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Research article

From point particles to body points†

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Abstract: Given a spacetime background against which to observe it, a material system in motion can be modeled discretely, as a collection of particles called 'point masses', or continuously, as a dense and deformable object (a *body*, in the language of continuum mechanics) occupying a region consisting of 'material points'. In that the discrete and continuous descriptions have a common conceptual framework, the scale gap can be got over, provided a coarsening procedure is devised. Here we restrict attention to kinematics, and consider four such bottom-up procedures, two statistical and two deterministic, to derive a macroscopic velocity field from a microscopic one. We show that, to do this, introducing space and time *mesoscopic* scales is of the essence. We also show under what assumptions a macroscopic motion of the given material system can be associated with a microscopically-informed velocity field. Interestingly, no matter what coarsening procedure one chooses, the points of the resulting continuous description of the system's motion carry intrinsic physical information and may be persistently labelled: we propose to call them *body points*.

Keywords: point mass; material point; discrete mechanics; continuum mechanics; statistical coarsening; deterministic coarsening

1. Introduction

Although the detailed analysis that is in principle possible in particle mechanics (PM) would be at times unpractical or of little use for many applications, to come up with a microscopically-informed continuum mechanics (CM) formulation of an evolutionary problem would be important in a number of circumstances. However, passing from a microscopic description in terms of *mass points* to a

macroscopic, but somehow and to some extent microscopically informed, description in terms of *material points* requires nontrivial changes of mathematical and thermodynamical formats which, whenever effective and of substantial reach, are necessarily intertwined. As to mathematical formats, a change is needed from a system of ordinary differential equations for the current positional parameters of all mass points in the collection at hand, to a system of partial differential equations for the pointwise evolution of mass density, shape and volume of the material region corresponding to the given mass-point collection. As to changes in thermodynamical formats, an issue which demands paramount attention is matching the intrinsic reversibility of PM processes studied within a Hamiltonian framework with the inherent dissipative nature of CM processes, where energy conservation is not a fundamental principle but, at best, a convenient approximation. Moreover, it is by no means clear what microscopic notion of entropy, if any, would lead to a form of CM entropy imbalance.

It is because of the many differences in format of PM and CM that coming up with a convincing scale-bridging procedure is such a demanding intellectual challenge. In the first place, it seems to us important to deal with a language issue. A notion of point is encountered and regarded as primitive in a number of formalized disciplines. As a rule, the introduction of points is accompanied by an adjectival specification of their role or of their peculiar character (see Sections A.1, A.2 of the Appendix). Within old and well-established disciplines like standard CM and classical PM, talking about, respectively, material points and point masses is an almost universal outcome of habit. However, it seems to us that the truly primitive notion of CM is rather that of *body* than that of *point*. Hence, we prefer to talk about *body points* rather than about material points. And, we draw *point particles* alongside body points because, in our opinion, 'point particle' does a better job than 'point mass' to capture the true peculiar character of the typical object of PM.

The purpose of this note is to discuss *how the CM notion of body point should be interpreted in terms of the PM notion of point particle*. While different, both notions are the result of similar modeling abstractions. The latter has a more transparent intuitive content and a lighter mathematical apparatus; for these reasons, it is often taken as a convenient springboard for cheap introductions to the former. Clean direct introductions to CM are available, where however generally the deep and tight relationships between the continuum and discrete models of physical reality are not discussed. This state of affairs needs to be overcome, any time some information transfer from PM to CM is attempted by way of a coarse-graining procedure.

We read in the introductory remarks of an authoritative treatise [1, p. 11] a statement having the form of an undisputed truth of reason:

> the macroscopic conservation laws of matter, momentum and energy are, from a microscopic point of view, consequences of the mechanical laws governing the motions of the constituent particles of the system.

Accordingly, those macroscopic conservation laws hold at body points as consequences of microscopic laws holding for point particles. Given our present purpose of interpreting body points in terms of point particles, we can restrict our discussion of the available bottom-up procedures to the necessarily preliminary issues of *consistency between discrete and continuum kinematics*. As we shall see, even in such a restricted context the resolution of those consistency issues is not achievable by means of purely kinematical arguments: also certain discrete and continuum accounts of the nature of the body at hand

play a role. In this connection, we find it appropriate to quote a few passages from a 1936 paper by Einstein [2], where he deals with foundational issues, beginning with this one on p. 350:

> I believe that the first step in the setting of a "real external world" is the formation of the concept of bodily objects and of bodily objects of various kinds . . . [a concept owing] its meaning and its justification exclusively to the totality of the sense impressions which we associate with it.

In fact, for Einstein, the early foundations of mechanics were laid by posing first the

> [c]oncept of a material point:* a bodily object which—as regards its position and motion—can be described with sufficient exactness as a point with coordinates X_1, X_2, X_3[, its motion being described] by giving X_1, X_2, X_3, as functions of the time. (p. 358)

And he insists that

> [t]he notion "material point" is fundamental for mechanics. If now we seek the mechanics of a bodily object which itself can not be treated as a material point—and strictly speaking every object "perceptible to our senses" is of this category—then the question arises: *How shall we imagine the object to be built up out of material points* [our italics], and what forces must we assume as acting between them? The formulation of this question is indispensable, if mechanics is to pretend to describe the object *completely*. (p. 360)

We maintain that even a single CM body point is "a bodily object which itself can not be treated as a material point." On paraphrasing Einstein modulo a change in space scale and terminology, in this paper we try and give an answer to a question—*How shall we imagine a body point to be built up out of PM point particles?*—that would seem to be at odds with his view of CM as a collection of theories, such as hydrodynamics and elasticity, "belong[ing] to the so-called "phenomenological" physics." To him, those theories

> avoid the consideration of a subdivision of matter down to "real" material points . . . by fictions which, in the light of the foundation of classical mechanics, can only have an approximate significance . . . [Although, i]n addition to their great *practical* significance, these categories of science have . . . created those formal auxiliary instruments (partial differential equations) which have been necessary for the subsequent attempts at formulating the total scheme of physics in a manner which is new as compared with that of Newton. (p. 361)

'Subdivisions' of body points into point particles are at least implicitly accepted truths of fact at the outset of all bottom-up scale-bridging procedures, including the four ones we hereafter consider—two probabilistic in nature and two deterministic. In all of them, 'gross' kinematic descriptors of mass and motion are defined in terms of corresponding 'fine' descriptors by way of some sort of averaging. What is in question is the physical interpretation of the space-like variable $\boldsymbol{x}$ on which the spacetime fields for CM mass density and velocity we arrive at depend. For us, in all four cases, that variable is to be understood as the place occupied at the present time t by the body point associated with a set of point particles which is in the need of case-by-case specification. That set consists of all particles

*By 'material point' Einstein means exactly what we call here 'point particle.'

in the system when the averaging procedure is statistical: only velocities count for the *Boltzmann coarsening* dealt with in Section 2.1, while (position, velocity) pairs count for the *Irving & Kirkwood coarsening* in Section 2.2. Position and velocity of a large number of particles also count for any of the deterministic coarsenings discussed in Sections 3.1 (via *localization functions*) and 3.2 (via *cell averaging*), because those deterministic procedures both propound averages over specks of matter being macroscopically small, although microscopically large, and occupying current neighborhoods of a prospective body point $\boldsymbol{x}$. The crop of Sections 2 and 3 is a set of four microscopically informed velocity fields, of the form $\mathbf{v} = \mathbf{v}(\boldsymbol{x}, t)$, over the open space region $\mathscr{B}_t$ where the point particles reside at time t. In Section 4.1 we briefly recall those basic notions of CM kinematics that are needed to show, in Section 4.2, how to make use of the information embodied in any of the mentioned velocity fields to construct the microscopically informed CM motion that takes pointwise onto $\mathscr{B}_t$ the region $\mathscr{B}_{t_0}$ where the point particles resided at some previous time t_0. This we achieve by the use of a well-known result about the solvability for the motion $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t)$ of the $\boldsymbol{X}$-family of initial-value Cauchy problems

$$\dot{\boldsymbol{\chi}}(\boldsymbol{X}, t) = \mathbf{v}(\boldsymbol{\chi}(\boldsymbol{X}, t), t), \qquad \boldsymbol{\chi}(\boldsymbol{X}, t_0) = \boldsymbol{X} \in \mathscr{B}_{t_0},$$

provided the field $\mathbf{v}$ is conveniently spacetime smooth in a spacetime neighborhood of $\mathscr{B}_{t_0} \times \{t_0\}$. The unique (local-in-time) solution is the motion $\boldsymbol{\chi}$ of the given material system when modeled as a continuous body in a microscopically informed manner, microscopic information being carried over by the field $\mathbf{v}$ according to the chosen coarsening method. We associate each space point $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t)$ in $\mathscr{B}_t = \boldsymbol{\chi}(\mathscr{B}_{t_0}, t)$ to a body point, persistently identified in a time interval $\mathcal{I}_{t_0}$ by the label $\boldsymbol{X}$ it gets in the configuration $\boldsymbol{\chi}(\cdot, t_0)$ (cf. also the discussion in Section A.3). We find it appropriate to anticipate, here from Section 5, our main conclusion: *the notion of body point we propose has a contingent, system-dependent physical content, the filtrate resulting from the adopted coarsening procedure.*

2. Statistical coarse-graining

The purpose of applying any coarse-graining procedure to PM is to arrive at one or more CM fields $\Psi = \widehat{\Psi}(\boldsymbol{x}, t)$, each furnishing some macroscopic mechanical information to be attached to the body point placed at $\boldsymbol{x}$ at instant t, the microscopic counterpart of that information being carried at the same instant by the collection of point particles involved into the individuation of that body point. When the procedure is statistical, that collection is the totality of point particles in the system associated with the continuous body at hand. Coarse-graining is achieved by averaging the relevant microscopic information carried by a field $\widehat{\psi}$, with the use of a time-dependent measure $d\mu$ that is absolutely continuous with respect to the relevant kinetic measure $d\kappa$:

$$d\mu = f\, d\kappa.$$

Precisely, as we shall see in the subsection to come,

$$\widehat{\Psi}_B(\boldsymbol{x}, t) := \int \widehat{\psi}_B(\boldsymbol{x}, \mathbf{c}, t)\, d\mu_B, \quad d\mu_B = f_B(\boldsymbol{x}, \mathbf{c}, t)\, d\mathbf{c}, \tag{2.1}$$

in case of Boltzmann coarsening, where particle velocity—the only relevant microscopic coordinate—is customarily denoted by $\mathbf{c}$ and where f_B is the number-density distribution which solves Boltzmann

equation. And, in case of the Irving & Kirkwood coarsening dealt with in Section 2.2,

$$\widehat{\Psi}_{IK}(\boldsymbol{x},t) \coloneqq \int \widehat{\psi}_{IK}(\boldsymbol{x},z)\, d\mu_{IK}\,, \quad d\mu_{IK} = f_{IK}(z,t)\, dz, \tag{2.2}$$

where z denotes a point of the state space and f_{IK} a probability distribution.*

As anticipated in the Introduction, both Sections 2.1 and 2.2 close with the explicit construction of a CM velocity field over the space region currently occupied by the continuous body associated with the particle system under study: a rarified gaseous body in the former case, a body whose aggregation state remains to be determined in the latter. We shall see in Section 4 how to make use of the information embodied in these velocity fields—in fact, in any velocity field—to arrive at an account of the corresponding CM motion.

2.1. The Boltzmann way to the CM notion of rarefied gas

In the discrete picture envisaged first by D. Bernoulli [3] in 1738, enriched by Clausius [4] in 1858 by the notion of mean free path, and for which Boltzmann [5] proposed a statistical description in 1872, a class of gaseous bodies of interest consists of a very large but finite, constant number N of particles in a container of volume V, of identical mass m, having no internal degree of freedom, and whose only relevant interactions are mutual collisions.

