Microscopic chaos and macroscopic entropy in fluids

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Abstract: *In nonequilibrium thermodynamics macroscopic entropy creation plays an important role. Here we study, from various viewpoints, its relation with the phase space contraction, which has been recently proposed as an apparently alternative quantity.*

Keywords: Entropy, Nonequilibrium Thermodynamics, Fluids, Navier-Stokes, Thermostats, Chaotic hypothesis

1. *Thermostats, entropy creation and phase space contraction*

Studying stationary states of mechanical systems in interaction with thermostats the latter are often modeled by systems of particles subject to anholonomic constraints. The equations of motion take the form $\dot{x} = f_{\underline{E}}(x)$ where x is a point in phase space and $\underline{E}$ are parameters controlling the size of the acting nonconservative forces.

It has appeared natural to define *entropy creation rate* as the divergence $\sigma(x) \overset{def}{=} -\sum_j \partial_{x_j} f_{\underline{E},j}(x)$. There are other natural definitions of entropy creation rate and here we study their relation with the above phase space divergence. The aim is to find such a relationship for a system that can be considered to be described by a continuum evolving under macroscopic equations.
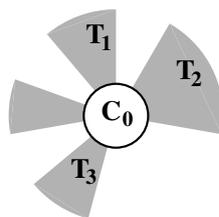

Fig1

Fig.1 Reservoirs occupy finite regions outside $\mathcal{C}_0$, *e.g.* sectors $\mathcal{C}_i \subset R^3$, $i = 1, 2 \ldots$. Their particles are constrained to have a *total* kinetic energy K_i constant, by suitable forces, so that the reservoirs "temperatures" T_i are well defined.

To be concrete and in rather ample generality we imagine a system $\mathcal{C}_0$ of particles enclosed in a container, also called $\mathcal{C}_0$, with elastic boundary conditions surrounded by a few thermostats which consist of particles, all of unit mass for simplicity, interacting with the

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system via short range interactions, through a portion $\partial_i \mathcal{C}_0$ of the surface of $\mathcal{C}_0$, and subject to the constraint that the total kinetic energy of the N_i particles in the i-th thermostat is $K_i = \frac{1}{2}\underline{\dot{X}}_i^2 = \frac{3}{2}N_i k_B T_i$. A symbolic illustration is in Fig.1. The equations of motion will be

$$\underline{\ddot{X}}_0 = -\partial_{\underline{X}_0}\Big(U_0(\underline{X}_0) + \sum_{j>0} W_{0,j}(\underline{X}_0, \underline{X}_j)\Big) + \underline{E}(\underline{X}_0),$$

$$\underline{\ddot{X}}_i = -\partial_{\underline{X}_i}\Big(U_i(\underline{X}_i) + W_{0,i}(\underline{X}_i, \underline{X}_j)\Big) - \alpha_i \underline{\dot{X}}_i \tag{1}$$

with α_i such that K_i is a constant. Here $W_{0,i}$ is the interaction potential between particles in $\mathcal{C}_i$ and in $\mathcal{C}_0$, while U_0, U_i are the internal energies of the particles in $\mathcal{C}_0, \mathcal{C}_i$ respectively. We imagine that the energies $W_{0,j}, U_j$ are due to *smooth* translation invariant pair potentials; repulsion from the boundaries of the containers will be elastic reflection. It is assumed, in Eq.(1) that there is no direct interaction between different thermostats: their particles interact directly only with the ones in $\mathcal{C}_0$. Here $\underline{E}(\underline{X}_0)$ denotes possibly present external positional forces stirring the particles in $\mathcal{C}_0$.

