and Fried (2011), Capriz et al. (2012), Capriz and Giovine (2016, 2017), Capriz and Mariano (2014, 2018, 2019, 2020), and Mariano (2020). We refine and clarify those works, adding new matter. With respect to those references, specific contributions of the present work are as follows:

- In constructing macroscopic fields on a statistical basis, we eliminate in Section 3 an indeterminacy in the definition (and thus selection) of the affine component of velocity fluctuations that emerged in the quoted proposals.
- We modify the evolution equation of the inertial tensor of $\mathfrak{e}$ underlining in Section 4 the influence of the mass exchange through the boundary of $\mathfrak{e}$ along the motion.
- We extend in Section 8 the integral balance of tensor kinetic energy to a form that eliminates an indeterminacy on the identification of inertial terms implied by previous existing versions in Capriz and Giovine (2017), Capriz and Mariano (2014, 2018, 2019). Then, we prove the existence of a hyperstress entering the balance of actions governing the evolution of Reynolds' tensor associated with fluctuations; this hyperstress has been previously only postulated in Capriz and Giovine (2017), Capriz and Mariano (2014, 2018, 2019).
- We connect in Section 11 the path followed with the general dynamical system based approach to continuum thermodynamics. We propose versions of energy balance and Clausius–Duhem's inequality in terms of C-derivatives – time variations computed by following the motion associated with the affine component of fluctuations and accounting for the relative rate at which the molecular cluster volume changes in $\mathfrak{e}$. What emerges is a structure naturally compatible with finite speed heat propagation; so, a description far from Fourier's paradox.

1.3. Something more on the approaches to discrete-to-continuum transition

As already mentioned, at variance of the common use we consider the Cauchy–Born rule in terms of velocities rather than placements. The traditional version, however, does not preclude dynamics as shown by J. Braun (Braun, 2017), who proved the H^1-convergence of long-time solutions of atomistic elastodynamics as the interatomic distance tends to zero (the convergence involves the one of velocities with respect to the L^2-norm).

In statics, rigorous scaling analyses make sense in various physical circumstances and can be carried out with different techniques (see, e.g., Müller and Schlömerkemper, 2002; Schlömerkemper, 2005).

A particularly powerful tool is E. De Giorgi's $\Gamma-$convergence of energies depending on the lattice scale. By varying that scale we have a parametrization of both a family of functionals and a corresponding set of possible (meaning when they exist) minimizers; the question is whether the limit of minimizers is a minimizer of the limit energy, assuming convergence of both sequences in some appropriate sense. $\Gamma-$convergence is a way of making sense of this question (for its use in the lattice-to-continuum description see, e.g., Braides and D'Elia (2023), Braides and Gelli (2016), and Braides (2014) for an extended view on the scenario).

Of course, in the various approaches, the resulting continuum depends on the interactions considered: specifically, whether they are spring or beam like and/or first or higher-order neighbors are considered. Averages on lattices are computed on finite-size regions, so they can imply strong or weakly non-local continuum representations; a rather general view leading to finite-length averages has been proposed by Kunin (1982), Kunin (1983) (specific circumstances related to this issue are analyzed from different perspectives – averages and/or interpolations, exploiting also pseudo-differential operators – in Bacigalupo and Gambarotta, 2001; Challamel et al., 2014; Giovine, 2002, 1993; Rizzi et al., 2019). Once again, the rigorous scaling that account for some forms of non-locality requires non-trivial analyses (pertinent results are in Bach et al., 2020; Braides, 2000).

Not always, or not necessarily, the Cauchy–Born rule is adopted; however, thinking in terms of it may also address the construction of effective finite element schemes (Makridakis and Süli, 2013). In any case, the combination of molecular or atomistic approaches in a cell and a continuum view on the whole body can lead to efficient numerical schemes because it allows consideration of fine properties of the matter while exploiting advantages of continuum schemes in terms of computational cost (Liu et al., 2004). Among possible numerical approaches that adopt a mixing between discrete and continuum schemes is the quasicontinuum method (Shenoy et al., 1999), formulated first in conservative setting and re-discussed later in order to include dissipative structures (Beex et al., 2014).

At quantum scale, the same Kohn–Sham's theory, constructed starting from Thomas–Fermi's approach, addresses the formulation of computational schemes from a variational structure, for the purpose of developing macroscopic analyses on the basis of quantum-scale information (Suryanarayana et al., 2013; Wang et al., 2016).

The scenario goes well beyond the previous incomplete sketch and offers multiple approaches, analyses, and methods (remarks on the concurrency between atomistic and continuum models are in Chakraborty and Ghosh, 2021; Markesteijn et al., 2014). For this reason, we do not review further the matter and focus on the statistically-based discrete-to-continuum transition discussed here.

2. Notations

With $\mathfrak{X}$ a finite-dimensional linear space over the fields of real numbers, we indicate by $\{\mathbf{e}_i\}$ a basis in it and by $\{\mathbf{e}^j\}$ the corresponding basis in the dual counterpart of $\mathfrak{X}$, namely $\mathfrak{X}^*$, the space of linear maps over $\mathfrak{X}$. Every $\mathbf{e}^j$ is defined to be such that $\mathbf{e}^i \cdot \mathbf{e}_j = \delta^i{}_j$, where $\delta^i{}_j$ is the Kronecker delta and the interposed dot indicates from now on the duality pairing. It corresponds to the standard scalar product when we refer to orthonormal reference frames, as we assume here, to within a few circumstances in which we indicate the appropriate generalization to non-trivial metrics.

For $a \in \mathfrak{X}$ and $b \in \mathfrak{X}^*$, a second-rank linear operator from $\mathfrak{X}$ onto itself is given by the dyad $a \otimes b$, defined to be such that for every $h \in \mathfrak{X}$, $(a \otimes b)h = (b \cdot h)a$. Dyadic products $\mathbf{e}_i \otimes \mathbf{e}_j$, $\mathbf{e}_i \otimes \mathbf{e}^j$, $\mathbf{e}^i \otimes \mathbf{e}_j$, $\mathbf{e}^i \otimes \mathbf{e}^j$ constitute bases of different second-rank tensor spaces on $\mathfrak{X}$. Let A be a linear operator from $\mathfrak{X}$ onto itself. With respect to a basis $\{\mathbf{e}_i\}$ in $\mathfrak{X}$, we have $A = A^i{}_j \mathbf{e}_i \otimes \mathbf{e}^j$, where we adopt here and throughout this paper the usual summation over repeated indices.

For A and B two linear maps from $\mathfrak{X}$ onto itself (two tensors indeed), in short $A, B \in \mathrm{Hom}(\mathfrak{X}, \mathfrak{X})$, we indicate by $A \cdot B$ the scalar given by $A^i{}_j B^j{}_i$, and by AB the second rank tensor $AB = A^i{}_k B^k{}_j \mathbf{e}_i \otimes \mathbf{e}^j$. Analogous notations hold for linear maps from $\mathfrak{X}$ onto its dual $\mathfrak{X}^*$ and vice versa, or from $\mathfrak{X}^*$ onto itself. Every second-rank tensor like A admits the decomposition $A = \mathrm{sym}A + \mathrm{skw}A$, with $\mathrm{sym}A = \frac{1}{2}(A + A^\top)$ and $\mathrm{skew}A = \frac{1}{2}(A - A^\top)$, where the apex $\top$ denotes standard transposition.

Consider another finite-dimensional real linear space $\mathfrak{Y}$, and a linear operator G from $\mathfrak{X}$ onto $\mathfrak{Y}$. Two linear operators are naturally associated with G. One is the transpose $G^\top \in \mathrm{Hom}(\mathfrak{Y}, \mathfrak{X})$; the other operator is the adjoint $G^* \in \mathrm{Hom}(\mathfrak{Y}^*, \mathfrak{X}^*)$.

If $G \in \mathrm{Hom}(\mathfrak{X}, \mathfrak{X})$ is non-singular, that is $\det G \neq 0$, its inverse G^{-1} belongs also to $\mathrm{Hom}(\mathfrak{X}, \mathfrak{X})$ but is in general different from $G^\top$; when $G^\top = G^{-1}$, itself G is said to be orthogonal and we write $G \in O(\mathfrak{X}, \mathfrak{X})$; in this case $\det G = \pm 1$.

If g and $\tilde{g}$ are non-singular metrics in $\mathfrak{X}$ and $\mathfrak{Y}$ respectively, for $G \in \mathrm{Hom}(\mathfrak{X}, \mathfrak{Y})$ we have $G^\top = g^{-1} G^* \tilde{g}$. If the two metrics are flat and trivial, namely they are related to orthonormal frames of reference, G^* and $G^\top$ coincide.

When $G \in \mathrm{Hom}(\mathfrak{X}, \mathfrak{X})$ is non-singular, there exist two second-rank symmetric tensors U and V, and a unique orthogonal linear map $R \in O(\mathfrak{X}, \mathfrak{X})$ such that $G = RU = VR$; also, when $\det G > 0$, R is simply a rotation and does not involve reflections, that is $R \in SO(\mathfrak{X}, \mathfrak{X}) = SO(m)$, with $m = \dim \mathfrak{X}$, which means $\det Q = 1$. This is Automne's polar decomposition theorem. We commonly call RU and VR as right and left polar decomposition of G, respectively. Automne's theorem can be considered for $G \in \mathrm{Hom}(\mathfrak{X}, \mathfrak{Y})$, provided that the two spaces $\mathfrak{X}$ and $\mathfrak{Y}$ are identified.

Let $\mathbf{m}$ be a third-rank tensor, for example $\mathbf{m} = \mathbf{m}^{ijk} \mathbf{e}_i \otimes \mathbf{e}_j \otimes \mathbf{e}_k$. We denote by ${}^t\mathbf{m}$ its *minor-left transpose*, namely a tensor with components $\mathbf{m}^{jik}$, by $\mathbf{m}^t$ its *minor-right transpose*, a tensor with components $\mathbf{m}^{ikj}$, and by $\mathbf{m}^\top$ its *major transpose*, a tensor with components $\mathbf{m}^{kji}$.

3. Local and gross motions

3.1. Within the space window $\mathfrak{e}$

A cluster of molecules occupies at time τ the space window $\mathfrak{e}$, a cube of edge size δ, a multiple of the mean free path, and has instantaneous mass center at x. Every other point in $\mathfrak{e}$ is indicated by a position vector y issued by $x \in \mathcal{B}$. The generic molecule crossing at the instant τ a point in $\mathfrak{e}(x)$ indicated by y is endowed with velocity w. Sometimes we will write $\mathfrak{e}(x)$ to recall that we attribute to x the instantaneous statistical properties of $\mathfrak{e}$; and this is for every $x \in \mathcal{B}$. For such properties we presume to know the (integrable) distribution $\Theta(\tau, x; y, w)$, which indicates the number of molecules per unit volume, $\Theta\, \mathrm{d}w$, endowed with velocities w within the infinitesimal ball $(w + \mathrm{d}w)$ around w. Fig. 2 offers a perceptible example of the viewpoint.