In the first instance, particles may be visualized as hard spheres of diameter d, whose number density N/V and separation $(V/N)^{1/3}$ with respect to their container are, respectively, very small (in the sense that $(N/V)\, d^3 \ll 1$) and large enough that these particles can be regarded as Newtonian (because, at temperatures T of interest, their separation is much larger than the de Broglie wavelength: $\hbar\,(2mk_BT)^{-1/2} \ll (V/N)^{1/3}$, where $\hbar$ is Planck's constant and k_B is Boltzmann's; see [6, p. 52]. For v the average speed of particles, the collision rate—that is, the number of collisions experienced by a particle per unit time—is of the order of $w = (N/V)\, d^2 v$; $\tau = 1/w$ is the flight time of a particle, i. e., the time lapse between two collisions; τv is a particle's mean free path.†

In fact, Boltzmann equation is laid down under the drastic modeling assumption that particles are so small that it makes sense not only to regard them as punctiform but also to think of two of them as occupying one and the same place $\boldsymbol{x}$ at the instant t when a collision occurs. Collisions are supposed to entail no instantaneous positional discontinuities, only velocity jumps; accordingly, for $t \mapsto \boldsymbol{x}(t)$ the piecewise rectilinear trajectory leading a particle to a collision at time t_c, it is assumed that $\boldsymbol{x}(t_c - 0) = \boldsymbol{x}(t_c + 0)$; the pre- and post-collision velocities of that particle are denoted by $\mathbf{c} = \dot{\boldsymbol{x}}(t_c - 0)$ and $\mathbf{c}' = \dot{\boldsymbol{x}}(t_c + 0)$, respectively; and it is assumed that both momentum and kinetic energy of two particles with pre-collision velocities $\mathbf{c}$ and $\mathbf{c}^1$ are conserved:

$$\mathbf{c} + \mathbf{c}^1 = \mathbf{c}' + \mathbf{c}^{1\prime},$$
$$|\mathbf{c}|^2 + |\mathbf{c}^1|^2 = |\mathbf{c}'|^2 + |\mathbf{c}^{1\prime}|^2.$$

*Note that both coarsening transformations (2.1) and (2.2) preserve tensorial order.

†Rarefaction increases while preserving a desired interparticle collision rate $w>0$ when it so happens that $(N/V)d^3 \to 0$ as $N \to \infty$ and $d \to 0$. This conditioned passage to the limit is known as *Grad's limit*; for the total mass of gas in the container not to vanish in such a limit, it is presumed that a particle's mass diverges as $1/d$. Were instead the collision rate let to vanish as $N \to \infty$ and $d \to 0$ (the case of *Knudsen's gas*), then the gas motion would be determined exclusively by collisions of particles with the container's walls (cf., e. g., [7, Section 7.1.1]). For a gentle introduction to collision formulas, see [8].

Boltzmann's *kinetic theory* is based on a postulated time evolution for the scalar-valued function $f_B = f_B(\boldsymbol{x}, \mathbf{c}, t)$, driven by the source term s_{f_B} and ruled by the equation

$$\partial_t f_B + \partial_{\boldsymbol{x}} f_B \cdot \mathbf{c} = s_{f_B}. \tag{2.3}$$

According to a standard interpretation (see, e. g., [9, Chapter 3], or [10, p. 23]), f_B delivers the number density of particles with velocity $\mathbf{c}$ to be found about $\boldsymbol{x}$ at time t: that is to say, $f_B(\boldsymbol{x}, \mathbf{c}, t)\, d\boldsymbol{x}\, d\mathbf{c}$ is the number of particles with velocities ranging from $\mathbf{c}$ to $\mathbf{c} + d\mathbf{c}$ to be found at time t in a volume element about $\boldsymbol{x}$. Were there no collisions, the same number of particles would be found in a volume element about $\boldsymbol{x} + \mathbf{c}\,\delta t$ at time $t + \delta t$; otherwise,

$$\big(f_B(\boldsymbol{x} + \mathbf{c}\,\delta t, \mathbf{c}, t + \delta t) - f_B(\boldsymbol{x}, \mathbf{c}, t)\big) d\boldsymbol{x}\, d\mathbf{c} \simeq s_{f_B}\, d\boldsymbol{x}\, d\mathbf{c}\, \delta t,$$

where the right side is "the net gain of molecules" [9] with velocities between $\mathbf{c}$ and $\mathbf{c} + d\mathbf{c}$ per volume element, in the considered time interval; granted smoothness, the above relation yields *Boltzmann equation* (2.3).* In that equation, the source term $s_{f_B} = s_{f_B}(\boldsymbol{x}, t, \mathbf{c})$ is the *collision integral*

$$s_{f_B} = \int (f'_B f^{1\prime}_B - f_B f^1_B)\, \widehat{w}(\mathbf{c}, \mathbf{c}^1; \mathbf{c}', \mathbf{c}^{1\prime})\, d\mathbf{c}^1 d\mathbf{c}' d\mathbf{c}^{1\prime} \tag{2.4}$$

(where $f'_B = f_B(\boldsymbol{x}, \mathbf{c}', t)$, $f^1_B = f_B(\boldsymbol{x}, \mathbf{c}^1, t)$, and $f^{1\prime}_B = f_B(\boldsymbol{x}, \mathbf{c}^{1\prime}, t)$), which accounts for the binary interactions of particle pairs having velocities $(\mathbf{c}, \mathbf{c}^1)$ before they collide at $(\boldsymbol{x}, t)$. Boltzmann's assumption about the number density of collisions—his *Stoßzahlansatz*—and its account in (2.4) reflect the crucial modeling approximation that in a rarefied gas individual particles perform statistically independent motions until they happen to collide. Then, since a collision involves the simultaneous occurrence of two statistically independent occupation events, it changes the product $f_B f^1_B$ into $(f_B f^1_B)' = f'_B f^{1\prime}_B$. Moreover, the effectiveness of a collision is measured by the scalar-valued mapping $\widehat{w}$, which is stipulated to be insensitive to both time reversal and particle exchange:

$$\widehat{w}(\mathbf{c}', \mathbf{c}^{1\prime}; \mathbf{c}, \mathbf{c}^1) = \widehat{w}(\mathbf{c}, \mathbf{c}^1; \mathbf{c}', \mathbf{c}^{1\prime}),$$
$$\widehat{w}(\mathbf{c}', \mathbf{c}^{1\prime}; \mathbf{c}, \mathbf{c}^1) = \widehat{w}(\mathbf{c}^{1\prime}, \mathbf{c}'; \mathbf{c}^1, \mathbf{c}).$$

The Boltzmann equation permits a coarse-graining of the prohibitive particle model of rarefied gaseous matter into a tractable continuous model. How this is doable has been demonstrated multiple times. On borrowing, e. g., the developments in Section 3.2 of [10], one can quickly show how with the use of (2.3) *equations of transfer* (or *of transport*) are deduced, having the form of partial differential equations which capture certain probabilistic consequences of the Newtonian equations of motion holding for systems of particles; such equations can be put in term-by-term correspondence with the CM *balance equations* of identical physical meaning. Quoting from [11, pp. 40–41]:

*Were particles subject also to an external force field $\mathbf{f}$ that would make them move, in the absence of collisions, according to Newton's prescriptions, their velocity would change by $\mathbf{f}\delta t$ in the considered time interval. Then, equation (2.3) would be generalized into

$$(f_B)^{\cdot^B} = s_f, \quad \text{with} \quad (\cdot)^{\cdot^B} := \partial_t(\cdot) + \partial_x(\cdot) \cdot \mathbf{c} + \partial_{\mathbf{c}}(\cdot) \cdot \mathbf{f}.$$

We point out that, contrary to a diffuse and facile habit, neither the transport operator $(\cdot)^{\cdot^B}$ nor its reduced version appearing in Boltzmann equation should be regarded as material time derivatives.

> What is the motivation for setting up and solving the Boltzmann equation? We can distinguish two main kinds of application. The first one is concerned with deducing the macroscopic behaviour of gases from the microscopic model, when the mean free path ... is much smaller than other typical lengths of the problem. These applications are therefore a particular instance of the basic problem of statistical mechanics, which is to bridge the gap between the atomic structure of matter and its continuum-like behaviour at a macroscopic level. Typical results of these researches are the explanation of the macroscopic behaviour of gases, and computations of viscosity and heat conduction coefficients from postulated laws of interaction between pairs of molecules .... Besides their intrinsic importance, these researches are of interest because they constitute *a model of what one should be able to do for other states of aggregation of matter* [our italics] (liquids, solids, many phase systems).

The basic tool of Boltzmann coarse-graining is definition (2.1), which associates any tensor-valued mapping $\psi_B = \widehat{\psi}_B(\boldsymbol{x}, \mathbf{c}, t)$ with its average $\Psi_B = \widehat{\Psi}_B(\boldsymbol{x}, t)$ with respect to the Boltzmann measure $d\mathbf{c}$. As far as deciding what notion of body point applies for rarefied gases, two special choices of the microscopic observable ψ_B suffice:
(i) $\widehat{\psi}_B(\boldsymbol{x}, t, \mathbf{c}) = m$, the particle mass per unit volume, leading to the identification of the macroscopic observable

$$\widehat{\Psi}_B(\boldsymbol{x}, t) = \int m f_B(\boldsymbol{x}, \mathbf{c}, t) d\mathbf{c} = m\widehat{n}(\boldsymbol{x}, t) \tag{2.5}$$

as the counterpart of microscopic origin for the CM *gas mass density*

$$\varrho(\boldsymbol{x}, t) \leftarrow m\widehat{n}(\boldsymbol{x}, t); \tag{2.6}$$

(ii) $\widehat{\psi}_B(\boldsymbol{x}, t, \mathbf{c}) = m\mathbf{c}$, the particle momentum per unit volume of a particle having velocity $\mathbf{c}$, leading to the identification of the macroscopic observable

$$\widehat{\Psi}_B(\boldsymbol{x}, t) = \int m\mathbf{c} f_B(\boldsymbol{x}, \mathbf{c}, t) d\mathbf{c} \tag{2.7}$$

as the counterpart of microscopic origin for the CM gas momentum density $\mathbf{p}$. On recalling the CM relation between velocity, mass and momentum densities, we arrive at the identification

$$\varrho(\boldsymbol{x}, t)^{-1}\mathbf{p}(\boldsymbol{x}, t) =: \mathbf{v}(\boldsymbol{x}, t) \leftarrow \widehat{n}(\boldsymbol{x}, t)^{-1} \int \mathbf{c} f_B(\boldsymbol{x}, \mathbf{c}, t) d\mathbf{c} \tag{2.8}$$

as the counterpart of microscopic origin for the CM *gas velocity* (*streaming velocity*) $\mathbf{v}$. The difference

$$\mathbf{w} := \mathbf{c} - \mathbf{v}$$

is the *fluctuation velocity* (*thermal velocity*). In view of (2.8), this definition implies that

$$\int \mathbf{w} f_B(\boldsymbol{x}, \mathbf{c}, t) d\mathbf{c} = \mathbf{0}. \tag{2.9}$$

Taking $\widehat{\psi}_B(\boldsymbol{x},t,\mathbf{c})=\frac{1}{2}m|\mathbf{c}|^2$, the atomic kinetic energy per unit volume, leads to the identifications

$$\begin{gathered}\widehat{\Psi}_B(\boldsymbol{x},t)=\int\tfrac{1}{2}|\mathbf{c}|^2 f_B\,d\mathbf{c}\ \to\ \varrho(\boldsymbol{x},t)(\kappa(\boldsymbol{x},t)+\upsilon(\boldsymbol{x},t)),\\ \kappa(\boldsymbol{x},t)\coloneqq\tfrac{1}{2}|\mathbf{v}(\boldsymbol{x},t)|^2,\quad \upsilon(\boldsymbol{x},t)\coloneqq\int\tfrac{1}{2}|\mathbf{w}|^2 f_B\,d\mathbf{c}\,,\end{gathered}\tag{2.10}$$

where $\varrho\kappa$ and $\varrho\upsilon$ are, respectively, the *gas kinetic-energy density* and the *gas internal-energy density*.* Interestingly, both these CM energies are nonnegative-valued, the kinetic energy depending on the streaming velocity, the internal energy on the thermal velocity.

With the use of the developments in Section 4, acceptance of the correspondence postulated by (2.8) provides spacetime-local information sufficient to uniquely determine the macroscopic motion presumably associated with the microscopic motion of a rarefied gas, as it is described within the Boltzmann framework.

2.2. The Irving & Kirkwood way to 'the equations of hydrodynamics'

In statistical mechanics (SM), a pair (q,p) individuates a microstate of the system at hand, visualized as a point $z\equiv(q,p)$ of a $6N$-dimensional (micro)state space $\mathcal{Z}$, a region of $\mathbb{R}^{6N}$; precisely,

$$(\boldsymbol{q}_1,\boldsymbol{q}_2,\dots,\boldsymbol{q}_N)\equiv q,\quad (\mathbf{p}_1,\mathbf{p}_2,\dots,\mathbf{p}_N)\equiv p,$$

where $\boldsymbol{q}_i$ denotes the current position of the i-th particle in the three-dimensional Euclidean space $\mathscr{E}$, and where $\mathbf{p}_i=m_i\mathbf{v}_i$ denotes its momentum, with $m_i>0$ its mass and $\mathbf{v}_i=\dot{\boldsymbol{q}}_i$ its velocity. According to Irving & Kirkwood's procedure, macroscopic observables of microscopic origin which are to correspond to spacetime fields of interest in CM are obtained by drawing average information about the individual properties of the particles in a statistical system, with the use of a non-equilibrium probability distribution function

$$f=f(z,t)\geq 0,\qquad \int_{\mathcal{Z}} f(z,t)\,dz=1,\tag{2.11}$$

defined over $\mathcal{Z}$ for all t in a chosen time interval, whose time dependence is ruled by Liouville equation.

