



## Role of thermodynamics in multiscale physics

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### ARTICLE INFO

#### Keywords:

Thermodynamics  
Hamiltonian and gradient dynamics  
Contact geometry

### ABSTRACT

One way to deal with complexity is to recognize important features, concentrate on them, and ignore everything else. A useful strategy for the recognition process is to carry out the investigation on several levels involving different amounts of detail and then compare the results. The comparison is, in its essence, thermodynamics. We formulate such abstract thermodynamics (we call it the Dynamical Maximum Entropy Principle) and show that the equilibrium and nonequilibrium thermodynamics as well as the equilibrium and nonequilibrium statistical mechanics are all its particular representations.

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### 1. Introduction

It is easier (less complex) to understand and predict the behavior of water encountered in our everyday experience than the behavior of biological liquids in living tissues. An explanation of this statement may proceed as follows.

There is a large family of observations of water that are of practical importance and that can be organized, understood and predicted with a single theoretical framework, namely with classical fluid mechanics. On the other hand, any analysis of practical interest of flows of biological fluids in living tissues seems to require microscopic details as well as an overall macroscopic analysis. In other words, we know what we can afford to ignore in the theoretical framework (e.g. microscopic details of water molecules or larger structures emerging in turbulent flows) and still obtain results of practical interest in the case of water but we do not have such certainty in the case of biological fluids.

To establish the terminology that we shall use throughout this paper, classical fluid mechanics represents a level of description with a relatively large domain of applicability. In general, a *level of description* is a theoretical framework providing an organization and an explanation for our experience accumulated in a certain class of experimental observations of a certain class of macroscopic systems. The family of observations and the family of macroscopic systems form the domain of applicability of the level of description. Problems that can be investigated on a single level of description will be considered in this paper to be *simple* and the problems requiring several different levels will be seen as *complex*. Taking this viewpoint, an analysis of complexity becomes an analysis of the relation between two different levels of description. Only this type of analysis can show what is essential and when and what can be ignored in order to simplify.

To begin the multilevel analysis, we briefly recall its history. The first example in which macroscopic and microscopic viewpoints have been combined is equilibrium thermodynamics. In this theory the classical mechanics represents both the macroscopic (e.g. movements of a piston) and also the microscopic (heat seen as an action of external forces of microscopic origin—e.g. electromagnetic waves in microwave ovens) levels. The microscopic level appears implicitly in the classical equilibrium thermodynamics (its mechanical origin is however expressed explicitly in the “First Law of Thermodynamics”), explicitly then in Gibbs’ equilibrium thermodynamics – called equilibrium statistical mechanics – (in the form of mechanics of particles composing macroscopic systems), and explicitly in another form (namely the form of the classical fluid mechanics) in the classical nonequilibrium thermodynamics. The most fundamental contribution that has emerged in these investigations is the concept of *entropy*. It has been realized that a passage from a level to a more macroscopic (i.e. involving

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less details) level is done by maximizing a potential subjected to constraints [1] (so-called “Second Law of Thermodynamics” or Maximum Entropy Principle or also MaxEnt). The potential, called an entropy, measures disorder, while the constraints are the state variables used on the more macroscopic level.

In this paper we formulate first (in Section 2) the Maximum Entropy Principle (MaxEnt) in the mathematical setting (namely the setting provided by the contact structure geometry and by the variational formulation) that is suitable for applications in the more general context of complexity theory. A mesoscopic time evolution is seen in this setting as a continuous sequence of Legendre transformations maximizing the entropy, or alternatively, the trajectories generated by the mesoscopic time evolution are seen as trajectories for which the entropy production reaches its extremum. This dynamical extension of the Maximum Entropy Principle is called in this paper a Dynamical Maximum Entropy Principle (DynMaxEnt). Subsequently, in Section 3, we illustrate the abstract formulation in the context of multilevel analysis of heat transfer.

## 2. Maximum entropy principle and dynamic maximum entropy principle

We recall three well known and important examples of the passage from a level to a more macroscopic level by maximizing entropy.

First, we consider a gas whose time evolution is described on the level of the Boltzmann kinetic theory (i.e. the state variable is the one particle distribution function whose time evolution is governed by the Boltzmann kinetic equation). The passage to the more macroscopic level of classical equilibrium thermodynamics (in which state variables are two scalars, namely the energy and the number of moles, and no time evolution takes place) is made by maximizing the entropy (the famous Boltzmann H-function) subjected to two constraints (the total energy and the total number of particles, both expressed in terms of the one particle distribution function). It is the time evolution that carries the entropy to its maximum (this is the subject of the famous Boltzmann H-theorem).

In the second example the more microscopic level is represented by classical fluid mechanics (i.e. state variables are the same as the ones used on the level of classical thermodynamics except that they are local and they are supplemented by local velocity; their time evolution is governed by the Navier–Stokes Fourier equations) and the more macroscopic level is again the level of classical thermodynamics. The passage from the level of fluid mechanics to the level of classical thermodynamics is made by maximizing the entropy (that is in this case the local entropy – here enters the so-called local equilibrium assumption – integrated over the position vector). It is again the time evolution itself that brings the entropy to its maximum value. Classical fluid mechanics supplemented with the analysis of the passage to the level of classical thermodynamics is called classical nonequilibrium thermodynamics.

The passage involved in the third example is the passage from the level of the Boltzmann kinetic theory to the level of the classical fluid mechanics. This passage is known as the Chapman–Enskog method of solving the Boltzmann kinetic equation. We shall show in Section 3 that the Chapman–Enskog approach can also be interpreted as maximization of entropy.

The common features extracted from the above three examples (and from many other examples that we are not mentioning in this paper but are discussed for example in [2]) are the following. (i) The time evolution on a level of description (Level 1) proceeds in two stages: in the first stage a more macroscopic level (Level 2) is approached, this stage is then followed by the time evolution taking place on the more macroscopic level. We shall call the time evolution taking place in the first stage a *fast time evolution* and the one taking place in the second stage a *slow time evolution*. In the first two examples the fast time evolution is the complete time evolution, the “slow” in the second stage means, in fact, “still” in these two examples. (ii) The fast time evolution has universal features that reflect the universality of thermodynamics. In Section 2.1 we shall assume that the two levels, Level 1 and Level 2, are known and formulate the fast time evolution providing the passage from Level 1 to Level 2. We pay attention in particular to the mathematical aspects of the formulation. In Section 2.2 we make another assumption, namely we assume that the complete time evolution on Level 1 is known and we discuss the problem of splitting it into fast and slow.

### 2.1. Contact structure geometry formulation of the fast time evolution

Let the symbol  $x$  denote the state variables used on one level of description (Level 1) and the symbol  $y$  state variables used on a second, more macroscopic level (Level 2). The state space used on Level 1 will be denoted by  $M$  (i.e.  $x \in M$ ) and the state space used on Level 2 by  $N$  (i.e.  $y \in N$ ). Some examples of  $x$  and  $y$  are presented in Section 3.

Our objective is to formulate the fast time evolution of  $x$  in which Level 2 is approached as the time goes to infinity. The formulation presented below has emerged from an attempt to identify a common mathematical structure in the three examples mentioned in the beginning of this section and also in other examples (some of which are discussed in Section 3). Its full physical content will be revealed in the illustrations discussed in Section 3 and in the references cited therein.

We begin by introducing certain structures into the spaces  $M$  and  $N$ .

#### 2.1.1. Energy

The space  $N$  will always be composed of two components:

$$\begin{aligned} N &= \mathbb{R} \times Z \\ N \ni y &= (e, z); \quad e \in \mathbb{R}, z \in Z. \end{aligned} \tag{1}$$

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