We indicate by $\mathbb{V}$ the space of velocities w, here identified with $\mathbb{R}^3$; also $\mathrm{d}w$ is a measure in $\mathbb{V}$. Knowledge of Θ renders available the *average velocity*

$$v(\tau, x) := \left(\int_{\mathfrak{e}} \theta(\tau, x; y)\, \mathrm{d}y \right)^{-1} \int_{\mathfrak{e}} \theta w_*(\tau, x; y)\, \mathrm{d}y,$$

where

$$\theta(\tau, x; y) := \int_{\mathbb{V}} \Theta(\tau, x; y, w)\, \mathrm{d}w,$$

and w_* is the *local average velocity* given by

$$w_*(\tau, x; y) := \frac{1}{\theta} \int_{\mathbb{V}} \Theta(\tau, x; y, w)\, w\, \mathrm{d}w.$$

The cluster of molecules within the window $\mathfrak{e}$ associated with x has, at an instant τ, *Euler's inertia tensor* $\mathcal{I}$ per unit mass given by

$$\mathcal{I} := \delta^{-3} \int_{\mathbb{V} \times \mathfrak{e}} \Theta(\tau, x; y, w)\, |y|^2 I\, \mathrm{d}w\, \mathrm{d}y - \delta^{-3} \int_{\mathbb{V} \times \mathfrak{e}} \Theta(\tau, x; y, w)\, y \otimes y\, \mathrm{d}w\, \mathrm{d}y,$$

where I is the second-rank unit tensor. We indicate by Y the second integral, namely

$$Y := \delta^{-3} \int_{\mathbb{V} \times \mathfrak{e}} \Theta(\tau, x; y, w)\, y \otimes y\, \mathrm{d}w.$$

By using Y, here referred to as the *inertia binor*, we can construct a second-rank symmetric tensor N in the present configuration, given by

$$N := \delta^{-2} \bar{Y}.$$

When the metric over $\tilde{\mathbb{R}}^3$ is not referred to an orthonormal reference frame, $\bar{Y} := Y\bar{g}$, with $\bar{g}$ the metric in $\tilde{\mathbb{R}}^3$; otherwise we identify Y with $\bar{Y}$, as we do in what follows.

We then consider another copy $\hat{\mathbb{R}}^3$ of $\mathbb{R}^3$ and take it as a *comparison space*, without selecting in it a reference configuration. Once again we exploit the identification: $\hat{\mathbb{R}}^3$ and $\mathbb{R}^3$ are identical although distinguished. The arbitrariness of $\hat{\mathbb{R}}^3$ avoids the need of calling upon Truesdell's retrogression technique as done in Capriz and Giovine (2016, 2017), Capriz and Mariano (2014, 2018, 2019, 2020) (see also Remark 3, below). Such a new space has only momentary instrumental role. With reference to $\hat{\mathbb{R}}^3$ we define a second-rank tensor field, with values G, which maps vectors in $\hat{\mathbb{R}}^3$ to those in $\tilde{\mathbb{R}}^3$. We choose it to be such that

$$Y = \delta^2 G G^\top. \tag{1}$$

We assume that

- G is differentiable with respect to time.
- $\det G > 0$, meaning G is non-singular and preserves the local space orientation.

The last assumption implies that we imagine more than only one molecule in $\mathfrak{e}$ at every x so that Y does not degenerate.

We have

$$G := N^{\frac{1}{2}} R, \tag{2}$$

with $R \in SO(\hat{\mathbb{R}}^3, \tilde{\mathbb{R}}^3)$.

Through G we define another linear operator B to be such that

$$\dot{G} = BG, \tag{3}$$

where from now on the superposed dot indicates total time derivative. B is a linear map from $\tilde{\mathbb{R}}^3$ on itself and depends on x and τ. We will use B to select the local affine component of fluctuations beyond the average velocity $v(\tau, x)$. Previous definition of B, the value of a field depending only on τ and x, is affected by the arbitrariness in selecting the comparison space and, thus, by an orthogonal factor R. In fact, by the relation (2), Eq. (3) implies

$$N^{\frac{1}{2}} \dot{R} + \overline{\dot{N^{\frac{1}{2}}}} R = B N^{\frac{1}{2}} R.$$

So, we get

$$B = N^{\frac{1}{2}} \dot{R} R^\top N^{-\frac{1}{2}} + \overline{\dot{N^{\frac{1}{2}}}} N^{-\frac{1}{2}},$$

where $N^{\frac{1}{2}}$ is invertible by the definition of Y. In the previous equation, N is presumed to be known as a consequence of the analogous assumption on Θ, while the spin $\dot{R} R^\top$ is unknown at this stage.

Then, we impose as a modeling choice that B is also such that

$$\omega(\tau, x)^{-1} \int_{\mathfrak{e}} \theta(\tau, x; y)\, y \otimes w_*\, \mathrm{d}y = Y B^\top, \tag{4}$$

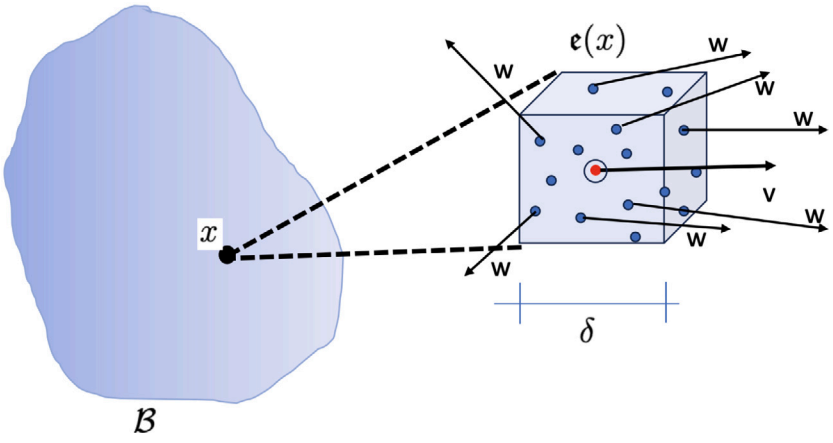

Fig. 2. The molecular cluster in the space window associated with a point x in the continuum. Arrows evidence the peculiar velocities w and the average velocity v of the cluster.

where

$$\omega(\tau,x) := \int_{\mathfrak{e}} \theta(\tau,x;y)\,\mathrm{d}y.$$

The combination of relations (3) and (4) defines uniquely B and avoids the ambiguity implied by choices made in Brocato and Capriz (2011), Capriz (2003, 2006, 2008, 2019), Capriz and Fried (2011), Capriz et al. (2012), Capriz and Giovine (2016, 2017), Capriz and Mariano (2014, 2018, 2019, 2020). So, we adopt the decomposition

$$w_* = v + By + c, \tag{5}$$

distinguishing three scales: the *macroscopic* (or gross) view described by $v(\tau,x)$, the *mesoscopic* rate $B(\tau,x)$, and the *microscopic* fluctuations c. To allow the previous decomposition to be significant – meaning the elements involved have components in the same space – we exploit often tacitly, but also systematically, the identification of $\mathbb{R}^3$ with $\mathbb{R}^3$. We also consider w_* to be differentiable.

Proposition 1. *Condition (4) and decomposition (5) imply that the average and the first tensor momentum of the microscopic (spurious) fluctuations c vanish, namely*

$$\int_{\mathfrak{e}} \theta c\,\mathrm{d}y = 0 \quad \textit{and} \quad \int_{\mathfrak{e}} \theta y \otimes c\,\mathrm{d}y = 0.$$

Such a proposition has been already proven in Capriz and Mariano (2018). We report here the proof only for reader's convenience.

Proof. Since v is the average of w_*, we have

$$\begin{aligned} v(\tau,x) &:= \omega^{-1}\int_{\mathfrak{e}} \theta w_*(\tau,x;y)\,\mathrm{d}y = \omega^{-1}\int_{\mathfrak{e}} \theta(v+By+c)\,\mathrm{d}y \\ &= v + B\omega^{-1}\int_{\mathfrak{e}} \theta y\,\mathrm{d}y + \omega^{-1}\int_{\mathfrak{e}} \theta c\,\mathrm{d}y = v + \omega^{-1}\int_{\mathfrak{e}} \theta c\,\mathrm{d}y, \end{aligned}$$

because y is evaluated in a reference frame having its origin in the (instantaneous) mass center of the window $\mathfrak{e}(x)$, so that

$$\int_{\mathfrak{e}} \theta y\,\mathrm{d}y = 0.$$

Also, we compute

$$\begin{aligned} 0 = -YB^{\top} + \omega^{-1}\int_{\mathfrak{e}} \theta\, y \otimes w_*\,\mathrm{d}y &= -YB^{\top} + \omega^{-1}\left(\int_{\mathfrak{e}} \theta\, y\,\mathrm{d}y \otimes v \right. \\ &\left. + \int_{\mathfrak{e}} \theta\, y \otimes y\,\mathrm{d}y\, B^{\top} + \int_{\mathfrak{e}} \theta\, y \otimes c\,\mathrm{d}y\right) = \omega^{-1}\int_{\mathfrak{e}} \theta\, y \otimes c\,\mathrm{d}y, \end{aligned}$$

which concludes the proof. ■

Remark 1. The left-hand-side term of the (definitory) assumption (4) can be written obviously, to within ω, as

$$\int_{\mathfrak{e}} \theta\, y \otimes w_*\,\mathrm{d}y = \int_{\mathfrak{e}} \theta\, y \otimes (w_* - v)\,\mathrm{d}y.$$

So, the right-hand-side integral represents (to within the factor ω^{-1}) the tensor moment of momentum inside the window $\mathfrak{e}(x)$ of fluctuations $By+c$. Of course, condition (4) is more stringent than the only moment of momentum constraint. In fact, it includes also the symmetric component of the dyad $y \otimes c$. However, such a component is not essential in fixing a rotation that defines completely B once Θ (thus Y) is known.

Remark 2. The conditions expressed in Proposition 1 do not exhaust all the fluctuations. Those described by the sum $By+c$ are fluctuations *with respect to* v and w_*, the latter per se a local average around y at the instant τ. There are *remaining fluctuations* described by the vector field $\tilde{c} := w - w_*$. They do not satisfy necessarily the constraints emerging in Proposition 1.

By taking into account definitions (1) and (3), we compute

$$\dot{Y} = \delta^2(\dot{G}G^{\top} + G\dot{G}^{\top}) = \delta^2(BY + YB^{\top}).$$

Also, since Y is symmetric, by setting from now on $\delta = 1$ for the sake of simplicity (or – that is the same – by normalizing lengths with respect to δ), we get

$$\dot{Y} = 2\mathrm{sym}(BY).$$

3.2. Looking at the space window as a whole

Assuming v to be known and setting $L := D\tilde{v}(\tau,x)$, where D indicates derivative with respect to x, we write F for a linear map from $\hat{\mathbb{R}}^3$ to $\mathbb{R}^3$ such that

$$\dot{F} = LF, \tag{6}$$

with the constraint

$$\det F > 0. \tag{7}$$

By left polar decomposition, we write $F = VR$, with V a symmetric tensor from $\mathbb{R}^3$ to $\mathbb{R}^3$ and $R \in SO(3)$, thanks to the constraint. We also take R to be coincident with the orthogonal factor appearing in Eq. (2). Thus, once Y and B are known, which implies knowledge of R, the unknown factor V emerges from Eq. (6), which can be rewritten as

$$\dot{V} - V(N^{-\frac{1}{2}}\dot{N}^{\frac{1}{2}} - N^{-\frac{1}{2}}BN^{\frac{1}{2}}) = LV,$$

reasonably supplemented by the initial condition $V(0,x) = I$.

We stress once again that we are directly working with velocity fields and do not refer at first to standard one-to-one deformations, in

order to maintain free the possibility of material elements not uniquely and permanently identifiable, an aspect – this one – detaching us from the standard format of continuum mechanics.

3.3. Measuring relative volume variations in the space window

Proposition 2. *The time rate of relative change in volume between the gross motion and the local homogeneous component of molecular rearrangements within every space window is the scalar*

$$\sigma := \operatorname{tr} L - \operatorname{tr} B.$$

The following proof is a mild refinement of the one proposed in Capriz and Mariano (2018).