The procedure of Irving & Kirkwood to derive the target equations holds irrespective of the macroscopic aggregation state, not only for fluids, as the title of [12] suggests to readers accustomed to the CM terminology.† It features a representation for microscopic observables $\widehat{o}$ associated with a

*Note that

$$\int m\mathbf{w}\cdot\mathbf{v}\,f_B\,d\mathbf{c}=\left(\int m\mathbf{w}\,f_B\,d\mathbf{c}\right)\cdot\mathbf{v}=0,$$

because, in view of (2.5) and (2.7),

$$\int m\mathbf{w}\,f_B\,d\mathbf{c}=\int m\mathbf{c}\,f_B\,d\mathbf{c}-\left(\int m\,f_B\,d\mathbf{c}\right)\mathbf{v}=\mathbf{0}.$$

† Those readers, however, should take into account that in the SM jargon 'hydrodynamics' is not contrasted to 'solid mechanics' but rather to 'thermodynamics'—the former discipline being concerned with *non*-equilibrium properties, the latter with statistical equilibrium properties. This being said, it is also true that the 'transport processes' Irving & Kirkwood have in mind are primarily diffusion, heat transfer, and fluid flow. In [13], the first paper of the series of which [12] is the fourth item, Kirkwood writes explicitly: " The most common transport processes are macroscopically described by the hydrodynamic equations of continuity, motion, and energy transport, supplemented by certain empirically established relations connecting the mass and heat currents and the stress tensor with the gradients of the molar variables or functions of those variables, for example, the chemical potential gradients, temperature gradient, and rate of strain."

property $\widetilde{o}_i$ of the i-th particle, in which an all-important space dependence appears:

$$\widehat{o}(\boldsymbol{x}, z) = \textstyle\sum_i \widetilde{o}_i(z)\, \delta(\boldsymbol{q}_i - \boldsymbol{x}), \quad \boldsymbol{x} \in \mathscr{E} \tag{2.12}$$

(here and henceforth $\sum_i$ is shorthand for $\sum_{i=1}^N$, and δ denotes the Dirac measure supported at $\mathbf{0}$); the relative macroscopic observable is

$$\langle o \rangle(\boldsymbol{x}, t) \coloneqq \int_{\mathcal{Z}} f(z, t)\, \widehat{o}(\boldsymbol{x}, z)\, dz.^* \tag{2.13}$$

A combination of (2.13) and (2.12),

$$\langle o \rangle(\boldsymbol{x}, t) = \langle \textstyle\sum_i \widetilde{o}_i(z) \delta(\boldsymbol{q}_i - \boldsymbol{x}) \rangle, \tag{2.14}$$

yields the $(\widetilde{o}_i, \langle o \rangle)$ pairing which conveys the physical nature of $\widetilde{o}_i$ to $\langle o \rangle$, the spacetime field of fully microscopic origin that will be identified with one of the macroscopic fields entering CM balance laws. Note that all $\langle o \rangle$s inherit their time dependence from the distribution function f, in some sense a constitutive characteristic of the system at hand. The Dirac space localization can be disposed of by using an *ad hoc* notation that we now introduce, implementing a proposal of Noll's [14, Engl. transl. [15]]. For $\mathcal{Z} \ni z = (q, p) \in \mathcal{Q} \times \mathcal{P} = \mathcal{Z}$, let

$$(\boldsymbol{q}_1, \ldots, \boldsymbol{q}_{i-1}, \boldsymbol{q}_{i+1}, \ldots, \boldsymbol{q}_N) =: \boldsymbol{q}_{\setminus i} \in \mathcal{Q}_{\setminus i} \coloneqq \mathcal{Q}_1 \times \ldots \mathcal{Q}_{i-1} \times \mathcal{Q}_{i+1} \times \ldots \times \mathcal{Q}_N$$

and

$$(q_{\setminus i}, p) =: z_{\setminus i} \in \mathcal{Z}_{\setminus i} \coloneqq \mathcal{Q}_{\setminus i} \times \mathcal{P};$$

moreover, let:

$$z_{/i}(\boldsymbol{x}) \coloneqq (\boldsymbol{q}_1, \ldots, \boldsymbol{q}_{i-1}, \boldsymbol{x}, \boldsymbol{q}_{i+1}, \ldots, \boldsymbol{q}_N, p).$$

With the use of this notation, relation (2.14) reads

$$\langle o \rangle(\boldsymbol{x}, t) = \int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i \widetilde{o}_i(z_{/i}(\boldsymbol{x}))\, f(z_{/i}(\boldsymbol{x}), t)\, dz_{\setminus i}\,. \tag{2.15}$$

The kinematic descriptors of a particle are $\widetilde{o}_i(z) = m_i$ for mass and $\widetilde{o}_i(z) = m_i \mathbf{v}_i$ for momentum. Hence, on making use of (2.15), the 'bottom-up' macroscopic kinematic descriptors for the CM mass-density field ρ and momentum-density field $\mathbf{p}$ are, respectively,

$$\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i\, f(z_{/i}(\boldsymbol{x}), t)\, dz_{\setminus i} \;\to\; \varrho(\boldsymbol{x}, t), \tag{2.16}$$

$$\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i\, \dot{\boldsymbol{q}}_i(t)\, f(z_{/i}(\boldsymbol{x}), t)\, dz_{\setminus i} \;\to\; \mathbf{p}(\boldsymbol{x}, t). \tag{2.17}$$

*To stay reasonably close to the notation used in [12], in this subsection we have chosen to depart from the notation we introduced in (2.2). This is why we have used $\widehat{o}$ instead of $\widehat{\psi}_{IK}$ in (2.12), and $\langle o \rangle$ instead of $\widehat{\Psi}_{IK}$ in (2.13). For using f instead of f_{IK} in (2.11) there is one more reason: at variance with Boltzmann's, the Irving & Kirkwood procedure needs no specific choice of probability distribution (in fact, a dependence on the underlying ensemble might be traceable in the numerical predictions of the balance equations it yields).

In the procedure of Irving & Kirkwood, a notion derived by combining (2.16) and (2.17) is meant to correspond to the CM velocity field over the region $\mathscr{B}_t \subset \mathscr{E}$ currently occupied by the continuous body under study:

$$\varrho(\boldsymbol{x},t)^{-1}\mathbf{p}(\boldsymbol{x},t) =: \mathbf{v}(\boldsymbol{x},t) \leftarrow \left(\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}\right)^{-1} \int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i \dot{\boldsymbol{q}}_i(t) f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}. \tag{2.18}$$

Just as in the case of rarefied gases, a notion of *thermal velocity* can be introduced, here measured *per particle*:

$$\mathbf{w}_i \coloneqq \mathbf{v}_i - \mathbf{v}\,;$$

in view of (2.18), this definition implies that

$$\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i \mathbf{w}_i f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i} = \mathbf{0}, \qquad \mathbf{w}_i(\boldsymbol{x},t) = \dot{\boldsymbol{q}}_i(t) - \mathbf{v}(\boldsymbol{x},t). \tag{2.19}$$

For $\widetilde{o}_i(z) = K_i \coloneqq \frac{1}{2} m_i |\mathbf{v}_i|^2$, the kinetic energy per particle, a further use of (2.14) leads to

$$\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i K_i(t) f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i} \;\rightarrow\; (\varrho\kappa)(\boldsymbol{x},t), \qquad K_i(t) = \frac{1}{2} m_i |\dot{\boldsymbol{q}}_i(t)|^2,$$

a bottom-up coarsening identification of the CM *kinetic-energy density* field. Since

$$\begin{aligned}\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i K_i(t) f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i} = {}& \tfrac{1}{2}\left(\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}\right)|\mathbf{v}(\boldsymbol{x},t)|^2 \\ & + \tfrac{1}{2}\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i |\mathbf{w}_i(\boldsymbol{x},t)|^2 f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}\,,\end{aligned} \tag{2.20}$$

the field $\varrho\kappa$ splits additively into two nonnegative-valued fields, the *'mechanical' kinetic-energy density*

$$(\varrho\kappa_{mech})(\boldsymbol{x},t) \coloneqq \tfrac{1}{2}\varrho(\boldsymbol{x},t)|\mathbf{v}(\boldsymbol{x},t)|^2 \leftarrow \tfrac{1}{2}\left(\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}\right)|\mathbf{v}(\boldsymbol{x},t)|^2$$

and the *'thermal' kinetic-energy density*

$$(\varrho\kappa_{th})(\boldsymbol{x},t) \leftarrow \tfrac{1}{2}\int_{\mathcal{Z}_{\setminus i}} \textstyle\sum_i m_i |\mathbf{w}_i(\boldsymbol{x},t)|^2 f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i};$$

the quantities κ_{mech} and κ_{th} of Irving & Kirkwood are analogous to Boltzmann's gas kinetic-energy density κ and gas internal-energy density υ in (2.10).

Acceptance of the bottom-up correspondence between microscopic and macroscopic velocity distributions postulated by (2.18) provides us—again by the use of a line of reasoning to be expounded in Section 4—with a spacetime-local information sufficient to determine the macroscopically-observable motion we presume associated *à la* Irving & Kirkwood with the given microscopic motion $z = z(t)$.

3. Deterministic coarse-graining

In their compilation of results in [12, p. 827], Irving & Kirkwood state:

> The equations of *phenomenological hydrodynamics* for a single component, single phase system are relations about certain macroscopic observables—mass density, fluid velocity, body force density, energy density, stress tensor, and heat current density. Using classical statistical mechanics, we have found that it is possible to define the corresponding microscopic observables and that *equations identical in form* to the hydrodynamical equations relate these quantities. The macroscopic equations may be obtained from the microscopic (or *point function*) equations *by averaging over a microscopically large though macroscopically small space domain determined by the resolution of one's measurements and averaging over a time interval of the order of the relaxation time of one's measuring instruments*.

All italicizations in this quote are ours. The first recalls Einstein's "phenomenological physics" quoted in the Introduction. The others are meant to stress that to Irving & Kirkwood their macroscopic observables—their "point functions," spacetime fields, in our terminology—and their equations need some averaging to become accredited correspondents of phenomenological observables and equations. Indeed, the equations of "phenomenological hydrodynamics" deal with macroscopic observables, whose microscopically-based definition should involve not only ensemble averages, but also spacetime averages, determined by the spatial and temporal resolution of the available measuring instruments.

Over forty years after the publication of [12], in their first joint paper [16] Murdoch & Bedeaux rightly remarked that the task of performing the appropriate spacetime averages should have not been dismissed, and set out to determine physically significant conditions under which Irving & Kirkwood's hydrodynamical-like equations are form-invariant under the secondary spacetime averaging advocated by them (cf. quote above).* In a different section of the same paper, Murdoch & Bedeaux review and improve the cell-averaging method Murdoch [19, 20] had propounded ten years before and applied to diverse CM issues during the intervening decade in relative isolation [21–25]. The paper closes with a lucid discussion of the respective strengths and weaknesses of Murdoch's and Irving & Kirkwood's methods, which we summarize hereafter. Murdoch's method concerns macroscopic measurements, whose values are assumed to be reproducible—*within a tolerated error*—experiment by experiment; it has the merit of emphasizing the scope of CM and its limitations, and helps in gaining insight into the physical interpretation of CM fields; its downside is that the assumptions implicit in CM modeling are accounted for via the introduction of so-called "ε-limits."†

*In 1986, Pitteri [17, erratum [18]] had showed that unwanted microscopic fluctuations can be filtered out by replacing the probability—in the notations of (2.11)—by

$$\overline{f}(z,t)=\fint_{-\tau}^{+\tau} f(z,t+\theta)\,d\theta,\quad \text{and (2.14) by}\quad \langle o\rangle(\boldsymbol{x},t)=\left\langle \textstyle\sum_i \widetilde{o}_i(z)\displaystyle\fint_{\mathscr{C}_{\boldsymbol{x}}}\delta(\boldsymbol{q}_i-\boldsymbol{\xi})\,d\boldsymbol{\xi}\right\rangle,$$

where τ is a mesoscopic time span and $\mathscr{C}_{\boldsymbol{x}}$ is an $\boldsymbol{x}$-centered cube with mesoscopic edge length.

