ON THE MODELING OF TRANSPORT PHENOMENA IN CONTINUUM AND STATISTICAL MECHANICS

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Dedicated to Tomáš Roubíček on the occasion of his sixtieth birthday

Abstract. The formulation of balance laws in continuum and statistical mechanics is expounded in forms that open the way to revise and review the correspondence instituted, in a manner proposed by Irving and Kirkwood in 1950 and improved by Noll in 1955 and 2010, between the basic balance laws of Cauchy continua and those of standard Hamiltonian systems of particles.

1. Introduction. When equipped with suitable initial and boundary conditions, the archetypal parabolic equation
\[ \partial_t u = \Delta u \] (1)
delivers the space distribution and time evolution of the scalar-valued field \( u = \hat{u}(x, t) \). Interestingly, beside the standard approach to modeling macroscopic thermal and mechanical phenomena by introducing conveniently smooth fields, this deterministic equation can be arrived at by taking a probabilistic modeling approach consistent with a discrete microscopic picture of matter. In fact, both Continuum Mechanics (CM) and Statistical Mechanics (SM) provide mathematical descriptions of the basic transport phenomena, diffusion and convection, under form of balance laws that, when coupled with constitutive information, take the form of evolution equations: e.g., when the target phenomenology is heat conduction, the evolution equation for temperature is induced by energy balance modulo constitutive choices of Fourier type for energy itself and heat flux. CM balances are deterministic and SM balances probabilistic: the purpose of the present paper is to revise, review, and compare, these two modeling approaches. The probabilistic/stochastic modeling approach stemming from two famous papers by Einstein [6] and Langevin [14] is the subject of a companion paper, where special attention is given to the case of diffusion, normal, anomalous, and drift.

In CM, both convection and diffusion enter the general balance equation for a given field of interest: convection takes place in every body in motion, independently of its constitution and proportionally, as a rule, to the velocity field; diffusion does depend on material constitution, and generally vanishes only over those body parts.

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where the field is spatially uniform, just as observed experimentally by Fourier in 1822 for the temperature of a heat-conducting solid at rest and by Fick in 1855 for the concentration of solute particles migrating in a still liquid.

Likewise, in SM both transport mechanisms enter the Liouville evolution of a given observable. Indeed, the Liouville operator is modulated in terms of the system’s Hamiltonian: in the standard case when kinetic and potential energies only depend, respectively, on momenta and on Lagrangean coordinates, kinetic energy generally determines the convective part, and potential energy the diffusive part, of the Liouville evolution. Moreover, as Irving and Kirkwood have shown in their path-breaking 1950 paper if a Liouville’s equation is written for certain SM observables associable with the CM densities of, respectively, mass, momentum and energy, then it takes forms that can be regarded as counterparts of the relative CM balances.

Quick but fairly complete accounts of the general formats of balance laws are given in Sections 2, according to CM, and 3, according to SM; what probabilistic SM balances parallel the basic deterministic CM balances is the subject of Section 4, the relevant preparatory manipulations being relegated to the final Appendix; our main findings are recapitulated in the conclusive Section 5.

2. The format of CM balance laws. A difference between CM and SM is that there is no role in the latter for the notion of referential placement of a material system: SM invariably considers material systems in their current placement. Now, this is the standard CM practice for fluids, but not for solids, whose deformational vicissitudes are customarily described by comparing their current placement with a referential placement chosen once and for all. For an easier comparison with the SM balance laws to be dealt with in the next section, we here derive the current versions of the CM balance laws.

Two transport phenomena are in order at the boundary of the space region currently occupied by a typical part of a continuous body in motion, namely, diffusion and convection; we give a quick description of both.

Let \( \rho \) denote the current mass density; moreover, let \( \psi \) denote the density per unit mass of a physical field of interest, so that \( \rho \psi \) is the corresponding density per unit current volume. The part-wise balance law of field \( \psi \) at time \( t \) has the following standard form:

\[
\left( \int_{P_t} \rho \psi \right)' = - \int_{\partial P_t} i_\psi [n] + \int_{P_t} s_\psi,
\]

where \( i_\psi \) and \( s_\psi \) are, respectively, the diffusive influx and the source of \( \psi \). An influx has always tensorial order bigger by 1 than the field it is associated with; thus, the outcome of the contraction product \( i_\psi [n] \) of the influx of \( \psi \) and the outer unit normal \( n \) to the boundary \( \partial P_t \) of \( P_t \) is a field of the same tensorial order as \( \psi \)

1 This paper is the fourth in a series of fourteen, whose general title is “The statistical mechanical theory of transport phenomena”. I am indebted to E. Fried for pointing out to me two other papers in this series of relevance for the matters that I here treat, the eleventh [12] and the fourteenth [13].

2 In this connection, recall the title purpose of [12], namely, to derive “[t]he equations of hydrodynamics”, not of elastodynamics, say, although the equations they derive are common to both theories. Indeed, we know of no precise SM distinction between material aggregation states such as fluidity and solidity. Not surprisingly, a distinction between fluids and solids is also absent in MD, the brachium saeculare of SM, whose role is to provide a numerical realization of the processes studied by standard SM.
and \( s_\psi \); the symbol \([ \cdot ]\) is meant to convey the idea that in a contraction product the first factor acts linearly on the second.

We now give (2) a form that makes patent the mechanism of transport by convection. Preliminary, note that, for \( \psi(x,t) \equiv 1 \), \( i_\psi \equiv 0 \) and \( s_\psi \equiv 0 \), (2) gives the part-wise form of the *mass conservation law*:

\[
\left( \int_{P_t} \rho \right)^\cdot = 0, \tag{3}
\]

whose point-wise formulation is:

\[
\dot{\rho} + \rho \text{div } \mathbf{v} = 0 \tag{4}
\]

(a superposed dot, just as a superscript dot in (2) and (3), signifies time differentiation). We recall here for later reference that in any volume-preserving motion the velocity field is everywhere divergenceless:

\[
\text{div } \mathbf{v} = 0, \tag{5}
\]

so that (4) becomes

\[
\dot{\rho} = 0 \quad \text{or rather, equivalently,} \quad \partial_t \rho + \text{grad } \rho \cdot \mathbf{v} = 0. \tag{6}
\]

If mass is conserved, then

\[
\left( \int_{P_t} \rho \psi \right)^\cdot = \int_{P_t} \rho \dot{\psi}. \tag{7}
\]