Proof. Take a vector $\hat{a}$ in the comparison space $\hat{\mathbb{R}}^3$. Its image through G, namely $a := G\hat{a}$, belongs to $\tilde{\mathbb{R}}^3$, which we may shift into $\mathbb{R}^3$, the space of x's, where we select $\mathcal{B}$. The shifter is precisely the linear map associated with the identification $\imath : \tilde{\mathbb{R}}^3 \longrightarrow \mathbb{R}^3$. So, we may compare the vector $\imath(a) \in \mathbb{R}^3$ with $F\hat{a} \in \mathbb{R}^3$. Then, the square modulus $|\imath(a) - FG^{-1}a|^2$ quantifies the difference in length between the two vectors, and the second-rank tensor

$$\tilde{X} := FG^{-1}$$

accounts for the discrepancy between strain induced by G and the one by F. Incidentally, by considering the left polar decomposition $F = VR$, with the orthogonal factor R appearing also in $G = N^{\frac{1}{2}}R$, by definition, we eventually have $\tilde{X} = VN^{-\frac{1}{2}}$. So, we rightly loose in $\tilde{X}$ any reference to the comparison space, which is arbitrarily chosen. Then, we get

$$\frac{\dot{\det \tilde{X}}}{\det \tilde{X}} = \frac{\dot{\det F}}{\det F} + \frac{\dot{\det G^{-1}}}{\det G^{-1}} = \operatorname{tr} L + \frac{\dot{\det G^{-1}}}{\det G^{-1}},$$

and compute

$$\begin{aligned}\dot{\det G^{-1}} &= \frac{\mathrm{d}(\det G^{-1})}{\mathrm{d}G^{-1}} \cdot \dot{G^{-1}} = (\det G^{-1})G^{\top} \cdot \frac{\mathrm{d}G^{-1}}{\mathrm{d}G}[\dot{G}] \\ &= -(\det G^{-1})G^{\top} \cdot G^{-1}\dot{G}G^{-1} = -(\det G^{-1})G^{-\top}G^{\top} \cdot BGG^{-1} \\ &= -(\det G^{-1})I \cdot B = -(\det G^{-1})\operatorname{tr} B,\end{aligned}$$

so that

$$\frac{\dot{\det \tilde{X}}}{\det \tilde{X}} = \operatorname{tr} L - \operatorname{tr} B = \sigma. \quad \square$$

When all molecules in the cluster occupying $\mathfrak{e}(x)$ at the instant τ have equal mass, the scalar σ measures mass loss or gain.

Remark 3. Although written in a slightly different form that involves the right-hand-side term in the formula in Remark 1, condition (4) has been used by G. Capriz as a definition for B (see Capriz, 2003, 2006, 2008, 2019; Capriz and Fried, 2011; Capriz et al., 2012; Capriz and Giovine, 2016, 2017; Capriz and Mariano, 2014, 2018, 2019). Then, a fictitious reference environment has been constructed in those references by a retrogression – that is a backwards time integration – of the equation $\frac{\mathrm{d}\hat{x}(\tau,x)}{\mathrm{d}\tau} = v(\tau, x)$, with $\hat{x}(\bar{\tau}, x) = x$, varying x, once we consider the time τ running in the interval $[\tau_0, \bar{\tau}]$. A solution was the field determining F after differentiation with respect to x. An analogous argument was used for G. Now, even if the retrogression at every x would assure existence in the same interval of time for every point, so that a fictitious reference frame could be available, we would be in general not assured a priori that the same time interval would occur for the backwards integration of By, leading to a differentiable field from which we could derive G. The definition of B discussed in the present paper overcomes such potential difficulty.

4. C-derivatives

According to decomposition (5), and taking into account that $\dot{G^{-1}} = -G^{-1}B$, we define time derivatives of second-rank tensors, vectors, and scalars along the homogeneous component of the motion around x, the one with rate B. We indicate by a superposed circle such derivatives. Their definition depends on the type of fields involved.

- For a *second-rank-valued fully contravariant tensor field* $(\tau, x) \longmapsto A := \tilde{A}(\tau, x) = A^{ij}\tilde{\mathbf{e}}_i \otimes \tilde{\mathbf{e}}_j$, with $\tilde{\mathbf{e}}_i$ the ith vector of the basis in $\tilde{\mathbb{R}}^3$, the space where we place $\mathfrak{e}(x)$. We define $\mathring{A}$, calling it the C-derivative of A, by

$$\begin{aligned}\mathring{A} := \frac{1}{\det \tilde{X}} G\left(\dot{\overline{(\det \tilde{X})G^{-1}AG^{-*}}}\right)G^{*} &= G\dot{\overline{G^{-1}}}A + \dot{A} + A\dot{\overline{G^{-*}}}G^{*} + \sigma A \\ &= \dot{A} - BA - AB^{*} + \sigma A,\end{aligned}$$

  where $\dot{A} := \frac{\partial A}{\partial \tau} + (\nabla A)v$.
- For a *second-rank-valued 1-contravariant, 1-covariant tensor field* $(\tau, x) \longmapsto A := \tilde{A}(\tau, x) = A^{i}{}_{j}\tilde{\mathbf{e}}_i \otimes \tilde{\mathbf{e}}^j$, with $\tilde{\mathbf{e}}^j$ the jth element of the basis dual to $\{\tilde{\mathbf{e}}_i\}$. We define $\mathring{A}$ by

$$\begin{aligned}\mathring{A} := \frac{1}{\det \tilde{X}} G\left(\dot{\overline{(\det \tilde{X})G^{-1}AG^{-\top}}}\right)G^{\top} &= G\dot{\overline{G^{-1}}}A + \dot{A} + A\dot{\overline{G^{-\top}}}G^{\top} + \sigma A \\ &= \dot{A} - BA - AB^{\top} + \sigma A.\end{aligned}$$

When $\sigma = 0$, $\mathring{A}$ reduces to the Oldroyd derivative along the vector field By, a Lie derivative, indeed. When $\sigma \neq 0$, we could think of interpreting $\mathring{A}$ as a Lie derivative of $A \otimes \mu_r$, where μ_r is a volume measure with time rate σ, analogously of what we do with Truesdell's objective derivative. However, since at first μ_r (a measure of volume differences, indeed) is not available and, if so, at least in principle, its time rate following By would not account directly only for L, we do not identify the C-derivatives above with Truesdell's one.

- For a *two-point tensor field*, say $(\tau, x) \longmapsto P := \tilde{P}(\tau, x) = P^{i}_{\hat{k}}\tilde{\mathbf{e}}_i \otimes \hat{\mathbf{e}}^{\hat{k}}$, where $\hat{\mathbf{e}}^{\hat{k}}$ is the $\hat{k}$-th element of the dual basis over the comparison space $\hat{\mathbb{R}}^3$, while $\tilde{\mathbf{e}}_i$ is as above the ith element of a basis in $\tilde{\mathbb{R}}^3$, where we place the window $\mathfrak{e}$, we define

$$\mathring{P} := \frac{1}{\sqrt{\det \tilde{X}}} G\dot{\overline{(\sqrt{\det \tilde{X}})G^{-1}P}} = \dot{P} - BP + \frac{\sigma}{2}P.$$

The covariant component of P lives in the comparison space, which is left invariant by the flow By, defined on the current configuration after shifting through the map $\imath$ already defined the first contravariant component of $B^{i}{}_{j}$ into $\mathbb{R}^3$. As a special case, G itself is the value of a two-point tensor field with components of the type $G^{i}{}_{A}$. Consequently, we can write for it

$$\mathring{G} := \dot{G} - BG + \frac{\sigma}{2}G.$$

- For the gross *velocity field* $(\tau, x) \longmapsto v := \tilde{v}(\tau, x)$ we also define $\mathring{v}$ to be

$$\mathring{v} := \frac{1}{\sqrt{\det \tilde{X}}}\dot{\overline{(\sqrt{\det \tilde{X}})v}} = \dot{v} + \frac{\sigma}{2}v.$$

Here B does not appear because v is the mass center velocity of $\mathfrak{e}(x)$ and is not affected by the affine motion dictated by B. Consequently, we set

$$\mathring{\overline{v \otimes v}} = \dot{\overline{v \otimes v}} + \sigma(v \otimes v) = 2\operatorname{sym}(v \otimes \mathring{v}). \tag{8}$$

- For a *scalar field* $(\tau, x) \longmapsto a := \tilde{a}(\tau, x)$, we define

$$\mathring{a} := \frac{1}{\det \tilde{X}}\dot{\overline{(\det \tilde{X})v}} = \dot{a} + \sigma a.$$

Remark 4. In references Capriz and Giovine (2016, 2017), Capriz and Mariano (2014, 2018, 2019), Y is defined by the product $\bar{G}\bar{G}^{\top}$, where $\bar{G}$ is solution to the equation $\dot{\bar{G}} + \frac{\sigma}{2} = B\bar{G}$, so that $\mathring{Y} = 0$. Our choice, expressed by relation (2), describes, *at variance*, the intuitive

circumstance that the inertial tensor of the molecular cluster in $\mathfrak{e}$ varies depending how many molecules are gained or lost in time. In fact, by computing the C-derivative of Y, we get

$$\mathring{Y} = \dot{Y} - BY - YB^{\top} + \sigma Y = \dot{Y} - 2\mathrm{sym}(BY) + \sigma Y = \sigma Y. \tag{9}$$

5. Observers and their changes

We focus here attention on observers because we pave the way to an invariance requirement under a class of observer changes for the external power alone, the entity defining at a continuum scale the actions that summarize in a determinate sense the molecular interactions.

Observers are reference frames assigned to all spaces selected to represent the body morphology and its time variation. Here, beyond the time scale, we take frames of reference in all the identical copies of $\mathbb{R}^3$ involved.

We consider isometric-type changes of observer in both $\mathbb{R}^3$ and $\tilde{\mathbb{R}}^3$. We leave invariant the time scale, an admissible choice because we are in classical space–time. We also leave invariant the comparison space $\hat{\mathbb{R}}^3$.

Consider two observers in $\mathbb{R}^3$, namely $\mathcal{O}$ and $\mathcal{O}'$. Assume that they are related by a rigid-body motion. So, the first observer evaluates a place x, while the second one checks a place $x' := r(\tau) + Q(\tau)(x - x_0)$, where $r(\tau) \in \mathbb{R}^3$, $Q(\tau) \in SO(3)$, and x_0 is an arbitrary point fixed in space. The maps $\tau \longmapsto r(\tau)$ and $\tau \longmapsto Q(\tau)$ are assumed to be smooth. With v the velocity evaluated by $\mathcal{O}$ and v' the one recorded by $\mathcal{O}'$, given by $v' = \dot{r} + \dot{Q}(x - x_0) + Qv$, to compare them in the same frame of reference, say $\mathcal{O}$, by considering v' as a free vector, we pull back v' to $\mathcal{O}$, obtaining a vector $v^{\diamond}$ given by

$$v^{\diamond} = v + \hat{\mathrm{c}} + \hat{\mathrm{W}}(x - x_0), \tag{10}$$

where $\hat{\mathrm{c}} := Q^{\top}\dot{r}$ and $\hat{\mathrm{W}} = Q^{\top}\dot{Q}$ is a skew-symmetric tensor. By differentiating with respect to x, we get

$$Dv^{\diamond} = Dv + \hat{\mathrm{W}}. \tag{11}$$

A relation similar to (11) occurs for B. Since the two observers $\mathcal{O}$ and $\mathcal{O}'$ are defined as systems of reference frames in both $\mathbb{R}^3$ and $\tilde{\mathbb{R}}^3$, we have to consider what happens in terms of changes of observers in the window $\mathfrak{e} \subset \tilde{\mathbb{R}}^3$. Indeed, although $B(\tau, x)$ is the value of a field defined on $\mathcal{B}$, its first component is in $\tilde{\mathbb{R}}^3$ because y is defined in $\mathfrak{e}$. Specifically, at τ and x, the second rank tensor B has components $B^i_{\ \tilde{j}}$ and is $B = B^i_{\ \tilde{j}}\mathbf{e}_i \otimes \tilde{\mathbf{e}}^{\tilde{j}}$, where $\mathbf{e}_i$ is the $i-$th element of a vector basis in $\mathbb{R}^3$, while $\tilde{\mathbf{e}}^{\tilde{j}}$ belongs to the dual vector basis over $\tilde{\mathbb{R}}^3$. In its physical essence, although not further specified, B has to be intended as a velocity gradient, so, given two values B and B' recorded by the two observers involved above, the value $B^{\diamond}$ of the pull-back of B' into $\mathcal{O}'$ can be considered to be something like

$$B^{\diamond} = B + Y,$$

with Y a skew-symmetric second rank tensor mapping $\tilde{\mathbb{R}}^3$ onto $\mathbb{R}^3$, according to the relation (11).