†In [20, pp. 293–94] these "limits" are introduced as follows:

> Let g_i denote a quantity associated with a particle (point mass) P_i: for example, its mass. Consider $\sum_i g_i/V_\varepsilon$, where the sum is taken over an ε-cell of volume V_ε, centred at $\boldsymbol{x}$. If this volume average is $d(\boldsymbol{x})(1+\beta)$ for some fixed quantity $d(\boldsymbol{x})$, with $|\beta|\ll 1$, over a range of ε values macroscopically small yet microscopically large, quite independently of the shape

On the contrary, Irving & Kirkwood's method is mathematically well-defined, but its precision, which is made possible by subsuming the basic modeling assumptions in the choice of a probability distribution function, gets lost under a secondary spacetime averaging operated *à la* Murdoch.

In Section 3.2 a recent, strengthened version of the cell-averaging method will be presented, as applied only to assess consistency between discrete and continuum kinematics, in line with the often recalled restricted goal of this paper. In the next Section 3.1, we premise a presentation of another deterministic coarse-graining method, in which spatial-localization functions are essential tools.

3.1. Coarse-graining via localization functions

Almost simultaneously and altogether independently of the seminal proposal [19] by Murdoch, in 1982 Hardy [26] had introduced a different coarse-graining method, based on spatial localization functions. His reservations against the Irving-Kirkwood method were mostly pragmatic:

> [One motive for] using the methods of molecular dynamics ... is to test the validity of the continuum description of the phenomenon. Continuum theory considers local properties such as the mass density ϱ, momentum density $\mathbf{p}, \ldots$. Thus, to test continuum theory one needs formulas that relate these local properties to the masses, positions, and velocities of the particles whose motion is simulated. Irving and Kirkwood presented formulas of this type [whose] resulting densities and fluxes exactly satisfied continuity equations for mass, momentum, and energy conservation. Difficulties arise, however, when one attempts to use their formulas in a molecular-dynamics simulation: (1) The validity of the resulting conservation laws appears to depend on an ensemble average being taken. ... (3) The position at which a particle contributes to the macroscopic properties is determined with a Dirac δ-function, which would ... need to be approximated.

His declared purpose was "to present formulas for the densities and fluxes that exactly satisfy the usual continuity equations for mass, momentum, and energy conservation and avoid the above mentioned difficulties. In particular, the formulas are easily implemented in molecular-dynamics simulations, and there are no restrictions on the interparticle force range."

In 1994, Murdoch & Bedeaux [27] independently reinvented Hardy's method (under the label of 'weighting-function method'), implementing also weighted time averages. Remarkably, the combination of spacetime averaging and formal exactness was the most praised feature of the method also for its re-discoverers; in their view, the weighting-function method supplanted the cell-averaging method, preserving its pluses while eliminating its negatives. In fact, after 1994 Murdoch abandoned the older method, systematically adopting the newer one [28–35].* In the 2012 summa of his

of the cell, then $d(\boldsymbol{x})$ is termed the *ε-limit* of the volume average at $\boldsymbol{x}$ and we write

$$d(\boldsymbol{x}) =: \lim_{\varepsilon} \{\textstyle\sum_i' g_i / V_\varepsilon\}$$

(Here, and in what follows, a summation sign with superposed prime indicates that the sum is taken over an ε-cell). If such limits exist everywhere in a region R then d will be a field on R. Hereafter, in working with any given ε-limit, $1+\beta$ will be approximated by 1 for any $|\beta| \ll 1$. It follows that any ε-limit, within this approximative scheme, is unique and expressible as a volume average for some cell.

*Murdoch firstly mentioned Hardy's work in [33, p. 114], where he wrote: "Unaware of Hardy's work, Murdoch & Bedeaux [...] adopted a similar approach [...] to obtain molecular expressions for stress and heat flux together with relevant balance relations."

thirty-year-long pioneering and mostly solitary efforts, Murdoch recalls [36, pp. 223–24] that the cell-averaging method he had introduced in 1983

> was based upon an assumed insensitivity of volume and surface densities of additive molecular quantities to modest changes in geometry and scales of length and time. … This … approach was developed [and used] by the author before he was made aware of weighting-function methodology by Dick Bedeaux …. However, the precision, and absence of assumptions of scale insensitivity, associated with weighting function analysis make the latter approach both simpler and more general.

In [26], Hardy accepts as a *localization function* any non-negative real-valued function ψ on space vectors that is peaked at $\mathbf{0}$, tends to 0 away from it, and is normalized so that

$$\int_{\mathscr{E}} \psi(\mathbf{r})\, d\mathbf{r} = 1\,,$$

where $\mathbf{r} = \boldsymbol{x} - \boldsymbol{o}$ and $\boldsymbol{o}$ is a chosen point of $\mathscr{E}$. The Gaussian $\psi_{G}(\mathbf{r}) = \pi^{-3/2} L^{-3} \exp(-|\mathbf{r}|^2/L^2)$, where L characterizes the size of the averaged-over region, is given as an example; another example is

$$\psi_{C}(\mathbf{r}) = V_{C}^{-1} 1_{C}(\boldsymbol{o} + \mathbf{r}), \tag{3.1}$$

where 1_{C} is the indicator function of a parallelepipedal cell centered at $\boldsymbol{o}$, of volume V_{C}. In [27], Murdoch & Bedeaux require that *weighting functions* be C^1-continuous, in essence mollifications of ψ_{C} in (3.1) which decay monotonically to zero in a thin boundary layer. Both in [26] and in [27], once an averaging measure $\psi(\mathbf{r})d\mathbf{r}$ is chosen, the microscopically-informed CM density $\mathfrak{f}_{\psi}$ of a physical quantity $\mathfrak{f}$ is constructed as

$$\mathfrak{f}_{\psi}(\boldsymbol{x}, t) \leftarrow \textstyle\sum_i \psi(\boldsymbol{q}_i(t) - \boldsymbol{x})\, \mathfrak{f}_i(t) = \displaystyle\int_{\mathscr{E}} \textstyle\sum_i \psi(\boldsymbol{q}_i(t) - \boldsymbol{x})\, \mathfrak{f}_i(t)\, \delta(\boldsymbol{q}_i(t) - \boldsymbol{y})\, d\boldsymbol{y} \tag{3.2}$$

where $\boldsymbol{q}_i(t)$ denotes the position of the i-th particle at the current time t and $\mathfrak{f}_i(t)$ denotes the current value of $\mathfrak{f}$ associated with that particle. Interestingly, Murdoch & Bedaux introduce the additional requirement that a so-obtained density field $\mathfrak{f}_{\psi}$ be invariant under repeated spatial averaging, that is, they privilege those ψ which, whatever $\mathfrak{f}$, guarantee that

$$\mathfrak{f}_{\psi} = (\mathfrak{f}_{\psi})_{\psi}, \quad \text{with} \quad (\mathfrak{f}_{\psi})_{\psi}(\boldsymbol{x}, t) := \int_{\mathscr{E}} \psi(\boldsymbol{y} - \boldsymbol{x})\, \mathfrak{f}_{\psi}(\boldsymbol{y}, t)\, d\boldsymbol{y}\,. \tag{3.3}$$

A non-negative ψ cannot satisfy this requirement. In fact, the simplest ψ complying with (3.3) is

$$\psi_{MB}(\mathbf{r}) = \frac{1}{2\pi^2 |\mathbf{r}|^3} \left(\sin \frac{|\mathbf{r}|}{L} - \frac{|\mathbf{r}|}{L} \cos \frac{|\mathbf{r}|}{L} \right),$$

where L is the length scale associated with ψ_{MB}.

Once a localization function ψ has been selected, the relative CM fields of *mass density* ϱ, *momentum density* $\mathbf{p}$, and *velocity* $\mathbf{v}$, are identified with the use of (3.2):

$$\begin{aligned} \varrho(\boldsymbol{x}, t) &\leftarrow \textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x}, t)) m_i\,, \\ \mathbf{p}(\boldsymbol{x}, t) &\leftarrow \textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x}, t)) m_i\, \dot{\boldsymbol{q}}_i(t)\,, \\ \varrho(\boldsymbol{x}, t)^{-1} \mathbf{p}(\boldsymbol{x}, t) =: \mathbf{v}(\boldsymbol{x}, t) &\leftarrow \big(\textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x}, t)) m_i\big)^{-1} \textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x}, t)) m_i\, \dot{\boldsymbol{q}}_i(t)\,, \end{aligned} \tag{3.4}$$

where $\mathbf{r}_i(\boldsymbol{x},t) \coloneqq \boldsymbol{q}_i(t) - \boldsymbol{x}$. Identifications (3.4), along with the definition of *thermal velocities*

$$\mathbf{w}_i(\boldsymbol{x},t) \coloneqq \dot{\boldsymbol{q}}_i(t) - \mathbf{v}(\boldsymbol{x},t),$$

imply that the thermal momentum density is null:

$$\textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x},t)) m_i \mathbf{w}_i(\boldsymbol{x},t) = \mathbf{0}, \tag{3.5}$$

and that the microscopic kinetic energy density equals the sum of the macroscopic 'mechanical' and 'thermal' kinetic-energy densities:

$$\tfrac{1}{2}\textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x},t)) m_i |\dot{\boldsymbol{q}}_i(t)|^2 = \tfrac{1}{2}\varrho |\mathbf{v}(\boldsymbol{x},t)|^2 + \tfrac{1}{2}\textstyle\sum_i \psi(\mathbf{r}_i(\boldsymbol{x},t)) m_i |\mathbf{w}_i(\boldsymbol{x},t)|^2, \tag{3.6}$$

an additive decomposition which compares with Boltzmann's (2.10) and Irving & Kirkwood's (2.20).

With the use of the developments in Section 4, acceptance of the correspondence between microscopic and macroscopic velocity distributions postulated by $(3.4)_3$ provides us with spacetime-local information sufficient to uniquely determine the macroscopic motion ψ-associated with the microscopic motion $\boldsymbol{q}_i = \boldsymbol{q}_i(t)$.

3.2. Coarse-graining via cell averaging

After a long eclipse, about a dozen years ago the cell-averaging method was resumed in a new direction, brought about by ideas and capabilities coming from Molecular Dynamics (MD)—the computer-spawned brainchild of SM, whose beginnings date back to the sixties.* The novelty introduced by molecular simulations was to make it possible, thanks to electronic computers, to calculate concretely the hitherto abstract concepts of SM, thus providing a way to make realistic predictions about the behavior of previously intractable molecular systems.†

Its growing and momentous application within a SM framework notwithstanding, MD remained remote from potential application to the cell-averaging method for coarse-graining until Andersen [39] had the idea of allowing the *volume* of the computational cell to change in time, thus introducing a CM-like extra *scalar* degree of freedom (DOF), whose dynamics was coupled with the particle DOFs. Until then, the MD cell had been thought of as an inert space window of fixed volume and shape (a rectangular parallelepiped, typically a cube, suitably replicated periodically to mimic bulk conditions) within which an as large as feasible sample of point particles was let evolve according to Newtonian rules, on keeping its numerousness and total energy fixed. To perform MD computations under fixed

*The conventional birthdate of MD *sensu stricto* is considered to be 1964, the publication year of Rahman's groundbreaking paper [37], whose abstract starts with the plain statement: "A system of 864 particles interacting with a Lennard-Jones potential and obeying classical equations of motion has been studied on a digital computer (CDC 3600) to simulate molecular dynamics in liquid argon at 94.4°K and a density of 1.374 g cm^{-3}."

†In the words of Verlet—one of the founding fathers of MD—as quoted in translation by Levesque and Hansen [38, p. 43]:

> Immediately after World War II, the increase in power of computers allowed to reconsider the basis of the question raised by the atomistic hypothesis and addressed by Maxwell and Boltzmann in the 19th century: how to determine the macroscopic properties of gases and liquids, knowing that they are composed by large numbers of atoms obeying Newton's equations of motion and assuming that they interact via a given force law? … The situation changed in the fifties due to the advancement of powerful computers. It became possible to follow, over a sufficiently long time span, the trajectories of several tens or even hundreds of particles behaving like billiard balls. A few years later it became feasible to tackle a more realistic model, namely about one thousand particles interacting via pairwise Lennard-Jones forces.

pressure, such a microcanonical-ensemble setting had to be changed, which is what Andersen did in his 1980 paper [39]. In the very same year, Parrinello & Rahman [40, 41], whose goal was to simulate stress-driven phase transitions in crystals, extended Andersen's cell dilation to a general *homogeneous deformation* described by an extra *tensorial* DOF, thus gaining the ability to prescribe a general applied *stress*.* In this way, the quintessential CM notions of stress and strain entered explicitly the MD arena in 1980–1981, thus predating by a couple of years Murdoch's earliest paper on coarse-graining by means of cell averaging [19]. However, despite the fast success enjoyed by the Andersen–Parrinello–Rahman (APR) method within the MD community, it took several decades for it to percolate and touch a tiny minority within the CM community.† The first journal paper where the APR method was discussed from a CM perspective appeared in 2010 [48]. Significantly, this paper gave also the first deterministic analysis, and partial justification, of the Parrinello–Rahman dynamics as an authentic proxy for Newtonian dynamics, strongly reminiscent of the Cauchy–Born rule to study the elastic deformations of crystalline matter at zero temperature.