Moreover, an application of the divergence lemma yields:

\[
\int_{\partial P_t} i_\psi \left[ \mathbf{n} \right] = \int_{P_t} \text{div } i_\psi. \tag{8}
\]

With (8) and (7), (2) takes, via localization, the following form:

\[
\rho \dot{\psi} = -\text{div } i_\psi + s_\psi, \tag{9}
\]

the *point-wise balance law* of field \( \psi \). This basic equation can be given the form:

\[
\partial_t (\rho \psi) = -\text{div } (i_\psi + j_\psi) + s_\psi, \tag{10}
\]

where

\[
j_\psi := \rho \psi \otimes \mathbf{v}. \tag{11}
\]

the part-wise version of (10) is

\[
\int_{P_t} \partial_t (\rho \psi) = -\int_{\partial P_t} (i_\psi + j_\psi)[\mathbf{n}] + \int_{P_t} s_\psi. \tag{12}
\]

The triplet \((i_\psi, j_\psi, s_\psi)\) specifies the *inflow* of \( \psi \) into \( P_t \).

*Convection*, the phenomenon of boundary transport of \( \psi \) due to body motion, is brought into the open by the formulation (12) of the balance law for \( \psi \): under the assumption that mass is conserved, a material element in motion with velocity \( \mathbf{v} \) *conveys* \( \psi \) in that a convective current \( j_\psi \), whose representation (11) is *material-independent*, is observed at the boundary of each body part.

*Diffusion*, the phenomenon of migration of a substance through a material body, generally independent of the motion of the latter and inducing in the region it

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The *dyadic product* \( \otimes \) of two quantities \( \psi, a \) of arbitrary tensorial orders is defined by its linear action on quantities of the same tensorial order as the second factor:

\[
(\psi \otimes a)[b] := (a[b])\psi \quad \text{for all } b.
\]

If \( \psi \) is a scalar, then the dyadic product of \( \psi \) and \( a \) reduces to scalar multiplication: \( \psi \otimes a \equiv \psi a \), whatever the tensorial order of \( a \).
occupies the evolution of the field \( \psi \), is manifested by the presence of the diffusive current \( i_\psi \) in whatever version the balance of field \( \psi \) is given. A constitutive prescription is needed to specify diffusion, the following being a fairly general and thermodynamically-consistent prescription of the diffusive current:

\[
\begin{align*}
    i_\psi &= -\hat{D}(\psi, \text{grad } \psi)[\text{grad } \psi], \\
    \langle \hat{D}(\psi, \text{grad } \psi)[\text{grad } \psi] \rangle[\text{grad } \psi] &\geq 0; \\
\end{align*}
\]

(13)

\( D \) is called the \textit{diffusivity tensor}.\footnote{For a derivation of representation (13) see ([7], App. B).} Diffusion is \textit{isotropic} if \( \langle \hat{D}(\psi, \text{grad } \psi)[a] \rangle[a] \propto a \), that is to say, if the diffusivity tensor is a scalar multiple of the identity map over the linear space where \( \text{grad } \psi \) takes its values, so that (13) specializes into

\[
\begin{align*}
    i_\psi &= -\hat{d}(\psi, \text{grad } \psi)\text{grad } \psi, \\
    \hat{d}(\psi, \text{grad } \psi) &\geq 0; \\
\end{align*}
\]

(14)

with this, in the absence of motion, (10) reduces to the following general antecedent of (1):

\[
\partial_t (\rho \psi) = \text{div} (\hat{d}(\psi, \text{grad } \psi)\text{grad } \psi) + s_\psi.
\]

(15)

\textbf{Remark 1.} In the literature, balance equations of this form are often called \textit{continuity equations} and, if the source term depends functionally on the unknown field \( \psi \) (because, say, a chemical reaction entails creation or annihilation of a certain amount of \( \psi \)), \textit{reaction-diffusion equations}; mathematical analysts, whose interest for the mechanical well-posedness of the equations they study is oftentimes modest, refer to them either as to \textit{gradient flows} of Dirichlet-type functionals or as to \textit{relaxation laws} of the relative Euler-Lagrange equations.

The presumptions underlying gradient-flow derivations of evolution PDEs of type (1) are that minimization of a given functional characterizes equilibrium states; that any evolution process can be regarded as the consequence of some initial perturbation of an equilibrium state; and that one or another equilibrium state is to be more and more approached as a consequence of a built-in isotropic dissipation mechanism. For the simplest exemplification of an \( L^2 \)-gradient flow, pick equation (1) and observe that the associated Dirichlet integral over the referential space region \( R \):

\[
F\{u\} := \int_R \frac{1}{2} |\nabla u|^2
\]

plays the role of a Liapunov function, because

\[
\frac{d}{dt} F\{u\} = -\int_R \hat{u}^2 \leq 0
\]

along whatever process that solves (1). This suggests that, as \( t \to \infty \), the field \( u \) tends to coincide with the minimizer of the energy functional (10), that is to say, with the solution of the corresponding Euler-Lagrange equation. Thus, in a manner of speaking, a gradient-flow derivation induces an orientation of the time arrow, in that it postulates an intrinsic irreversibility due to the simplest – but by no means the only one – dissipation mechanism compatible with the Second Law of thermodynamics.

\footnote{For a more general example, consider the functional \( G\{u\} = \int_R g(u, \nabla u) \), with \( u = (u_1, u_2, \ldots, u_m) \). The associated system of relaxation laws:

\[
\beta_i \partial_t u_i = -\left( \partial_{u_i} g - \partial_{x_j} (\partial_{u_i,j} g) \right) \quad (i = 1, 2, \ldots, m; \text{ no sum on } i),
\]

with \( (\beta_1, \beta_2, \ldots, \beta_m) \) a list of positive \textit{mobility constants}, is nothing but the gradient flow of functional \( G \).}
3. **The format of SM balance laws.** For \((q, p)\) a pair of \(n\)-strings of Hamiltonian coordinates, let \(z = (q, p)\) denote a point in the state space \(Z\); moreover, let 

\[
\{(z, t) \mapsto \tilde{\rho}(z, t) : t \in \mathbb{R}\}
\]

denote the time evolution of a chosen probability measure over \(Z\).