Since the work per unit time that particles outside the thermostat $\mathcal{C}_i$ (hence in $\mathcal{C}_0$) exercise on the particles in it, is $Q_i \overset{def}{=} -\partial_{\underline{X}_i} W_{0,i}(\underline{X}_0, \underline{X}_i) \cdot \underline{\dot{X}}_i$ and it can be interpreted as the "amount of heat Q_i entering" the thermostat $\mathcal{C}_i$, energy conservation yields

$$\frac{d}{dt}\Big(\frac{1}{2}\underline{\dot{X}}_i^2 + U_i\Big) \equiv \dot{U}_i = -\alpha_i \underline{\dot{X}}_i^2 + Q_i \tag{2}$$

and the contraints on the thermostats kinetic energies give $\alpha_i \equiv \frac{Q_i - \dot{U}_i}{3N_i k_B T_i}$.

Set $x = (\underline{X}_i, \underline{\dot{X}}_i)_{i=0,\ldots}$ and write Eq.(1) as $\dot{x} = f_{\underline{E}}(x)$. The divergence $\sigma(x) = -\sum_j \partial_{x_j} f_{\underline{E},j}(x)$ of the equations of motion in phase space is readily computed from Eq.(1), see also [1], and is $\sigma(x) = \sum_{i>0} \frac{Q_i}{k_B T_i} + \dot{R}$ or

$$\sigma(x) = \varepsilon(x) + \dot{R}, \qquad \text{with}$$
$$\varepsilon(x) = \sum_{i>0} \frac{Q_i}{k_B T_i} \tag{3}$$

where $R = \sum_{i>0} \frac{U_i}{k_B T_i}$: here and $\frac{Q_i}{k_B T_i}, \frac{U_i}{k_B T_i}$ should really be multiplied by $(1 - \frac{1}{3N_i})$: this neglection of $O(N_i^{-1})$ is made just to simplify the formulae as, in any event, we shall be interested in cases in which $N_0, N_i \gg 1$.

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Remark: (i) $\varepsilon(x) \stackrel{def}{=} \sum_{i>0} \frac{Q_i}{k_B T_i}$ can be called naturally the *entropy creation rate* and, therefore, Eq.(3) has a physical meaning: *entropy is created at the boundary of the system.* Creation *really* takes place where the walls get in contact with the thermostats, where the temperatures T_i are defined.

(ii) Note that if particles in $\mathcal{C}_0$ were *also* subject to an isokinetic constraint $\frac{1}{2}(\dot{\underline{X}}_0)^2 = \frac{3}{2} N_0 k_B T_0$ phase space contraction would simply be changed by the addition of $\frac{Q_0}{k_B T_0}$ with Q_0 being the work done per unit time by the thermostats in $\mathcal{C}_i$, $i > 0$, on particles in $\mathcal{C}_0$; also R will contain an extra term proportional to $\dot{U}_0$.

(iii) The divergence $\sigma(x)$ is *different* from the entropy creation rate $\varepsilon(x)$. Their difference is a "total time derivative", see Eq.(3), therefore there is a relation between the time averages $a \stackrel{def}{=} \frac{1}{\tau} \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \sigma(S_t x) \, dt$ and $a_0 \stackrel{def}{=} \frac{1}{\tau} \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} \varepsilon(S_t x) \, dt$, namely

$$a = a_0 + \frac{1}{\tau}(R(S_{\frac{\tau}{2}} x) - R(S_{-\frac{\tau}{2}} x)). \tag{4}$$

This means that the observables a and a_0 will have the *same* distribution with respect to any stationary distribution in the limit $\tau \to \infty$ if R is a bounded function (as in our case). More general and "singular" interaction potentials could be considered and would lead to essentially equivalent conclusions, following the results in [2].

(iv) Note that also phase space contraction of a system in contact with isokinetic thermostats has a precise physical meaning as it *equals minus the sum of the dimensionless free energy creation rates* $-\frac{\dot{U}_i}{k_B T_i} + \frac{Q_i}{k_B T_i}$ of the thermostats.