By exploiting once again the identification of $\tilde{\mathbb{R}}^3$ with $\mathbb{R}^3$, we take $Y = \hat{\mathrm{W}}$, so that for $B^{\diamond}$ we have the expression

$$B^{\diamond} = B + \hat{\mathrm{W}}. \tag{12}$$

6. Mass density and its time variation

Let $\mu(\tau, x; y)$ be the mass at $y \in \mathfrak{e}(x)$ at the instant τ. We may define a continuous mass density $\rho(\tau, x)$ by

$$\rho(\tau, x) := \delta^{-3} \int_{\mathfrak{e}} \theta\,(\tau, x; y)\,\mu(\tau, x; y)\,\mathrm{d}y.$$

(We explicit here δ for the sake of generality, although we have chosen $\delta = 1$ as always it can be done by scaling lengths.)

When all molecules have equal mass μ, the previous formula obviously reduces to

$$\rho(\tau, x) := \mu\delta^{-3} \int_{\mathfrak{e}} \theta\,(\tau, x; y)\,\mathrm{d}y.$$

Assume that, globally, the whole region $\mathcal{B}$ at the instant τ does not loose or gain mass. However, the freedom of molecules to relatively fly, since the phase is sparse (say particulate), implies local mass loss or gain. When molecules are all of the same mass, as we accept here for the sake of simplicity, the density variation is due to the rate at which (pointwise at macroscopic scale) the volume of the molecular cluster varies locally along the gross motion with average velocity v, so that we write

$$\dot{\rho} = -\rho\mathrm{tr}B,$$

that is

$$\dot{\rho} + \rho\mathrm{tr}L - \rho\mathrm{tr}L = -\rho\mathrm{tr}B,$$

or

$$\frac{\partial \rho}{\partial \tau} + \mathrm{div}(\rho v) - \sigma\rho = 0.$$

This last equation reduces to the standard local balance of mass when $\sigma = 0$.

7. External power, invariance, and balance

Take any arbitrary compact control volume $\mathfrak{b}$ in $\mathbb{R}^3$ with diameter much larger than δ and piecewise smooth surface boundary. Based on the previous analyses, we can leave apart (in a sense) the particulate nature of the bodies under analysis and may think in terms of continuous fields, in particular those considered here to be basic ingredients in describing pertinent mechanical processes, namely, v and B. We associate mechanics to what is described by these fields, and leave to thermal-like effects what is associated with the fluctuations represented by c, which are spurious with respect to w_*, v, and B.

As usual in continuum mechanics, we distinguish actions into two classes: bulk and contact ones. They are defined by the power that they develop on the velocity fields considered, namely v and B. Since v is a vector, the actions performing power on it are naturally covectors so their pairing with v is well-defined without the need to specify a metric. Also, since B is a second-rank tensor, actions defined by the power that they develop over it are thus second-rank tensors too, with dual character with respect to B. So, bulk actions are indicated by $b^{\ddagger}$, a covector in $\mathbb{R}^{3*}$, and $O^{\ddagger}$, a second-rank tensor over $\mathbb{R}^3$. Contact actions are indicated by t_{∂}, once again a covector in $\mathbb{R}^{3*}$, and a second-rank tensor $\hat{\mathrm{M}}_{\partial}$ over $\tilde{\mathbb{R}}^3$. All depend on time τ and space x. The subscript ∂ indicates that t_{∂} and $\hat{\mathrm{M}}_{\partial}$ depend also on the boundary $\partial\mathfrak{b}$. Given an arbitrary part $\mathfrak{b}$ of $\mathcal{B}$, we write the power that *external* agencies perform over it – and we call it the *external power*, indicating it by $\mathcal{P}^{ext}_{\mathfrak{b}}$ – as

$$\mathcal{P}^{ext}_{\mathfrak{b}}(v, B) := \int_{\mathfrak{b}} (\rho b^{\ddagger} \cdot v + \rho O^{\ddagger} \cdot B)\,\mathrm{d}x + \int_{\partial\mathfrak{b}} (\mathrm{t}_{\partial} \cdot v + \hat{\mathrm{M}}_{\partial} \cdot B)\,\mathrm{d}\mathcal{H}^2(x). \tag{13}$$

Since $\partial\mathcal{B}$ is open, the arbitrariness in choosing $\mathfrak{b}$ does not imply the need of discussing what happens on $\partial\mathcal{B}$, which deserves a specific treatment not tackled here. Notice that we *do not* postulate the internal power expression: it will be deduced as a consequence of the subsequent developments.

We require that $\mathcal{P}^{ext}_{\mathfrak{b}}$ must be invariant under isometric-type changes of observer described by the relations (10) and (12). So, we formally impose an *axiom of external power invariance*:

$$\mathcal{P}^{ext}_{\mathfrak{b}}(v, B) = \mathcal{P}^{ext}_{\mathfrak{b}}(v^{\diamond}, B^{\diamond}) \tag{14}$$

for any choice of $\hat{\mathrm{c}}$, $\hat{\mathrm{W}}$, and $\mathfrak{b}$. Also, we recall that $\hat{\mathrm{W}} = \mathfrak{e}q = q\times$, with $\mathfrak{e}$ the third-rank Ricci's alternating index in $\mathbb{R}^3$ and $q \in \mathbb{R}^3$; precisely, in component form, we have $\hat{\mathrm{W}}^i_{\ j} = \mathfrak{e}^i_{\ jk}q^k$.

An immediate consequence is the standard integral balance of forces

$$\int_{\mathfrak{b}} \rho b^{\ddagger}\,\mathrm{d}x + \int_{\partial\mathfrak{b}} \mathrm{t}_{\partial}\,\mathrm{d}\mathcal{H}^2(x) = 0. \tag{15}$$

and a non-standard integral balance of couples in tensor form, given by

$$\int_{\mathfrak{b}} \mathbf{e}((x-x_0)\otimes\rho b^{\ddagger} + \rho O^{\ddagger})\,\mathrm{d}x + \int_{\partial\mathfrak{b}} \mathbf{e}((x-x_0)\otimes \mathrm{t}_{\partial} + \hat{\mathsf{M}}_{\partial})\,\mathrm{d}\mathcal{H}^2(x) = 0. \tag{16}$$

- If $\left|\rho b^{\ddagger}\right|$ is bounded over $\mathcal{B}$ and t_{∂} is a continuous function of x, on the basis of Cauchy's theorem we have $\mathrm{t}_{\partial} = \mathfrak{t} := \tilde{\mathfrak{t}}(\tau, x, n)$, with n the normal to $\partial\mathfrak{b}$ and $\tilde{\mathfrak{t}}(\tau, x, n) = -\tilde{\mathfrak{t}}(\tau, x, -n)$, that is the action–reaction principle. Also, as a function of n, $\tilde{\mathfrak{t}}$ is homogeneous and additive, meaning there exists a second-rank tensor field $x \longmapsto T(\tau, x)$ such that $\tilde{\mathfrak{t}}(x, n) = T(x)\,n(x)$ (see, e.g., Truesdell, 1977; Dafermos, 2005); T is the common *Cauchy stress*.

- Since $\mathcal{B}$ is taken to be bounded, we may choose x_0 in a way such that the boundedness of $\left|\rho b^{\ddagger}\right|$ implies the one of $\left|(x-x_0)\otimes\rho b^{\ddagger}\right|$. Then, if in addition $\left|\rho O^{\ddagger}\right|$ is bounded over $\mathcal{B}$, and $\hat{\mathsf{M}}_{\partial}$ depends continuously on x, we may reproduce the arguments above showing that $\hat{\mathsf{M}}_{\partial}$ depends on $\partial\mathfrak{b}$ only through the normal n to it in all points where n is well-defined, meaning there is a tensor-valued function $\tilde{\mathsf{M}}$ such that $\tilde{\mathsf{M}}_{\partial}(\tau, x) = \tilde{\mathsf{M}}(\tau, x, n)$ and

  $$\mathrm{skw}(\tilde{\mathsf{M}}(\tau, x, n) - \tilde{\mathsf{M}}(\tau, x, -n)) = 0. \tag{17}$$

  Also, as a function of n, $\tilde{\mathsf{M}}$ is homogeneous and additive, meaning there exists a third-rank tensor field $x \longmapsto \mathbf{m}(\tau, x)$ such that $\tilde{\mathsf{M}}(\tau, x, n) = \mathbf{m}(\tau, x)\,n(x)$.

- If the stress field T is in $C^1(\mathcal{B})\cap C\left(\bar{\mathcal{B}}\right)$ and $x \longmapsto b^{\ddagger}$ is continuous over $\mathcal{B}$, the point-wise balance of forces

  $$\mathrm{div}T + b^{\ddagger} = 0 \tag{18}$$

  holds due to the arbitrariness of $\mathfrak{b}$. Also, by exploiting Eq. (18) and the arbitrariness of $\mathfrak{b}$ in the integral balance (16), when $\rho O^{\ddagger}$ is continuous and $\mathbf{m}$ is in $C^1(\mathcal{B})\cap C\left(\bar{\mathcal{B}}\right)$, we may read the pointwise version of Eq. (16) by saying that there exists a field $x \longmapsto A(\tau, x) \in \mathbb{R}^3\otimes\mathbb{R}^3$ such that

  $$\mathrm{skw}T = \mathrm{skw}A. \tag{19}$$

  and

  $$\rho O^{\ddagger} - A + \mathrm{div}\mathbf{m} = 0. \tag{20}$$

The items above refine a theorem in Capriz and Mariano (2018).

Remark 5. If, at variance of what we do here, we had chosen the virtual power principle as a basic axiom, we would have had to hypothesize the existence of the self-stress A and the hyperstress $\mathbf{m}$ (a third-rank tensor), because that principle is in essence nothing more that the prescription of a weak form of the balance equations, so of all the ingredients entering them, without proving their necessity.

Remark 6. Cauchy–Born's rule helps in determining explicit expressions of T, A, and $\mathbf{m}$ in terms of the intermolecular interactions at discrete scale. In particular, second-neighbor interactions at discrete scale appear in identifying the third-rank tensor $\mathbf{m}$, as proven in Capriz and Mariano (2019). We do not investigate further the issue here and address to the quoted reference.

8. Tensor kinetic energy balance

We presume that $b^{\ddagger}$ and $O^{\ddagger}$ admit additive decompositions into inertial and non-inertial components, the former indicated by a superscript in:

$$b^{\ddagger} = b + b^{in} \qquad , \qquad O^{\ddagger} = O + O^{in}.$$

The inertial components are determined by the kinetic energy expressed in an appropriate form to account more directly for anisotropy in the kinetics within $\mathfrak{e}(x)$ at the instant τ. So, we call upon for the kinetic energy a second-rank tensor form $\bar{\mathcal{W}}$, defined by

$$\bar{\mathcal{W}} = \frac{1}{2\omega}\int_{\mathfrak{e}(x)} \theta w_*\otimes w_*\,\mathrm{d}y = \frac{1}{2\omega}\int_{\mathfrak{e}(x)} \theta(v+By+c)\otimes(v+By+c)\,\mathrm{d}y.$$

By computing the products and integrating, we get

$$\begin{aligned}\bar{\mathcal{W}} =& \frac{1}{2\omega}\int_{\mathfrak{e}(x)} \theta(v\otimes v + By\otimes yB^{\top} + c\otimes c)\,\mathrm{d}y + \frac{1}{2\omega}\int_{\mathfrak{e}(x)} \theta 2\mathrm{sym}(v\otimes By)\,\mathrm{d}y\\ &+ \frac{1}{2\omega}\int_{\mathfrak{e}(x)} \theta(2\mathrm{sym}(v\otimes c) + 2\mathrm{sym}(By\otimes c))\,\mathrm{d}y\\ =& \frac{1}{2}(v\otimes v + BYB^{\top} + H),\end{aligned} \tag{21}$$

due to Proposition 1 and the circumstance that y is by assumption computed from the mass center of $\mathfrak{e}(x)$ so that $\int_{\mathfrak{e}(x)}\theta y\,\mathrm{d}y = 0$. In the previous expression, H is a second-rank symmetric tensor given by

$$H(\tau, x) := \omega^{-1}\int_{\mathfrak{e}(x)} \theta c\otimes c\,\mathrm{d}y,$$

which plays here the role of a Reynolds tensor.