3.1. **Liouville’s theorem and Liouville’s equation.** Let

\[
\text{grad}_z(\cdot) := (\partial_q(\cdot), \partial_p(\cdot))
\]

(17)
denote the state-space gradient operator. For an evolving Hamiltonian system, *Liouville’s Theorem* can be stated as follows:

*the state-velocity field \(\dot{z} = (\dot{q}, \dot{p})\) is divergenceless:

\[
\text{div}_z \dot{z} = 0.
\]

(18)

Note the formal identity with (5): just as an incompressible continuous body is constitutively capable solely of divergenceless motions, a Hamiltonian system is constitutively capable only of divergenceless evolutions in the state space. Moreover, just as the mass-conservation condition (4) takes the alternative special forms (6) whenever (5) prevails, it follows from (18) that

*the probability measure is materially constant in time at each point of the state space:

\[
\dot{\tilde{\rho}} = 0 \quad \text{or rather, equivalently,} \quad \partial_t \tilde{\rho} + \text{grad}_z \tilde{\rho} \cdot \dot{z} = 0 .^6
\]

(19)

The conservation condition (19) is often called the *Liouville equation* and written as

\[
\partial_t \tilde{\rho} + \ell[\tilde{\rho}] = 0,
\]

(20)

where

\[
\ell[\cdot] := \sum_i \left( (\partial_{p_i} H) \partial_{q_i} [\cdot] - (\partial_{q_i} H) \partial_{p_i} [\cdot] \right)
\]

(21)

is the *Liouville operator* for a system whose Hamiltonian is \(H\). The Liouville equation evolves a given initial value \(\tilde{\rho}(z, t_0) = \tilde{\rho}_0(z)\) of the probability measure at a given point of the state space into its current value \(\tilde{\rho}(z, t)\) at the same point. The kernel of Liouville operator \(\ell\) consists of all probability measures that do not depend explicitly on time; in particular, it contains all stationary probability measures of Gibbsian type, that is to say, probability measures having the general form apparently first brought to attention by Gibbs himself, namely,

\[
\tilde{\rho}(z) = \phi(H(z)) \geq 0.
\]

Since we are interested in the modeling of transport phenomena, which in the SM parlance are studied by *non-equilibrium thermodynamics*, all probability measures we deal with do depend explicitly on time.

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6 The distinction between ‘material’ and ‘spatial’ time derivatives is essential in the CM of solids, where a central role is played by a comparison between the current placement and an arbitrarily chosen reference placement, which needs not but may very well be the initial placement. In SM, the only special state of the system under study is the initial state; accordingly, by ‘materially constant in time’ we mean ‘the same as in the initial state’.

7 Here and henceforth we presume it understood over what set of integers the summation index runs; accordingly, in (21) \(\sum_i\) signifies \(\sum_{i=1}^n\).
3.2. Liouville evolution of a macroscopic observable. A microscopic observable is a function \( z \mapsto o = \tilde{o}(z) \) defined over the whole state space; the corresponding macroscopic observable is delivered by a weighted-average mapping:

\[
\langle o \rangle(t) := \int_Z \tilde{o}(z)\tilde{\rho}(z,t)\,dz,
\]

and is referred to as the expected value of \( \tilde{o} \) at time \( t \) with respect to the chosen probability measure.

An important usage of the Liouville equation is to compute the time derivative of the expected value of a microscopic observable: under the assumption that \( \int_Z \ell[\tilde{o}(z)\tilde{\rho}(z,t)]\,dz = 0 \)

\[
\partial_t \langle o \rangle = \langle \ell[\tilde{o}] \rangle.
\]

We read (23) as the assertion that, given a Hamiltonian system, the time rate of the expected value \( \langle o \rangle \) of a microscopic observable \( \tilde{o} \) equals the expected value of the Liouville operator evaluated at \( \tilde{o} \); on recalling (21), relation (23) can be written as

\[
\partial_t \langle o \rangle = \langle \partial_q \tilde{o} [\partial_p H] - \partial_p \tilde{o} [\partial_q H] \rangle.
\]

Whenever \( H = \tilde{H}(q,p) = \tilde{K}(p) + \tilde{U}(q) \), as is the case for the systems of mass points on which we are going to focus, (24) becomes:

\[
\partial_t \langle o \rangle = \langle \partial_q \tilde{o} [\partial_p K] - \partial_p \tilde{o} [\partial_q U] \rangle.
\]

As we shall see next, for any chosen density field \( \psi \) and for a suitable choice \`a la Irving-Kirkwood-Noll (IKN) of a related macroscopic observable \( \langle o_\psi \rangle \), a striking correspondence between the CM evolution law (10) for \( \psi \) and the SM evolution law (25) for \( \langle o_\psi \rangle \) can be found. Precisely, whatever \( \psi \), the kinetic-convective term \( -\text{div} \mathbf{j}_\psi \) in (10) is paralleled by a kinetic-convective contribution to the balance of the related macroscopic observable \( \langle o_\psi \rangle \): convection is a universal transport mechanism, no matter if modelled deterministically, as is done in CM, or probabilistically, as in SM. Concerning transport by diffusion, the CM constitutive-diffusive term \( -\text{div} \mathbf{j}_\psi \) finds an SM counterpart both in the case when \( \psi \) is momentum and in the case when \( \psi \) is internal-energy density.

4. How to find the SM equivalent of a CM balance law. First Navier in 1823, then Cauchy, Lamé, and others (see the “Historical Introduction” in [15] and [24], Section 301), tried to answer the following fundamental question:

*Given that matter has a discrete structure, what is the discrete counterpart of its continuous description?*

All those great men had modest success in furnishing an answer, chiefly because their ‘molecular physics’ was based on the naive picture of matter available at their time. In fact, the question stands, although today more than one attempt to give it a convincing answer has been made; we begin by rephrasing it in a less encompassing but more specific form, borrowed from [12]:

*What are the discrete counterparts*

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8It can be shown that this condition is fulfilled if the potential energy is reasonably regular and has a sufficiently fast decay at infinity.
of the CM notions of mass density, velocity, stress, kinetic energy, internal energy, and heat flux?

- of the ‘equations of hydrodynamics’, that is, of the CM balance laws of mass, momentum, and total energy?

These three equations are called in [12] the equations of, respectively, ‘continuity’, ‘motion’, and ‘transport of energy’; interestingly, Irving and Kirkwood’s “equations of hydrodynamics” became Noll’s “Grundgleichungen der Thermomechanik der Kontinua” [17]. All these authors ignored a balance that, although irrelevant in Newtonian mechanics, should be listed among the basic equations of continuum thermomechanics, that is, the balance of moment of momentum. In the case of Cauchy’s continua, this equation can be stated as the requirement that the Cauchy-stress field be symmetric-valued; under reasonable constitutive assumptions to be specified later on, the discrete counterpart of the Cauchy stress constructed according to the IKN method turns out to be symmetric. The balance of moment of momentum plays a crucial role in the case of continua whose discrete counterparts are systems of massy particles more structured than the standard IKN system: to imagine such microscopic structures becomes the main modeling issue [21, 22, 3].

