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# **The architecture of thermodynamics and its future developments**

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## **Abstract**

The way contemporary thermodynamics works is based on hypotheses and measurements, both at the microscopic level of individual particles and at the macroscopic level of the “large” systems. The first kind of hypotheses and measurements are based on mechanical concepts such as position, mass, velocity, forces, kinetic/potential energy, or Newton’s Laws. The second kind are based on the definition of new quantities such as temperature, amount of heat, entropy, and of their assumed properties. Statistical hypotheses complete this ensemble and explain how it is possible to go from the microscopic level to the macroscopic level (extensivity property, postulate of ergodicity, whether or not individual particles are discernable, definition and equiprobability of the microstates, etc.). The number of microscopic particles in the overall system has an effect on how we consider the transition between levels. The overall architecture of thermodynamics must allow these different hypotheses and measurements to co-exist in the four aspects. Different authors propose different ways to understand this overall architecture, as a function of whether or not sets of hypotheses are put forward, independently or not, at one or another level (or whether the question of scale even arises). This article touches upon these possibilities and, in a very general way, discusses the consistencies among these architectures and the potential degrees of freedom in their construction, based on the premise that any paths to progress in thermodynamics (or to refreshing our knowledge in this field) must be placed within this framework. A few examples are given to open up avenues for research.

**Keywords:** thermodynamics; mechanics; hypotheses; microscopic; macroscopic; statistics; architecture; recursivity; number of particles; heat; work; entropy; uncertainty; arbitrary; degree of freedom; concepts

## Introduction

Here, we lay out our understanding of how the different components and concepts of thermodynamics fit together. This view is necessarily general, and tends towards the “philosophy of science”. It could be filled in with specific examples that there is not room here to include. We believe that understanding this architecture is one of the conditions for developing thermodynamics in the new directions mentioned at the end of the article.

In the historical view, elementary thermodynamic concepts (the transfer of a quantity of heat, temperature, entropy, internal energy, and the associated laws) were defined at the macroscopic level of steam engine reservoirs. Thermodynamics could operate at this scale independently. However, an understanding of the corpuscular structure of matter came later, giving the discipline a new perspective linking the concepts and quantities associated with microscopic corpuscles (i.e. those of rational mechanics) to those associated with the above-mentioned macroscopic level. So today, the science of thermodynamics structures a dialogue between two scales for studying reality. These scales are presumed to have already been given: one microscopic, the other macroscopic. The microscopic approach (statistical thermodynamics) enables making quantitative forecasts that eliminate the need for a large number of macroscopic measurements and which join what is known and measured at the macroscopic scale. Note that this elementary presentation of thermodynamics (dialogue between the microscopic and macroscopic levels) does not exclude various technical adjustments that define many different types of thermodynamics (irreversible thermodynamics, non-equilibrium thermodynamics, extended irreversible thermodynamics, rational thermodynamics, endoreversible thermodynamics, finite time thermodynamics, quantum thermodynamics, etc.; see the works of W. Muschik on this subject). Without discussing these many variations here, we will presume for the moment that they do not fundamentally change the elementary conceptual architecture reviewed above (it could be interesting in the future, however, to see how each one accommodates the degrees of liberty that are discussed further on in the text).

Because the topic of interest is today’s thermodynamics, we must examine both the hypotheses made at the microscopic and macroscopic levels and the rules for going from one level to the other. We can also discuss our choice of proportion between the size of the macroscopic system and that of a microscopic entity, or the number of microscopic particles

N in the macroscopic system. In all, there seems to be four instances of hypotheses where the organization enables the whole to function. Each of these groups of statements contains its own degrees of arbitrariness and can potentially change the whole theory by making new choices as a function of new requirements or new understanding. With this in mind, we need to highlight the following points.