2. *Macroscopic fluids*

The above analysis shows that the two notions of entropy creation rate $\varepsilon(x)$ in Eq.(3) and of phase space contraction $\sigma(x)$ are *related but different.*

They have *in particular* the same stationary average, as they differ by a total derivative $\dot{R}$. As a consequence, not only the averages of σ and ε are equal but also that the fluctuations of their finite time averages, *i.e.* of a and a_0 in Eq.(4), are the same in the limit $\tau \to \infty$: so that properties known for the fluctuations of σ imply corresponding properties for the fluctuations of the physically meaningful entropy creation rate ε. This is relevant because, in the literature, several results have been derived concerning the fluctuations of the time averages of the phase space contraction, see [4].

Therefore it is of some interest to see what the above mechanical notion of entropy creation rate becomes in a system which can be considered as a continuum in a stationary state and in local equilibrium. In fact for such a system an independent definition of entropy creation is classical, [3]. We check that the two notions coincide up to a total derivative.

Consider, in $\mathcal{C}_0$, a system of particles which can be regarded as a Navier-Stokes (NS) continuum in a stationary state and in contact with fixed walls on which, at each boundary point $\boldsymbol{\xi} \in \partial \mathcal{C}_0$, temperature is prescribed at a value $T(\boldsymbol{\xi})$ because the surface element $ds_{\boldsymbol{\xi}}$ is in contact with a thermostat (as idealized in Fig.1) whose internal potential energy per unit surface is $U_{ext}(\boldsymbol{\xi})$. Then the entropy creation rate according to Eq.(3) will be

$$\varepsilon = \int_{\partial \mathcal{C}_0} \frac{Q(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}}, \tag{5}$$

where $Q(\boldsymbol{\xi})$ is the amount of work per unit time and unit surface that the fluid performs on the thermostat in contact with the surface element $ds_{\boldsymbol{\xi}}$, while phase space contraction σ will differ from this by $-\frac{d}{dt} \int_{\partial \mathcal{C}_0} \frac{U_{ext}(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}}$.

There are no complete derivations of the NS equations from molecular models: however all attempts (which achieve the result under reasonable extra assumptions) deal with limiting regimes implying restrictions on initial data and involving a length scaling of $O(\delta^{-1})$, a time scaling of $O(\delta^{-2})$, (hence) a velocity scaling $O(\delta)$ and become exact in the limit as $\delta \to 0$ (δ being a dimensionless scaling parameter).

Here we shall assume that the NS equations can be also obtained from a molecular model under a suitable scaling of space and time variables. We shall therefore consider microscopic initial data with velocity and position distributions with average fields (of density $\rho(\underline{x})$, of kinetic energy, *i.e.* temperature, $T(\underline{x})$ and velocity $\underline{u}(\underline{x})$) consistent with initial values corresponding to a continuum. And we shall suppose that they evolve so that average velocity, density, kinetic energy satisfy NS with good approximation, and exactly in the limit in which some scaling parameter $\delta \to 0$. The temperature field is identified with the average kinetic energy per particle, with velocities measured with respect to the average velocity $\underline{u}$.

Physically δ is a parameter measuring "how far from a continuum the microscopic structure is"; it can be identified with the ratio between the molecular free path and the length scale of the variation of the macroscopic velocity and temperature fields.

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Therefore in the limit $\delta \to 0$ each volume element will contain an infinite number of particles and fluctuations will be suppressed; however the *average* entropy creation will be defined and, by Eq.(3), be

$$\langle \varepsilon \rangle_\mu = - \int_{\partial \mathcal{C}_0} \kappa \frac{\underline{n}(\boldsymbol{\xi}) \cdot \underline{\partial} \, T(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}} \qquad (6)$$

where κ is the thermal conductivity, $\underline{n}$ is the outer normal to $\partial \mathcal{C}_0$ and *the average is intended over a time scale long compared to the microscopic time evolution but macroscopically short.*

The subscript μ indicates that the time average $\langle \varepsilon \rangle_\mu$ of Eq.(5) coincides with the average with respect to a probability distribution μ that is defined on the microscopic phase space and that we assume to be identified with a kind of evolving SRB distribution representing local stationarity. *I.e.* we assume the validity of a "Chaotic hypothesis", [1], not only globally and asymptotically in time but also locally and over times long compared to the microscopic time evolution but macroscopically short. This means that μ may change with time over macroscopic time scales and is, therefore, in general different from the true SRB distribution that would describe the system over time scales very long with respect to macroscopic times.