To answer the questions above, we use a version – cleansed and generalized by Noll in 1955 [17] and, more recently, in [18] – of the method proposed by Irving and Kirkwood [12], in line with the XIX century views about the discrete-to-continuum passage: working in a SM framework, to deduce the macroscopic equations of classic thermomechanics by phase-space averaging of the Hamiltonian version of the microscopic Newtonian equations ruling the motion of a standard system of massy particles.

4.1. Prelims. We set:

\[ q = (r_1, \ldots, r_N), \quad p = (p_1 = m_1 \dot{r}_1, \ldots, p_N = m_N \dot{r}_N), \]  

where \( r_n = x_j - x_o \) is the current position vector with respect to a fixed origin \( x_o \) of the \( J \)-th particle in a collection of \( N \). The total kinetic energy reads:

\[ \hat{K}(p) = \sum_j K_j, \quad K_j := \frac{\|p_j\|^2}{2m_j}; \]  

particle interactions are ruled by a potential energy of the form:

\[ \hat{U}(q) = \sum_j U_j, \quad U_j := \frac{1}{2} \sum_K V(r_{JK}), \quad r_{JK} := |r_j - r_K|, \quad V(0) = 0. \]  

Consequently,

\[ \partial_{p_j} K = \partial_{p_j} K_j = \frac{p_j}{m_j} = v_j, \quad \partial_{r_j} U = 2 \partial_{r_j} U_j = \sum_K V'(r_{JK}) \frac{r_j - r_K}{|r_j - r_K|}. \]  

\[ ^9 \text{The IKN method has been recently re-exposed and generalized by a number of authors (see e.g. [23, 4, 3, 5]). The basic concepts and equations of CM can also be derived from a discrete picture of matter by the use of weighted space-time averages of molecular quantities being suitably indifferent to changes in observer (see [16] and the earlier papers quoted therein by the author and coworkers). A similar approach was developed in [11], with the use of a space-localization function easier to handle mathematically than the Dirac localization adopted by Irving and Kirkwood.} \]

\[ ^{10} \text{For simplicity, we ignore both external contributions to the system’s potential energy and internal contributions that are not reducible to pair-wise form.} \]
so that the Liouville equation (25) for the evolution of a macroscopic observable becomes:

\[ \partial_t \langle o \rangle = \sum J \langle \partial_r \hat{o} [\partial_p J, K] - 2 \partial_p J \hat{o} [\partial_r U_J] \rangle, \]

(cf. equation (2.7) of [12]), or rather

\[ \partial_t \langle o \rangle = \sum J \langle \partial_r \hat{o} [v_J] + \partial_p J \hat{o} [f_J] \rangle, \]

where we let

\[ f_J := \sum K f_{JK}, \quad f_{JK} := -\partial_r J V(r_{JK}) = -V'(r_{JK}) \frac{r_J - r_K}{|r_J - r_K|}, \]

and we identify \( f_{JK} \) as the force exerted by particle \( K \) on particle \( J \), and \( f_J \) as the total force exerted on particle \( J \) by all other particles. Note that \( f_{JK} = -f_{KJ} \), and that \( f_{JK} \) is attractive (repulsive) for \( V'(r_{JK}) > 0 \) (for \( V'(r_{JK}) < 0 \)).

4.2. The target CM balances. The IKN method consists of three steps:

(i) mass density, momentum, and total energy, are associated with the expectations of certain suitable microscopic observables;

(ii) each of the above expectations, in the order, is evolved \( \text{`a la} \) Liouville with the use of (31)-(32);

(iii) the so-obtained Liouville flows are identified term by term with their CM counterparts for Cauchy bodies, which are conveniently cast in the format (10)-(11):

- (mass conservation)
  \[ \partial_t \rho + \text{div} (\rho v) = 0; \]  

- (momentum balance)
  \[ \partial_t (\rho v) + \text{div} (\rho v \otimes v - T) = 0; \]  

- (total-energy balance)
  \[ \partial_t (\rho \tau) + \text{div} (\rho \tau v + q - T^T v) = 0, \quad \tau = \varepsilon + \kappa, \quad \kappa = \frac{1}{2} \dot{v} \cdot v. \]

Here, \( T, \tau, \varepsilon, \text{and} \kappa \), denote Cauchy’s stress and, respectively, total, internal, and kinetic, energy densities; for simplicity, in line with what we did when we specified the discrete potential energy mapping \( \hat{U} \), external momentum sources (that is to say, external noninertial distance forces) have been left out from (34), as well as external energy sources from (35); the convective contributions to the boundary inflows of mass, momentum and total energy, are:

\[ \rho v, \quad \rho v \otimes v, \quad \text{and} \quad \rho \tau v; \]

the relative diffusive contributions are:

\[ 0, \quad -T, \quad \text{and} \quad q; \]

an internal source term – namely, \( \text{div} (T^T v) \) – is needed to balance energy. Since external non-inertial sources are irrelevant to our present purpose, we have set them all to null.

With the help of (33), equation (34) can be given the usual form

\[ \rho \dot{v} = \text{div} T, \]
where the inertial distance force $d^{in} := -\rho \ddot{v}$ appears. Moreover, this time with the help of both (33) and (34), equation (35) can be reduced to the *internal-energy balance* familiar in thermomechanics:

$$\rho \dot{\varepsilon} + \nabla \cdot \mathbf{q} - \mathbf{T} \cdot \nabla \mathbf{v} = 0,$$

or rather, equivalently but in the format (10)-(11),

$$\partial_t (\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \mathbf{v} + \mathbf{q}) - \mathbf{T} \cdot \nabla \mathbf{v} = 0. \quad (39)$$

Finally, on subtracting (39) from (35) and making use of (38), we arrive at the *kinetic-energy balance*:

$$\partial_t (\rho \kappa) + \nabla \cdot (\rho \kappa \mathbf{v}) - \mathbf{v} \cdot \nabla \mathbf{T} = 0; \quad (40)$$

on accounting for (38), equation (40) is equivalent to

$$\rho \dot{\kappa} - \rho \dot{\varepsilon} \mathbf{v} \cdot \mathbf{v} = 0. \quad (41)$$