By setting $K := YB^{\top}$ and considering the formula (8), we compute

$$\mathring{\bar{\mathcal{W}}} = \mathrm{sym}(v\otimes\mathring{v}) + \frac{1}{2}B\mathring{K} + \frac{1}{2}\dot{B}K + \frac{1}{2}\dot{H} - \mathrm{sym}(BH) + \frac{1}{2}\sigma H. \tag{22}$$

Remark 7. The expression of $\mathring{\bar{\mathcal{W}}}$ differs from the one indicated in Capriz and Giovine (2016), Capriz and Giovine (2017), Capriz and Mariano (2018) by the presence of $\frac{1}{2}\dot{B}K$, which is justified as follows:

$$\begin{aligned}\overline{\mathring{BYB^{\top}}} = \overline{\mathring{BK}} &= \overline{\dot{BK}} - BBK - BKB^{\top} + \sigma BK\\ &= \dot{B}K + B\dot{K} - BBK - BKB^{\top} + \sigma BK = \dot{B}K + B\mathring{K},\end{aligned} \tag{23}$$

and $\overline{\mathring{BYB^{\top}}}$ is the term pertaining to B in the C-derivative of $\bar{\mathcal{W}}$.

In common treatments of continuum mechanics, with the aim of deriving the representation of inertial terms from a first principle, we may assume as an axiom that the sum of (scalar) kinetic energy time rate and power of inertial bulk actions vanishes for any choice of the velocity fields and the body part considered.

If we would opt to do the same here for the integral of $\rho\mathring{\bar{\mathcal{W}}}$ over a given region in space, equating it to the negative tensor power of b^{in} and O^{in}, we would face the difficulty that $\mathrm{sym}(v\otimes\mathring{v})$ is symmetric while $v\otimes b^{in}$ is not; also BO^{in} has no correspondent term in the energy derivative that is one made by the product of B with something else. So, we define

$$\begin{aligned}\mathring{\bar{\mathcal{W}}} :&= \mathring{\bar{\mathcal{W}}} + \mathrm{skew}(v\otimes\mathring{v}) - \frac{1}{2}\dot{B}K + \frac{1}{2}B\mathring{K} - \mathrm{skew}(BH)\\ &= (v\otimes\mathring{v}) + B(\mathring{K} - H) + \frac{1}{2}\dot{H} - \frac{1}{2}\sigma H\end{aligned} \tag{24}$$

and assume that

$$\begin{aligned}\int_{\mathfrak{b}} \rho\mathring{\bar{\mathcal{W}}}\,\mathrm{d}x + \int_{\mathfrak{b}} \rho(v\otimes b^{in} + BO^{in})\,\mathrm{d}x - \frac{1}{2}\int_{\mathfrak{b}}(\rho J - Z)\,\mathrm{d}x\\ - \frac{1}{2}\int_{\partial\mathfrak{b}} \hat{\mathrm{J}}_{\partial}\,\mathrm{d}\mathcal{H}^2(x) = 0,\end{aligned} \tag{25}$$

for every part $\mathfrak{b}$ and all rate fields involved. In the previous equation, J and Z are (respectively outer and inner) sources and $\hat{\mathrm{J}}_{\partial}$ a flux. In principle they are needed to compensate the time variation of fluctuations described by H that are beyond the power developed by b^{in} and O^{in}. Even in this case the subscript ∂ indicates that $\hat{\mathrm{J}}_{\partial}$ depends on the boundary of $\mathfrak{b}$ besides instant τ and place x.

The arbitrariness of rate fields implies

$$\rho b^{in} = -\rho\mathring{v}, \qquad \rho O^{in} = -\rho\mathring{K} + \rho H, \tag{26}$$

to within powerless terms, and the residual integral balance

$$\int_{\mathfrak{b}} \rho(\dot{H}+\sigma H)\,\mathrm{d}x - \int_{\mathfrak{b}} (\rho J - Z)\,\mathrm{d}x - \int_{\partial\mathfrak{b}} \hat{\jmath}_{\partial}\,\mathrm{d}\mathcal{H}^2(x) = 0. \tag{27}$$

Remark 8. The inclusion of $\mathring{\tilde{\mathcal{W}}}$ in the balance (25) marks a difference with how the same balance has been used in Capriz and Mariano (2018), Capriz and Mariano (2019), where a form of the balance (25) accepting $\mathring{\mathcal{W}}$ and only the symmetric part of the current second integral is involved, so that the resulting identifications (26) are only compatible with that balance, while here they are implied necessarily.

When the volume integral densities in Eq. (27) are bounded and $\hat{\jmath}_{\partial}$ is continuous with respect to x, Cauchy's theorem implies that $\hat{\jmath}_{\partial}$ depends on $\partial\mathfrak{b}$ only through the boundary n to $\partial\mathfrak{b}$ at the points where n is well-defined. Precisely, there is a function $\tilde{\jmath}$ such that we get

$$\hat{\jmath}_{\partial} = \jmath := \tilde{\jmath}(\tau, x, n) = -\tilde{\jmath}(\tau, x, -n). \tag{28}$$

Also, $\tilde{\jmath}$ is linear with respect to n, meaning that there exists a third-rank tensor field with values $\mathbf{j} = \tilde{\mathbf{j}}(\tau, x)$ such that

$$\hat{\jmath} := \tilde{\jmath}(\tau, x, n) = \tilde{\mathbf{j}}(\tau, x)n = \mathbf{j}n.$$

The existence of $\tilde{\jmath}$ and related properties is, at variance, assumed a priori in Capriz and Mariano (2018) and Capriz and Mariano (2019). In contrast, here we prove the emergence of $\tilde{\mathbf{j}}(\tau, x)$.

When the difference $\rho\dot{H} - (\rho J - Z)$ is continuous in space and $\tilde{\mathbf{j}}(\tau, \cdot)$ is C^1, the arbitrariness of Ω and Gauss' theorem imply the local balance

$$\rho(\dot{H} + \sigma H) = \rho J - Z + \operatorname{div}\mathbf{j}.$$

Remark 9. Indeed, continuity with respect to x of all the boundary fluxes considered above is superabundant according to Cauchy's theorem (see Dafermos (2005, p. 3)). However, we accept here such a regularity only for the sake of simplicity, due to our focus on conceptual issues, rather than on analytical aspects.

9. Summary of the balance equations and related inner power

The analyses in the previous section furnish the following balance equations in local form:

- Density of mass:

$$\dot{\rho} + \rho \operatorname{div} v - \sigma\rho = 0. \tag{29}$$

- Momentum:

$$\rho\mathring{v} = \operatorname{div} T + b. \tag{30}$$

- Moment of momentum:

$$\operatorname{skw} T = \operatorname{skw} A. \tag{31}$$

- Interactions associated with the affine component of fluctuations:

$$\rho\mathring{K} - \rho H = \rho O - A + \operatorname{div}\mathbf{m}. \tag{32}$$

- Interactions associated with the fluctuations c:

$$\rho(\dot{H} + \sigma H) = \rho J - Z + \operatorname{div}\mathbf{j}. \tag{33}$$

Multiply by $v\otimes$ the balance of momentum and by B the one of interactions associated with the affine component of fluctuations. Take the symmetric part of the results and multiply them and the balance associated with H by $\frac{1}{2}$. If we sum the results and integrate over a control volume $\mathfrak{b}$, we get

$$\int_{\mathfrak{b}} \rho\mathring{\tilde{\mathcal{W}}}\ \mathrm{d}x - \frac{1}{2}\int_{\mathfrak{b}} \dot{B}K\,\mathrm{d}x = \int_{\mathfrak{b}} \rho\left(\operatorname{sym}(v\otimes b + BO) + \frac{1}{2}J\right)\mathrm{d}x + \int_{\partial\mathfrak{b}} \left(\operatorname{sym}(v\otimes Tn + \mathbf{m}(Bn)) + \frac{1}{2}\mathbf{j}n\right)\mathrm{d}\mathcal{H}^2(x)$$

$$- \int_{\mathfrak{b}} \left(\operatorname{sym}\left((\nabla v)T^{\top} + BA + \mathbf{b}\mathbf{m}^t\right) + \frac{1}{2}Z\right)\mathrm{d}x.$$

We interpret

$$\mathfrak{p}^{inn} := \operatorname{sym}\left((\nabla v)T^{\top} + BA + (DB)^t\mathbf{m}\right) + \frac{1}{2}Z, \tag{34}$$

as a *tensor density of internal power*.

Remark 10. The integral balance above corrects an analogous relation in Capriz and Giovine (2016) (Capriz and Giovine, 2017), Capriz and Mariano (2018), where the term involving $\dot{B}K$ does not appear.

10. A special class of constrained motions

For the sake of simplicity we still refer to orthonormal reference frames. The results in this section hold also, as those above, for metrics associated with other type of reference frames, provided a few formal adjustments.

F and G differ from each other in general. With them, we construct pertinent right Cauchy–Green tensors, $C := F^{\top}F$ and $N := G^{\top}G$, respectively at macroscopic and window-size scales. They allows us to define a tensor, say P, called a *distemper* (Capriz and Giovine, 2017) and defined to be

$$\mathsf{P} := \frac{1}{\operatorname{tr} CN^{-1}} N^{-\frac{1}{2}} C N^{-\frac{1}{2}} - \frac{1}{3} I,$$

with I the second-rank unit tensor. It measures the discrepancy between macroscopic and window-scale affine motions. Assuming appropriate regularity at a first glance, we also consider the symmetric tensor $M := \Delta\mathsf{P}$. Then, we choose

$$Z = \mathbf{Z}\dot{M}, \qquad \text{and} \qquad \mathbf{j} = \Gamma\nabla\dot{M},$$

with $\mathbf{Z}$ and Γ fourth-rank and rank-6 tensors, respectively.

Also, we impose the *internal constraint*

$$F = G. \tag{35}$$

It implies $\nabla v = B$ and $\sigma = 0$ (it is possible to write Eq. (35) due to the identification accepted from the beginning of $\mathbb{R}^3$ with $\tilde{\mathbb{R}}^3$, and also with $\hat{\mathbb{R}}^3$). The immediate consequence is $\mathsf{P} = 0$. Then, $Z = 0$ and $\mathbf{j} = 0$. Also, in this special case the tensor density of internal power reduces to

$$\mathfrak{p}^{inn} := \operatorname{sym}\left((\nabla v)T^{\top} + BA + (\nabla B)\mathbf{m}^{\top}\right).$$

Its trace is

$$\operatorname{tr}(\mathfrak{p}^{inn}) := \nabla v\cdot(T + A^{\top}) + {}^t\mathbf{m}\cdot\nabla^2 v,$$

where ∇^2 indicates the second gradient.

