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GENERIC guide to the multiscale dynamics and thermodynamics

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Abstract

GENERIC is an abstract equation collecting the mathematical structure guaranteeing agreement of its solutions with results of certain basic experimental observations (conservations of mass and energy and the approach to equilibrium at which the classical equilibrium thermodynamics applies). In the unifying framework provided by GENERIC we present recent developments and open challenges in the fundamental aspects of the multiscale dynamics and thermodynamics.

1. Introduction

GENERIC (an acronym for General equation for Non-Equilibrium Reversible-Irreversible Coupling) is an abstract mesoscopic time evolution equation

$$\dot{x} = L\frac{\delta E}{\delta x} + \left[\frac{\delta \Psi(x, x^*)}{\delta x^*}\right]_{x^*=\frac{\delta S}{\delta x}} \tag{1}$$

collecting the structure that guarantees its physical pertinence. Alternatively, in particular when the geometrical aspects of the time evolution are in the center of attention, equation (1) is also called a metriplectic time evolution equation in order to emphasize the presence of both the symplectic and the Riemannian (metric) geometry. The symbol x stands for a mesoscopic state variable (e.g. one particle distribution function in kinetic theory or hydrodynamic fields in fluid mechanics), $\dot{x}$ is the time derivative of x, the first term on the right hand side represents mechanics (symplectic geometry), the second term is the thermodynamical (Riemannian geometry) contribution appearing due to the mesoscopic (i.e. not keeping all the microscopic details) nature of the state variable x. The structure of (1), that we shall present and discuss below, guarantees that its solutions agree with the experimentally observed approach to equilibrium at which the classical equilibrium thermodynamics, obtained by solving (1), provides an excellent description of the observed behavior. The archetype example of the GENERIC equation (1) is the Boltzmann kinetic equation presented in section 2.4.

In applications, the GENERIC equation provides a framework (a scaffold) for constructing mesoscopic dynamical models. The modeling process begins with a partial validation (with the requirement of the compatibility with thermodynamics that is expressed already in the framework (1)) and continues with specifying the modules (building blocks) represented by the symbols appearing in (1). The modules can be specified individually on the basis of a physical insight into the macroscopic system under consideration. If they satisfy all the required properties (listed in sections 2.1, 2.2, and 2.3) and are put together as prescribed in (1), the overall compatibility is guaranteed. The validation can then continue with different types of experimental observations. In this paper we do not discuss applications. Their recent review can be found in [1]. We only emphasize again the important difference between the standard and the GENERIC modeling. The former begins with microscopic mesoscopic physical insights into the system under investigation that is then expressed mathematically in governing equations. Finally, the model is validated by comparing solutions to the governing equations with results of experimental observations. The GENERIC modeling begins on the other hand with the GENERIC structure (1) that by itself is already a partial validation since it guarantees that solutions of the model agree with certain basic experimental observations (namely with the experimentally observed approach of externally unforced systems to equilibrium states at which the classical equilibrium thermodynamics is found to provide a good description of the observed behavior). The physical insight enters the GENERIC modeling in the process of the specification of the modules (in other words, in the process of constructing a particular realizations of (1). After solving the governing equations, the validation of the model continues with the comparison of solutions with results of more specific experimental observations. The GENERIC structure (1) thus provides both a scaffold for the modeling and a partial validation of the resulting models.

In the fundamentally oriented investigations of the mesoscopic dynamics and thermodynamics of macroscopic systems, the GENERIC equation (1) has provided a motivation and an inspiration. Our objective in this paper is to investigate the fundamental aspects of mesoscopic dynamics from a unifying multiscale viewpoint. The unifying context invites new insights and new viewpoints. For the completeness of the presentation, we repeat some well known results but our focus is put on the recent developments. Our intention is to show that this field is full of new ideas and open challenges. In section 2 we make comments about physical interpretations and about the methods used in specifications of the quantities appearing in (1). We also answer several frequently asked questions about the GENERIC equation (1). In section 3 we show new directions and new challenges in the investigation of the mesoscopic dynamics that are inspired by GENERIC.

2. Physical and mathematical aspects

From the physical point of view, equation (1) describes, on a mesoscopic level of description (we shall denote it by the symbol *MESO*), a preparation process for using another level of description that is called an equilibrium thermodynamics level (we shall denote it by the symbol *equilibrium*). The time evolution governed by (1) brings the macroscopic systems under consideration to equilibrium states at which the classical equilibrium thermodynamics describes well their behavior. In the standard formulation of the classical equilibrium thermodynamics [2], the existence of such states is the Postulate 0 of thermodynamics. We begin our presentation of thermodynamics with this postulate and continue to investigate it more. We are not satisfied with only the existence of equilibrium states but we ask the question of how they are reached. From this investigation unfolds then the whole thermodynamics. We postulate equation (1) to be the equation governing the approach to equilibrium. Postulate 1 and Postulate 2 of Callen become statements (in sections 2.1, 2.2, 2.3) about the structure and consequently about the properties of solutions of equation (1).

Symbolically, we regard (1) as representing the passage $MESO \to equilibrium$. A generalization to the passage $MESO \to meso$, where *meso* is another mesoscopic level that involves less details than the level *MESO*, is discussed in section 3.

From the mathematical point of view, GENERIC (1) represents a combination of symplectic dynamics (the first term on the right hand side of (1)), with gradient dynamics (the second term on the right hand side of (1)). While separately, the symplectic and the gradient dynamics are well understood, their combination (1), arising in mesoscopic dynamics, is not. Some of the challenges are discussed below.

2.1. Mechanics

In the Hamiltonian viewpoint of mechanics, the vector field (i.e. the arrows that give the order to the motion) is a covector, that is a gradient E_x of the energy $E(x)$, transformed into a vector by a Poisson bivector L (see the first term on the right hand side of (1)). The energy E is a real valued and sufficiently regular function of x, $E\colon \mathbf{M} \to \mathbb{R}$, where $\mathbf{M}$ denotes the state space. i.e. $x \in \mathbf{M}$, used on the level *MESO*. We use hereafter the shorthand notation $E_x = \frac{\delta E}{\delta x}$. If $\mathbf{M}$ is an infinite dimensional space, for example if x is a distribution function or a field, then $\frac{\delta}{\delta x}$ is an appropriate functional derivative (see more in section 2.5), if $\mathbf{M}$ is a finite dimensional space then $\frac{\delta}{\delta x}$ is a standard partial derivative.

The bivector L is a Poisson bivector if the bracket $\{A, B\} = \langle A_x, LB_x\rangle$ is a Poisson bracket (i.e. $\{A, B\}$ is linear in A_x and B_x, $\{A, B\} = -\{B, A\}$, the Leibnitz and the Jacobi identities hold; by $\langle,\rangle$ we denote pairing in the state space $\mathbf{M}$; A and B are real valued functions of x). If L is degenerate then there exist functions $C(x)$, called Casimirs, for which $\{A, C\} = 0, \forall A$. The above requirements imply immediately that solutions to $\dot{x} = LE_x$ obey the conservation laws $\dot{E} = \{E, E\} = 0, \dot{C} = \{C, E\} = 0$.

From the physical point of view, the bivector L represents kinematics of x. For example, the kinematics of the classical continuum is expressed mathematically in the Lie group $\mathcal{G}^{(cont)}$ of the transformations $\mathbb{R}^3 \to \mathbb{R}^3$. The momentum field can be seen as an element of the dual of the Lie algebra corresponding to the Lie group $\mathcal{G}^{(cont)}$. The Lie-Poisson bracket, arising canonically on duals of Lie algebras, provides then the bivector L expressing kinematics of the classical continuum. As for the fields of the mass density and the entropy density, that join the momentum field to form the complete set the state variables of the classical continuum, their kinematics is determined by letting them to be passively advected by the momentum field and by using the concept of the semi-direct product to express it mathematically. In the mesoscopic theories in which distribution functions serve as state variables, the group representing kinematics is the Lie group $\mathcal{G}^{(kin)}$ of canonical (i.e. the symplectic structure preserving) transformation of the particle mechanics. The distribution function can then be seen as an element of the dual of the Lie algebra corresponding to $\mathcal{G}^{(kin)}$.

The fact that the Euler fluid mechanics equation (i.e. a mesocopic time evolution equation with $x = \textit{hydrodynamic fields}$) can be cast into the form $\dot{x} = LE_x$ with $\langle A_x, LB_x\rangle$ being the Poisson bracket has been noted first by Alfred Clebsch [3]. With the relation between Lie groups and the bivector L, noted in [4], the presence of the term LE_x has been recognized in many other mesoscopic time evolution equations (see [5]). For instance the Liouville reformulation of the time evolution equations of classical mechanics (i.e. a formulation of the classical mechanics in which x is the $\mathfrak{N}$-particle distribution function, $\mathfrak{N} \sim 10^{23}$ known as the Liouville equation) can also be cast into the form $\dot{x} = LE_x$ with $\langle A_x, LB_x\rangle$ being the Poisson bracket.

Let the state variable x be chosen (on the basis, for example, of our physical insight into the system under consideration and on the basis of our interest in particular applications), what is L expressing its kinematics?. A general answer to this question is not known. The interested reader can find some partial results, for example, in [6, 7]. Very useful is also the computer assisted verification of the Jacobi identity developed in [8]. We shall return to this question in several different contexts later in this paper. A useful strategy for finding L may be to invert the whole process of selecting the state variables. Instead of starting with choosing x we start with choosing a Lie group representing the mesoscopic kinematics. Making such choice, we then arrive at both the mesoscopic state variables x and L representing their kinematics.

2.2. Thermodynamics

If the state space $\mathbf{M}$ includes all the data needed in the classical mechanics (i.e. if $x \in \mathbf{M}$ includes position vectors and velocities of all the particles composing the macroscopic system under investigation) then equation (1) without the second term on its right hand side governs the time evolution. If however some data are missing (i.e. when we are ignoring in x some details that do not interest us) then the time evolution of x is not governed by $\dot{x} = LE_x$. This is because the ignored details, however unimportant in the context of the chosen *MESO* viewpoint of macroscopic systems, still influence the *MESO* time evolution of x. How does one take into account such influence? For the answer we turn to the classical thermodynamics. We introduce a new potential $S(x)$, called an entropy, that tends always to its maximum allowed by constraints. This entropy maximization process (called MaxEnt principle) represents then the influence of the ignored details on the behavior of x. If we interpret $S(x)$ as a measure of disorder then MaxEnt is the process in which the ignored details are causing maximum disorder, allowed by constraints, in $\mathbf{M}$.