We see from (39) that $\mathbf{q}$ is indeed a diffusive contribution specific of internal energy, and from (40) that there is no diffusive contribution to the balance of kinetic energy. In view of the identity

$$\nabla \cdot (\mathbf{T} \mathbf{v}) = \mathbf{T} \cdot \nabla \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{T},$$

we also see that the internal source of total energy splits into a source of internal energy, equal to the stress-power expenditure $\mathbf{T} \cdot \nabla \mathbf{v}$, plus a source of kinetic energy, equal to the negative of the power expended by the inertial distance force, $\mathbf{v} \cdot \nabla \mathbf{T} = -d^{in} \cdot \mathbf{v}$.\(^{11}\)

In preparation for the identifications of their SM counterparts to be made in Sections 4.4.3 and 4.4.4, we state the partial balances (40) and (39) in the following more general forms of type (10)-(11):

- *(kinetic-energy balance)*

$$\partial_t (\rho \kappa) + \nabla \cdot (\rho \kappa \mathbf{v}) - \mathbf{v} \cdot \nabla \mathbf{T} - s^{extra}_\kappa = 0; \quad (42)$$

- *(internal-energy balance)*

$$\partial_t (\rho \varepsilon) + \nabla \cdot (\rho \varepsilon \mathbf{v} + \mathbf{q}) - \mathbf{T} \cdot \nabla \mathbf{v} - s^{extra}_\varepsilon = 0, \quad (43)$$

with

$$s^{extra}_\kappa + s^{extra}_\varepsilon = 0 \quad (44)$$

(note that introducing the additional internal sources $s^{extra}_\kappa$ and $s^{extra}_\varepsilon$ leaves the total-energy balance (35) unchanged).\(^{11}\)

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\(^{11}\)That for whatever chosen class of massy continuous bodies the constitutive choices for the two manifestations of inertial interactions, kinetic energy and inertia force, should be consistent in the following sense:

$$\frac{d}{dt} (\text{kinetic energy}) + (\text{inertial power}) = 0$$

has been pointed out in [19]; the discovery power intrinsic to this balance requirement has been exemplified in [5, 9, 10, 20].
4.3. The IKN counterparts of the CM fields. The identifications mentioned under step (iii) of the IKN method are successful because of a shrewd choice for the common form of microscopic observables, namely,
\[ \hat{o}(z, x) = \sum_J \hat{o}_J(z) \delta(r_J - r), \quad r = x - x_0; \] (45)
according to (22), the associated macroscopic observables have the common form:
\[ \langle o \rangle(x, t) = \langle \sum_J \hat{o}_J(z) \delta(r_J - r) \rangle, \] (46)
or rather, equivalently,
\[ \langle o \rangle(x, t) = \sum_J \langle o_J \rangle(x, t), \quad \langle o_J \rangle(x, t) = \int_Z \hat{o}_J(z, x) \delta(r_J - r) \tilde{\rho}(z, t) dz. \] (47)

For mass, momentum, kinetic energy, and internal energy, of a particle, Irving and Kirkwood chose:
\[ \hat{o}_J(z) = \begin{cases} m_J, \\
p_J, \\
K_J, \\
U_J, \end{cases} \] (48)
whence they deduced the following macro/micro identifications of type (46):
- for mass density,
\[ \rho \equiv \langle \sum J m_J \delta(r_J - r) \rangle; \] (49)
- for momentum,
\[ p(x, t) \equiv \sum_J \langle p_J \delta(r_J - r) \rangle; \] (50)
- for motion velocity,
\[ v(x, t) = (p^{-1} p)(x, t) \equiv \left( \langle \sum J m_J \delta(r_J - r) \rangle \right)^{-1} \sum_J \langle p_J \delta(r_J - r) \rangle; \] (51)
- for kinetic-energy density,
\[ (\rho K)(x, t) \equiv \sum_J \langle K_J \delta(r_J - r) \rangle; \] (52)
- for internal-energy density,
\[ (\rho U)(x, t) \equiv \sum_J \langle U_J \delta(r_J - r) \rangle. \] (53)

The calculations leading to the relative discrete balances have been detailed by Irving and Kirkwood [12], implemented by Noll [17, 18], and repeated many times, with minor variants, in recent times (see, e.g., Section 8.2 of [23]). We relegate to the Appendix our own version of those calculations.

12The expectation of finding the J-th mass point at x at time t is:
\[ \langle \delta(r_J - r) \rangle(x, t) = \int_Z \delta(r_J - r) \tilde{\rho}(z, t) dz. \]
4.4. The SM counterparts of the target CM balances.

4.4.1. Mass conservation. To begin with (see Section 6.1), the probabilistic SM counterpart of the deterministic CM statement of mass conservation is easily found to be the boxed equation here below:

$$\partial_t \rho \equiv \partial_t \left( \sum_J m_J \delta(r_J - r) \right) = -\partial_r \left( \sum_J p_J \delta(r_J - r) \right) \equiv -\text{div} (\rho v); \quad (54)$$

in both theories, the mass-transport mechanism is exclusively convective.

4.4.2. Momentum balance. The SM counterpart of the CM momentum balance is:

$$\partial_t \left( \sum_J p_J \delta(r_J - r) \right) + \sum_J \left( \partial_r (p_J \delta(r_J - r))[v_J] - \sum_J f_J \delta(r_J - r) \right) = 0, \quad (55)$$

that is, equation (70) in Section 6.2. In view of the developments in that section, it follows from (55) that

$$\partial_t (\rho v) + \text{div} (\rho v \otimes v) = \text{div} T \equiv -\partial_r \left( \sum_J m_J \delta(r_J - r)(v_J - v) \otimes (v_J - v) \right) + f, \quad (56)$$

where, in line with (45)-(46), we have introduced the force field

$$f \equiv \langle f \rangle (x, t) := \langle \sum_J f_J(z) \delta(r_J - r) \rangle; \quad (57)$$

the emerging issue is to identify the discrete counterpart of the Cauchy stress $T$.