Hence suppression of fluctuations will not mean that the μ-averages, over times long with respect to microscopic scales, defining $\underline{u}(\underline{x}), T(\underline{x})$ or the average $U(\underline{x}) \stackrel{def}{=} \langle U \rangle_\mu (\underline{x}), \underline{x} \in \mathcal{C}_0$, of the microscopic energy density U or the average energy per unit surface of the external thermostats $U_{ext}(\boldsymbol{\xi}) \stackrel{def}{=} \langle U_{ext} \rangle_\mu (\boldsymbol{\xi}), \boldsymbol{\xi} \in \partial \mathcal{C}_0$, over such scales will not continue to vary over macroscopic times.

In other words we are saying that there are two basic time scales: at times long with respect to the microcopic time scale (determined by the molecular free path) the volume elements of the fluid are in a stationary state and the distribution μ used to compute the averages can be thought as being locally stationary on times short compared to the macroscopic times. As time evolves on the macroscopic time scale the distribution μ also changes: to average, asymptotically, to the true SRB distribution for the global stationary state.

Eq.(6) is the expression corresponding to Eq.(3) derived from molecular dynamics and it must be compared, for compatibility, with the familiar expressions for the entropy creation rate in systems described by macrosopic continua equations, [3].

We consider here a viscous and thermally conducting NS-fluid in local equilibrium. Thus

the local equilibrium entropy density s depends on the local temperature and density: $s = s(T, \rho)$. Let $\underset{\sim}{\tau}'$ be the stress tensor $\tau'_{ij} = (\partial_i u_j + \partial_j u_i)$ in terms of the velocity field $\underline{u}$, η be the dynamical viscosity and $U(\underline{x}) = \langle U \rangle_\mu(\underline{x})$ be the internal energy density (sum of the potential energy density and the kinetic energy density evaluated with respect to the average velocity $\underline{u}$). Then the NS equation are, [4, p.2,3,6,18],

$$
\begin{aligned}
&(1) & \partial_t \rho + \underline{\partial} \cdot (\rho \underline{u}) &= 0 \\
&(2) & \partial_t \underline{u} + \underline{u} \cdot \underline{\partial}\,\underline{u} &= -\tfrac{1}{\rho}\underline{\partial} p + \tfrac{\eta}{\rho}\Delta \underline{u} + \underline{g} \\
&(3) & \partial_t U + \underline{\partial} \cdot (\underline{u} U) &= \eta\,\underset{\sim}{\tau}'\,\underline{\partial}\,\underline{u} + \kappa \Delta T - p\,\underline{\partial} \cdot \underline{u} \\
&(4) & T\left(\partial_t s + \underline{\partial} \cdot (\underline{u} s)\right) &= \eta\,\underset{\sim}{\tau}'\,\underline{\partial}\,\underline{u} + \kappa \Delta T
\end{aligned}
\tag{7}
$$

here $\underline{g}$ is a (nonconservative) external force generating the fluid motion and p is the physical pressure. The conditions at the boundary of the fluid container $\mathcal{C}_0$ will be time independent, $T = T(\boldsymbol{\xi})$ and $\underline{u} = \underline{0}$ (no slip boundary).

As mentioned, Eq.(7) are macroscopic equations that can be valid only in some limiting regime. Given a system of particles with short range pair interactions let δ be the mentioned natural dimensionless scaling parameter; then a typical conjecture is: for suitably restricted and close to local equilibrium initial data (see [4, p.21] for examples) *on time scales of $O(\delta^{-2})$ and space scales $O(\delta^{-1})$ the evolution of $\rho, \underline{u}, T, U, s$ follows the incompressible NS equation*, [4, p.30].

