

MULTISCALE MESOSCOPIC DYNAMICS AND THERMODYNAMICS

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EXTENDED ABSTRACT

Dynamics is primary and statics secondary in investigations of macroscopic systems. It is in the time evolution where explanations for their behavior, both static and dynamics, have to be searched. By the time evolution we mean either the microscopic time evolution of $\sim 10^{23}$ microscopic particles composing them or a multiscale mesoscopic time evolution. In this investigation we concentrate on the latter.

Different types of observations of macroscopic systems have led to different experiences that in turn have led to different theoretical frameworks providing settings for their organization and understanding. As an example we mention fluid mechanics (FM) and kinetic theory (KT), both involving the time evolution, and a static theory known as classical equilibrium thermodynamics (CET). We recall that all these three theories (we shall call them levels of description) have arisen (recall their well known history) independently one of the other and all three are completely self-contained (i.e. they do not need others to be applied). Depending on the amount of details involved on the levels, a hierarchical order can be established. We say that KT is more microscopic (i.e. involving more details) than FM and CET and that FM is more microscopic than CET. Instead of saying that KT is more microscopic than FM we can also equivalently say that FM is more macroscopic than KT. Formally, we shall denote the levels by the symbol \mathcal{L} and we shall say that a level \mathcal{L}_j is more microscopic than \mathcal{L}_i if $j > i$.

Having a family of levels (that are initially completely independent and unrelated) equipped with the hierarchical order, we can attempt to recognize a level \mathcal{L}_i as a pattern emerging in an analysis of the time evolution on a more microscopic level $\mathcal{L}_j; j > i$. I make now the following proposition: **Passages from \mathcal{L}_j to $\mathcal{L}_i; i < j$ share a universal structure that I will call Multiscale Mesoscopic Dynamics (MMD)**. This abstract dynamics encompasses both classical as well as mesoscopic equilibrium and nonequilibrium thermodynamics. Below, I will make a few comments about MMD. A more detailed presentation can be found for instance in [1],[2],[3],[4].

We begin with CET. Its essence is maximization of entropy known as MaxEnt principle. The entropy is a potential (a real valued function of state variables satisfying certain requirements). Its specification is called a fundamental thermodynamic relation. Two questions arise: Where does the fundamental thermodynamic relation come from, and why is the entropy maximized. For answers we turn to the time evolution taking place on a more microscopic level (e.g. KT). The entropy is a potential (or one of the potentials) generating the (fast) time evolution bringing the macroscopic system under consideration to states at which the more macroscopic level (e.g. CET) applies. The maximization of the entropy during the fast time evolution is a manifestation of the approach to the more macroscopic level on which either no time evolution takes place (as it is in the case of CET) or a slow time evolution takes place (as it is for example in the case of the passage $\text{KT} \rightarrow \text{FM}$).

The main challenge in the mathematical formulation of the abstract thermodynamics is to identify a geometry in which the Hamiltonian (i.e. time reversible and nondissipative) dynamics (formulated in the setting of *symplectic geometry*) naturally coexists with the gradient (i.e. time irreversible and dissipative) dynamics (formulated in the setting of *Riemannian geometry*). Such geometry appears to be a *contact structure geometry*. This conclusion arises also from the following argument. We ask the question of what is the group of transformations playing a dominant role in thermodynamics. The answer is: it is a group of Legendre transformations (since these are the transformations arising in MaxEnt). It is then well known that the contact structure geometry provides a natural setting for Legendre transformations.

REFERENCES

- [1] M. Grmela, "Multiscale Equilibrium and Nonequilibrium Thermodynamics in Chemical Engineering: Adv. Chem. Engineering **39**, 75-128 (2010)
- [2] M. Grmela, "Fluctuations in Extended Mass-Action-Law Dynamics", Physica D, **241**, 976-986 (2012)
- [3] M. Grmela, "Role of Thermodynamics in Multiscale Physics", Computers and Mathematics with Appl. DOI. org/10.1016/j.camwa.2012.11.019 (2013).
- [4] M. Grmela, "Extensions of Nondissipative Continuum Mechanics Toward Complex Fluids and Complex Solids" Cont.Mech.Themod. **25**, 55-57 (2013)