We show in Section 6.2 that, to within a divergenceless addendum, we may take

$$T \equiv K + R, \quad (58)$$

with the kinetic stress

$$K = -\langle \sum_J m_J \delta(r_J - r)(v_J - v) \otimes (v_J - v) \rangle \quad (59)$$

and the reaching stress

$$R = -\frac{1}{2} \int_V \left( \int_0^1 \gamma(x - (1 - \alpha)v, x + \alpha v)d\alpha \right) v \otimes v dv, \quad (60)$$

$$\gamma(x, y) = -|x - y|^{-1} \sum_J \sum_K \langle V'(r_{JK}) \delta(x_J - x) \delta(x_K - y) \rangle,$$

such that

$$\text{div} R = f. \quad (61)$$

Both $K$ and $R$ are symmetric. Both $\text{div} K$ and $\text{div} R$ play the role of SM momentum sources, the first kinetic and the second constitutive, while $\text{div} T$, the only CM momentum source, is constitutive in nature.

Identification (58)-(60) completes our juxtaposition of CM and SM momentum balances; on recalling equations (35), (43), and (42), this identification must not be forgotten when it comes to search for similar juxtapositions for balances of energy, kinetic, internal, or total.
4.4.3. Kinetic-energy balance. In view of equations (75) and (76) in Section 6.3, the IKN kinetic-energy balance is:
\[
\partial_t \langle \sum J K J \delta(r J - r) \rangle + \partial_r \langle \sum J K J \delta(r J - r) v J \rangle - \langle \sum J \delta(r J - r) f J \cdot v J \rangle = 0
\] (62)
(cf. equation (6.4) in [12]). Irving and Kirkwood leave this discrete balance as is, we do not.

To see whether (62) does indeed qualify as a counterpart of the CM balance (42), just as we did for the balances of mass and momentum, we try and juxtapose them piece by piece:
\[
\partial_t (\rho \kappa) + \text{div} (\rho \kappa v) = \partial_t \langle \sum J U J \delta(r J - r) \rangle + \partial_r \langle \sum J U J \delta(r J - r) v \rangle + \partial_r \langle \sum J U J \delta(r J - r) (v J - v) \rangle + (v \cdot \text{div} R) = 0
\]

Given (58), the question mark in the last line of the above relation chain could be removed if the following juxtaposition were tenable:
\[
v \cdot \text{div} K + s^\text{extra} = -\partial_r \langle \sum J K J \delta(r J - r) (v J - v) \rangle + \sum J \delta(r J - r) f J \cdot (v J - v).
\]

We make the reasonable assumption that \( f \) is equipowerful to the force system \( \{|f J| J = 1, 2, \ldots, N\} \):
\[
\langle \sum J \delta(r J - r) f J \cdot v J \rangle \equiv f \cdot v
\]
(recall definition (57)). Consequently, the SM counterpart of \( s^\text{extra}_\kappa \) is identified by posing
\[
s^\text{extra}_\kappa \equiv v \cdot \partial_r \langle \sum J \delta(r J - r) (v J - v) \rangle
\]
\[
- \partial_r \langle \sum J K J \delta(r J - r) (v J - v) \rangle.
\]

4.4.4. Internal-energy balance. It is shown in Section 6.4 that the IKN internal-energy balance is:
\[
\partial_t \langle \sum J U J \delta(r J - r) \rangle + \partial_r \langle \sum J U J \delta(r J - r) v \rangle + \partial_r \langle \sum J U J \delta(r J - r) (v J - v) \rangle + \frac{1}{2} \langle \sum J \sum K (v J - v) \cdot f J K (\delta(r J - r) + \delta(r K - r)) \rangle = 0.
\]

With a view toward paralleling equation (43), we set
\[
\partial_t (\rho \varepsilon) + \text{div} (\rho \varepsilon v) \equiv \partial_t \langle \sum J U J \delta(r J - r) \rangle + \partial_r \langle \sum J U J \delta(r J - r) v \rangle,
\]
and we remain with
\[
\text{div } q - T \cdot \nabla v - s^\text{extra}_e \equiv \partial_r \left( \sum J U_J \delta(r_J - r)(v_J - v) \right)
+ \frac{1}{2} \sum J \sum K (v_J - v) \cdot f_{JK} \left( \delta(r_J - r) + \delta(r_K - r) \right).
\]

We move further by setting:
\[
q \equiv \left( \sum U_J \delta(r_J - r)(v_J - v) \right) + q^{\text{add}},
\]
where the vector field \(q^{\text{add}}\), on accounting for (44) and (65), is to be chosen consistent with
\[
\text{div } q^{\text{add}} - R \cdot \nabla v \equiv \frac{1}{2} \sum J \sum K (v_J - v) \cdot f_{JK} \left( \delta(r_J - r) + \delta(r_K - r) \right)
- \partial_r \left( \sum m_J \delta(r_J - r)(v_J - v) \otimes (v_J - v) \right) v + \left( \sum K J \delta(r_J - r)(v_J - v) \right);
\]
this juxtaposition makes visible the twofold, constitutive and kinetic, nature of \(q^{\text{add}}\).

4.4.5. Total-energy balance. The IKN total-energy balance is arrived at by summing up the kinetic- and internal-energy balances (62) and (66). On juxtaposition of the result with (35), and on accepting (64), one finds that
\[
\text{div } (q - T^T v) \equiv \partial_r \left( \sum J (U_J + K_J) \delta(r_J - r)(v_J - v) \right)
+ \frac{1}{2} \sum J \sum K (v_J - v) \cdot f_{JK} \left( \delta(r_J - r) + \delta(r_K - r) \right).
\]

5. Conclusions. In the first part of this paper we have revised the modeling of transport phenomena in both continuum and statistical mechanics. In the second part we have dealt, in a manner proposed by Irving and Kirkwood [12] and improved by Noll [17, 18], with a correspondence instituted between the basic balance laws of Cauchy – aka ‘simple’ – continua and those of standard discrete systems of massy particles.\(^{13}\) In particular, we have identified the discrete counterparts of the fields entering the continuum description of diffusion mechanisms, namely, the Cauchy stress \(T\) and the heat flux \(q\) (cf., respectively, equations (58)-(59)-(60) and (67)-(68)). Now, while in continuum mechanics both \(T\) and \(q\) are specified solely by constitutive prescriptions, their discrete identifications both come out consisting of constitutive and kinetic parts, the kinetic parts being Galilean-invariant manifestations of the particles’ random fluctuation motion.