In order to implement the MaxEnt principle in the context of the time evolution, we have to introduce new dynamics that maximizes $S(x)$. It is quite straightforward to suggest three candidates for such dynamics. The first one is

$$\begin{aligned}&\dot{x} = M(x)S_x\\ &\quad M(x)\ \textit{is a symmetric and positive definite operator}\end{aligned}\tag{2}$$

the second is

$$\begin{aligned}&\dot{x} = [M(x, x^*)x^*]_{x^*=S_x}\\ &\quad M(x, x^*)\ \textit{is a symmetric and positive definite operator}\end{aligned}\tag{3}$$

and the third is

$$\begin{aligned}&\dot{x} = [\Psi_{x^*}(x, x^*)]_{x^*=S_x}\\ &\quad \Psi(x, 0) = 0\\ &\quad \Psi(x, x^*)\ \textit{reaches its minimum},\ \ \textit{as a function of}\ \ x^*\ \textit{at}\ x^* = 0\\ &\quad \Psi(x, x^*) \textit{is a convex function of}\ \ x^*\ \textit{in a neighborhood of}\ \ x^* = 0\end{aligned}\tag{4}$$

We note that all three time evolution equations imply $\dot{S} \geqslant 0$. We also note that (3) is the most general among them (see [9]), and (2) is a particular case of (4) corresponding to $\Psi(x, x^*) = \frac{1}{2}\langle x^*, M(x)x^*\rangle$. The potential Ψ, introduced in (4), is called a dissipation potential.

The relaxation equation (2) is known as the Ginzburg-Landau [10] and also Cahn-Hilliard [11] equation. Its physical and geometrical significance has recently been investigated in [12].

The dissipation potential as well as the entropy will be discussed in the rest of this section (see in particular sections 2.9 and 2.8) .

2.3. Mechanics & thermodynamics

We look for equations whose solutions represent the experimentally observed approach to equilibrium states at which the classical equilibrium thermodynamics describes well the observed behavior. We therefore begin with equilibrium thermodynamics. The quantities serving as state variables in classical equilibrium thermodynamics are (E, N), where E is the energy per unit volume and N the number of moles per unit volume. The fundamental thermodynamic relation is given by

$$S = S(E, N);\;\; E = E;\;\; N = N \tag{5}$$

where $S \in \mathbb{R}$ is the equilibrium thermodynamic entropy per unit volume. It is in the function $S(E, N)$ where the individual nature of the macroscopic system under consideration is expressed.

On the *MESO* level the state variables are x and the fundamental thermodynamic relation is

$$S = S(x);\;\; E = E(x);\;\; N = N(x) \tag{6}$$

We obtain (5) from (6) by MaxEnt, i.e. by maximizing $S(x)$ with constraints $E(x)$ and $N(x)$, or in other words, by making a reducing Legendre transformation. We introduce

$$\Phi(x, T, \mu) = -S(x) + \frac{1}{T}E(x) - \frac{\mu}{T}N(x) \tag{7}$$

called a thermodynamic potential. The symbols T and μ stand for the equilibrium temperature and the equilibrium chemical potential respectively. Next, we solve the equation $\Phi_x = 0$. Let its solutions be $x_{eq}(T, \mu)$. Finally, we evaluate the thermodynamic potential Φ at x_{eq} and obtain

$$\Phi(x_{eq}(T, \mu), T, \mu) = -S(x_{eq}(T, \mu)) + \frac{1}{T}E(x_{eq}(T, \mu)) - \frac{\mu}{T}N(x_{eq}(t, \mu) = -\frac{P}{T}(T, \mu) \tag{8}$$

where P is the thermodynamic pressure. For later use, we introduce the following notation: $E^* = S_E$; $N^* = S_N$; $x^* = S_x$; $\Phi(x_{eq}(E^*, N^*), E^*, N^*) = S^*(E^*, N^*)$. In terms of the standard notation used in the classical equilibrium thermodynamics we thus have $E^* = \frac{1}{T}$; $N^* = -\frac{\mu}{T}$; $S^* = -\frac{P}{T}$.

So far, we have succeeded to pass from the fundamental thermodynamic relation (6) to the relation $S^* = S^*(E^*, N^*)$. From this relation we then pass to the fundamental thermodynamics relation (5) by the standard Legendre transformation (i.e. we introduce $\Phi^*(E^*, N^*, E^{**}, N^{**}) = -S^*(E^*, N^*) + E^{**}E^* + N^{**}N^*$, solve the equations $\Phi^*_{E^*} = \Phi^*_{N^*} = 0$, evaluate Φ^* at the solutions and make the identifications: $S^{**} = S$; $E^{**} = E$; $N^{**} = N$).

Now we turn to the time evolution. We require that the time evolution that we seek has the following properties: (i) it makes the passage from the fundamental thermodynamic relation (6) to the relation $S^* = S^*(E^*, N^*)$ that we made above by applying the reducing Legendre transformation, (ii) it combines the Hamiltonian and the gradient dynamics discussed in the previous sections and implies

$$\dot{S}(x) \geqslant 0;\;\; \dot{E}(x) = 0;\;\; \dot{N}(x) = 0 \tag{9}$$

We note that (1) satisfies both these requirements provided L and Ψ are appropriately degenerate. The degeneracy of L is mathematically expressed by

$$\langle S_x, Lx^*\rangle = 0, \forall x^*;\;\; \langle N_x, Lx^*\rangle = 0, \forall x^* \tag{10}$$

The degeneracy requirements on Ψ and alternatively on M take the form

$$\langle E_x, \Psi_{x^*}\rangle = 0, \forall x^*;\;\; \langle N_x, \Psi_{x^*}\rangle = 0, \forall x^* \tag{11}$$

and

$$\langle E_x, Mx^*\rangle = 0, \forall x^*;\;\; \langle N_x, Mx^*\rangle = 0, \forall x^* \tag{12}$$

In the commonly accepted terminology, a real valued function $C(x)$ satisfying $\{C, A\} = \langle C_x, LA_x\rangle \forall A$ is called a Casimir. We suggest to call it a symplectic Casimir and to call a real valued function $C(x)$ satisfying $\langle C_x, \Psi_{x^*}\rangle = 0, \forall x^*$ a metric Casimir.

It is easy to verify that with these additional requirements on L and Ψ, equation (1) describes indeed the preparation process for applying the equilibrium thermodynamics. The relations (9) are verified, the thermodynamic potential (7) plays the role of the Lyapunov function (provided the potentials in (6)) are convex) for the approach to the equilibrium state x_{eq}, and the passage from (6) to the equilibrium fundamental thermodynamics relation $S^* = S^*(E^*, N^*)$ is made by following the time evolution to its conclusion.

In order to address the question of uniqueness of the split of the right hand side of (1) into the sum of two terms, we introduce (see more in [13]) two properties of vector fields: dissipativity and time reversibility. We say that a vector field $\mathcal{V}$ is dissipative if $\langle S_x, \mathcal{V}\rangle \geqslant 0$ and nondissipative if $\langle S_x, \mathcal{V}\rangle = 0$. In order to define the time reversibility we need an idempotent mapping $\mathcal{I}$: $N \to N$. We say that the vector field $\mathcal{V}$ is time reversible if $T\mathcal{I}\mathcal{V}(\mathcal{I}x) = -\mathcal{V}(x)$ and time irreversible if $T\mathcal{I}\mathcal{V}(\mathcal{I}x) = \mathcal{V}(x)$. By the symbol $T\mathcal{I}$ we denote the action induced on the tangent space of $\boldsymbol{N}$ by the mapping $\mathcal{I}$ in $\boldsymbol{N}$. For example, in fluid mechanics, where x are hydrodynamic fields, the operator $\mathcal{I}$ changes the sign of the velocity field. Some authors make an additional requirement on (1) (e.g. [13]), namely that the first term on the right hand side of (1) is always nondissipative, Hamiltonian and time reversible, and the second term always dissipative, gradient or generalized gradient in the sense of (4) and time irreversible. This and the choice between (3) and (4) (see also section 2.9) have been and continue to be probably the most contested elements of the GENERIC structure (see also section 2.13).

Time evolution equations involving both the Hamiltonian and the gradient part have appeared first in [14], in [15] (that was presented at the AMS-IMS-SIAM Joint Summer Research Conference in the Mathematical Sciences on Fluids and Plasmas: Geometry and Dynamics, held at the University of Colorado, Boulder, CO, USA, 17–23 July 1983) and in [16–22]. In [20, 21] the abstract equation (1) has been called GENERIC. The adaptation of (1) to quantum systems has been discussed in [23].