The presence of an internal constraint implies the decomposition of interactions into active (indicated by a subscript a) and reactive components (those with r):

$$T = T_a + T_r, \quad A = A_a + A_r, \quad \mathbf{m} = \mathbf{m}_a + \mathbf{m}_r.$$

Since the assumed internal constraint is holonomic, the reactive components of interactions do not perform power along *any* motion allowed by the constraint, so that we must have

$$\nabla v\cdot(T_r + A_r^{\top}) + {}^t\mathbf{m}_r\cdot\nabla^2 v = 0,$$

for *any* choice of ∇v and $\nabla^2 v$, taken as independent entities because they belong to linear spaces and are not constrained. Such an arbitrariness implies

$$T_r = -A_r^{\top}, \quad \mathbf{m}_r + \mathbf{m}_r^{\top} = 0, \tag{36}$$

which give

$$\operatorname{skw} T_r = \operatorname{skw} A_r, \quad \operatorname{div}((\operatorname{div}\mathbf{m}_r)^{\top}) = 0.$$

The first equation and the additive decomposition of stresses into active and reactive component imply in addition

$$\operatorname{skw} T_a = \operatorname{skw} A_a. \tag{37}$$

From the transpose of Eq. (32) we obtain

$$T_r = \rho\left(\left(\frac{\partial\nabla v}{\partial\tau} + (\nabla^2 v)v\right)Y - H - O^\top\right) + A_a^\top - (\mathrm{div}(\mathbf{m}_r + \mathbf{m}^\top))^\top.$$

Eventually, we get the following balance laws:

$$\frac{\partial\rho}{\partial\tau} + \mathrm{div}(\rho v) = 0, \tag{38}$$

$$\rho\left(\frac{\partial v}{\partial\tau} + (\nabla v)v\right) + \mathrm{div}\left(\rho\left(H - \left(\frac{\partial\nabla v}{\partial\tau} + (\nabla^2 v)v\right)Y\right)\right) = \rho b - \mathrm{div}(\rho O^\top) + \mathrm{div}\left(\mathrm{sym}(T_a + A_a) - (\mathrm{div}\mathbf{m}_a)^\top\right), \tag{39}$$

$$\rho\left(\frac{\partial H}{\partial\tau} + (\nabla H)v\right) = \rho J, \tag{40}$$

where Y satisfies now

$$\mathring{Y} = 0$$

because $\sigma = 0$ with the adopted constraint (see Eq. (9)); in other words the assumption $F = G$ implies that each material element is a canonical ensemble from a statistical viewpoint.

We do not add details about the path from balance Eqs. (29)–(33) to (38)–(40), granted by the constraint (35) because they are in Capriz and Giovine (2017) where Eqs. (29)–(33) are only postulated.

We may specify further the issue.

10.1. Case 1

Assume that there exists a differentiable vector field u such that $G = \nabla u$ and $|\nabla u| \ll 1$. The adopted identification between $\hat{\mathbb{R}}^3$ and $\mathbb{R}^3$ allows us to avoid distinguishing x from x_*. We also have

$$Y = \nabla u \nabla u^\top.$$

Consider the motion to be incompressible, namely

$$\mathrm{div} v = 0.$$

Take also

$$T_a + A_a = \bar{\mathbb{C}}\nabla u - \pi I,$$

where I is the unit tensor, $-\pi$ a pressure implied by the incompressibility constraint, and $\bar{\mathbb{C}}$ a fourth-rank tensor with at least major symmetries. Finally, consider

$$\mathbf{m}_a = 2r_1\nabla\mathrm{sym}\nabla u + 2r_2\nabla\mathrm{sym}\nabla v, \tag{41}$$

with r_1 and r_2 positive constants. Such choices imply considering elastic-type interactions of first and second neighbor type among the flowing molecules. Consequently, the system (38)–(40) reduces to

$$\mathrm{div} v = 0,$$

$$\rho\left(\frac{\partial v}{\partial\tau} + (\nabla v)v\right) + \mathrm{div}\left(\rho\left(H - \left(\frac{\partial\nabla v}{\partial\tau} + (\nabla^2 v)v\right)Y\right)\right) + \nabla\pi = \mathrm{div}\left(\bar{\mathbb{C}}\nabla u\right) + f - 2\,\mathrm{div}\left(\left(\mathrm{div}(r_1\nabla\mathrm{sym}\nabla u + r_2\nabla\mathrm{sym}\nabla v)\right)^\top\right),$$

$$\rho\left(\frac{\partial H}{\partial\tau} + (\nabla H)v\right) = \rho J,$$

with the additional relation

$$\frac{\partial Y}{\partial\tau} + (v\cdot\nabla)Y = \nabla v Y + Y\nabla v^\top,$$

since $\sigma = 0$, as already recalled. The vector $f := \rho b - \mathrm{div}(\rho O^\top)$ and the second-rank tensor J are data.

10.2. Case 2

As already mentioned, the term $\bar{\mathbb{C}}\nabla u$ accounts for first-neighbor interactions of (say) "elastic" nature, while $r_1\nabla\mathrm{sym}\nabla u$ describes second-neighbor interactions (a hyperstress-type component indeed). If we assume that these contributions vanish and the stresses have essentially viscous-type nature, the right-hand-side term of the balance of momentum reduces to

$$-2r_2\mathrm{div}\left(\mathrm{div}\nabla\mathrm{sym}\nabla v\right)^\top + f,$$

so the equation simplifies in structure but its analysis remains far from being trivial once initial and boundary conditions are prescribed because the greatest analytical difficulty essentially lies in the term $((\nabla^2 v)v)Y$, a portion of what can be considered a non-local inertial effect due to fluctuations as a consequence of the presumed internal constraint. Experimental analyses on avalanches or flows of wheat, for example, should investigate this theoretically foreseen effect, above all its weight on the whole motion.

Other constraints can be introduced (see Capriz et al., 2012; Capriz and Giovine, 2016). In special cases, the balance of forces reduces to the $\alpha\beta$−regularization of Navier–Stokes' equations (Capriz and Fried, 2011).

11. Heat and fluctuations

11.1. Heat-like processes

Notions of temperature for sparse phases have been discussed by looking directly at the distribution Θ even if only in some its special specifications (Capriz and Mariano, 2018, 2019, 2020).

However, temperature can be viewed as a field over $\mathcal{B}$, defined indirectly by the equations it satisfies. We start from such a view and develop a notion of heat and temperature moving along a dynamical system based view on thermodynamics (Šilhavy, 1997).

For the sake of simplicity, we consider the state at y, inside $\mathfrak{e}(x)$ as determined only by the velocity w_* of molecules crossing y at the instant τ in the window pertinent to x. At macroscopic scale (that is outside the window), the state space Σ is a finite-dimensional set of triples (v, B, s), where s is a list of appropriate variables such as the distemper mentioned above or analogous choices (see for them proposals in Capriz and Giovine (2017)).

In what follows, we continue to neglect the remaining fluctuations $w - w_*$ and attribute to c alone and its spatial variations inside $\mathfrak{e}(x)$ the origin of what we can consider heat. This is *different* from what W. Noll proposed in Noll (1955) (and also Lehoucq and Von Lilienfeld-Toal, 2010), where *all* fluctuations beyond v enter what is considered to be heat.

Let C_x be a space of integrable vector fields over $\mathfrak{e}(x)$, each their value a vector with the same dimension of the space where $\mathfrak{e}(x)$ is chosen (say $3D$ or $2D$ vector fields).

Definition 1. A *heat-like process* for a window $\mathfrak{e}$ at x is a path in C_x that is parameterized by τ, namely a map $\pi_c(\cdot, x) : [0, d_\pi] \longrightarrow C_x$ (d_π the process duration), such that $\pi_c(\tau, x) = c(\tau, x; \cdot)$.

We write C for the disjoint union $\sqcup_{x\in\mathcal{B}} C_x$ and extend the notion of $\pi_c(\cdot, x)$ to the process $\pi_c : [\tau_1, \tau_2]\times\mathcal{B} \longrightarrow C$ so that $\pi_c(\tau, x) = c(\tau, x; \cdot)$.

Let Π_C denote the space of such field-valued maps π_c. By assumption we take it to be closed with respect to sub-processes: for every choice of τ_1 and τ_2 such that $0 < \tau_1 < \tau_2 < d_\pi$, Π_C contains a process $\pi_{c,x} : [\tau_1, \tau_2] \longrightarrow C_x$. The property holds for every choice of d_π.

A general process is thus a map $\pi : [0, d_\pi]\times\mathcal{B} \longrightarrow \Sigma\times C$ with values

$$\pi(\tau, x) = (v(\tau, x), B(\tau, x), s(\tau, x), \pi_c(\tau, x)),$$

whose value at τ and $y \in \mathfrak{e}(x)$ is given by

$$\pi(\tau, x)|_y = (v(\tau, x), B(\tau, x), s(\tau, x), c(\tau, x; y)).$$

Π indicates the space of such processes, assumed to be closed with respect to sub-processes, as its component Π_C is. When a process $\bar{\pi}$ is such that $\pi(d_\pi) = \bar{\pi}(0)$, we say that $\bar{\pi}$ is a *continuation* of π_c; we write $\bar{\pi}\circ\pi$ for the compound process. We say that π is cyclic when its value

at 0 coincides with the one at d_π (a superscript $cycl$ will identify cyclic processes and their sub-space into Π).

Definition 2. We say that two elements of $\bar{\Sigma} := \Sigma \times C$ are *accessible* when there is an admissible process connecting them, admissibility defined every time we select a class of motions in $\mathfrak{e}(x)$ while here left unspecified.

11.2. Work-heat pairs

We define the (scalar) *work density done* in apart $\mathfrak{b}$ of $\mathcal{B}$ along π by the functional

$$\mathfrak{w}(\pi, \mathfrak{b}) := -\int_0^{d_\pi} \mathrm{tr} \int_{\mathfrak{b}} \mathfrak{p}^{inn} \, \mathrm{d}x \, \mathrm{d}\tau,$$

where $\mathfrak{p}^{inn}$ is the one in Eq. (34).

We also introduce a scalar

$$\mathfrak{r}(\tau, x) := \int_{\mathfrak{e}(x)} \theta(\tau, x; y) \hat{\mathfrak{r}}(c; B(x)) \, \mathrm{d}y$$

and a $3D$ vector

$$\mathfrak{q}(\tau, x) := \int_{\partial\mathfrak{e}(x)} \theta(\tau, x; y) \hat{\mathfrak{s}}(c, \nabla_y c; B(x)) \, \mathrm{d}\mathcal{H}^2(y),$$

where ∇_y indicates the gradient with respect to y within the window $\mathfrak{e}(x)$; $\hat{\mathfrak{r}}$ and $\hat{\mathfrak{s}}$ indicate formally heat sources and fluxes densities in $\mathfrak{e}(x)$.

We call *neat heat gained* by $\mathfrak{b}$ in a process π the functional

$$\mathcal{Q}(\pi, \mathfrak{b}) := \int_0^{d_\pi} \left(\int_{\mathfrak{b}} \mathfrak{r}(\tau, x) \, \mathrm{d}x + \int_{\partial\mathfrak{b}} \mathfrak{q}(\tau, x) \cdot n \, \mathrm{d}\mathcal{H}^2(x) \right) \mathrm{d}\tau.$$

Consider the space of cyclic processes Π^{cycl} in Π. With respect to them, we can accept two versions of *the first law of thermodynamics* (see Šilhavy, 1997). The first version states that *for every cyclic process and every body part* $\mathfrak{b}$

$$\mathcal{Q}(\pi, \mathfrak{b}) = 0 \Longrightarrow \mathfrak{w}(\pi_g, x) = 0.$$

The second version states, instead, that *for every cyclic process and every body part* $\mathfrak{b}$

$$\mathfrak{w}(\pi, \mathfrak{b}) > 0 \Leftrightarrow \mathcal{Q}(\pi, \mathfrak{b}) > 0.$$

Definition 3. $\mathfrak{e}(x)$ admits *Joule's relation* with proportionality coefficient $\mathrm{J} \in \mathbb{R}$ if for every cyclic process and every body part $\mathfrak{b}$

$$\mathfrak{w}(\pi, \mathfrak{b}) = \mathrm{J}\mathcal{Q}(\pi, \mathfrak{b}).$$

We call each $(\mathfrak{w}, \mathcal{Q}) : \Pi^{cycl} \times \mathcal{B} \longrightarrow \mathbb{R}$ a *cyclic work-heat pair*. $\mathbb{CP}(\mathcal{B})$ is the *space of all such pairs pertaining to* $\mathcal{B}$. Let $\mathcal{U}$ a class of bodies like $\mathcal{B}$: a pertinent universe.