These manifestations are not the only ones. In fact, in continuum mechanics the internal sources of both kinetic and internal energy have the well-known representations in terms of \(T\) shown in the relative balances, equations (40) and (39); moreover, the discrete counterpart of \(T\) is fixed (to within a non-influential divergenceless addendum) so as to achieve the juxtaposition of the continuum and discrete momentum balances. Thus, when the continuum balances of kinetic and internal energies are juxtaposed with their putative discrete counterparts, it becomes convenient to relax the rigidity induced by the previous identification of a

\(^{13}\)As remarked in the opening of Section 4, complex – aka ‘non-simple’ – continua call for discrete systems more structured than the standard one.
discrete counterpart for $T$. This is done by generalizing (39) into (43), where the additional internal source of internal energy $s^\text{extra}_c$ appears; at the same time, so as to let the balance statement of total energy (35) unaffected, the kinetic-energy balance (40) is generalized into (42) by the introduction of the additional internal source $\kappa^\text{extra} = -s^\text{extra}_c$. The occurrence of such a purely kinetic contribution to internal-energy production is a macroscopic consequence of microscopic motion randomness that continuum mechanics could not predict were it not IKN-hybridized with statistical mechanics.

6. Appendix. The IKN derivation of SM balances. The common format we use for SM balances is that of equation (31), namely,

$$\partial_t \langle o \rangle = \sum_J \langle \partial_{r_J} \tilde{o} [v_J] + \partial_{p_J} \tilde{o} [f_J] \rangle. \quad (69)$$

6.1. Mass balance. With the choice (48) for observables, (45) becomes:

$$\tilde{o}(z,x) = \sum_K m_K \delta (r_K - r),$$

whence

$$\partial_{r_J} \tilde{o} = -m_J \partial_r \delta (r_J - r), \quad \partial_{p_J} \tilde{o} = 0 \quad (14)$$

moreover, (46) becomes:

$$\langle o \rangle (x,t) = \langle \sum_J m_J \delta (r_J - r) \rangle.$$ 

Consequently, (69) takes the following form:

$$\partial_t \langle o \rangle = -\sum_J \langle p_J \cdot \partial_r \delta (r_J - r) \rangle = -\text{div}_r \langle \sum_J p_J \delta (r_J - r) \rangle.$$

6.2. Momentum balance. In the case of (48) for $z$, (45) becomes:

$$\tilde{o}(z,x) = \sum_K p_K \delta (r_K - r)$$

and implies that

$$\partial_{r_J} \tilde{o} [v_J] = -\partial_r (p_J \delta (r_J - r))[v_J], \quad \partial_{p_J} \tilde{o} [f_J] = f_J \delta (r_J - r);$$

moreover,

$$\langle o \rangle (x,t) = \langle \sum_J p_J \delta (r_J - r) \rangle.$$

Accordingly, equation (69) takes the following form:

$$\partial_t \langle \sum_J p_J \delta (r_J - r) \rangle = -\sum_J \langle \partial_r (p_J \delta (r_J - r))[v_J] - f_J \delta (r_J - r) \rangle; \quad (70)$$

we proceed to manipulating the first addendum in the right-hand side. To begin with, we note that

$$\partial_r (p_J \delta (r_J - r))[v_J] = \text{div}_r (m_J \delta (r_J - r) v_J \otimes v_J);$$

next, we note that

$$(v_J - v) \otimes (v_J - v) = v_J \otimes v_J + v \otimes v - v \otimes v_J - v_J \otimes v,$$

14Here we have used for the first time the following relation:

$$\partial_x f(x - y) = -\partial_y f(x - y).$$
where \( \langle v_j - v \rangle \) is the velocity fluctuation of the \( J \)-th particle; hence,

\[
\sum_j m_j \delta(r_j - r) v_j \otimes v_j = \sum_j \delta(r_j - r) \left( m_j (v_j - v) \otimes (v_j - v) \right)
\]

\[
- \sum_j m_j \delta(r_j - r) v \otimes v + v \otimes \left( \sum_j p_j \delta(r_j - r) \right) + \sum_j p_j \delta(r_j - r) \otimes v
\]

\[
= \sum_j m_j \delta(r_j - r) (v_j - v) \otimes (v_j - v) + \rho v \otimes v.
\]

We then arrive at

\[
- \sum_j \partial_r (p_j \delta(r_j - r)) \langle v_j \rangle = - \text{div}_r \left( \left( \sum_j m_j \delta(r_j - r) v_j - v \right) \otimes (v_j - v) + \rho v \otimes v \right),
\]

and we re-write equation (70) as follows:

\[
\partial_t \langle \rho \rangle + \partial_r (\rho v \otimes v) = - \text{div}_r \left( \left( \sum_j m_j \delta(r_j - r) v_j - v \right) \otimes (v_j - v) + \sum_j \delta(r_j - r) f_j \right).
\]

Given that our target CM balance is:

\[
\partial_t (\rho v) + \text{div} (\rho v \otimes v) = \text{div} \mathbf{T}
\]

(cf. (34)), and that

\[
\partial_t (\rho v) + \text{div} (\rho v \otimes v) \equiv \partial_t \langle \rho \rangle + \text{div}_r (\rho v \otimes v),
\]

it remains for us to search for a definition of a discrete counterpart of the Cauchy stress \( \mathbf{T} \) such that

\[
\text{div} \mathbf{T} = - \text{div}_r \left( \sum_j m_j \delta(r_j - r) (v_j - v) \otimes (v_j - v) + \sum_j \delta(r_j - r) f_j \right).
\]

To within a divergenceless tensor field, we set:

\[
\mathbf{T} = \mathbf{K} + \mathbf{R},
\]

with

\[
\mathbf{K} := - \langle \sum_j m_j \delta(r_j - r) (v_j - v) \otimes (v_j - v) \rangle,
\]

\[
\text{div} \mathbf{R} := \sum_j \delta(r_j - r) f_j.
\]  (71)

Note that the kinetic stress \( \mathbf{K} \) – that is, the part of \( \mathbf{T} \) depending on velocity fluctuations – is symmetric; such kinetic part would be all of \( \mathbf{T} \) in the case of an ideal gas, whereas we expect it to be often (but not always, see the discussion in Section 8.1.3 of [23]) negligible in the case of liquid-like or solid-like matter, especially at low temperatures. We now construct a symmetric-valued representation for the tensor field \( \mathbf{R} \) in terms of the interparticle forces analyzed in Section 4.1.