The classical entropy creation rate in nonequilibrium thermodynamics of an *incompressible fluid* is, [4, p.6],

$$
k_B \varepsilon_{classic} = \int_{\mathcal{C}_0}\left(\kappa\,(\frac{\partial T}{T})^2 + \eta\,\frac{1}{T}\underset{\sim}{\tau}'\,\underline{\partial}\,\underline{u}\right) d\underline{x}.
\tag{8}
$$

By integration by parts and use of the first and fourth of Eq.(7), $k_B \varepsilon_{classic}$ becomes, if $S \stackrel{def}{=} \int_{\mathcal{C}_0} s\, d\underline{x}$ is the total thermodynamic entropy of the fluid,

$$
\begin{aligned}
\int_{\mathcal{C}_0}\left(-\kappa\,\underline{\partial} T \cdot \underline{\partial} T^{-1} + \eta\,\frac{1}{T}\underset{\sim}{\tau}'\,\underline{\partial}\,\underline{u}\right) d\underline{x} = \\
= -\int_{\partial \mathcal{C}_0} \kappa\,\frac{\underline{n} \cdot \underline{\partial} T}{T}\, ds_{\boldsymbol{\xi}} + \int_{\mathcal{C}_0}\frac{(\kappa \Delta T + \eta\,\underset{\sim}{\tau}'\underline{\partial}\underline{u})}{T} d\underline{x} =
\end{aligned}
\tag{9}
$$

$$= -\int_{\partial \mathcal{C}_0} \kappa \frac{\underline{n} \cdot \partial T}{T} \, ds_{\boldsymbol{\xi}} + \dot{S} + \int_{\mathcal{C}_0} \underline{u} \cdot \underline{\partial} s \, d\underline{x} =$$

$$= -\int_{\partial \mathcal{C}_0} \kappa \frac{\partial T \cdot \underline{n}}{T} \, ds_{\boldsymbol{\xi}} + \dot{S}$$

i.e. this *still leads to* the expression Eq.(6), "local on the boundary" or "localized at the contact between system and thermostats", since $\underline{u} \cdot \underline{n} \equiv 0$ by the boundary conditions, *plus the time derivative of the total "thermodynamic entropy" of the fluid.*

Remarks: (i) An identical analysis can be performed for *Rayleigh's convection model*, widely used to test ideas on turbulence since [5]: the result is the same because the extra term that would appear in Eq.(9), see [4, p. 47], would be proportional to $\int_{\mathcal{C}_0} u_z d\underline{x}$ which vanishes because the motion has no net momentum in the z direction.

(ii) It should be noted that in the limit $\delta \to 0$, *i.e.* when the NS equations are expected to become rigorously exact, the Eq.(8) simplifies: only the first term in *r.h.s.* remains because the velocity $\underline{u}$ scales as $O(\delta)$, [4, p.26].

3. *Incompressible continua viewpoint*

The above analysis leads to a further natural question: whether the phase space contraction and the entropy creation rate can be computed if we consider an incompressible fluid *in local equilibrium and observed on a short but macroscopic time scale* and imagine, as it is tempting to do and often done, [3, 4], its small macroscopic volume elements as a collection of small thermostats in contact with reservoirs consisting in the neighboring volume elements: if we apply the general theory of Sec.1 would the results be consistent with the ones in Sec.2?

In establishing a comparison it should, however, be noted that the volume elements $E = d\underline{x}$ are not separated by walls, hence they can exchange particles, and they also move. In order to be able to treat volume elements as systems on their own we imagine that their size is λ with λ macroscopically small but microscopically large: certainly such length scale λ is $\ll L \sim (\frac{1}{T} \frac{\partial T}{\partial x})^{-1}$ where L is the macroscopic scale of the container $\mathcal{C}_0$.

Furthermore we have to assume that molecules diffuse, in a characteristic evolution time, over a distance $\ll \lambda$. The diffusion coefficient is $D = O(\frac{k_B T}{mr^2 \rho v})$ with v the average speed, $v = O(v_{sound})$, m the mass of the molecules, r their radius and ρ the numerical density, and a characteristic time scale is $\theta = \frac{mD}{k_B T}$. The distance traveled by diffusion in the latter time scale is $(D\theta)^{\frac{1}{2}}$ ($\sim 10^{-2}$cm in air at normal conditions).