As reported in [49, 50], the APR method affords the key idea that makes it possible to revive and strengthen the cell-averaging procedure for coarse-graining PM into CM, by surmounting the alleged inconsistencies that led its first originator to abandon that procedure since 1994. Moreover, current MD capabilities make an APR-hybridized cell-averaging procedure computable. The basic novelty of the revised cell-averaging method expounded in [49, 50] consists in equating a deforming APR-like cell—endowed also with translational DOFs—with a piece of a CM body, small enough that CM fields are well-represented by their affine approximation at the cell center. The essentials of the relative kinematical setup are presented in the rest of this section, starting by making explicit the fundamental role played by a three-level scale separation in space and time.

3.2.1. Space and time scale separation

Coarse-graining a PM dynamics into a CM field theory depends crucially upon the all-important presumption that an adequate separation of space and time scales is possible. On condition that (i) the involved scales are made quantitatively explicit, the cell-averaging method (ii) provides specific conditions under which a CM picture is feasible, and (iii) emphasizes the essential role played by well-tuned mesoscopic tolerances in constructing and using a microscopically-informed CM theory.

As to item (i), three pairs of well-separated length and time scales—*micro-*, *meso-* and *macro-scopic*—must be introduced. For definiteness, their typical orders of magnitude are shown in Table 1; there, and in what follows, the symbols $\approx$, $\gtrsim$, and $\gg$ denote, respectively, the relations 'is of the same order of magnitude of', 'is at least of the order of magnitude of', and 'is of greater order of magnitude than'. The microscopic length scale L_μ is set by the effective range of short-ranged interactions (or, in a rarefied Boltzmann gas and in hard-sphere solids and dense fluids [51], by the mean free path), the microscopic time scale T_μ by the precision required to resolve the fine details of particle motion. The mesoscopic length scale L_m and space scale T_m correspond, respectively, to the linear size of a typical MD cell and to the time span covered by a typical MD simulation. The macroscopic length scale L_M and time scale T_M characterize the coarseness of a typical spacetime

*What Andersen first, and then Parrinello & Rahman, did was to change the microcanonical protocol by introducing *ad hoc* Lagrangians to govern the *coupled* dynamics of particles' and cell's DOFs. In the eighties, Parrinello & Rahman's 'molecular dynamics at constant applied stress' [42] was variously criticized, and several variants were proposed [43–46].

†A thorough account of the early beginnings and developments of molecular simulation from the mid fifties to the mid eighties is given by Battimelli, Ciccotti & Greco [47]. In particular, the birth of the APR method is treated on pp. 118–23.

sampling grid allowing for a satisfactory reconstruction of the CM fields of interest.* The feasibility conditions alluded to in item (ii) will surface in Section 3.2.4, where the macroscopic fields of velocity and mass density are constructed by assigning them the values of cell-wise average densities, and where the mesoscopic tolerances mentioned in item (iii) are introduced through the notion of 'equality to within a mesoscopically negligible error.'

The Cartesian structure of the ambient spacetime suggests and permits to proceed to the simpler (and general) time averaging in Section 4.2, after the more delicate (and specific) space averaging procedure has been detailed in the forthcoming Sections 3.2.2 to 3.2.5.

Table 1. Typical length (L) and time (T) scales: $L_{\mathsf{M}} \gg L_{\mathsf{m}} \gg L_\mu$, $T_{\mathsf{M}} \gg T_{\mathsf{m}} \gg T_\mu$.

	length scale	time scale
macroscopic	$L_{\mathsf{M}} \gtrapprox 1\mu\mathrm{m}$	$T_{\mathsf{M}} \gtrapprox 1\mu\mathrm{s}$
mesoscopic	$L_{\mathsf{m}} \gtrapprox 10\mathrm{nm}$	$T_{\mathsf{m}} \approx 1\mathrm{ns}$
microscopic	$L_\mu \approx 1\mathrm{nm}$	$T_\mu \approx 1\mathrm{fs}$

3.2.2. Mean mass density and velocity of a cell

By a *mesoscopic space cell* $\mathscr{C}$ we mean an open convex set in $\mathscr{E}$ (say, a parallelepiped) having inner and outer diameters of the same order of magnitude of the mesoscopic length scale:

$$D_{\mathsf{in}} \approx D_{\mathsf{out}} \approx L_{\mathsf{m}}.^{\dagger}$$

The *presence index in* $\mathscr{C}$ *of a particle is*

$$\varphi_i^{\mathscr{C}}(t) := \begin{cases} 1 & \text{if } \boldsymbol{q}_i(t) \in \mathscr{C}, \\ 0 & \text{otherwise}. \end{cases}$$

For each time t, (i) the instantaneous *cell mass* is the sum of the masses of all particles contained in $\mathscr{C}$ at that time:

$$M_{\mathscr{C}}(t) := \textstyle\sum_i \mu_i^{\mathscr{C}}(t), \quad \text{with} \quad \mu_i^{\mathscr{C}}(t) := \varphi_i^{\mathscr{C}}(t) m_i; \tag{3.7}$$

(ii) the instantaneous *cell mass-center* is

$$\boldsymbol{c}_{\mathscr{C}}(t) := M_{\mathscr{C}}(t)^{-1} \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\, \boldsymbol{q}_i(t), \tag{3.8}$$

subject to the proviso that $M_{\mathscr{C}}(t)$ be nonzero; and (iii) the instantaneous *cell momentum* is

$$\boldsymbol{p}_{\mathscr{C}}(t) := \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\, \dot{\boldsymbol{q}}_i(t).$$

*The mesoscopic length scale L_{m} plays a role analogous to the length L associated in Section 3.1 with Hardy's Gaussian localization function ψ_G or with Murdoch & Bedeaux's weighting function ψ_{MB}. In most cases, the relevant values of L_{M} and T_{M} are much larger than those given in Table 1, possibly pertinent to micromechanical applications.

†By definition, D_{in} and D_{out} are, respectively, the sup/inf of the diameters of the in/circumscribed spheres.

The *cell-averaged velocity* $\boldsymbol{v}_{\mathscr{C}}(t)$ and the *cell-averaged mass density* $\rho_{\mathscr{C}}(t)$ are defined to be, respectively,

$$\boldsymbol{v}_{\mathscr{C}}(t) \coloneqq M_{\mathscr{C}}(t)^{-1}\,\boldsymbol{p}_{\mathscr{C}}(t) \tag{3.9}$$

and

$$\rho_{\mathscr{C}}(t) \coloneqq V_{\mathscr{C}}^{-1} M_{\mathscr{C}}(t), \tag{3.10}$$

with $V_{\mathscr{C}}$ the volume of the space cell $\mathscr{C}$. It is instructive to compare and contrast Eq (3.9) with (2.8), (2.18), and $(3.4)_3$, and Eq (3.10) with (2.6), (2.16), and $(3.4)_1$: the velocity $\boldsymbol{v}_{\mathscr{C}}(t)$ and the mass-density $\rho_{\mathscr{C}}(t)$ are associated not with a single space point but with a mesoscopically extended space cell $\mathscr{C}$. The conditions under which these quantities may be meaningfully associated with the cell centroid will be discussed in Sections 3.2.4 and 3.2.5.

3.2.3. $\mathscr{C}$-streaming velocity field and $\mathscr{C}$-thermal velocities

With a view to extracting collective mesoscopic information about the individual kinetic state of particles happening to be in $\mathscr{C}$ at time t, we consider

$$\boldsymbol{\alpha}(\boldsymbol{x}) = \boldsymbol{v} + \boldsymbol{L}(\boldsymbol{x}-\boldsymbol{o}),$$

a family of affine vector fields on $\mathscr{E}$ parameterized by the pair $(\boldsymbol{v}, \boldsymbol{L})$, with $\boldsymbol{o}$ a chosen point of $\mathscr{E}$, $\boldsymbol{v}$ a vector and $\boldsymbol{L}$ a double tensor, and we seek the one such vector field that best approximates the particle velocities, in the sense that it minimizes the kinetic quantity[*]

$$\mathscr{K}_{\mathscr{C}}(\boldsymbol{v}, \boldsymbol{L}; t) \coloneqq \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\left|\dot{\boldsymbol{q}}_i(t) - \boldsymbol{\alpha}(\boldsymbol{q}_i(t))\right|^2. \tag{3.11}$$

It turns out that the minimizer is the instantaneous *$\mathscr{C}$-streaming velocity field*

$$\boldsymbol{\alpha}_{\mathscr{C}}(\boldsymbol{x}; t) = \boldsymbol{v}_{\mathscr{C}}(t) + \boldsymbol{L}_{\mathscr{C}}(t)\big(\boldsymbol{x} - \boldsymbol{c}_{\mathscr{C}}(t)\big),$$

with $\boldsymbol{v}_{\mathscr{C}}(t)$ the cell-averaged velocity (3.9), $\boldsymbol{c}_{\mathscr{C}}(t)$ the cell mass-center (3.8), and with

$$\boldsymbol{L}_{\mathscr{C}}(\,t) \coloneqq \boldsymbol{P}_{\mathscr{C}}(t)\,\boldsymbol{E}_{\mathscr{C}}(t)^{-1}, \tag{3.12}$$

where, for

$$\mathbf{r}_i^{\mathscr{C}}(t) \coloneqq \boldsymbol{q}_i(t) - \boldsymbol{c}_{\mathscr{C}}(t) \tag{3.13}$$

the instantaneous central radius vector of the i-th particle,[†]

$$\boldsymbol{P}_{\mathscr{C}}(t) \coloneqq \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,\mathbf{r}_i^{\mathscr{C}}(t)\otimes\dot{\boldsymbol{q}}_i(t) \quad \text{and} \quad \boldsymbol{E}_{\mathscr{C}}(t) \coloneqq \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,\mathbf{r}_i^{\mathscr{C}}(t)\otimes\mathbf{r}_i^{\mathscr{C}}(t) \tag{3.14}$$

are, respectively, the instantaneous central *moment of momentum* and *Euler tensor*.[‡] Symmetric by construction, $\boldsymbol{E}_{\mathscr{C}}(t)$ is assumed to be positive definite, and hence invertible: strict positive definiteness fails if and only if, at time t, all particles in $\mathscr{C}$ lie on a plane—an occurrence ruled out in Section 3.2.5. Note in particular that $\boldsymbol{\alpha}_{\mathscr{C}}(\boldsymbol{c}_{\mathscr{C}}(t); t) = \boldsymbol{v}_{\mathscr{C}}(t)$.

[*] Note that, at each time t, $\mathscr{K}_{\mathscr{C}}(\cdot,\cdot;t)$ is a convex quadratic function of the pair $(\boldsymbol{v}, \boldsymbol{L})$.

[†] It follows from definitions (3.7), (3.8), and (3.13), that $\sum_i \mu_i^{\mathscr{C}}(t)\mathbf{r}_i^{\mathscr{C}}(t) = \mathbf{0}$.

[‡] We define the tensor product is such a way that $(\mathbf{a}\otimes\mathbf{b})\mathbf{u} \coloneqq (\mathbf{a}\cdot\mathbf{u})\mathbf{b}$ for all vectors $\mathbf{a}$, $\mathbf{b}$, $\mathbf{u}$. Consequently, $(\mathbf{a}\otimes\mathbf{b})_{\alpha\beta} = a_\beta b_\alpha$ in Cartesian index notation, and $(\mathbf{L}\,\mathbf{a})\cdot\mathbf{b} = \mathbf{L}\cdot(\mathbf{a}\otimes\mathbf{b})$ and $(\mathbf{L}\,\mathbf{a})\otimes\mathbf{b} = (\mathbf{a}\otimes\mathbf{b})\mathbf{L}^\top$ for all double tensors $\mathbf{L}$.