2.4. Boltzmann kinetic equation

We concentrate in this paper on the fundamental aspects of equation (1). It is nevertheless useful to have in mind at least one of its specific realizations. The archetype example of a particular realization of (1) is the Boltzmann kinetic equation

$$\begin{aligned}\frac{\partial f(\boldsymbol{r},\boldsymbol{v})}{\partial t} = -\frac{\boldsymbol{v}}{m}\frac{\partial f(\boldsymbol{r},\boldsymbol{v})}{\partial \boldsymbol{r}} + \int d\boldsymbol{v}' \int d\boldsymbol{v}_1 W^{(B)}(f;\boldsymbol{v},\boldsymbol{v}_1,\boldsymbol{v}'\boldsymbol{v}_1')\\ \times [f(\boldsymbol{r},\boldsymbol{v}')f(\boldsymbol{r},\boldsymbol{v}_1') - f(\boldsymbol{r},\boldsymbol{v})f(\boldsymbol{r},\boldsymbol{v}_1)]\end{aligned} \tag{13}$$

$f(\boldsymbol{r},\boldsymbol{v})$ is the one particle distribution function, $\boldsymbol{r}$ is the position vector, and $\boldsymbol{v}$ momentum of a particle with the mass m. The first term on the right hand side of (13) represents the free flow, the second term binary collisions taking place at $\boldsymbol{r}$ and transforming the momenta $(\boldsymbol{v},\boldsymbol{v}_1)$ of the incoming two particles into the momenta $(\boldsymbol{v}',\boldsymbol{v}_1')$ of the outcoming two particles, $W^{(B)}$ is a real valued non negative function that is symmetric with respect to the exchange $(\boldsymbol{v},\boldsymbol{v}') \rightleftarrows (\boldsymbol{v}_1,\boldsymbol{v}_1')$ of the particle and its partner in the collision, and the exchange $(\boldsymbol{v},\boldsymbol{v}_1) \rightleftarrows (\boldsymbol{v}',\boldsymbol{v}_1')$ between the momenta before and after the collision. Moreover, W remains unchanged if the signs of all the velocities are reversed and is different from zero (and positive) only if $\boldsymbol{v}+\boldsymbol{v}_1 = \boldsymbol{v}'+\boldsymbol{v}_1'$ and $(\boldsymbol{v})^2+(\boldsymbol{v}_1)^2 = (\boldsymbol{v}')^2+(\boldsymbol{v}_1')^2$ expressing the conservations of the momentum and the energy in the binary collisions. The form of the Boltzmann collision term appearing in (13) comes from considering binary collisions as chemical reactions of species parametrized by the momentum coordinate $\boldsymbol{v}$ (see more in [24]).

The modules of (1) corresponding to (13) are the following: the state variable x is the one particle distribution function $f(\boldsymbol{r},\boldsymbol{v})$, $\{A,B\} = \int d\boldsymbol{r}\int d\boldsymbol{v} f\left[\frac{\partial A_f}{\partial \boldsymbol{r}}\frac{\partial B_f}{\partial \boldsymbol{v}} - \frac{\partial B_f}{\partial \boldsymbol{r}}\frac{\partial A_f}{\partial \boldsymbol{v}}\right]$
$\Phi(f,T,\mu) = k_B\int d'rr\int d\boldsymbol{v} f(\boldsymbol{r},\boldsymbol{v})\ln f(\boldsymbol{r},\boldsymbol{v})_{\frac{1}{T}}\int d\boldsymbol{r}\int d\boldsymbol{v} f(\boldsymbol{r},\boldsymbol{v})\frac{\boldsymbol{v}^2}{2m} - \frac{\mu}{T}\int d\boldsymbol{r}\int d\boldsymbol{v} f(\boldsymbol{r},\boldsymbol{v})$
$\Psi(f,f^*) = \int d\boldsymbol{r}\int d\boldsymbol{v}\int d\boldsymbol{v}'\int d\boldsymbol{v}_1\int d\boldsymbol{v}_1' W(f;\boldsymbol{v},\boldsymbol{v}_1,\boldsymbol{v}'\boldsymbol{v}_1')(e^X+e^{-X}-2)$, where
$X = -f^*(\boldsymbol{r},\boldsymbol{v}) - f^*(\boldsymbol{r},\boldsymbol{v}_1) + f^*(\boldsymbol{r},\boldsymbol{v}') + f^*(\boldsymbol{r},\boldsymbol{v}_1')$ is the thermodynamic force driving the binary collisions and $W^{(B)}$ appearing in (13) and W appearing in the dissipation potential are related by
$W^{(B)} = \frac{1}{2}W[f(\boldsymbol{r},\boldsymbol{v})f(\boldsymbol{r},\boldsymbol{v}_1)f(\boldsymbol{r},\boldsymbol{v}')f(\boldsymbol{r},\boldsymbol{v}_1')]^{\frac{1}{2}}$. It is easy to verify that the GENERIC equations (1) with the modules specified above becomes indeed the Boltzmann kinetic equation (13).

The Poisson bracket expressing the kinematics of the one particle distribution function $f(\boldsymbol{r},\boldsymbol{v})$ is the Lie-Poisson bracket (see section 2.1) that can be obtained from the Lie group of canonical transformations in the one particle phase space with coordinates $(\boldsymbol{r},\boldsymbol{v})$ or alternatively by a reduction [6]. The dissipation potential corresponding to the binary collisions is a particular case of the dissipation potential arising in chemical kinetics [24].

2.5. Mathematical rigor

In mesoscopic theories, the state variable x is typically a collection of fields (as it is in fluid mechanics) or a distribution function (as it is in the kinetic theory). This is because x characterizes only a part (the part that directly interests us) of the full microscopic state characterization. The interesting part is often of the statistical nature and thus it is expressed in terms of a distribution function. Moments of the distribution function are then the fields. The state space **M** is thus typically infinite dimensional. This means that the mathematically rigorous discussion has to include many elements that are not needed in the case when **M** is a finite dimensional space. In particular, we have to choose in the rigorous analysis the topology that gives a precise meaning to the notion of a limit and is thus also essential for a rigorous use of the calculus. From the physical point of view, these extra requirements could play the role of additional tools that can be used to express the physics involved. This type of interaction of physics and mathematics is not yet however very developed. There are only a few particular realizations of (1) with infinite dimensional spaces **M** for which the questions arising in the mathematically rigorous analysis have been addressed. We recall below some examples.

The question of the global (in time and space) existence of solutions to the Boltzmann kinetic equation has been answered in [25]. The topology used in the proof has not received yet, to the best of our knowledge, a physical interpretation. We will not therefore discuss the physical significance of this result. There is however another mathematically rigorous result about solutions of the Boltzmann equation, obtained by Grad [26] and Villani and Devillettes [27], that does provide a new physical insight. The problem studied in [26, 27] is the approach of solutions to the Boltzmann equation to the spatially homogeneous Maxwell distribution. Their rigorous analysis shows that the thermodynamic potential (7), satisfying the properties (9), can play the role of the Lyapunov function for the approach. There is an important physical insight revealed in the analysis. The second term on the right hand side of (1), called in the context of the Boltzmann equation the Boltzmann collision term, drives, if considered only by itself, the distribution function to the local (i.e. spatially inhomogeneous) Maxwellian distribution. If it is however considered together with the first term (called, in the context of the Boltzmann equation, a free flow term), that by itself leaves the entropy unchanged, then solutions approach, as $t\rightarrow\infty$, the total (spatially homogeneous) Maxwell distribution. This means that just by changing the manifold of the local Maxwellian distributions from an exact invariant manifold to an approximate invariant manifold (by adding to the vector field a term that by itself leaves the entropy invariant) we in fact enhance the dissipation. In other words, just by following the time evolution generated by both the collision term and the free flow term, the dissipation increases. We believe that this result has a profound significance for understanding the emergence of the dissipation and the time irreversibility. Originally a very small dissipation (for example created by making the microscopic particle indistinguishable—see [28])—may gradually increase into the dissipation needed for the approach to equilibrium states.

The Vlasov kinetic equation (addressing the time evolution of a collisionless gas with long range attractive interactions) is a particular realization of (1) without the second term on its right hand side. In spite of the complete absence of the dissipation in the vector field, solutions to the Vlasov equations are shown to approach a spatially homogeneous distribution. This property is called a Landau damping. Villani and Mouhot [29] have shown in their rigorous analysis that the dissipation emerges as the loss of regularity of the solutions. A physical interpretation, in the context of the multiscale GENERIC dynamics, has been recently given to this result in [30].

Another example where the mathematical rigor appears to be very closely associated with the physical content arises in the investigation of the system of partial differential equations known as the system of Godunov local conservation laws [31–33]. Existence of the companion local conservation law (from the physical point of view, the local conservation of entropy) implies that the initial value problem for the partial differential equations is well posed.

A rigorous analysis of the interplay between GENERIC dynamics and stochastic processes investigated in [34, 35] are also contributing to a deeper understanding of the physics involved in the GENERIC structure.

The GENERIC equations arising in the rheological modeling of complex fluids have also attracted attention of the rigorous functional analysis [36, 37]. The physical interpretation and the physical significance of these investigations remain to be clarified.

2.6. Contact geometry

The classical equilibrium thermodynamics is mathematically expressed in the fundamental thermodynamics relation (5) and the MaxEnt principle. How can we formulate it geometrically? Gibbs has suggested [38] to regard (5) as a two dimensional manifold, called Gibbs manifold, imbedded by the mapping $(E, N)\hookrightarrow(S(E, N), E, N)$ in the three dimensional space with coordinates (S, E, N). But this geometrical formulation does not include the MaxEnt principle. How can we include it? This question has been answered by Hermann in [39]. The chain of arguments leading to Hermann's answer can be formulated as follows (see [40]). MaxEnt with constraints is, from the mathematical point of view, a Legendre transformation. The group of Legendre transformations is thus the fundamental group of thermodynamics. Following now the reasoning developed mainly in the elementary particle physics, we look for the geometry in which the transformations in the fundamental group appear as natural transformations. This leads us to the contact geometry since the 1-form specifying the contact structure is preserved in the Legendre transformations. In the context of the classical thermodynamics, the passage to the contact formulation means to lift the two dimensional Gibbs manifold imbedded in the three dimensional space with coordinates (S, E, N) to another two dimensional manifold, denoted $\mathcal{M}^{(GL)}$, imbedded in the five dimensional space with coordinates (S, E^*, N^*, E, N) by the mapping $(E, N)\hookrightarrow(S(E, N), S_E(E, N), S_N(E, N), E, N)$. Such lift is also called a 1-jet extension of the function $S=S(E,N)$. The five dimensional space with coordinates (S, E^*, N^*, E, N), called a contact thermodynamic space, is, from the mathematical point of view, $T^*\mathbf{N}_{eq}\times\mathbb{R}$, where $\mathbf{N}_{eq}$ is the space of equilibrium thermodynamics, (i.e. $(E, N)\in\mathbf{N}_{eq}$), and $T^*\mathbf{N}_{eq}$ is the cotangent bundle of $\mathbf{N}_{eq}$ with coordinates (E, N, E^*, N^*). The contact thermodynamic space is naturally equipped with the 1-form $\theta=dS-E^*dE-N^*dN$. This form is preserved in Legendre transformations. The manifold on which the contact 1-form equals zero is called a Legendre manifold. On the manifold $\mathcal{M}^{(GL)}$ the 1-form θ equals zero and it is thus a Legendre manifold. In the context of thermodynamics we call it a Gibbs-Legendre manifold since it is a natural lift of the Gibbs manifold from the space with coordinates (S, E, N) to the contact thermodynamic state space with coordinates (S, E^*, N^*, E, N).