## **1. The relative nature of what is called microscopic and macroscopic**

“Microscopic” and “macroscopic” refer to something at a given moment and in no way corresponds to the fundamental levels of reality that always elude us: the microscopic level can itself be considered as macroscopic in relation to an even finer microscopic level, and the opposite can be true for the macroscopic level in relation to an even larger-scale level, which we might call megascopic. The two scales are considered in opposition to each other or in combination. In the drift of the above discussion, the proportion between the two sizes is crucial in determining how the thermodynamics operate.

## **2. Comparing the microscopic and macroscopic levels**

Comparison of the microscopic et macroscopic levels can be understood in two different ways: 1) Historically, it started by establishing *identifications* between the concepts and quantities of the two levels without changing their respective sizes, i.e. without changing the size of the macroscopic level (or more specifically without changing the proportion between the sizes of the two levels: this is what we call the thermodynamic limit of  $N \rightarrow \infty$ , see L. Boltzmann’s works). 2) Another approach would be to examine how to go from one level to the other by progressively increasing the size of microscopic systems (N no longer starts out as infinity, but is made to vary from 1 to a larger number). This is not just the expression of correspondences between the two levels: it is the genesis itself of the thermodynamic concepts based on those of mechanics, which can be taken up again in this way.

### **3. The concepts and laws posited at the microscopic level**

First and foremost, to build the theory at the microscopic level, you have to posit the space and time concepts, and write out the corresponding mathematical variables. The concepts at the microscopic level are usually those of Newton's rational mechanics: mass, position, velocity, quantity of motion, expression of forces, kinetic and potential energy, work; the link between force and acceleration, the energy conservation law for changes affecting the elementary particles, etc. You can add to that, or replace it with, the concepts and laws of electromagnetism, of special or general relativity, and/or of quantum mechanics if required. You'll notice that the concept of corpuscle (to which will be added mass, energy, etc.) comes to us from the macroscopic scale (billiard balls are not microscopic!) and by shrinking the corpuscle and associated concepts down to the elementary scale, we've already made a hidden transition from macroscopic to microscopic. Measurements made at the microscopic level on individual particles are relatively rare and are in reality derived from macroscopic measurements (see next section). When you posit a wave function for an individual particle in quantum mechanics, you lose the microscopic locality and also establish a hidden transition from the macroscopic level to the microscopic level.

### **4. The constraints imposed by the macroscopic level**

Some of the concepts and quantities at the macroscopic level are the same as for the microscopic level. Thus, it is possible to postulate that the basic space and time concepts are the same as for the microscopic level, even if some authors reflect on the emergence of time at the macroscopic level based on phenomena at the microscopic level, without associating time with the latter level. Another hypothesis is that the energy for microscopic transformations is the same as at the macroscopic level. To the usual concepts for the microscopic level, it is possible, as mentioned in the introduction, to add specific concepts such as temperature, pressure, the quantity of heat, entropy, etc., and their inferred properties (expressed synthetically in the principles of thermodynamics). We try to show how we identify these concepts with those derived from the microscopic level. But it would be an intellectual error to present things in a uniquely "upward" way from the microscopic to the macroscopic, using summation and averaging procedures as is often done. We already mentioned the transfer of the mental image of corpuscle from the macroscopic level to the

microscopic level. But even if all useful concepts were defined “independently” at the microscopic level, it remains that we know almost nothing about the value of quantities! It is not possible, for the multitude of microscopic particles, to know the mechanical data (positions, velocities) that are usually known for macroscopic mechanical objects (or one is dealing with a system where the number  $N$  is fairly small: either one is leaving the realm of thermodynamics, or has already; this point is rediscussed further on). The macroscopic level we are measuring imposes the values of the average quantities to be calculated at the microscopic level: i.e. part of the information is transferred from the macroscopic level to the microscopic level. The energy conservation expressed at and linking the two levels enables the transfer; a more detailed description of the microscopic quantities also requires statistical assumptions that we will discuss in the following section.

A look at the energy levels of elementary particles within the framework of quantum mechanics shows that their quantification is a result of the boundary conditions for the entire system, and not an essential property of each particle. The properties assigned to individual particles are often determined on macroscopic measurements of systems with a large number of particles; by hypothesizing an absence of interaction among them, it is possible to assign the measured properties to individual particles.