By definition, the instantaneous $\mathscr{C}$*-thermal velocity* of the i-th particle is the difference

$$\mathbf{w}_i^{\mathscr{C}}(t) := \dot{\boldsymbol{q}}_i(t) - \boldsymbol{\alpha}_{\mathscr{C}}(\boldsymbol{q}_i(t);t) = \dot{\boldsymbol{q}}_i(t) - \big(\boldsymbol{v}_{\mathscr{C}}(t) + \boldsymbol{L}_{\mathscr{C}}(t)\,\mathbf{r}_i^{\mathscr{C}}(t)\big). \tag{3.15}$$

Minimization of (3.11) with respect to the pair $(\boldsymbol{v}, \boldsymbol{L})$ ensures that thermal velocities have null cell-wise zeroth and first moments of momentum:

$$\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,\mathbf{w}_i^{\mathscr{C}}(t) = \mathbf{0}, \qquad \sum_i \mu_i^{\mathscr{C}}(t)\,\mathbf{r}_i^{\mathscr{C}}(t)\otimes\mathbf{w}_i^{\mathscr{C}}(t) = \mathbf{0}. \tag{3.16}$$

In fact, $(3.16)_1$ and $(3.16)_2$ are the stationarity conditions of (3.11) with respect to $\boldsymbol{v}$ and $\boldsymbol{L}$.*

3.2.4. Space-averaged fields of mass density, velocity, and velocity gradient

At each time t, we consider a macroscopic open region $\mathscr{D}_t$ of the ambient space $\mathscr{E}$ that can be covered by an L_M-coarse sampling grid consisting of L_m-sized space cells and is *densely populated by particles*, in the following sense:
(i) for each pair $(\boldsymbol{x}, t) \in \mathscr{D}_t$, there is a mesoscopic space cell $\mathscr{C}$ whose instantaneous mass center $\boldsymbol{c}_{\mathscr{C}}(t)$ differs from $\boldsymbol{x}$ by a *mesoscopically negligible* offset, a relation that we denote by

$$\boldsymbol{c}_{\mathscr{C}}(t) \cong \boldsymbol{x};$$

hereafter, we denote '$\cong$-equal' any two quantities satisfying an equality relation to within a mesoscopically negligible error, and we denote by $\mathscr{C}_{(\boldsymbol{x},t)}$ a cell, whenever we wish to emphasize that its mass center $\cong \boldsymbol{x}$ at time t;
(ii) the number of particles in $\mathscr{C}$ at time t is large enough that—given the Voronoi tessellation associated with the set $\{\boldsymbol{q}_j(t)\,|\,\varphi_j^{\mathscr{C}} = 1\}$, whose typical cell $\mathscr{C}_i(t)$ has volume $V_i(t)$—it so happens that

$$\int_{\mathscr{C}} \mathfrak{f}(\boldsymbol{y})\,d\boldsymbol{y} \cong \textstyle\sum_i \varphi_i^{\mathscr{C}}(t)\,\mathfrak{f}(\boldsymbol{q}_i(t))\,V_i(t) \tag{3.17}$$

for all fields $\mathfrak{f}$ defined in $\mathscr{C}$ which *vary slowly on the microscopic length scale* L_μ, in the sense that, for all $\mathscr{C}_i(t)$,

$$\int_{\mathscr{C}_i(t)} \mathfrak{f}(\boldsymbol{y})\,d\boldsymbol{y} \cong \mathfrak{f}(\boldsymbol{q}_i(t))\,V_i(t);$$

(iii) for whatever mesoscopic space cell $\mathscr{C}'$ whose mass center satisfies $\boldsymbol{c}_{\mathscr{C}'}(t) \cong \boldsymbol{x}$, the cell averages $\rho_{\mathscr{C}'}(t), \boldsymbol{v}_{\mathscr{C}'}(t), \boldsymbol{L}_{\mathscr{C}'}(t)$ satisfy, respectively,

$$\rho_{\mathscr{C}'}(t) \cong \rho_{\mathscr{C}}(t), \quad \boldsymbol{v}_{\mathscr{C}'}(t) \cong \boldsymbol{v}_{\mathscr{C}}(t), \quad \boldsymbol{L}_{\mathscr{C}'}(t) \cong \boldsymbol{L}_{\mathscr{C}}(t).$$

We say that a field $\mathfrak{f}(\cdot, t)$ defined in $\mathscr{D}_t$ *varies slowly on the mesoscopic length scale* L_{m} if it so happens that, for whatever mesoscopic cell $\mathscr{C}$,

$$\int_{\mathscr{C}} \mathfrak{f}(\boldsymbol{y},t)\,d\boldsymbol{y} \cong \mathfrak{f}(\tilde{\boldsymbol{c}}_{\mathscr{C}},t)\,V_{\mathscr{C}}, \qquad \text{with} \quad \tilde{\boldsymbol{c}}_{\mathscr{C}} := V_{\mathscr{C}}^{-1}\int_{\mathscr{C}} \boldsymbol{y}\,d\boldsymbol{y}$$

*In [20, p. 298] two equalities essentially equivalent to (3.16) (labeled as T. M. 1 and T. M. 2) were *postulated* as expressing the assumed "random character" of thermal velocities. This terminology needs at least qualification so as not to be misleading, since thermal velocities may exhibit a highly organized "randomness," as in plastic flow of crystalline solids [52].

the centroid (center of volume) of $\mathscr{C}$.

In conclusion, we consider the following construction:

$$\varrho(\boldsymbol{x},t) \leftarrow \rho_{\mathscr{C}_{(\boldsymbol{x},t)}}, \qquad \mathbf{v}(\boldsymbol{x},t) \leftarrow \boldsymbol{v}_{\mathscr{C}_{(\boldsymbol{x},t)}}, \qquad \mathbf{L}(\boldsymbol{x},t) \leftarrow \boldsymbol{L}_{\mathscr{C}_{(\boldsymbol{x},t)}}, \tag{3.18}$$

and regard it as satisfactory when each of the macroscopic fields $\varrho(\cdot,t)$, $\mathbf{v}(\cdot,t)$, and $\mathbf{L}(\cdot,t)$ is mesoscopically slow-varying. Since $\mathbf{v}(\cdot,t)$ varies slowly on the L_{m} scale, its restriction $\mathbf{v}(\cdot,t)|_{\mathscr{C}}$ to any mesoscopic space cell $\mathscr{C} \subset \mathscr{D}_t$ satisfies

$$\mathbf{v}(\cdot,t)|_{\mathscr{C}} \cong \boldsymbol{\alpha}_{\mathscr{C}}(\cdot\,;t). \tag{3.19}$$

Hence, (3.15) and (3.19) imply that, if $\boldsymbol{q}_i(t) \in \mathscr{C}$, then

$$\mathbf{w}_i^{\mathscr{C}}(t) \cong \dot{\boldsymbol{q}}_i(t) - \mathbf{v}(\boldsymbol{q}_i(t),t). \tag{3.20}$$

Moreover, since the right side of (3.20) does not depend on what cell $\mathscr{C} \ni \boldsymbol{q}_i(t)$ was chosen, the difference between the particle velocity $\dot{\boldsymbol{q}}_i(t)$ and the value of the macroscopic velocity field $\mathbf{v}$ at the particle position is $\cong$-equal to the thermal velocity with respect to any mesoscopic space cell $\mathscr{C} \ni \boldsymbol{q}_i(t)$:

$$\mathbf{w}_i^{\mathscr{C}}(t) \cong \mathbf{w}_i(t) \coloneqq \dot{\boldsymbol{q}}_i(t) - \mathbf{v}(\boldsymbol{q}_i(t),t).$$

At odds with all previously discussed coarse-graining methods, the present one delivers an extra tensor-valued field, $\mathbf{L}(\cdot,t)$, whose value at $\boldsymbol{x}$ is $\cong$-equal to the gradient of the $\mathscr{C}$-streaming velocity field $\boldsymbol{\alpha}_{\mathscr{C}}(\cdot\,;t)$ for any mesoscopic space cell $\mathscr{C}$ $\cong$-centered at $\boldsymbol{x}$ (cf. $(3.18)_3$). The assumption that both $\mathbf{v}(\cdot,t)$ and $\mathbf{L}(\cdot,t)$ vary slowly on the L_{m} scale implies that

$$\mathbf{L} \cong \operatorname{grad}\mathbf{v}, \tag{3.21}$$

where grad denotes the gradient operator.* Moreover, the spatial slowness property of $\mathbf{v}(\cdot,t)$ and $\mathbf{L}(\cdot,t)$ and the tolerances allowed by (3.19) and (3.21) may be exploited to select, among all the vector fields $\mathbf{v}(\cdot,t)$ satisfying (3.19), a velocity field which is (at least) continuous and piecewise C^1.† From now on, we assume that $\mathbf{v}$ denotes a streaming velocity field with such a spatial smoothness.

*In [50] this fact is proved by taking any two mesoscopic space cells, $\mathscr{C}_-$ and $\mathscr{C}_+$ in $\mathscr{D}_t$, such that their intersection $\mathscr{C} \coloneqq \mathscr{C}_- \cap \mathscr{C}_+$ is also a mesoscopic space cell, and considering that—due to the spatial slowness hypothesis—the velocity fields $\boldsymbol{\alpha}_{\mathscr{C}_-}(\cdot\,;t)$, $\boldsymbol{\alpha}_{\mathscr{C}_+}(\cdot\,;t)$ are mesoscopically indistinguishable on $\mathscr{C}$, in the sense that

$$\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\left|\boldsymbol{\alpha}_{\mathscr{C}_+}(\boldsymbol{q}_i(t);t) - \boldsymbol{\alpha}_{\mathscr{C}_-}(\boldsymbol{q}_i(t);t)\right|^2 \cong 0.$$

†We sketch a line of reasoning to prove this assertion. Consider, for simplicity, a space-filling tessellation $\mathscr{T}$ made up of mesoscopic cubic cells, and let $\mathscr{T}'$ be the dual tessellation. The intersection of a primal cell $\mathscr{C} \subset \mathscr{T}$ centered at $\boldsymbol{o}$ with the cell $\mathscr{C}_i' \subset \mathscr{T}'$ centered at the vertex $\boldsymbol{x}_i$ of $\mathscr{C}$ is also a cube of mesoscopic size. Then,

$$\boldsymbol{\alpha}_{\mathscr{C}}(\boldsymbol{x}_i) = \boldsymbol{v}_{\mathscr{C}} + \boldsymbol{L}_{\mathscr{C}}(\boldsymbol{x}_i - \boldsymbol{o}) \cong \boldsymbol{\alpha}_{\mathscr{C}_i'}(\boldsymbol{x}_i) = \boldsymbol{v}_{\mathscr{C}_i'},$$

where $\boldsymbol{\alpha}_{\mathscr{C}}$ ($\boldsymbol{\alpha}_{\mathscr{C}_i'}$) is the $\mathscr{C}$ ($\mathscr{C}_i'$)-streaming velocity field. Given the values $\boldsymbol{v}_{\mathscr{C}_1'}, \dots, \boldsymbol{v}_{\mathscr{C}_8'}$ at the 2^3 vertices of $\mathscr{C}$, there is a unique trilinear vector field $\boldsymbol{\tau}_{\mathscr{C}}$ such that $\boldsymbol{\tau}_{\mathscr{C}}(\boldsymbol{x}_i) = \boldsymbol{v}_{\mathscr{C}_i'}$ ($i = 1, \dots, 8$), which may be represented as

$$\boldsymbol{\tau}_{\mathscr{C}}(\xi,\eta,\zeta) = \mathbf{c}_0 + \xi\,\mathbf{c}_1 + \eta\,\mathbf{c}_2 + \zeta\,\mathbf{c}_3 + \xi\eta\,\mathbf{c}_{12} + \eta\zeta\,\mathbf{c}_{23} + \zeta\xi\,\mathbf{c}_{31} + \xi\eta\zeta\,\mathbf{c}_{123}$$

3.2.5. Mass, Euler tensor, and kinetic energy, of a cell

The assumption that the mass density field $\varrho(\cdot,t)$ varies slowly on the L_{m} scale, combined with (3.7), (3.10) and $(3.18)_1$, implies that

$$M_{\mathscr{C}}(t) = \varrho(\boldsymbol{c}_{\mathscr{C}}(t),t)V_{\mathscr{C}} \cong \int_{\mathscr{C}} \varrho(\boldsymbol{y},t)\,d\boldsymbol{y}\,.$$

Under the same assumption, the mass center $\boldsymbol{c}_{\mathscr{C}}(t)$ of a mesoscopic cell is $\cong$-equal to the centroid $\tilde{\boldsymbol{c}}_{\mathscr{C}}$, so that

$$\mathbf{r}_i^{\mathscr{C}}(t) \cong \tilde{\mathbf{r}}_i^{\mathscr{C}}(t) \coloneqq \boldsymbol{q}_i(t) - \tilde{\boldsymbol{c}}_{\mathscr{C}} \tag{3.22}$$