Following [40], we extend now the above contact formulation of classical thermodynamics to the mesoscopic thermodynamics expressed in the fundamental thermodynamic relation (6). We begin by introducing a space $\mathbb{M}^{(eq)} = \mathbf{M} \times \mathbf{M}^* \times \mathbf{N}_{eq} \times \mathbf{N}^*_{eq} \times \mathbb{R}$ with coordinates (x, x^*, y, y^*, ϕ). The space $\mathbf{M}^*$ with elements x^* is the dual space of the mesoscopic state space $\mathbf{M}$, similarly, $\mathbf{N}^*_{eq}$ with elements y^* is the dual space of the equilibrium state space $\mathbf{N}_{eq}$. The space $\mathbb{M}^{(eq)}$ is naturally equipped with the 1-form $\vartheta = d\phi - x^*dx - ydy^*$. The thermodynamic potential takes the form $\Phi(x, y^*) = -S(x) + \langle y^*, \mathcal{P}(x)\rangle$, where we use a shorthand notation $\mathcal{P}(x) = (E(x), N(x))$. The Gibbs-Legendre manifold $\mathcal{M}^{(GL)}_{(Meq)}$ expressing geometrically the fundamental thermodynamic relation (6) is now the image of the mapping $(x, y^*) \hookrightarrow (\Phi(x, y^*), x, \Phi_x(x, y^*), y^*, \Phi_{y^*}(x, y^*))$. This manifold displays the fundamental thermodynamic relation (6) in $[\mathcal{M}^{(GL)}_{(Meq)}]_{y^*=0}$ as well as the states x_{eq} representing the thermodynamic equilibrium in $[\mathcal{M}^{(GL)}_{(Meq)}]_{x^*=0}$.

As in section 2.3, we want to introduce time evolution, now it will be the time evolution in $\mathbb{M}^{(eq)}$, that makes the reducing Legendre transformation from the level *MESO* to the level *equilibrium*. However, we now have an extra requirement on this time evolution [41]. We want it to be the time evolution that preserves the contact structure, i.e. that leaves invariant the 1-form ϑ. We begin by asking the question of what is a general form of the time evolution equations preserving the 1-form θ. The answer to this question is well known (see e.g. [42]):

$$\begin{aligned} \dot{x} = \mathcal{H}_x; \quad \dot{x}^* &= -\Psi_x + x^*\mathcal{H}_\phi \\ \dot{y}^* = \mathcal{H}_y; \quad \dot{y} &= -\mathcal{H}_{y^*} + y\mathcal{H}_\phi \\ \dot{\phi} &= -\mathcal{H} + \langle x^*, \mathcal{H}_{x^*}\rangle + \langle \mathcal{H}_y, y\rangle \end{aligned} \tag{14}$$

where $\mathcal{H}$, called a contact Hamiltonian, is a real valued function of $(x, x^*.y.y^*, \phi)$.

It remains to find the contact Hamiltonian for which: (i) the Gibbs-Legendre manifold $\mathcal{M}^{(GL)}_{(Meq)}$ is an invariant manifold, and (ii) (equation (14)) $_{\mathcal{M}^{(GL)}_{(Meq)}}$ is the GENERIC equation (1). It is easy to verify (see more in [40, 41, 43, 44]) that

$$\mathcal{H}(x, x^*, y^*) = -\mathcal{S}(x, x^*, y^*) + \frac{1}{E^*}\mathcal{E}(x, x^*, y^*) \tag{15}$$

where

$$\begin{aligned} \mathcal{S}(x, x^*, y^*) &= \Psi(x, x^*, y^*) - [\Psi(x, x^*, y^*)]_{x^*=\Phi_x} \\ \mathcal{E}(x, x^*, y^*) &= \langle x^*, L\Phi_x\rangle \end{aligned} \tag{16}$$

is such contact Hamiltonian provided we put an extra requirement

$$\langle x^*, [\Psi_{x^*}]_{x^*=E_x}\rangle = \langle x^*, [\Psi_{x^*}]_{x^*=N_x}\rangle = 0 \tag{17}$$

on the degeneracy of the dissipation potential Ψ

The lift of the metriplectic equation (1) to the contact equation (14) makes the cohabitation of the two unfriendly vector fields appearing on the right hand side of (1), one symplectic and the other gradient, harmonious. In the contact equation (14) there is only one geometry, namely the contact geometry, transforming the covector (arising as a gradient of a generating potential) into a vector. The contact geometry is fixed and remains unchanged in the time evolution. The symplectic and the metric parts of the GENERIC dynamics (1) enter the contact dynamics (14) as two terms in the generating potential (15). Moreover, the thermodynamic aspects of the GENERIC time evolution enter the contact formulation (14) in the geometry of the Gibbs-Legendre manifold $\mathcal{M}^{(GL)}_{(Meq)}$ on which the time evolution takes place. Contact geometry has been recently discussed in the context of thermodynamics also in [45–50].

Among the interesting open problems we mention a few: (i) to clarify the physical meaning of the time evolution governed by (14) outside the Gibbs-Legendre manifold $\mathcal{M}^{(GL)}_{(Meq)}$, (ii) to lift the GENERIC equations discussed in section 3 to contact dynamics, (iii) to use the contact formulation for developing physically meaningful discretizations (an attempt in this direction is made in section 4.3.4 in [40]).

2.7. Variational formulation

It is well known that the Hamilton dynamics allows variational formulation (Hamilton's variational principle). Such formulation does not extend however to the metriplectic dynamics (1). An important advantage of the contact formulation (14) is that it allows the variational formulation and that the formulation has a very clear physical interpretation: the total entropy generated during the time evolution reaches its extremum.

We introduce a functional (see [40, 50–52])

$$\mathcal{I} = \int dt\, (\mathcal{H}(x, x^*, y^*) - \langle x^*, \dot{x} \rangle) \tag{18}$$

We see that $[\mathcal{I}]_{\mathcal{M}^{(GL)}_{(Meq)}}$ has the physical interpretation of the entropy generated during the time evolution. We also see that the Euler–Lagrange equations $\delta\mathcal{I} = 0$ (variations with respect to both x and x^*) on $\mathcal{M}^{(GL)}_{(Meq)}$ become equivalent to (1).

2.8. What is the nonequilibrium mesoscopic entropy?

In order to be able to apply equilibrium thermodynamics (i.e. the *equilibrium* level of description), the macroscopic systems have to be prepared. This is the Postulate 0 in Callen's formulation of thermodynamics [2] (see also [28] for the extension of this postulate to mesoscopic multiscale thermodynamics). The preparation process consists of leaving the macroscopic systems sufficiently long time free of external influences. The time evolution involved in the preparation process is governed by (1). The potential $S(x)$ entering this equation is the nonequilibrium mesoscopic entropy. This is our definition of the nonequilibrium mesoscopic entropy. We thus see the existence of the nonequilibrium mesoscopic entropy as a consequence of the Postulate 0. The question: does the nonequilibrium mesoscopic entropy exist and what it is? is the same question as: can the macroscopic system under consideration be prepared for using *equilibrium* level and what exactly is the time evolution involved in the preparation process?.

The terminology and the notation are also, at least partially, responsible for difficulties and confusions that are associated with the concept of entropy. For example $S(x)$ entering (1) and $S(x_{eq})$, where x_{eq} is $t \to \infty$ solution of (1), are two different quantities, having two different physical meanings, but they are both often called simply an entropy. Moreover, we note that the nonequilibrium mesoscopic entropy $S(x)$, defined above, depends on the initial level *MESO*. By changing the *MESO* level (i.e. by changing the way we see the macroscopic systems) we change the entropy. There are therefore as many entropies $S(x)$ as there are *MESO* levels. In section 3, where we consider the passages *MESO* → *meso*, we shall see in addition that the entropies also depend on the target level *meso*. The notation introduced in section 3 (used already in [28]) attempts to eliminate unnecessary disagreements when discussing the concept of entropy.

We emphasize that the entropy is an interscale (or in other words interlevel) concept (i.e. a concept that needs two different levels to be defined and that addresses the relation between them). This fundamental aspect of the entropy is not directly visible in the classical thermodynamics that is formulated only on a single level, namely the *equilibrium* level. The equilibrium entropy on the *equilibrium* level is $S^*(T, \mu)$, or its Legendre transform $S(E, N)$, that makes its appearance in the Postulates 1, 2, and 3 of Callen [2]. In the GENERIC viewpoint of thermodynamics, that we follow in this paper, the equilibrium entropy $S(E, N)$ arises as a Legendre transformation of $S^*(T, \mu) = \Phi(x_{eq}(T, \mu), T, \mu)$, where $x_{eq}(T, \mu)$ is the asymptotic ($t \to \infty$) solution of the GENERIC equation (1) in which the potential $S(x)$ appears as the potential generating the approach to $x_{eq}(T, \mu)$.