Axioms for $\mathbb{CP}(\mathcal{U})$ (Šilhavy, 1997, Chapter 5):

1 If $(\mathfrak{w}_1, \mathcal{Q}_1)$ and $(\mathfrak{w}_2, \mathcal{Q}_2)$ are cyclic work-heat pairs, their composition, namely the pair $(\mathfrak{w}_1 + \mathfrak{w}_2, \mathcal{Q}_1 + \mathcal{Q}_2)$ belongs to $\mathbb{CP}(\mathcal{U})$.
2 $\mathbb{CP}(\mathcal{U})$ contains elements $(\mathfrak{w}^+, \mathcal{Q}^+)$ and $(\mathfrak{w}^-, \mathcal{Q}^-)$ such that $\mathcal{Q}^+ > 0$ and $\mathcal{Q}^- < 0$.
3 $\mathbb{CP}(\mathcal{U})$ contains elements $(\mathfrak{w}^+, \mathcal{Q}^+)$ and $(\mathfrak{w}^-, \mathcal{Q}^-)$ such that $\mathcal{Q}^+ > 0$, $\mathcal{Q}^- < 0$ and $\alpha(\mathfrak{w}^+, \mathcal{Q}^+)$, $\alpha(\mathfrak{w}^-, \mathcal{Q}^-)$ are in $\mathbb{CP}(\mathcal{U})$ for every $\alpha \in (0, 1]$.

The first assumption states that work and heat gained are additive over processes. The second assumption prescribes the possibility of gaining or loosing heat along a process. The last one admits the existence of homogeneous processes.

Proposition 3 (*Šilhavy, 1997, Chapter 5*). *If $\mathcal{B}$ is such that the pertinent space of cyclic work-heat pairs satisfies assumptions 1 and 3 above, the first law first version is satisfied if and only if Joule's relation hold. Moreover, when assumptions 1 and 2 hold true, the first law second version is satisfied if and only if Joule's relation holds with* $\mathrm{J} > 0$.

11.3. Heat gained

Since $\mathcal{Q}$ involves an integral on the time interval of every process, it is additive over prolongations of processes. Also, if it is continuous over $\bar{\Sigma}$, it is per se an *action* in the sense of the dynamical-system-based foundational analysis of thermodynamics by Coleman and Owen (1974).

Proposition 4. *Assume that for every $\mathfrak{b} \subseteq \mathcal{B}$ there is an accessible state $\bar{\varsigma} \in \bar{\Sigma}$ from any other state $\varsigma \in \bar{\Sigma}$ in a way such that $\mathcal{Q}(\pi, \mathfrak{b}) \geq 0$ for every process π such that $\pi(0) = \varsigma$ and $\pi(d_\pi) = \bar{\varsigma}$. Then, for every cyclic process π^{cycl} at ς,*

$$\mathcal{Q}(\pi^{cycl}, \mathfrak{b}) \geq 0.$$

Proof. Let $\Pi_{\varsigma,\bar{\varsigma}}$ the set of processes connecting ς with $\bar{\varsigma}$. Take those constituted by an initial cycle different from the identity (namely the process $\pi(\tau, x) = \varsigma(0, x)$ for every τ) and followed by a state transformation ending at $\bar{\varsigma}$, namely a process $\bar{\pi} = \pi \circ \pi^{cycl}$, with π a process connecting ς with $\bar{\varsigma}$. Write $\Pi_{\varsigma,cycl,\bar{\varsigma}}$ for the set of type-$\bar{\pi}$ processes and $\Pi_{\varsigma,cycl}$ for the set of cyclic processes at ς. Clearly, $\Pi_{\varsigma,cycl,\bar{\varsigma}} \subset \Pi_{\varsigma,\bar{\varsigma}}$. Thus,

$$\inf_{\pi \in \Pi_{\varsigma,\bar{\varsigma}}} \mathcal{Q}(\pi, \mathfrak{b}) \leq \inf_{\bar{\pi} \in \Pi_{\varsigma,cycl,\bar{\varsigma}}} \mathcal{Q}(\bar{\pi}, \mathfrak{b}).$$

Since $\mathcal{Q}$ is additive over processes, we have

$$\inf_{\bar{\pi} \in \Pi_{\varsigma,cycl,\bar{\varsigma}}} \mathcal{Q}(\bar{\pi}, \mathfrak{b}) = \inf_{\pi^{cycl} \in \Pi_{\varsigma,cycl}} \mathcal{Q}(\pi^{cycl}, \mathfrak{b}) + \inf_{\pi \in \Pi_{\varsigma,\bar{\varsigma}}} \mathcal{Q}(\pi, \mathfrak{b}),$$

which proves the statement. ■

11.4. Heating measure and empirical temperature field

We distinguish between empirical and absolute temperature (Šilhavy, 1997).

We presume that $\mathbb{I} \subset \mathbb{R}$, an open set, is the range of *empirical temperature* field ϕ assumed to be continuous and differentiable over $\mathcal{B} \times \hat{I}$, with $\hat{I}$ a time interval to be specified. Every value $\phi(\tau, x)$ is interpreted as an average of local temperatures within $\mathfrak{e}(x)$ at time τ of effects due to the fluctuations c; such effects are summarized below into local source and flux of heat.

Let $\mathbb{B}(\mathbb{I})$ be the collection of Borel subsets of $\mathbb{I}$. Consider a signed Borel measure $\mathrm{Q} : \mathbb{B}(\mathbb{I}) \longrightarrow \mathbb{R}$. Then, Q admits positive and negative variations, namely $\mathrm{Q}^{\pm}(S) := \sup\{\pm\mathrm{Q}(E) \mid E \in \mathbb{B}(\mathbb{I}),\ E \subset S\}$, with S a measurable set in $\mathbb{I}$. Both Q^+ and Q^- are measures and, by Jordan decomposition (see Dobb, 1994, Chapter 9), $\mathrm{Q} = \mathrm{Q}^+ - \mathrm{Q}^-$, while the sum $\mathrm{Q}^+ + \mathrm{Q}^-$ defines the total variation $|\mathrm{Q}|$ of Q. Moreover, if $\mathrm{Q} = \lambda_1 - \lambda_2$ is a representation of Q as the difference between two measures, the inequalities $\mathrm{Q}^+ \leq \lambda_1$ and $\mathrm{Q}^- \leq \lambda_2$ hold true. For any Q, we call the support of Q, indicating it by $\mathrm{supp}\mathrm{Q}$, the smallest relatively closed subset of $\mathbb{I}$ such that $\mathrm{Q}(\bar{S}) = 0$ for any $\bar{S} \in \mathbb{B}(\mathbb{I})$ such that $\bar{S} \cap \mathrm{supp}\mathrm{Q} = \emptyset$.

A property of signed measures apply (see Dobb, 1994):

Proposition 5. *If* Q *and* Q′ *are such measures over $\mathfrak{I}$, there is a signed measure* Q∨Q′ *majorizing* Q *and* Q′ *and every other measure majorant of* Q *and* Q′.

Given $S \in \mathbb{B}(\mathbb{I})$, we write $\mathfrak{b}^S_{\hat{I}}$ for the set of pairs (τ, x), with $\tau \in \hat{I}$, $x \in \mathfrak{b}$, such that $\phi(\tau, x) \in S$. We also write $\partial\mathfrak{b}^S_{\hat{I}}$ for the analogous set of pairs evaluated on $\partial\mathfrak{b}$.

In this setting we call $\mathrm{Q}(\pi, \mathfrak{b}; \cdot)$ a *heating measure* (writing often shortly $\mathrm{Q}(\pi, \mathfrak{b})$ or $\mathrm{Q}(S)$ for it) when, with $S \in \mathbb{B}(\mathbb{I})$,

$$\mathrm{Q}(\pi, \mathfrak{b}; S) = \int_{\mathfrak{b}^S_{\hat{I}}} \mathfrak{r}(\tau, x) \, \mathrm{d}x \, \mathrm{d}\tau - \int_{\partial\mathfrak{b}^S_{\hat{I}}} \mathfrak{q}(\tau, x) \cdot n \, \mathrm{d}\mathcal{H}^2(x) \, \mathrm{d}\tau. \tag{42}$$

By the definition $\mathrm{Q}(\pi, \mathfrak{b})$ is additive on the continuation of processes and the union of disjoint parts. The real values

$$\mathrm{Q}^+(\mathbb{I}) = \mathcal{Q}^+(\pi, \mathfrak{b})$$

and

$$\mathrm{Q}^-(\mathbb{I}) = \mathcal{Q}^-(\pi, \mathfrak{b})$$

measure, respectively, *heat absorbed* and *heat emitted* by $\mathfrak{b}$ along π.

According to Šilhavy (1997), if $\mathrm{supp}\mathrm{Q}^{\pm}$ are two not empty and compact sets, we refer to the number

$$\phi^+ = \max \mathrm{supp}\mathrm{Q}^+$$

as the *maximum empirical temperature at which heat is absorbed*, and to the number

$$\phi^- = \min \mathrm{supp}\mathrm{Q}^-$$

as the *minimum empirical temperature at which heat is emitted*.

Let $\mathbb{M}(\mathbb{I})$ be the set of all Borel measures over $\mathbb{I}$. Not all its elements are of the form (42). Be $\mathbb{D}(\mathcal{B})$ the set of Q-type (according to (42)) measures over $\mathcal{B}$. When $\mathrm{Q}(\pi, \mathcal{B})$ and $-\mathrm{Q}(\pi, \mathcal{B})$ belong both to $\mathbb{D}(\mathcal{B})$, we say that $\mathcal{B}$ behaves reversibly along the process π, otherwise the behavior is irreversible along the same process.

The functionals $\mathfrak{w}$ and $\mathcal{Q}$ enter two possible expressions of the second law. Carnot's statement reads that, for every cyclic process π and every part $\mathfrak{b}$,

$$\mathfrak{w} > 0 \quad \Longrightarrow \quad \mathcal{Q}^- > 0.$$

Kelvin's statement reads that, for every cyclic process π and every part $\mathfrak{b}$,

$$\mathfrak{w} > 0 \quad \Longrightarrow \quad \mathrm{supp}\mathrm{Q} \text{ contains at least two temperatures.}$$

Both statements imply the existence of a smooth function $\tilde{\vartheta} : \mathbb{I} \longrightarrow \mathbb{R}^{++}$, with values ϑ, such that for every cyclic process π^{cycl}

$$\oint \frac{\mathrm{dQ}(\pi^{cycl}, \mathfrak{b})}{\vartheta} \geq 0.$$

In this case we say that $\mathfrak{b}$ satisfies the Clausius inequality with the absolute temperature scale $\tilde{\vartheta}$.

Carnot's and Kelvin's statements of the second law are equivalent if and only if the Clausius inequality holds for any cyclic process π^{cycl} and some universal temperature scale $\vartheta := \tilde{\vartheta}(\tau, x)$. In addition, when ϑ exists, it is unique to within a constant positive multiple (see also Šilhavy, 1997, Chapter 7, Prop. 7.5.2). In this way the absolute temperature ϑ appears as a state function of the empirical temperature ϕ.