We assume, as above, that the local quantities, velocity field and temperature field, $\underline{u}(\underline{x}), T(\underline{x})$, as well as the energy fields $\langle U \rangle_\mu(\underline{x}) = U(\underline{x}), \underline{x} \in \mathcal{C}_0$, and $\langle U_{ext} \rangle_\mu(\boldsymbol{\xi}) = U_{ext}(\boldsymbol{\xi}), \boldsymbol{\xi} \in \partial\mathcal{C}_0$, evolve on a time scale much slower than the microscopic time scale θ and can be considered constant on the latter time scale. The expression Eq.(8) should be regarded as an average over a long microscopic time (but over a short macroscopic time).

Suppose that the conditions allow us to consider a volume element in a fluid as a thermostated system in a stationary state in contact with thermostats made of the neighboring elements. *I.e.* suppose that the quantity δ introduced after Eq.(7) is small and the diffusion across the elements boundaries is not important enough to make the identity of the volume elements ill defined (*i.e.* $\delta \ll \lambda \ll L$). Then we can apply the analysis leading from Eq.(1) to Eq.(3) and conclude that *up to a total derivative* $\dot{R}$ the phase space contraction of the total system, *i.e.* fluid plus thermostats, is (see also remark (ii) in Sec1)

$$\varepsilon(x) = \sum_E \sum_{E'} \frac{Q_{E,E'}}{k_B T_{E'}} \tag{10}$$

where $Q_{E,E'}$ is the amount of work that the particles in a given volume element E perform over the neighboring elements E', see Eq.(3). The quantity $\varepsilon(x)$ will be the entropy creation rate defined by regarding the volume elements as small thermostats in stationary state.

If the average heat current is $-\kappa\,\underline{\partial}T$ and the element E is imagined with the bases orthogonal to the gradient of T, the average contribution to $Q_{E,E'}$ for E' adjacent to the upper base of E is $-\kappa\,\underline{\partial}T \cdot \underline{n}\,\lambda^2$ ($\lambda^2 =$ area of the base) and it is opposite to the contribution from the lower base; therefore the quantity $\sum_{E'} \frac{Q_{E,E'}}{T_{E'}}$ has average

$$-\kappa\,\underline{\partial}T \cdot \underline{n}\,\lambda^2 \left(\frac{1}{T_+} - \frac{1}{T_-}\right) = -\kappa\,\underline{\partial}T \cdot \underline{\partial}T^{-1}\lambda^3, \tag{11}$$

if $T_\pm$ are the temperatures at the two bases; hence summing over E: $k_B\langle\varepsilon\rangle_\mu = \int_{\mathcal{C}_0} \underline{\partial}(\frac{1}{T}) \cdot (-\kappa\,\underline{\partial}T)\,d\underline{x}$ which can be written in the more common and familiar form $\kappa \int_{\mathcal{C}_0} (\frac{\partial T}{T})^2 d\underline{x}$. Then if $\partial_t T = 0, \Delta T = 0$ and $\underline{u} = \underline{0}$ Eq.(8), therefore Eq.(6), follows by partial integration.

More generally in presence of time dependence and non vanishing velocity field there will be an extra amount of energy transferred to elements adjacent to E and due to diffusion across the bases: it can be evaluated in the same way as above to be $\eta\,\underline{\underline{\tau}}' \cdot \underline{n}\,(\underline{u}_+ - \underline{u}_-)\,\lambda^2$ if

$\underset{\sim}{\tau}'$ is the stress tensor and it changes $k_B \langle \varepsilon \rangle_\mu$ to Eq.(8), *hence to Eq.(6) plus $\dot{S}$* (see Eq.(9)) if account is taken of the fourth of Eq.(7).

The above viewpoint therefore also leads to the classical expression for the entropy creation rate.