The interscale nature of the entropy is, on the other hand, clearly visible in the Gibbs equilibrium statistical mechanics addressing the passage *MICRO* → *equilibrium*. The level *MICRO* (playing now the role of *MESO* in the passage *MESO* → *equilibrium*) is the microscopic level of description on which the state variable x consists of the position vectors and momenta of all $\mathfrak{N}$ microscopic particles composing the macroscopic system under investigation (or alternatively, in the Liouville representation, the distribution function $f_{\mathfrak{N}}$ of all $\mathfrak{N}$ particles)). The entropy on the *MICRO* level is the Gibbs entropy $S^{(Gibbs)}(f_{\mathfrak{N}}) = -k_B \int f_{\mathfrak{N}} \ln f_{\mathfrak{N}}$, where the integration is over the phase space of all $\mathfrak{N}$ particles. The minimization of the thermodynamic potential (7), with x being the distribution function $f_{\mathfrak{N}}$, $S(x)$ being the Gibbs entropy $S^{(Gibbs)}(f_{\mathfrak{N}})$, $E(x)$ being the average energy of the $\mathfrak{N}$ particles, and $N(x) = \int f_{\mathfrak{N}}$, provides the equilibrium entropy $S^*(T, \mu)$. This means that in the Gibbs equilibrium statistical mechanics we indeed obtain $S^*(T, \mu)$ as $S^*(T, \mu) = \Phi(x_{eq}(T, \mu), T, \mu)$, where $x_{eq}(T, \mu)$ is the distribution function $f_{\mathfrak{N}}$ at which the thermodynamic potential Φ reaches its minimum. What is missing in the Gibbs equilibrium statistical mechanics is the time evolution on the *MICRO* level in which $x_{eq}(T, \mu)$ is approached as $t \to \infty$. The microscopic dynamics on the *MICRO* level (governed by Hamilton's equations governing the time evolution of $\mathfrak{N}$ particles) is replaced in the Gibbs equilibrium statistical mechanics by: (i) the conservation of the total energy and the total number of particles, (ii) ergodic-type hypothesis about solutions of Hamilton's equations governing the time evolution of $\mathfrak{N}$ particles, and (iii) MaxEnt principle with the Gibbs entropy $S^{(Gibbs)}(f_{\mathfrak{N}}) = -k_B \int f_{\mathfrak{N}} \ln f_{\mathfrak{N}}$.

Summing up, we answer the question of how to extend the well known concept of the equilibrium entropy to nonequilibrium by reversing it. We ask the question of how to reduce the well known concept of the nonequilibrium entropy to the equilibrium entropy. The nonequilibrium entropy is well understood because it is the potential driving the process in which the macroscopic systems under investigation become prepared for using the equilibrium thermodynamics as a viable theory. The equilibrium entropy then arises simply by following the preparation process to its conclusion.

Attempts to answer directly the question of extending the concept of the equilibrium entropy to nonequilibrium have to begin with the question of how to understand the equilibrium entropy. There are indeed several very interesting and very useful ways to define the equilibrium entropy (e.g. through an analysis of the Carnot machines, or, inspired by the Gibbs equilibrium statistical mechanics, as a quantity proportional to the logarithm of the volume of the region in the $\mathfrak{N}$ particle phase space that corresponds to a single state on the *equilibrium* level, or others) the problem is that neither of these viewpoints of the equilibrium entropy extends well to other levels of description and to nonequilibrium.

2.9. Dissipation potential

The concept of the dissipation potential has appeared in [53] and [54]. From the geometrical point of view, (2) represents the gradient dynamics and (4) a generalized gradient dynamics. The generalization (4) of (2) has appeared in [15] in the context of the Boltzmann equation, in chemical kinetics [24], the diffusion theory [34], in stochastic processes [55] (in particular in the large deviation theory [35]), in the investigation of stochastic extensions of chemical kinetics (by lifting the chemical kinetics to the Fokker-Planck type kinetic theory [24]), in attempts to derive (1) from the microscopic dynamics [56], and in attempts to provide the most suitable geometrical setting for (1) (discussed in section 2.6) above. The GENERIC equation has appeared in the form (1) also in [20]) where the name GENERIC was introduced. It is therefore highly inappropriate to call (1) a generalized GENERIC equation.

As for choosing among (2), (3), and (4), we note that (2) is clearly insufficient to express the dissipation term that arises in many well known mesoscopic dynamical theories (for example in chemical kinetics and in the Boltzmann equation). Both forms (3) and (4) can be however used. For instance the chemical kinetics can be put into the form (3) (see [21, 57])) as well as to the form (4) (see [24]). Also the Boltzmann equation has been put into the form (3) in [58] and into the form (4) in [15, 28]. Strong arguments in favor of the choice (4) have been recalled in the previous paragraph.

In order to see more into the difference between (3) and (4), we make the following observation. Let us consider $x = (x_1, x_2, \ldots)$. The equality of (3) and (4) implies

$$M_{ij}(x, x^*)x_j^* = \frac{\partial\Psi(x, x^*)}{\partial x_i^*} \tag{19}$$

By differentiating this equation with respect to x_k^* we get

$$\frac{\partial M_{ij}(x, x^*)}{\partial x_k^*} + M_{ik}(x, x^*) = \frac{\partial^2\Psi(x, x^*)}{\partial x_i^*\partial x_k^*} \tag{20}$$

The $i \leftrightarrow k$ symmetry of the right hand side and the symmetry of M imply

$$\frac{\partial M_{ij}(x, x^*)}{\partial x_k^*} = \frac{\partial M_{kj}(x, x^*)}{\partial x_i^*} \tag{21}$$

This is the integrability condition that makes (3) identical to (4).

This integrability condition is clearly satisfied for M that is independent of x^* (i.e. a particular case of (4) for the quadratic dissipation potential). At this stage, we do not see any direct physical interpretation of the integrability condition (21). Indirectly however, there are many arguments, mentioned above, in favor of (4).

2.10. How many generating potentials are there?

In order to formulate the mesoscopic thermodynamics on the *MESO* level we need to specify the three potentials (6). In order to formulate the mesoscopic dynamics on the *MESO* level that is compatible with the mesoscopic thermodynamics we need to specify the same three potentials (6). The number of moles $N(x)$ enters the dynamics only indirectly (since it is both the symplectic and the metric Casimir), the energy $E(x)$ generates the Hamiltonian part of the time evolution and is the metric Casimir, the entropy $S(x)$ generates the thermodynamic part of the time evolution and is the symplectic Casimir. All three potentials (6) can be combined into one thermodynamic potential (7) that can serve as a single generating potential but then the GENERIC equation (1) takes the form

$$\dot{x} = TL\Phi_x - [\Psi_{x^*}]_{x^*=\Phi_x} \tag{22}$$

provided the requirement of degeneracy of Ψ includes also (17). In the case of the macroscopic systems that are kept at a constant temperature T, we can absorb the constant T into L and consider (1) as the time evolution equation involving only a single generating potential Φ. In general however, the GENERIC time evolution is always generated by the three potentials (6).

2.11. GENERIC statistical mechanics

We recall the Gibbs equilibrium statistical mechanics. The mathematical formulation of the classical equilibrium thermodynamics consists of the fundamental thermodynamic relation (5) and the MaxEnt principle. There is only one module that needs to be specified, namely the function $S = S(E, N)$. Given a macroscopic system, the specification can be made by following three routes: (i) by making experimental observations (results of the observations are collected in Thermodynamic tables), (ii) by starting on the *MESO* level with (6) that is specified by using a (mesoscopic) physical insight, and then applying the MaxEnt principle, and (iii) by turning to the Gibbs equilibrium statistical mechanics that provides a universal passage $MICRO \to equilibrium$ (see also section 2.8). By *MICRO* we denote the microscopic level of description on which the state variable x includes position vectors and momenta of all the microscopic particles composing the macroscopic system under investigation. The mapping is based on the assumption that the only thing that enters to the passage $MICRO \to equilibrium$ from the microscopic dynamics is the mass and energy conservation and the assumption that the microscopic trajectories are ergodic (in the sense that the time averages can be replaced by appropriate averages in the microscopic state space) together with the MaxEnt principle. The precise nature of the ergodicity that is sufficient for the validity of the equilibrium statistical mechanics passage $MICRO \to equilibrium$ has not yet been established.

Now we turn to the GENERIC equation (1). Instead of one module, we now have to specify all the modules (represented by the symbols (E, S, N, L, Ψ)) appearing in (1). Is there a universal passage $MICRO \to MESO$ that would provide a mapping between the microscopic Hamiltonian and the GENERIC modules, similarly as the passage $MICRO \to equilibrium$ introduced by Gibbs provides a mapping between the microscopic Hamiltonian and the fundamental thermodynamic relation (5)? The Gibbs passage $MICRO \to equilibrium$ is called an equilibrium statistical mechanics. We can correspondingly call the passage $MICRO \to MESO$ a *MESO* statistical mechanics or also GENERIC statistical mechanics (this name is used in [22]). It is clear that the universality of the mapping $MICRO \to MESO$, if it exists, must be limited since the mapping must depend on the choice of the *MESO* level. In addition, it seems to be also clear that in order to arrive at the modules (E, S, N, L, Ψ), the *MICRO* dynamics cannot be reduced only to the mass and the energy conservation and to the ergodicity hypothesis. Nevertheless, in particular if one considers only the version of (1) with the dissipation (2), very useful results in this direction have been obtained (see [22, 59]). The investigation described in [22] follows and extends the arguments introduced in Onsager's derivation of the Onsager relations [60, 61] and in the Green and Kubo investigations [62, 63] providing microscopic formulas for the Onsager coefficients.

2.12. Numerical methods preserving the GENERIC structure

If we want computers to assist us in solving the time evolution equations, the mathematical formulations have to be adapted to their abilities. In particular, the formulations have to be discrete and finite dimensional. From the physical point of view, we can see the discretization as a passage $MESO \to \mathbb{MESO}$, where $\mathbb{MESO}$ is the level of description suitable for computers. On the *MESO* level the time evolution is governed by a particular realization of the GENERIC equation (1) and on the $\mathbb{MESO}$ level the time evolution is governed by another particular realization of the same GENERIC equation (1). In other words, we require the general structure expressed in (1) to be preserved in the passage $MESO \to \mathbb{MESO}$. To make such passage is a big challenge from the mathematical point of view. Below, we mention a few examples.

Discretization in the finite dimensional state space that preserves the symplectic structure (i.e. only the time is discretized) has been extensively studied [64]. In the context of (1) this is the case when $\mathbf{M}$ is finite dimensional and the second term on the right hand side of (1) is missing. An extension of some of the methods developed in the symplectic-structure-preserving time discretization to the GENERIC-structure-preserving time discretization has been recently investigated in [65].