(cf. (3.13)). Consequently,

$$\boldsymbol{E}_{\mathscr{C}}(t) \cong \textstyle\sum_i \mu_i^{\mathscr{C}}(t)\tilde{\mathbf{r}}_i^{\mathscr{C}}(t)\otimes\tilde{\mathbf{r}}_i^{\mathscr{C}}(t) \cong \displaystyle\int_{\mathscr{C}} \varrho(\boldsymbol{y},t)\,\mathbf{u}(\boldsymbol{y})\otimes\mathbf{u}(\boldsymbol{y})\,d\boldsymbol{y}, \qquad \text{with} \quad \mathbf{u}(\boldsymbol{y}) \coloneqq \boldsymbol{y}-\tilde{\boldsymbol{c}}_{\mathscr{C}}\,,$$

where the first $\cong$-equality stems from $(3.14)_2$ and (3.22), and the second holds thanks to the integral approximation property (3.17) and the spatial slowness hypothesis. Under the same hypotheses, properties (3.16) of thermal velocities imply that

$$\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,\dot{\boldsymbol{q}}_i(t) \cong \sum_i \mu_i^{\mathscr{C}}(t)\,\mathbf{v}(\boldsymbol{q}_i(t),t) \cong \displaystyle\int_{\mathscr{C}} \varrho(\boldsymbol{y},t)\,\mathbf{v}(\boldsymbol{y},t)\,d\boldsymbol{y}, \tag{3.23}$$

$$\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\mathbf{r}_i^{\mathscr{C}}(t)\otimes\dot{\boldsymbol{q}}_i(t) \cong \sum_i \mu_i^{\mathscr{C}}(t)\tilde{\mathbf{r}}_i^{\mathscr{C}}(t)\otimes\mathbf{v}(\boldsymbol{q}_i(t),t) \cong \displaystyle\int_{\mathscr{C}} \varrho(\boldsymbol{y},t)\,\mathbf{u}(\boldsymbol{y})\otimes\mathbf{v}(\boldsymbol{y},t)\,d\boldsymbol{y}\,. \tag{3.24}$$

In these relations, the cell integrals on the right side are $\cong$-equal to their discrete microscopic correspondents on the left side. Equality (3.23) accords with (2.9), (2.19), and (3.5). In fact, this is a consequence of—and a strong motivation for—defining the macroscopic velocity as the ratio of the average microscopic momentum to the average microscopic mass, irrespective of the specific averaging procedure adopted. On the contrary, the microscopic kinetic energy is generally larger that its macroscopic correspondent:

$$\tfrac{1}{2}\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,|\dot{\boldsymbol{q}}_i(t)|^2 \cong \tfrac{1}{2}\displaystyle\int_{\mathscr{C}} \varrho(\boldsymbol{y},t)\,|\mathbf{v}(\boldsymbol{y},t)|^2 d\boldsymbol{y} + \tfrac{1}{2}\textstyle\sum_i \mu_i^{\mathscr{C}}(t)\,|\mathbf{w}_i(t)|^2, \tag{3.25}$$

since the second term on the right side, namely, the thermal kinetic energy, is strictly positive unless $\mu_i^{\mathscr{C}}(t)\mathbf{w}_i(t) = \mathbf{0}$ for all i. Again, equality (3.25) accords with (2.10), (2.20), and (3.6). Equality (3.24) is peculiar to the cell-averaging method, where not only the zeroth moments of particle masses and

in adapted Cartesian coordinates (ξ,η,ζ). Combination of the two relations just displayed yields

$$\boldsymbol{\tau}_{\mathscr{C}}(\boldsymbol{x}_i) \cong \boldsymbol{\alpha}_{\mathscr{C}}(\boldsymbol{x}_i)\ \ (i=1,\dots,8) \quad \Longrightarrow \quad \boldsymbol{\tau}_{\mathscr{C}}|_{\mathscr{C}} \cong \boldsymbol{\alpha}_{\mathscr{C}}|_{\mathscr{C}}\,.$$

Let a field $\boldsymbol{\tau}_{\mathscr{C}}$ be constructed for each $\mathscr{C}\subset\mathscr{T}$, and let a macroscopic velocity field $\mathbf{v}$ be defined cell-by-cell over $\mathscr{T}$ as

$$\mathbf{v}|_{\mathscr{C}} \coloneqq \boldsymbol{\tau}_{\mathscr{C}}|_{\mathscr{C}}\,;$$

then, $\mathbf{v}$ is a Lipschitz-continuous field which is $\cong$-equal to the $\mathscr{C}$-streaming velocity field $\boldsymbol{\alpha}_{\mathscr{C}}$ on each $\mathscr{C}\subset\mathscr{T}$. It is readily verified that $\mathbf{c}_0 = \boldsymbol{v}_{\mathscr{C}}$ and $\mathbf{c}_i = \boldsymbol{L}_{\mathscr{C}}\boldsymbol{e}_i$ $(i=1,2,3)$, with $(\boldsymbol{e}_1,\boldsymbol{e}_2,\boldsymbol{e}_3)$ the orthonormal adapted basis. This result is robust under the action of smooth space diffeomorphisms varying slowly on the L_{m} scale, such that the Cartesian coordinates (ξ,η,ζ) are transformed to curvilinear coordinates.

momenta, but also their first moments are taken into consideration (cf. (3.8) and $(3.14)_1$). This result adds motivation to definitions (3.9) and (3.12).

With the use of the developments in Section 4, acceptance of the correspondence between microscopic and macroscopic velocity distributions brought about in Section 3.2.4 provides us with spacetime-local information sufficient to uniquely determine—to within mesoscopically negligible errors—the macroscopic motion associated with the microscopic motion $\boldsymbol{q}_i = \boldsymbol{q}_i(t)$.

4. The macroscopic motion associated with a given velocity field

4.1. A quick recap of CM kinematics

In CM, a motion is customarily described as a conveniently spacetime-smooth family of deformations of the body under study, which is assumed to occupy a space region $\mathscr{B}_t$ at each t in the time interval of interest—in the sense that, at any given time t, each *space point* in $\mathscr{B}_t$ is occupied by one and only one *body point*. More precisely, when a material system is regarded as a continuous body, its motion can be described as a t-family of locally orientation-preserving maps $\boldsymbol{\chi}(\cdot, t)$ of the region $\mathscr{B}_{t_0}$ the body occupies at an 'initial' time t_0,* each $\boldsymbol{\chi}(\cdot, t)$ being bijective on its image $\mathscr{B}_t := \boldsymbol{\chi}(\mathscr{B}_{t_0}, t)$, the region the body occupies at time t. Granted the notations

$$(\boldsymbol{X}, t) \mapsto \boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t), \qquad \boldsymbol{\chi}_t(\boldsymbol{X}) := \boldsymbol{\chi}(\boldsymbol{X}, t), \qquad \boldsymbol{X} = \boldsymbol{\chi}_t^{-1}(\boldsymbol{x}), \tag{4.1}$$

three fields over $\mathcal{B}_{t_0}$ are introduced, the velocity $\dot{\boldsymbol{\chi}}$, the deformation gradient

$$\mathbf{F} := \mathrm{Grad}\,\boldsymbol{\chi}, \tag{4.2}$$

and its time rate $\dot{\mathbf{F}} = \mathrm{Grad}\,\dot{\boldsymbol{\chi}}$. At each t in the time interval on which the motion $(4.1)_1$ is defined, the space point $\boldsymbol{x} = \boldsymbol{\chi}(\boldsymbol{X}, t) \ni \mathscr{B}_t$ is interpreted as the current position of the body point placed in $\boldsymbol{X}$ at time t_0; conversely, $\boldsymbol{X}$ is the position at time t_0 of the body point currently placed in $\boldsymbol{x}$ (cf. $(4.1)_3$).† The quantities $\mathbf{B} := \mathbf{F}\mathbf{F}^\top$ and $\mathbf{C} := \mathbf{F}^\top\mathbf{F}$ are local exact strain measures. In view of $(4.1)_3$, the velocity may be regarded also as a field over the region currently occupied by the body:

$$\mathbf{v}(\boldsymbol{x}, t) := \dot{\boldsymbol{\chi}}(\boldsymbol{\chi}_t^{-1}(\boldsymbol{x}), t); \tag{4.3}$$

this relation, as we are going to argue here below, is of central importance to draw the main results of our former developments. Strain rate and vorticity are gauged by, respectively, the stretching $\mathbf{D}$ and the spin $\mathbf{W}$, the symmetric and skew parts of

$$\mathbf{L} := \mathrm{grad}\mathbf{v}. \tag{4.4}$$

*The region occupied by a continuous body in its reference configuration need not be occupied by the body at any instant of its motion. However, since it has to be diffeomorphic to each of the regions the body actually occupies, there is no loss in generality in assuming the actual configuration of the body at a certain (nominally initial) time t_0 as reference. Such a choice is mandatory, as we explain below, when extracting the information needed to determine the CM motion from an underlying PM motion. As a side note, we add a quote from Truesdell [55, p. 96]: "In the mid-eighteenth century Euler introduced the description that hydrodynamicists still call "Lagrangean." This is a particular referential description, in which the Cartesian coordinates of the position $\boldsymbol{X}$ of the body-point X at the time $t = 0$ are used as a label for that body-point."

†The smooth one-to-one correspondence between body points and space points in the reference region $\mathscr{B}_{t_0}$ should not obliterate the fact that any other space region diffeomorphic with $\mathscr{B}_{t_0}$ could equally be used as reference: CM body points are just *labeled* with space points, exactly as PM particles are labeled with natural numbers.

Finally, taking the gradient on both sides of (4.3) yields a well-know result of CM kinematics:

$$\mathrm{grad}\mathbf{v} = \dot{\mathbf{F}}\mathbf{F}^{-1}.$$

4.2. How to make CM kinematics PM-informed

All of the above account of CM kinematics, as in fact all of CM, is altogether independent of any PM foundation—notwithstanding the original atomistic motivations of the French founders of modern CM—Navier, Poisson, Cauchy, and Lamé [53]. However, in Sections 2 and 3, we have shown that every sound coarse-graining procedure of a PM dynamics—be it statistical or deterministic in nature—distills a spatially smooth streaming velocity out of a wiggling PM motion which, when time-smoothed as detailed below, delivers a velocity field of the same kind of the one that (4.3) *defines* in terms of a smooth CM motion. On this basis, one may ask whether it is possible to reverse roles in (4.3), so as to *generate* a CM motion from a *given* velocity field. This reversal of perspective was pointed out—though not pursued—by Murdoch in [30, p. 111], [32, pp. 73–75], [35, p. 5].

With a view toward associating a microscopically informed CM motion to a given PM account of the kinematics of a material system, we posit the $\boldsymbol{X}$-family of initial-value Cauchy problems

$$\dot{\boldsymbol{\chi}}(\boldsymbol{X},t) = \mathbf{v}(\boldsymbol{\chi}(\boldsymbol{X},t),t), \qquad \boldsymbol{\chi}(\boldsymbol{X},t_0) = \boldsymbol{X} \in \mathscr{B}_{t_0}, \tag{4.5}$$

where the field $\mathbf{v}$ is assumed to be defined in a spacetime neighborhood of $\mathscr{B}_{t_0}\times\{t_0\}$. Under the condition that $\mathbf{v}$ is Lipschitz-continuous with respect to its space argument and continuous with respect to time, the Picard–Lindelöf theorem guarantees existence and uniqueness of a solution $\boldsymbol{\chi}(\boldsymbol{X},\cdot)$ in some interval $\mathcal{I}_{t_0}$ centered at t_0 for all $\boldsymbol{X}\in\mathscr{B}_{t_0}$, possibly extending to the whole time line. It is only natural *to take for* $\mathbf{v}$ *any of the streaming velocity fields* obtained as end results of the coarse-graining procedures we exposed in Sections 2 and 3, provided it enjoys the requested spacetime smoothness. Let us shortly postpone dealing with this technical issue. For any time t within the time interval granted by the theorem, $\boldsymbol{\chi}(\boldsymbol{X},t)$ yields the position of the CM body point supposedly placed in $\boldsymbol{X}$ at time t_0 and driven along by the streaming velocity $\mathbf{v}$. A formal pointwise representation of the macroscopic motion induced by the motion of the particles, when coarse-grained as specified by the velocity field $\mathbf{v}$, is

$$\boldsymbol{\chi}(\boldsymbol{X},t) = \boldsymbol{X} + \int_{t_0}^{t} \mathbf{v}(\boldsymbol{\chi}(\boldsymbol{X},\tau),\tau)\,d\tau,$$

a suggestive reformulation of problem (4.5). Once this problem is solved, the deformation gradient $\mathbf{F}$ is obtained as in (4.2). This is equivalent to solving the subsidiary $\boldsymbol{X}$-family of initial-value problems

$$\dot{\mathbf{F}}(\boldsymbol{X},t) = \mathbf{L}(\boldsymbol{\chi}(\boldsymbol{X},t),t)\mathbf{F}(\boldsymbol{X},t), \qquad \mathbf{F}(\boldsymbol{X},t_0) = \mathbf{I},$$

with $\mathbf{L} = \mathrm{grad}\mathbf{v}$ (cf. (4.4)).