4. *Phase space contraction*

Finally it is interesting to remark that not only the entropy creation rate but also the phase space contraction can be computed along the above lines for macroscopic continua. Regarding each volume element E as a thermostated system in a stationary state with a fixed temperature, the average phase space contraction is deduced from Eq.(3) taking into account the $\dot{R}$ contribution.

Hence, setting $k_B e(\underline{x}) \overset{def}{=} \left(\kappa \left(\frac{\partial T}{T} \right)^2 + \eta \frac{1}{T} \underset{\sim}{\tau}' \underset{\sim}{\partial} \underline{u} \right)$, the average phase space contraction is $\int_{\mathcal{C}_0} \left(e(\underline{x}) - \frac{\dot{U}(\underline{x})}{k_B T(\underline{x})} \right) d\underline{x} - \int_{\partial \mathcal{C}_0} \frac{\dot{U}_{ext}(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}}$, where $U(\underline{x}) = \langle U \rangle_\mu(\underline{x})$ denotes the average potential energy density while with $U_{ext}(\boldsymbol{\xi}) = \langle U_{ext} \rangle_\mu(\boldsymbol{\xi})$ we denote the average potential energy density per unit surface of the thermostats.

Remark that the time derivative of the potential energy density $\dot{U}(\underline{x})$ could be replaced by the time derivative of the total energy density at $\underline{x}$: in fact the kinetic energies do not contribute to the total derivative of the energy density since they have been supposed to be constant because each volume element is regarded to have a constant kinetic energy, *i.e.* a well defined temperature, and in the above relations the energies appear through their time derivative). Hence energy conservation, $\dot{U}(\underline{x}) = \eta \underset{\sim}{\tau}' \cdot \underset{\sim}{\partial} \underline{u} + \kappa \Delta T$, see (3) in Eq.(7), for incompressible fluids and partial integration of the contribution $\kappa (\frac{\partial T}{T})^2$ to $e(\underline{x})$, see Eq.(8), in the integral $\int_{\mathcal{C}_0} \left(e(\underline{x}) - \frac{\dot{U}(\underline{x})}{k_B T(\underline{x})} \right) d\underline{x}$ leave us with a boundary term *which is just Eq.(6) minus* $\int_{\partial \mathcal{C}_0} \frac{\dot{U}_{ext}(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}}$ as it could be guessed from the expression for σ preceding Eq.(3).

Therefore even if we regard the fluid volume elements as thermostated systems in stationary nonequilibrium we are led to the expected relation between average entropy creation $\langle \varepsilon \rangle_\mu$ and average phase space divergence $\langle \sigma \rangle_\mu$, namely (if x denotes the fields determining the state of the fluid)

$$\langle \sigma \rangle_\mu = \langle \varepsilon \rangle_\mu - \int_{\partial \mathcal{C}_0} \frac{\dot{U}_{ext}(\boldsymbol{\xi})}{k_B T(\boldsymbol{\xi})} ds_{\boldsymbol{\xi}}. \tag{12}$$

Analysis of compressible fluids, unfortunately more difficult, should also be attempted:

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the first difficulty will be, of course, that it is not clear under which scaling the compressible NS equations should hold as a reasonable approximation.

5. *Conclusion*

The conclusion is that the *entropy creation rate* evaluated from the microscopic model, Eq.(1), and the microscopic definition of heat ceded to a thermostat (see Eq.(2))

(1) differs "by a total derivative", $\dot{R}$, from the microscopic phase space contraction (see Eq.(3)),

(2) if the system can be regarded as a NS continuum in stationary local equilibrium, its average coincides with the classical entropy creation rate up to a total derivative, $\dot{S}$, see Eq.(9),

(3) in the latter situation its average coincides with the entropy creation obtained by regarding the continuum as constituted by volume elements each of which is a thermostat in a stationary state exchanging heat with the neighboring volume elements, see Eq.(8), and differs by a total derivative from the average phase space contraction evaluated by regarding the continuum in the same way, see Eq.(12).

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