Another example of discretization, in this case in both the time and the space, in which a physically meaningful structure is preserved is the Godunov numerical method. The time evolution equations on the *MESO* level are the Godunov local conservation laws (the time derivative of a field equals gradient of a flux plus a source term), mentioned already in section 2.5. The discretized time evolution equations are again conservation laws but in discrete space elements and in discrete time. The limitation of the Godunov numerical method to local conservation laws is not severe since many time evolution equations (including for example many GENERIC equations arising in the context of complex fluids) can be cast, after appropriately extending them, into the form of the Godunov local conservation laws [66].

2.13. Why and how to make a non GENERIC model GENERIC?

As we have already mentioned in Introduction, modeling the time evolution of specific macroscopic systems consists of constructing specific particular realizations of (1), i.e. one needs to specifying all the modules appearing in (1). The specification is made by using the physical insight into the macroscopic system under investigation. The insight is acquired from seeing results of experimental observations and from a hypothetical microscopic picture of the physics involved. If the modules satisfy all the general properties listed in sections 2.1, 2.2, and 2.3 and are put together in accordance with (1), the compatibility with the equilibrium thermodynamics and all other properties of solutions of (1) discussed above in this section are guaranteed. Many models have been constructed in this way (see the review in [1]).

There are however also many models that have been constructed without the assistance of (1). Many of them have been validated with experimental observations and can be thus considered to be well established models. Examining their mathematical structure one finds that at least some of them do not possess the GENERIC structure. How shall we deal with this situation? There are two routes to take. The first one is to weaken the GENERIC structure so that the non-GENERIC but well established models will possess it. For example, we can abandon the requirement that the split of the vector field into dissipative and nondissipative is the same as the split into irreversible and reversible and also the same as the split into gradient (or generalized gradient) and Hamiltonian (see also the end in section 2.3). Some researches indeed have taken this route. We take the second route. We shall consider the well established models that do not possess the GENERIC structure as approximations of models (we shall call them extended GENERIC models) that do possess it. By constructing the extended GENERIC models (see also section 3.2) we provide: (i) an extra validation by proving the compatibility with the equilibrium thermodynamics, (ii) extra properties of solutions implied by the strong GENERIC structure, (iii) an extra physical insight that is revealed in the extension process (see section 3.2).

How shall we make the extension? Below, we shall provide two examples (see more in section 3.2). In the first one, in section 2.13.1, we show that a large class of well established but non GENERIC models can be seen as quasi-static approximations of extended GENERIC model in which a velocity type field has been adopted as an extra state variable. In the second example, in section 2.13.2, we present a well established non-GENERIC model (the Enskog kinetic equation) for which the problem of casting it, or its extension, to the GENERIC form (1) remains an open problem.

2.13.1. *Quasi-static approximation of GENERIC models*

We consider models in which the reversible part of the vector field is nondissipative but not Hamiltonian. The problem is to extend such model to a fully GENERIC model and illuminate in the process the physics involved. As an illustration, we consider a large family of models arising in the modeling of complex fluids. If the suspended particles or macromolecules are passively advected by the overall velocity (which is the only velocity type field included in the state variables) then the models are fully GENERIC. Due to the complex interactions on the fluid-particle interface or due to internal deformations of the particles, the particles do not follow exactly the overall flow, a slip emerges, [67]. With the slip, the reversible part remains nondissipative (this can be seen in fact as a condition determining the expression for the stress tensor, [68, 69]) but ceases to be Hamiltonian. From the physical point of view, that in the case of the slip, the velocity in the vicinity of the particle-fluid interface is different from the overall velocity. If such velocity is adopted as a new independent state variable, the model becomes GENERIC. By assuming that the extra velocity field evolves much faster than the rest of the state variables (the quasi-static approximation), the GENERIC model reduces to the original model. The interested reader can find details in [71] and a very simple finite dimensional illustration in section 3.2 in [70].

2.13.2. *Enskog kinetic equation*

In this example we recall an important modification of the Boltzmann kinetic equation (13), namely the Enskog kinetic equation. From the physical point of view, the collisions of point particles are replaced in the Enskog extension by collisions of a finite size hard core particles. This modification brings a new term into the time reversible part and a corresponding to it a new term into the Boltzmann entropy. With the modified entropy, the reversible part of the Enskog kinetic equation remains nondissipative [72]. As to wether the modified reversible part remains also Hamiltonian is an unsolved problem. To the best of our knowledge, the Hamiltonian structure that would make the Enskog kinetic equation (or its appropriate extension) GENERIC is not known.

If, in addition, the particles are let to interact also via long range attractive forces that are taken into account in the kinetic equation in the Vlasov mean field term (see [30]), the equilibrium thermodynamics implied by such Enskog-Vlasov equation is the equilibrium thermodynamics of the van der Waals gas [73]. The Vlasov kinetic equation is clearly GENERIC (see [30]) but the GENERIC structure of the Enskog-Vlasov (or its appropriate modification) is not known.

3. New Directions in GENERIC

The GENERIC equation (1) discussed in the previous section addresses the passage *MESO* → *equilibrium*. We now replace the *equilibrium* level with a *meso* level that is less detailed than the *MESO* level but still more detailed than the *equilibrium* level. An investigation of the $MESO \to meso$ passage (discussed in section 3.1 is an interesting and an important generalization of the investigation of the passage $MESO \to equilibrium$ since we can include into our consideration also externally driven systems that are prevented from reaching the equilibrium states (this means that the *equilibrium* level is not admissible to them) but still admit a mesoscopic level of description. For example, the observed behavior of the Rayleigh-Bénard system (a horizontal layer of a fluid heated from below) is known to be well described on the level of fluid mechanics. This means that any more detailed description of the Rayleigh-Bénard system (for example the description on the level of kinetic theory) has to approach, as $t \to \infty$, the level of fluid mechanics. The two external forces, namely the gravitational force and the imposed temperature gradient, prevent the approach to the complete thermodynamic equilibrium and consequently the equilibrium thermodynamics is not applicable.

In section 3.2 we then consider the passage $meso \to MESO$ that represents an extension of *meso* level to a more detailed *MESO* level.

3.1. Multiscale reductions

What new we meet in the investigation of $MESO \to meso$? First of all, there is no time evolution on the *equilibrium* level but there is a time evolution, at least in general, on the *meso* level. From the *MESO* level point of view, we call the dynamics involved in the passage $MESO \to meso$ a *reducing dynamics* and the dynamics on the *meso* level a *reduced dynamics*. This terminology has been introduced in [28]. By using it, the time evolution involved in the passage $MESO \to equilibrium$, that we have discussed in section 2, is the reducing time evolution and the reduced time evolution in the passage $MESO \to equilibrium$ is no time evolution.

Having the *MESO* time evolution, the problem that we are facing is to split it into the $MESO \to meso$ reducing time evolution and the *meso* reduced time evolution in such a way that the originally given *MESO* time evolution is well approximated by the reducing time evolution followed by the reduced time evolution. We can see the reformulation of the *MESO* dynamics into $MESO \to meso$ and *meso* dynamics as a nonlinear version of the block diagonalization known in the linear dynamics. The split of the *MESO* dynamics into the reducing is a result of a pattern-recognition investigation of solutions of the *MESO* dynamics. Collections of all the *MESO* trajectories (i.e. solutions, passing through all $x \in M$, to the governing equations of the *MESO* dynamics) form the *MESO* phase portrait (using the dynamical-system terminology). The problem of splitting the *MESO* dynamics into the reducing and the reduced dynamics is the problem of recognizing a pattern in the *MESO* phase portrait. The recognized pattern represents then the *meso* phase portrait and the process revealing it represents the reducing dynamics. We shall not discuss this very difficult problem here, we make only a few remarks that are inspired by its connection with thermodynamic.

Let us assume that we know the *meso* dynamics Moreover, we also know that the *meso* dynamics is found to describe well the experimentally observed behavior. This means that the split of the *MESO* dynamics into the reducing and the reduced dynamics must exist. The *meso* dynamics (that we assume to know) is the reduced dynamics. How do we find the reducing dynamics? We have seen in the previous section that the reducing dynamics making the passage $MESO \to equilibrium$ is GENERIC. *We assume that the reducing time evolution making the passage* $MESO \to meso$ *is also GENERIC*. Making this assumption, the problem that we face now is to adapt the GENERIC equation (1) to $MESO \to meso$ (i.e. an equations replacing (1) in the $MESO \to meso$ investigations) and then to construct its appropriate realizations. This problem has been discussed in [28]. Here we only recall a few essential points.

Before proceeding with the investigation of the GENERIC equation representing the passage $MESO \to meso$ we emphasize that in the context of externally forced systems (i.e. macroscopic systems that are prevented from reaching the *equilibrium* level) the governing equations of neither *MESO* dynamics nor the *meso* dynamics are GENERIC. What we assume however that the dynamics involved in the passage $MESO \to meso$ is always GENERIC (due to the fact that both the levels *MESO* and *meso* are found to describe well the experimentally observed behavior of the externally forced system under investigation).

The state space on the *meso* level is denoted by the symbol $\mathbf{N}$, the state variables are $y \in \mathbf{N}$. The time evolution of y, governed by

$$\dot{y} = Y(y) \tag{23}$$

is assumed to be known. The fundamental thermodynamic relation with which we replace (6) is

$$S^{(Mm)} = S^{(Mm)}(x); \quad y = y(x) \tag{24}$$

The upper index (Mm) makes reference to $MESO \to meso$. The potential $S^{(Mm)}(x)$ is the entropy associated with the passage $MESO \to meso$. Next, we introduce the $MESO \to meso$ thermodynamic potential

$$\Phi^{(Mm)}(x, y^*) = -S^{(Mm)}(x) + \langle y^*, y(x) \rangle \tag{25}$$

The simplest GENERIC equation representing the reducing *MESO* → *meso* dynamics is

$$\dot{x} = -M^{(Mm)}\Phi^{(Mm)}_x(x) \tag{26}$$

where $M^{(Mm)}(x)$ is degenerate in the sense that $M^{(Mm)}y_x = 0$ and positive semi-definite operator. As $t \to \infty$, solutions to (26) approach a manifold $\mathcal{M}^{(Mm)} \subset \mathbf{M}$ and $S^{*(Mm)}(y^*) = [\Phi^{(Mm)}(x, y^*)]_{\mathcal{M}^{(Mm)}}$ is the fundamental thermodynamic relation on the *meso* level corresponding to the reducing dynamics *MESO* → *meso*. This fundamental thermodynamic relation is a new addition to the *meso* level description that does not come from the *meso* dynamics itself but from the reducing dynamics describing the *MESO* → *meso* passage.