Due to the crucial role played by the Cauchy problem (4.5) in connecting PM and CM motions, it is essential to check whether the (relatively mild) conditions of the Picard–Lindelöf theorem are met by each of the candidate streaming velocity fields. We find it convenient to begin by listing them here below, as they are specified by (2.5) and (2.8) for Boltzmann gases:

$$\mathbf{v}_B(\boldsymbol{x},t) = \frac{\int \mathbf{c}\, f_B(\boldsymbol{x},\mathbf{c},t)\,d\mathbf{c}}{\int f_B(\boldsymbol{x},\mathbf{c},t)\,d\mathbf{c}}; \tag{2.8}_{\mathrm{rep}}$$

by (2.18) for Irving & Kirkwood's hydrodynamics:

$$\mathbf{v}_{IK}(\boldsymbol{x},t)=\frac{\int_{\mathcal{Z}_{\setminus i}}\sum_i m_i\,\dot{\boldsymbol{q}}_i(t)\,f(z_{/i}(\boldsymbol{x}),t)\,dz_{\setminus i}}{\int_{\mathcal{Z}_{\setminus i}}\sum_i f(z_{/i}(\boldsymbol{x}),t)\,m_i\,dz_{\setminus i}}; \tag{2.18$_{\text{rep}}$}$$

by $(3.4)_3$ in case of ψ-averaging:

$$\mathbf{v}_{\psi}(\boldsymbol{x},t)=\frac{\sum_i\psi(\boldsymbol{q}_i(t)-\boldsymbol{x})\,m_i\,\dot{\boldsymbol{q}}_i(t)}{\sum_i\psi(\boldsymbol{q}_i(t)-\boldsymbol{x})\,m_i}; \tag{3.4$_{3\,\text{rep}}$}$$

and by a spatially smooth $\mathbf{v}_{L_\mathsf{m}}$ satisfying (3.19) in case of cell averaging:

$$\mathbf{v}_{L_\mathsf{m}}|_{\mathscr{C}}\cong\boldsymbol{\alpha}_{\mathscr{C}} \tag{3.19$_{\text{rep}}$}$$

at all time $t\in\mathcal{I}_{t_0}$ for each mesoscopic space cell $\mathscr{C}\subset\mathscr{D}_t$. As to $\mathbf{v}_B$, its spacetime regularity depends ostensibly on that pertaining to $f_B(\cdot,\mathbf{c},\cdot)$, which in turn is the spacetime differentiability presumed on laying down Boltzmann equation (2.3). The requested smoothness in space of $\mathbf{v}_{IK}$ and $\mathbf{v}_{\psi}$ ensues from choosing conveniently smooth, respectively, the probability distribution f and the localization function ψ. In spite of this, their time course might suffer sudden discontinuities, whenever particle collisions were not negligible with respect to smooth at-a-distance particle interactions. As for $\mathbf{v}_{L_\mathsf{m}}$, the construction described in Section 3.2.4 ensures that it is uniformly L-Lipschitz (with L small) in space. However, it is discontinuous in time, due to the sudden jumps of the cell mass $M_{\mathscr{C}}$ and cell momentum $\boldsymbol{p}_{\mathscr{C}}$ whenever a particle enters/exits the cell.* Not only for preventing discontinuities, but also to filter out undesired fluctuations on the T_μ time scale, it is expedient to substitute $\mathbf{v}_{IK}$, $\mathbf{v}_{\psi}$, and $\mathbf{v}_{L_\mathsf{m}}$ with their mesoscopic time-averages

$$\overline{\mathbf{v}}(\boldsymbol{x},t):=\frac{1}{T_\mathsf{m}}\int_{t-T_\mathsf{m}/2}^{t+T_\mathsf{m}/2}\mathbf{v}(\boldsymbol{x},\tau)\,d\tau,$$

where $\mathbf{v}$ stands for either $\mathbf{v}_{IK},\mathbf{v}_{\psi}$, or $\mathbf{v}_{L_\mathsf{m}}$, under the assumption that microscopic fluctuations are integrated out with a proper choice of the mesoscopic time T_m. Such a measure is consistent both with "*averaging over a time interval of the order of the relaxation time of one's instruments*" advocated by Irving & Kirkwood in the passage from [12] we quote in the opening of Section 3, and with the weighted time-averages proposed by Murdoch & Bedeaux either in [16] or [27].

5. Conclusions: the physical content of the notion of body point

In CM, the notions of a body and its points are primitive. Bodies are observed against the background of a chosen spacetime structure, and consequentially granted a spatial extension. What makes a body and its points different from a space region and its points is the almost invariably accompanying adjective 'material', with its suggestive direct derivation from 'matter'. There is communal consensus that (i) among the many physical properties of matter, being massive is as basic as it is in particle mechanics, where the elementary objects of interest—our 'point particles'—are named 'point masses'; (ii) body parts of non-null volume—in fact, from our present perspective, of at

*Let the i-th particle enter/exit $\mathscr{C}$ at time t; then, $[\![M_{\mathscr{C}}]\!](t)=\pm m_i$, and $[\![\boldsymbol{p}_{\mathscr{C}}]\!](t)=\pm m_i\,\dot{\boldsymbol{q}}_i(t)$. While $m_i\ll M_{\mathscr{C}_\pm}$, generally $m_i|\dot{\boldsymbol{q}}_i|>|\boldsymbol{p}_{\mathscr{C}_\pm}|$, since typical *individual* thermal velocities are much larger than the streaming velocity.

least mesoscopic size—are body themselves, with the same material properties as the body they are parts of. But, what material quality should be attributed to a 0-dimensional material point? This is the question we have tried to answer. A widespread opinion holds that, at the very least, a 'body point'—as we prefer to call it—should be thought of as in some sense 'massy'. This is usually and more or less explicitly achieved by introducing a time-dependent mass density field ϱ, and by regarding the material point sitting at the space point $\boldsymbol{x}$ at time t as specified by the pair $(\boldsymbol{x}, \varrho(\boldsymbol{x}, t))$. The merit of the microscopically informed notion of body point we have proposed in this paper is that it *implicitly* conveys much more information about the physical properties of the CM body that point belongs to than just the spacetime-local value of mass density. In fact, the essential function of body points is to localize in space *all* mesoscopic physical properties, which, as such, are driven over time by collective—hence, average—features of the underlying microscopic dynamics.

Indeed, we have restricted ourselves to require consistency between discrete and continuum kinematics, that is, consistency between the description of the motion of a given material system when modeled either as a collection of point particles or as a continuous body. In so doing, we have emphasized the coarsening role played either by probability distributions, which embody generic a priori physical assumptions, or by deterministic averaging tools, whose mesoscopic resolving power mimics, in principle, that of the relevant measuring devices. The primary microscopic information that we have here manipulated conceptually, and that a numerical simulation would provide in practice, is a time-dependent collection of particle velocities, as determined by solving the Newtonian equations of motion, according to the nature of particle interactions and the action of the relevant external fields. Thus, both in principle and in practice, *the notion of body point we have proposed has a contingent, system-dependent physical content, the filtrate resulting from the adopted coarsening procedure.*

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Conflict of interest

The authors declare no conflict of interest.

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A. Appendix: Points are almost invariably in the need of an adjectival specification

A.1. The immaterial points of geometry and philosophical physics

Definition 1 in Book 1 of Euclid's *Elements* [54] (approximately 300 BC) concerns the geometrical notion of a *point*:

α'. σημεῖόν ἐστιν, οὗ μέρος οὐθέν ("a point is what has no parts")

or, in Fitzpatrick's translation,

1). “a point is that of which there is no part.”

Euclid’s Elements continue with these further definitions (Fitzpatrick’s translation again):

2). And a line is a length without breadth.
3). And the extremities of a line are points.
4). A straight-line is (any) one which lies evenly with points on itself.
5). And a surface is that which has length and breadth.*

Some 2200 years after, when geometry is axiomatized in Hilbert’s style, ‘point’ still is regarded as a primitive notion and, as such, needs no definition. In fact, Euclid’s definition is of an ostensive nature, in that it is meant to be directly and manifestly demonstrative of a character singling out points among other geometrical objects consisting of points, such as lines and surfaces. Euclid’s point is only superficially akin to Democritus’ ἄτομος (“uncuttable”), hence indivisible into parts.† In fact, cuttable objects have a latent material substance, which pre-qualifies them as objects of physics.

A.2. The massy points of mechanics

Mass is a primary property of matter. In PM, beginning with Newtonian’s, points are given both a position in space and a mass: they are termed *point masses*. In CM, a mass-density field is introduced and evaluated pointwise over the space region occupied by the observed body; it is customary to talk about *material points* for the points of such a region. The path from mass to material points is deducible from Truesdell’s introduction of point-related terminology in [55].

Firstly, in [55, Section I.3], where examples of universes of bodies are presented, the term *substantial point* is introduced “[t]o avoid any possible confusion with the term “particle” as used in physics”. From the dictionary, a ‘particle’ is a minute portion of matter; as such, at difference with any type of ‘point’, one expects a particle to occupy a space region with small but not null measure. Yet, in various influential expositions of continuum mechanics appeared in a fifty year span, from [56] in 1960 to [57] in 2010, the terms ‘particle’ and ‘material point’ are used interchangeably (cf., e. g., [57, Section 5.1]), a material point being as a rule identified by means of the space point it occupies in some chosen reference placement of the body it belongs to.

Interestingly, substantial points are introduced by Truesdell just before the notion of mass is given a measure-theoretic format in [55, Section I.4], where it is stated that “[t]he bodies of interest in mechanics have mass; as we may say, they are *massy*.” The hyphenated term *mass-point* is used for a substantial point when it is assigned a positive mass [55, p. 19]. The introduction of the term ‘material point’ is postponed until [55, Section IV.2], where the concept of ‘material’ is formalized by means of the notion of constitutive relation: a *material point* is a substantial point at which the stress response to a deformation history up to the current time has been specified by means of a constitutive mapping.

A.3. Should body points have a persistent physical identity?

Here is, reproduced from [58], Hellinger’s notion of a continuous medium and its points:

*A remarkable parallel with Euclid’s definitions 2 and 5 emerges in [55, p. 134], where the notions of *substantial line* and *substantial surface* are introduced, alongside with that of *substantial region*.

†Apropos of atom, Webster’s Dictionary says: “ORIGIN late Middle English (in the sense ‘indivisible’): from medieval Latin individualis, from Latin individuus, from in- ‘not’ + dividuus ‘divisible’ (from dividere ‘to divide’).” But, in our view, ‘to divide’ leaves unspecified the way a division into parts is achieved, not so ‘to cut’.

2. Der Begriff des Kontinuums.
2.a. Das Kontinuum and seine Deformation.
Das allgemeine *dreidimensionalen ausgedehnte kontinuierliche Medium*, auf das sich die folgenden Betrachtungen beziehen, bedeutet – unter Abstraktion von allen individuellen Eigenschaften der Materie – eine Gesamtheit von materiellen Teilchen, die erstens voneinander *unterscheidbar* sein und zweitens den Raum bzw. einem stetig begrenzten Raumteil *stetig ausfüllen* sollen.

2. The notion of continuum.
2.a. The continuum and its deformation.
The general *three-dimensionally extended continuous medium*, which is the object of the following considerations, consists—by abstraction from all individual properties of matter—of a collection of material points that firstly must be *distinguishable* the one for the other and, secondly, must *continuously fill* the whole space or, respectively, a continuous and bounded portion of space.

We see that, for Hellinger in 1914, having a persistent individual identity is the main defining feature of a material point—a body point, for us. Now, one may or may not care to carry out a microscopically-informed version of CM and, in particular, a microscopically informed notion of body point. In the second instance, as was noted in [59], Hellinger's presumption is a guaranteed consequence of restricting attention, as we did in Section 4.1, to globally invertible, smooth deformations, so that a continuous body evolves in spacetime in a way that can be tracked pointwise at each instant of the observation interval. This restriction precludes the analysis of many interesting motion classes; it also prohibits any study of body mutations involving creation or deletion of boundary points, as it happens with fracturing/healing processes or in drop splitting/coalescence. However, it is often expedient in CM, whenever comparing different *body shapes* (the space regions a body currently occupies) has importance, as it happens when guessing constitutive laws or checking their predictions. In the first instance, no matter the deterministic bottom-up notion of body point one seeks, it makes no sense to presume that one and the same collection of point particles is persistently associated with a given body point. Moreover, each of the four coarsening procedures we discussed yields a spatial velocity field, with the use of which the current body shape associated with the given material system is determined; the only persistent feature of each point of that shape is the label it is given in some reference shape.

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