Remark 11. In the definition of work density we use the trace of inner power, which includes Z, the self-action appearing in the fluctuation energy balance. That equation, however, governs the evolution of H, a tensor defined by c. On the other side, itself c determines $\mathcal{Q}(\pi, \mathfrak{b})$. Then, previous analyses underline implicitly that the balance of interactions associated with fluctuations described by H is the equation transferring mechanical effects into thermal processes.

By indicating by $\hat{\delta}$ the standard variation operator with respect to space, we link $\hat{\delta}\mathrm{Q}$ with the entropy density η, a differentiable real-valued state function, by the relation

$$\frac{\hat{\delta}\mathrm{Q}}{\vartheta} \leq \overset{\circ}{\eta} + \sigma\eta,$$

so that we get the pointwise inequality

$$\overset{\circ}{\eta} + \sigma\eta \geq \frac{\mathfrak{r}}{\vartheta} - \mathrm{div}\frac{\mathfrak{q}}{\vartheta}. \tag{43}$$

Although ϑ has been justified through ϕ in terms of fluctuations, namely those described by c and its gradient with respect to y, it enters the inequality above, which involve gross fields, defined by making averages over a window $\mathfrak{e}(x)$. Their knowledge does not allow a direct evaluation of how ϑ varies in time. To this aim we need a field-based first principle.

A form of such a principle has been introduced in Capriz and Mariano (2020) not accounting for the balance (33), while presuming that H is of the form χI, with χ a scalar depending on space and time, assumed to be differentiable with respect to τ and x, I the unit tensor.

At variance, here we maintain consideration of the balance (33) and presume the existence of a differentiable state function $e(\cdot)$ such that

$$\overset{\circ}{e} + \sigma e = \mathfrak{r} - \mathrm{div}\mathfrak{q} + \mathrm{tr}(\mathfrak{p}^{inn}). \tag{44}$$

In all cases, e depends on ϑ beyond other state variables included in the list s, based on how the molecules interact. We do not specify s, rather we focus attention on $\mathfrak{r}$ and $\mathfrak{q}$.

Both relations (43) and (44) are expressed here in Eulerian form. They are non-standard, indeed.

11.5. The local Clausius–Duhem inequality in Eulerian form

Since $\overset{\circ}{\eta} = \dot{\eta} - \sigma\eta$, $\overset{\circ}{e} = \dot{e} - \sigma e$, and

$$\mathrm{tr}\mathfrak{p}^{inn} = T \cdot \nabla v + A \cdot B + \nabla B \cdot \mathbf{m} + \frac{1}{2}\mathrm{tr}Z,$$

by introducing the free energy density $\psi = e - \vartheta\eta$, and combining the relations (43) and (44), we get a local version of the Clausius–Duhem inequality given by

$$\dot{\psi} + \dot{\vartheta}\eta - T \cdot \nabla v - A \cdot B - \nabla B \cdot \mathbf{m} - \frac{1}{2}\mathrm{tr}Z + \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta \leq 0, \tag{45}$$

an inequality presumed to hold for every choice of the time rates involved and their gradients (recall that B is also a time rate).

The bulk density $\dot{\vartheta}\eta - T \cdot \nabla v - A \cdot B - \nabla B \cdot \mathbf{m} - \frac{1}{2}\mathrm{tr}Z + \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta$ has counterpart over the comparison space $\bar{\mathbb{R}}^3$ given by

$$(\det F)(\dot{\vartheta}\eta - T \cdot \nabla v - A \cdot B - \nabla B \cdot \mathbf{m} - \frac{1}{2}\mathrm{tr}Z + \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta).$$

Thus, in that space, a counterpart of the inequality (45) reads

$$\dot{\psi}_R + (\det F)(\dot{\vartheta}\eta - T \cdot \nabla v - A \cdot B - \nabla B \cdot \mathbf{m} - \frac{1}{2}\mathrm{tr}Z + \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta),$$

where $\psi_R = (\det F)\psi$.

We assume that ψ_R, T, $\mathbf{m}$, A, Z, η depend all on the list $(F, G, \nabla_{x_*} G, \vartheta)$. By computing the time derivative of ψ_R, we thus get

$$\begin{aligned} &\left(\frac{1}{\det F}\frac{\partial\psi_R}{\partial G}G^\top + \frac{1}{\det F}\frac{\partial\psi_R}{\partial\nabla_{x_*}G}(\nabla_{x_*}G)^\top - A \right) \cdot B \\ &\quad + \left(\frac{1}{\det F}\frac{\partial\psi_R}{\partial F}F^\top - T \right) \cdot \nabla v \\ &\quad + \left(\frac{1}{\det F}\frac{\partial\psi_R}{\partial\nabla_{x_*}G}F^\top G^\top - \mathbf{m} \right) \cdot \nabla B \\ &\quad + \left(\frac{1}{\det F}\frac{\partial\psi_R}{\partial\vartheta} + \eta \right) - \frac{1}{2}\mathrm{tr}Z + \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta \leq 0. \end{aligned} \tag{46}$$

The assumed validity of the inequality for any (independent) choice of ∇v, B, and ∇B implies the identities

$$T = \frac{1}{\det F}\frac{\partial\psi_R}{\partial F}F^\top, \tag{47}$$

$$A = \frac{1}{\det F}\frac{\partial\psi_R}{\partial G}G^\top + \frac{1}{\det F}\frac{\partial\psi_R}{\partial\nabla_{x_*}G}(\nabla_{x_*}G)^\top, \tag{48}$$

$$\mathbf{m} = \frac{1}{\det F}\frac{\partial\psi_R}{\partial\nabla_{x_*}G}F^\top G^\top, \tag{49}$$

$$\eta = -\frac{1}{\det F}\frac{\partial\psi_R}{\partial\vartheta} \tag{50}$$

and the reduced dissipation inequality

$$\frac{1}{2}\mathrm{tr}Z - \frac{1}{\vartheta}\mathfrak{q} \cdot \nabla\vartheta \geq 0. \tag{51}$$

In terms of components, Eqs. (47), (48), (49) read

$$T^{ij} = \frac{1}{\det F}\left(\frac{\partial\psi_R}{\partial F}\right)^{iK}(F^\top)^{Kj},$$

$$A^{ij} = \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial G}\right)^{iK}(G^\top)^{Kj} + \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial \nabla_{x_*} G}\right)^{iKH}((\nabla_{x_*} G)^\top)^{HKj},$$

$$\mathbf{m}^{ikj} = \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial \nabla_{x_*} G}\right)^{iKH}(F^\top)^{Hk}(G^\top)^{Kj},$$

where capital indices indicate coordinates in the reference space $\hat{\mathbb{R}}^3$, while the lowercase ones refer to the physical space $\mathbb{R}^3$, and summation over repeated indices is adopted, as usual.

When we refer not to orthonormal frames of references, a few changes affect Eqs. (47), (48), (49): the adjoint operators substitute the transpose, so the derivative D_{x_*} substitutes $\nabla_{x_*} = D_{x_*}\hat{g}^{-1}$, with $\hat{g}$ the metric over $\hat{\mathbb{R}}^3$; so we distinguish between contravariant and covariant components. Eventually, we have

$$T_i{}^j = \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial F}\right)_i^K (F^*)_K{}^j,$$

$$A_i{}^j = \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial G}\right)_i^K (G^*)_K{}^j + \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial D_{x_*} G}\right)_i^{KH}((D_{x_*} G)^*)_{HK}{}^j,$$

$$\mathbf{m}_i{}^{j\ell} = \frac{1}{\det F}\left(\frac{\partial \psi_R}{\partial D_{x_*} G}\right)_i^{KH}(F^*)_H{}^j(G^*)_K{}^\ell,$$

with the relation (50) remaining invariant.

The reduced dissipation inequality (51) is compatible with a decomposition of the heat flux of the type

$$\mathfrak{q} = -\kappa\nabla\vartheta + \bar{\mathfrak{q}}. \tag{52}$$

The flux $\bar{\mathfrak{q}}$ is a perturbation of the Fourier component $\kappa\nabla\vartheta$ possibly induced by Z, that is by the fluctuations measured by H, so that we might presume

$$\bar{\mathfrak{q}} = \bar{\kappa}\nabla \mathrm{tr} H, \tag{53}$$

with $\bar{\kappa}$ a positive constant, leaving to the balance (33) a role analogous to the one kept by the Guyer–Krumhansl equation (Guyer and Krumhansl, 1966a,b) in several non-Fourier schemes adopted to avoid Fourier's paradox (see the treatise (Straughan, 2011)), that is the foreseen instantaneous propagation of temperature variations. More generally than the circumstances discussed here, we can say that the recorded finite speed temperature propagation in condensed matter is due to microstructural effects, as shown from two different viewpoints in Mariano (2017), Capriz et al. (2021), Mariano and Spadini (2022), and in general complex fluids in Mariano (2023).

Besides the specific choice (53), we could presume, for example,

$$\bar{\mathfrak{q}} = \ell(\vartheta, \nabla\vartheta), \tag{54}$$

with ℓ a vector-valued differentiable function. In this case, when also the thermal conductivity κ is constant, Eq. (44) reduces to

$$\hat{\mathfrak{c}}\dot{\vartheta} + \kappa\Delta\vartheta - \frac{\partial \ell}{\partial \nabla\vartheta}(\nabla\dot{\vartheta} - \nabla\vartheta\nabla v) = \mathfrak{r} + \mathrm{tr}(\mathfrak{p}^{inn}) - \mathfrak{k}, \tag{55}$$

where

$$\hat{\mathfrak{c}} := \frac{\partial e}{\partial \vartheta} - \frac{\partial \ell}{\partial \vartheta},$$

and

$$\mathfrak{k} := \frac{\partial e}{\partial F}\cdot\dot{F} + \frac{\partial e}{\partial G}\cdot\dot{G}\frac{\partial e}{\partial \nabla_{x_*} G}\cdot\dot{\nabla_{x_*} G} = \frac{\partial e}{\partial F}\cdot\dot{F} + \frac{\partial e}{\partial G}\cdot\dot{G}\frac{\partial e}{\partial \nabla_{x_*} G}\cdot\nabla_{x_*}\dot{G}.$$

12. Additional remarks

The scheme discussed here applies to various specific cases ranging from the dynamics of granular matter to the molecular transport in biological tissues.

For granular matter, in the present scheme each grain is represented only by its mass center. Beyond shuffling and/or expansion, tensor B accounts for spin of the entire cluster of grains in the window $\mathfrak{e}(x)$ rather than the spin of each single grain. For this last effect we need to add structure to each molecule. Specifically, beyond the velocity w of its mass center, we should consider a grain spin ϖ, which would involve appropriate balances of couples including averages of those performing power over ϖ. In this case, the distribution function Θ should depend on ϖ, namely we would have $\Theta(\tau, x; y, w, \varpi)$. Average over the vector space would produce at y a local averaged spin ϖ_* analogous to w_*. Then, further average of ϖ_* over $\mathfrak{e}(x)$ would produce a spin additional to the orthogonal factor entering the polar decomposition of B, which would affect the balance of moment of momentum together with pertinent actions. Also, we could account for fluctuations of the spin field, possibly decomposing them as we have done for w_*. Another possibility would be to consider other types of properties pertaining to each molecule, such as a freedom of having its own independent strain or suffering polarization, with the possibility of developing analogous pertinent analyses and re-interpretations of the Cauchy–Born rule. All these aspects, however, would require a work going beyond the limits of this specific paper.

We have already highlighted the awareness that our approach is useful for the description of particulate matter as the granular one. It applies also to phenomena involving biological matter; indeed, a simplified version of this approach, still based on Cauchy–Born's rule interpreted in terms of velocities (as we adopted here), has proven effective for the analysis of single protein translocation through biological tissues (Bacci and Mariano, 2021) and in modeling the mechanics of protein complexes (Mariano and Bacci, 2022).

CRediT authorship contribution statement

Paolo Maria Mariano: Conceptualization, Formal analysis, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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