The Nollian reaching stress \( \mathbf{R} \) corresponding to a given skew-symmetric volume-interaction density \( g \), in the sense that

\[
\int_E g(x, y) dy = \text{div} \mathbf{R}(x),
\]  (72)

has the following representation:

\[
\mathbf{R}(x) = \frac{1}{2} \int_V \left( \int_0^1 g(x - (1 - \alpha) w, x + \alpha w) d\alpha \right) \otimes w, dw
\]  (73)
interaction density $g$ such that
\[
\langle \sum_j \delta(r_J - r)f_J \rangle \equiv \int_{E} g(x, y)dy
\]
(we leave the dependence of $g$ on $t$ tacit). Now, whatever the observable $\hat{o}$ and whatever the indices $K, J$ ($K \neq J$),
\[
\langle \delta(r_J - r)\hat{o}(z) \rangle = \int_V \langle \delta(r_J - r)\delta(r_K - s)\hat{o}(z) \rangle ds, \quad s := y - x_o;
\]
hence,
\[
\langle \sum_j \delta(r_J - r)f_J \rangle = \int_V \langle \sum_j \sum_K f_{JK} \delta(r_K - r)\delta(r_J - s) \rangle ds,
\]
whence we deduce the form of the sought-for mapping $g$:
\[
g(x, y) = \frac{r - s}{|r - s|} \sum_j \sum_K \langle V'(r_{JK}) \delta(r_J - r)\delta(r_K - s) \rangle.
\]
Interestingly, this mapping is such that
\[
g(x, y) = \gamma(x, y)(x - y),
\]
\[
\gamma(x, y) := -|r - s|^{-1} \sum_j \sum_K \langle V'(r_{JK}) \delta(r_J - r)\delta(r_K - s) \rangle = \gamma(y, x).
\]
Then,
\[
g(x - (1 - \alpha)v, x + \alpha v) = -\gamma(x - (1 - \alpha)v, x + \alpha v)v,
\]
and Noll’s representation (73) yields the symmetric-valued field
\[
R(x) = -\frac{1}{2} \int_0^1 \left( \int_0^1 \gamma(x - (1 - \alpha)v, x + \alpha v)d\alpha \right) v \otimes v dv.
\]
6.3. Kinetic-energy balance. In view of (48), (45) and (46) become, respectively,
\[
\hat{o}(z) = \sum_j K_{jJ} \delta(r_J - r) \quad \text{and} \quad \langle o \rangle(x, t) = \langle \sum_j K_{jJ} \delta(r_J - r) \rangle;
\]
the first of these relations implies, in view also of (27), that
\[
\partial_{r_J} \hat{o} = -\partial_J (K_{jJ} \delta(r_J - r)) \quad \text{and} \quad \partial_{p_J} \hat{o} = \delta(r_J - r)v_J.
\]
Consequently, equation (69) becomes:
\[
\partial_t \langle o \rangle = -\text{div}_r \langle \sum_j K_{jJ} \delta(r_J - r)v_J \rangle + \langle \sum_j \delta(r_J - r)f_J \cdot v_J \rangle.
\]
6.4. **Internal-energy balance.** In the case of \( \text{(48)} \), equations \( \text{(45)} \) and \( \text{(46)} \) become, respectively,

\[
\partial(z, x) = \sum_K U_K \delta(r_K - r) \quad \text{and} \quad \langle \rho \rangle(x, t) = \sum_K U_K \delta(r_K - r);
\]

the first of these relations implies that

\[
\partial_p \partial \partial = 0,
\]

so that equation \( \text{(69)} \) reduces to:

\[
\partial_t \langle \rho \rangle = (\sum_J \mathbf{v}_J \cdot \partial r) \partial \partial.
\]  

(77)

Now, in view also of \( \text{(28)} \),

\[
\partial_J \partial \partial = -U_J \partial r \partial J - r + \sum_K \left( \partial_J U_K \right) \delta(r_K - r)
\]

\[
= -U_J \partial_J \partial J - r + \sum_K \partial_J \left( \sum_L V(r_{KL}) \delta(r_K - r) \right)
\]

\[
= -U_J \partial_J \partial J - r + \sum_K \partial_J \left( \sum_L V(r_{KL}) \delta(r_K - r) \right) + \sum_K \left( \partial_J V(r_{KL}) \delta(r_K - r) \right)
\]

\[
= -U_J \partial_J \partial J - r + \sum_K \left( \sum_L f_{JL} \delta(r_J - r) - \sum_K f_{JL} \delta(r_K - r) \right)
\]

\[
= -U_J \partial_J \partial J - r + \sum_K \left( \sum_L f_{JL} \delta(r_J - r) - \sum_K f_{JL} \delta(r_K - r) \right)
\]

Consequently, equation \( \text{(77)} \) becomes:

\[
\partial_t \langle \rho \rangle = -\left( \sum_J \mathbf{v}_J \cdot U_J \partial r \partial J - r \right)
\]

\[
- \frac{1}{2} \left( \sum_J \mathbf{v}_J \cdot \left( \sum_K f_{JK} \delta(r_J - r) - \sum_K f_{JK} \delta(r_K - r) \right) \right).
\]  

(78)

Furthermore, given that

(i) \( \sum_J \mathbf{v}_J \cdot U_J \partial r \partial J - r \) =

\[
\text{div} \left( \sum_J U_J \delta(r_J - r) (\mathbf{v}_J - \mathbf{v}) \right) + \text{div} \left( \sum_J U_J \delta(r_J - r) \mathbf{v} \right);
\]

(ii) \( \sum_J \mathbf{v}_J \cdot \left( \left( \sum_K f_{JK} \right) \delta(r_J - r) + \sum_K f_{JK} \delta(r_K - r) \right) \) =

\[
\sum_J \sum_K \mathbf{v}_J \cdot f_{JK} (\delta(r_J - r) + \delta(r_K - r)));
\]

(iii) \( \sum_J \sum_K f_{JK} \left( \delta(r_J - r) + \delta(r_K - r) \right) \) = \( \mathbf{0} \);

equation \( \text{(78)} \) becomes:

\[
\partial_t \langle \rho \rangle + \text{div} \left( \sum_J U_J \delta(r_J - r) \mathbf{v} \right) + \text{div} \left( \sum_J U_J \delta(r_J - r) (\mathbf{v}_J - \mathbf{v}) \right)
\]

\[
+ \frac{1}{2} \left( \sum_J \sum_K (\mathbf{v}_J - \mathbf{v}) \cdot f_{JK} (\delta(r_J - r) + \delta(r_K - r)) \right) = 0.
\]  

(79)
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