Given the *MESO* dynamics, the *meso* dynamics, and $y = y(x)$, how do we find $S^{(Mm)}(x)$ and $M^{(Mm)}(x)$? A very extensive (pattern-recognition type) investigation of solutions to the *MESO* time evolution equations is needed to answer this question (see e.g. [74, 75]). We can also ask another question. Given the *MESO* dynamics, $y = y(x)$, and the entropy $S^{(Mm)}(x)$, what is the corresponding to it *meso* dynamics? This is in fact the question asked by Dreyer in [76] in the context of *MESO* dynamics being the Boltzmann kinetic theory and $y = y(x)$ being the projection on Grad's moments (see [77, 78]) does not consider the passage to the manifold $\mathcal{M}^{(Mm)} \subset \mathbf{M}$ (called a closure manifold in this context) as a result of the reducing dynamics (26) but simply as the MaxEnt principle. The governing equations of the *meso* dynamics are the governing equations of the *MESO* dynamics restricted to $\mathcal{M}^{(Mm)}$ with the vector field projected on $\mathcal{M}^{(Mm)}$ by the mapping induced on the tangent spaces by the mapping $y = y(x)$. The entropy $S^{(Mm)}(x)$ chosen by Dreyer is the classical Boltzmann entropy arising in the passage *MESO* → *equilibrium*. This entropy can, at best, be only an approximation of the entropy $S^{(Mm)}(x)$ arising in the reducing passage from the Boltzmann equation to the equation governing the time evolution of a finite number of Grad's moments.

If the macroscopic system under investigation is free from external influences then the *micro* dynamics is GENERIC since it describes the passage *meso* → *equilibrium*. In such case we have three types of the approach to equilibrium: (1) *MESO* → *equilibrium*, (2) *MESO* → *meso* → *equilibrium*, and (3) *meso* → *equilibrium*. How they are related? This is one of the open questions (see more open questions in section 3.3).

An alternative consideration of the *MESO* → *meso* passage has also been developed in [28]. We replace (24) with

$$\mathfrak{S}^{(Mm)} = \mathfrak{S}^{(Mm)}(x);\;\; y = y(x);\;\; Y = Y(x) \tag{27}$$

This means that we do not only specify the state variables *y* used on the *meso* level as functions of *x* (that is the state variable used on the *MESO* level) but we also specify the vector field (constitutive relations) governing the time evolution of *y* as a function of *x*.

The reducing time evolution (26) is replaced by

$$\dot{x} = -\mathfrak{M}^{(Mm)}\mathfrak{P}^{(Mm)}_x(x, Y^*) \tag{28}$$

where $\mathfrak{M}^{(Mm)}(x)$ is degenerate in the sense that $\mathfrak{M}^{(Mm)}y_x = 0$, $\mathfrak{M}^{(Mm)}Y_x = 0$, and positive semi-definite operator, $\mathfrak{P}^{(Mm)}$ is the thermodynamic potential

$$\mathfrak{P}^{(Mm)}(x, Y^*) = -\mathfrak{S}^{(Mm)}(x) + \langle Y^*, Y(x)\rangle \tag{29}$$

The quantities Y^* are the external forces acting on the *meso* level or, as functions of y^*, thermodynamic forces determining the constitutive relations. The time evolution governed by (28) approaches the vector field (constitutive relations) on the *meso* level (see (23)). For this reason the equations of the type (28) have been called in [28] CR-GENERIC (CR stands for Constitutive Relations). It has been shown in [28] that $\mathfrak{S}^{(mM)}(Y^*)$ (which is $\mathfrak{S}^{(Mm)}(x)$ evaluated at the $t \to \infty$ solution to (28)) has the physical interpretation of the entropy production on the *meso* level. The maximization of $\mathfrak{S}^{(Mm)}(x)$ achieved in the reducing time evolution (28) is thus a version of the Maximum Rate Entropy principle (MaxREnt).

3.2. Multiscale extensions

Until now, we have looked in this paper down toward levels that involve less details. Our intention was to identify a simpler description that more directly addresses the overall properties of solutions of the governing equations that are of our principal interest. In this section we shall look in the opposite direction. The need for looking at the passage *meso* → *MESO* (that we shall call an ***extension of the meso** level*) comes from an unsuccessful validation of the *meso* models and/or from the need to obtain an additional thermodynamic information on the *meso* level that arises from the reduction process *MESO* → *meso* as the fundamental thermodynamic relation $S^{(mM)}(y)$ (see section 3.1).

The validation is unsuccessful if the results of experimental observations cannot be satisfactory seen in solutions of the *meso* models. It becomes obvious that the *meso* description is incomplete. Some details ignored on the *meso* level must be actually important for arriving at a satisfactory agreement with results of our experimental observations. Where and how shall we look for the important physics that is missing in *meso*?

In the case of externally unforced systems (i.e. the systems that are allowed to reach the *equilibrium* level) the *meso* dynamics is GENERIC and we shall, of course, require that the equation governing the time evolution on the extended *MESO* level is also a GENERIC equation (1). For externally forced systems that are prevented from reaching the *equilibrium* level neither the *meso* nor the extended *MESO* dynamics is GENERIC.

There are essentially three different routes that have been explored in the search for the extra physics involved in the extended *MESO* theory . We shall briefly describe them in the three following sections.

3.2.1. Langevin extensions

The experimental evidence driving this route to extensions is the observation of fluctuations. Results of the experimental measurements are not found to be always the same. This is because the state characterized by one y is in fact a family of states. Results of the experimental measurements are different for different states in the family. This then means that one value of y is associated with a family of experimental values.

In the Langevin extension one does not try to identify the microscopic causes of the fluctuations (i.e. the missing physics on the *meso* level). The objective is to appropriately describe the observed fluctuations. Following Langevin, we turn to the mathematics of random variables and stochastic processes [34, 35, 55]. The physical aspects of the Langevin extension are discussed for example in [79–83]. Below, we shall briefly recall the GENERIC formulation in a simple setting. A more complete GENERIC formulation is discussed in [34, 35].

Our objective is to extend the *meso* level to a *MESO* level that takes into account fluctuations seen on the *meso* level. First, we turn to the choice of state variables. The quantity y serving as the state variable on the *meso* level is either replaced by $\hat{y}$ that is a random variable or by $f(y)$ that is a distribution function. Below, we shall follow the latter extension. The state variable x on the *MESO* level is thus $f(y)$.

Next, we need to formulate a GENERIC equation (1) with $f(y)$ serving as state variable on the extended *MESO* level from a known GENERIC equation (1) with y serving as the state variable on the *meso* level. We shall restrict ourselves in this paper to the *meso* dynamics with the quadratic dissipation potential $\Psi^{(m)}(y, y^*) = \frac{1}{2}\langle y^*, M^{(m)}(y)y^*\rangle$, where $M^{(m)}$ is a positive definite operator. No restrictions are placed on the Poisson bracket $\{A^{(m)}, B^{(m)}\}^{(m)} = \langle A_y^{(m)}, L^{(m)}B_y^{(m)}\rangle$, and the thermodynamic potential $\Phi^{(m)}(y)$.

Now we proceed to the extension $y \mapsto f(y) = x$. In kinematics, we make the extension $\{A^{(m)}, B^{(m)}\}^{(m)} \mapsto \{A^{(M)}, B^{(M)}\}^{(M)} = \int dyf(y)\{A_{f(y)}^{(M)}, B_{f(y)}^{(M)}\}^{(m)}$, in the dissipation potential $\Psi^{(m)}(y, y^*) = \frac{1}{2}\langle y^*, M^{(m)}(y)y^*\rangle \mapsto \frac{1}{2}\int dyf(y)\langle\frac{\partial f^*(y)}{\partial y}, M^{(m)}(y)\frac{\partial f^*(y)}{\partial y}\rangle = \Psi^{(M)}(x, x^*)$, and in the thermodynamic potential $\Phi^{(m)}(y) \mapsto \int dyf(y)(\Phi^{(m)}(y) + k_B \ln f(y)) = \Phi^{(M)}(x)$, where $f^*(y) = \Phi_{f(y)}^{(M)}$ and k_B is the Boltzmann constant. The equation governing the time evolution on the *MESO* level is thus

$$\frac{\partial f(y)}{\partial t} = -\frac{\partial}{\partial y}(f(y)TL^{(m)}\Phi_y^{(m)}(y)) + \frac{\partial}{\partial y}(M^{(m)}(y)f(y)\Phi_y^{(m)}(y)) + \frac{\partial}{\partial y}\left(k_B M^{(m)}(y)\frac{\partial f(y)}{\partial y}\right) \tag{30}$$

The first term on the right hand side is the term arising in the Liouville formulation of the time evolution equation on the *meso* level. The last two terms on the right hand side represent the dissipative part of the *MESO* time evolution. The first one is the Liouville formulation of the dissipation term on the *meso* level, the second is a new (Fokker-Planck like) term that arises due to the presence of fluctuations. The fact that the operator $M^{(m)}(y)$ is the same in both terms is a formulation of the fluctuation-dissipation theorem. We thus see that in this GENERIC formulation the fluctuation-dissipation theorem is a simple consequence of the requirement that the GENERIC structure is preserved in the extension.

3.2.2. Kirkwood extensions

The prime example of the experimental evidence motivating this type of extensions is the observation of the flow behavior of complex fluids (for example the flow behavior of the egg white). Flow of the egg white is manifestly different from the flow of water. Since the main difference between water and the egg white is the size of the molecules composing them, it is natural to suggest that the reason for the difference in the flow behavior is the strong coupling between the motion of the large macromolecules composing the egg white (involving all types of deformations and rotations) with the overall fluid motion. Such coupling is on the other hand absent in water where the molecules composing it are small. The deformations and rotations of the small water molecules enter the classical fluid mechanics (representing in this example the *meso* level) only in unchanging with time material parameters like viscosity and heat conductivity coefficients.

Motivated by the example of polymeric fluids, we choose x (serving as the state variables on the extended *MESO* level) as y (serving as state variable on the *meso* level) supplemented with quantities characterizing the internal structure. With such extended state variables we have to then construct the equation governing their time evolution. By requiring it to be GENERIC, we face the problem of constructing appropriate new particular realizations of the GENERIC equation (1). Many such realizations have indeed been made and many are reviewed in [1]. In the standard approach to modeling, the equations of fluid mechanics that are extended by taking into account the internal structure have appeared first in the Kirkwood investigation of the reduction of the fully microscopic Liouville equation (formulated in the form of the BBGKY hierarchy) to the level of fluid mechanics [84]. This is the reason why we call this extension a Kirkwood extension. The Kirkwood investigation have been then followed systematically in rheology [85]. With the internal structure created in the flow (the turbulence type structure), the Kirkwood like extension of the Vlasov kinetic equation has been explored in [30]. In the context of the nonequilibrium thermodynamics the extensions involving internal state variables have been introduced in [86, 87].

An alternative way to include the internal structure into the state variables is to increase the dimension of the space of the variables on which the fields forming the *meso* state variables depend.

This has been introduced in the continuum theory in [88], in kinetic theory in [89] and in [90] (where the one particle distribution function, depending on the position vector $\boldsymbol{r}$ and the velocity $\boldsymbol{v}$, is let to depend also on another scalar parameter that addresses the internal structure of the gas particle and that enters the dynamics in collisions), and in in chemical kinetics in [92] where the mass concentrations of species (forming the *meso* state variables in chemical kinetics) are let to depend on a scalar parameter labeling the intermediate states in the chemical reactions (the parameter enters the dynamics in the energy).

Still another extension of this type has been introduced in [91]. The physical systems under investigation in [91] are polymeric fluids. The setting in which the modeling in [91] begins is already extended classical fluid mechanics in which a new field, namely the one dumbbell distribution function (the macromolecules are modeled as dumbbells) has been adopted as an extra state variable. A more realistic model of macromolecules is a chain composed of dumbbells. The problem is now to extend the one dumbbell model to a chain model. De Gennes suggested to formulate mathematically the more realistic chain view of macromolecules by letting the one dumbbell distribution function to depend on an extra scalar parameter having the physical interpretation of the coordinate on the string on the chain. In dynamics, this parameter enters the de Gennes analysis in a new diffusion term having the physical interpretation of the snake-like motion (called reptation by de Gennes) of the macromolecular chain. In this way de Gennes has succeeded to express (while still keeping the one chain distribution function as the state variable) the strong chain-chain interactions influencing the overall flow properties of polymeric fluids. Still unexplored possibility is to include the chain coordinate also in the energy. Such modification would allow to consider the influence of the curvature of the chain and of its elastic deformations on the overall motion of polymeric fluids. In the GENERIC form, the de Gennes reptation theory has been discussed in [93] and, on a more macroscopic level on which the states of macromolecules are characterized by an internal deformation tensor, in [94].

3.2.3. Grad extensions

The extra state variables are found on this route to extensions in the vector fields appearing on the *meso* level. We begin with a simple motivating example. Let the state variable y on the *meso* level be the position vector $\boldsymbol{r}$ and the equation governing its time evolution $\dot{\boldsymbol{r}} = \boldsymbol{v}(\boldsymbol{r})$. The vector field $\boldsymbol{v}(\boldsymbol{r})$ on this *meso* level is called a velocity (or alternatively a flow of $\boldsymbol{r}$), its specification, i.e. the specification of the function $\boldsymbol{v}(\boldsymbol{r})$, is called a constitutive relation. Now we proceed to the extension. We consider $\boldsymbol{v}$ as a new state variable. The state variable x on the extended *MESO* level is thus $(\boldsymbol{r}, \boldsymbol{v})$. The equations governing its time evolution is $\dot{\boldsymbol{r}} = \boldsymbol{v}$; $\dot{\boldsymbol{v}} = \frac{\boldsymbol{F}(\boldsymbol{r})}{m} - \frac{\xi \boldsymbol{v}}{m}$, where $\boldsymbol{F}(\boldsymbol{r})$ has the physical interpretation of a force, $\xi > 0$ is a friction coefficient, and $m > 0$ is another parameter having the physical interpretation of mass. The *meso* $\rightarrow$ *MESO* extension that we have just described is an extension of mechanics without inertial into mechanics with inertia and with friction. The limit $m \rightarrow 0$ is a reduction *MESO* $\rightarrow$ *meso* leading back to $\dot{\boldsymbol{r}} = \boldsymbol{v}(\boldsymbol{r})$ with the constitutive relation $\boldsymbol{v}(\boldsymbol{r}) = \frac{\boldsymbol{F}(\boldsymbol{r})}{\xi}$.

The Grad hierarchy formulation of the Boltzmann kinetic equation provides an excellent setting for making this type of extension in the classical fluid mechanics. Such extension has been considered in [77, 90] (where the extended fluid dynamics theories are called Extended Thermodynamics (ET)), and in [95] (where the extended theories are called Extended Irreversible Thermodynamics (EIT)). The main difference between ET and EIT is that ET remains to be closely attached to the Grad hierarchy and thus to the gas dynamics (including however both the monoatomic and the polyatomic gases [90]), while the extensions that have been developed in EIT are more motivated by fluid-mechanics type considerations and the intended applications reach beyong the gas dynamics. Both ET and EIT extensions are however extensions in which the constitutive relations are replaced by time evolution equations and thus extensions introducing a higher order inertia.

The GENERIC approach to this type of extensions has recently been explored in [78]. We have also already used the introduction of an extra inertia in section 2.13 as a way to bring the GENERIC structure to non GENERIC models.

3.3. Questions

Many questions arise in the investigations of multiscale reductions and extensions. We mention below four such questions. Detailed investigation of applications in specific physical contexts (e.g. heat transfer, dynamics of complex fluids and complex solids) will certainly help to answer them (see also [96]).

Question 1

The reducing and the reduced dynamics are different and appear to be independent one of the other. The former takes place on the *MESO* level and the latter on the *meso* level. The two dynamics cannot be however completely independent since they both represent the *MESO* dynamics. We conjecture that their dependence manifests itself in particular in the following two features.

(i) Let the system under investigation be externally unforced. As $t \to \infty$, the system reaches the complete thermodynamic equilibrium state and the *equilibrium* level is thus applicable. We have therefore three levels on which we can describe the observed behavior of the system, namely *MESO*, *meso*, and *equilibrium*. In such setting we are in position to investigate three passages to the *equilibrium* level: $MESO \to equilibrium$, $meso \to equilibrium$, and $MESO \to meso \to equilibrium$. We conjecture that the relation between the reducing and the reduced dynamics will manifests itself in the transitivity of the passages. In other words, we conjecture that the fundamental thermodynamic relation obtained by following all three passages are the same. If we denote the entropy arising in the passage $MESO \to equilibrium$ by the symbol $S^{(Me)}(x)$ and $S^{(eM)}(E,\ N))$ the Legendre transform of $[S^{(Me)}(x)]_{x=x_{eq}(T,\mu)}$ then the conjecture takes the form $S^{(eM)}(E,\ N) = S^{(em)}(E,\ N) = S^{(emM)}(E,\ N)$.

(ii) The emergence of a new pattern on the *meso* level (e.g. the emergence of convection in the Rayleigh-Bénard system) is seen as a bifurcation in the reduced dynamics (i.e. the *meso* dynamics) and as a phase transition in the *meso*-fundamental thermodynamic relation $S^{(mM)}(y)$. This conjecture is based on the observation according to which an emergence of new features on the *meso* level is always associated with an emergence of large fluctuations on the *meso* level. This then indicates that the emergence of new features on the *meso* level is seen also as an emergence of new features on the more microscopic *MESO* level. New features in the reduced *meso* dynamics are seen as bifurcations, new features in the reducing dynamics are seen as a loss of convexity (i.e. as a phase transition) of the generating potential.

Question 2

Another interesting question that remains unanswered is of what is the relation between the *meso*-level fundamental thermodynamic relation $S^{*(Mm)} = S^{*(Mm)}(y^*)$ implied by the reducing thermodynamic potential (25) and another *meso*-level fundamental thermodynamic relation $\mathfrak{S}^{*(Mm)} = \mathfrak{S}^{*(Mm)}(Y^*)$ implied by the CR reducing thermodynamic potential (29).

Question 3

An interesting problem that arises in extensions is the relation between the Kirkwood and the Grad extensions. On the first sight, they are very different. The former brings new interactions (i.e. the potentials $E(y)$ and $S(y)$ are extended) while the latter is extending the kinematics (bringing the extra inertia). However, if we realize that the flux bringing the extra inertia to the velocity has the physical interpretation of a force, we see that both extensions follow a similar route.

Question 4

In section 2.13.2 we have described another open problem, namely the problem of casting the Enskog kinetic equation, or its appropriate extension, into the GENERIC form (1).

4. Concluding remarks

If we take a very detailed viewpoint of macroscopic systems (e.g. the viewpoint taken in microscopic numerical simulations) then we see details but we lose the overall picture. If, on the other hand, we choose a mesoscopic viewpoint that ignores details (e.g. the viewpoint taken in fluid mechanics description) then the picture that we are getting is incomplete if some of the ignored details play an important role in determining the overall view. This happens, for example, in macroscopic systems arising in nanotechnology and biotechnology. The best solution is to regard complex macroscopic systems simultaneously on several different levels that take into account different amounts of details. Such a multilevel (multiscale) viewpoint can be however useful only if the relations among the levels is understood. Such understanding is the objective of the GENERIC thermodynamics and dynamics discussed in this paper.

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