There are other constraints in passing from the macroscopic level to the microscopic level: we can posit that the microscopic evolutions must keep the value of certain macroscopic integrals (this calls to mind principles like the least action principle or the minimum entropy production principle; these extremal principles, along with various constraints, are a way to express something that we know about the whole system, and appear to establish a “finality” at the microscopic level). One can speculate as to the equivalent or supplementary nature of the hypotheses made at the macroscopic level with respect to those made at the microscopic level: we know, for example, the equivalence between certain local formulations of mechanics (in the form of differential equations) and global integral formulation (see end of text).

## **5. The rules for passing from the microscopic to the macroscopic level**

With respect to the rules for going from one level to another, we have already mentioned energy conservation and postulated that it is the “same” energy at both levels. Other rules

have to be added, e.g. the one that allows adding small systems together to arrive at the larger one by scaling up various associated quantities: this is called the extensivity property (for what are called extensive quantities), which assumes certain implicit conditions that cannot always be verified. This is the case when the interaction forces between elementary particles are long-distance interactions, as for stellar systems and gravitational forces.

There are also all of the statistical hypotheses, which are sometimes very technical. We will mention only a few:

- the postulate of ergodicity, or ergodic postulate, and its many formulations, establishing a link between the knowledge about small systems and the knowledge about large systems, both specifically and with respect to predicting their “average” changes over time;
- hypotheses on whether or not elementary particles are discernable, which can depend on particle and system type;
- the ensuing rules that posit the different microscopic states as equiprobable. You still have to define these states, know how to list the energy levels, how to differentiate in placing the particles on the different levels – i.e. to what extent these particles are to be considered as discernable or not – and how to take degeneracy into account. Different statistical distribution laws proceed as a function of the choices made, making it possible to average out the microscopic quantities and to access all types of macroscopic sizes, thereby establishing the correspondences sought between the two levels.

Certain hypotheses appear to be specific to the macroscopic level, e.g. the rules of symmetry between forces and fluxes (especially useful for non-equilibrium thermodynamics) or extending the second thermodynamic principle on closed systems to open systems, but it is generally possible to reach these rules without additional hypotheses based on the microscopic level if you are using this approach (this could require verification for some cases). The local microreversibility hypothesis is covered by the same procedure.

## **6. Talking points, avenues of research**

Any paths to progress in thermodynamics require the possibility to discuss the choices made concerning the four “drivers” for this overall architecture (hypotheses at the microscopic level, hypotheses at the macroscopic level, rules for passing from one level to the other, the



number  $N$  of particles). Could one hypothesis be replaced by another? Here are a few proposals within this framework. To a large extent, these should be considered as “research projects” and could be specified in more extensive developments on the subject, with calculations.

### *6.1. Discussion of hypotheses made at the microscopic level*

If you come back to an in-depth examination of time and space concepts posited as a framework for the movement of microscopic particles, these two concepts do not refer to separate, pre-existing substances from reality, but are constructed in opposition to or in combination with each other. Understanding this construction affects our understanding of certain thermodynamic concepts, e.g. the irreversibility of time. The first problem with time is not its irreversibility, but its construction; the concepts of reversibility and irreversibility must be treated in opposition to one another, and their limit is subject to arbitrariness and uncertainty (see works by Guy). Likewise, the notions of equilibrium or disequilibrium are not absolute, but relative to the time and space scales under consideration (these discussions also concern Section 6.2).

At the microscopic level, you can also discuss the nature of the fundamental forces or interactions to be taken into account, and the laws governing them. Within the community of physicists, there are ongoing debates on everything that concerns gravitation (revisiting Newton’s laws, special and general relativity laws, etc.); you could also add what concerns electromagnetism. Incorporating new laws will have consequences on the formalism of thermodynamics. Choosing to assign a specific position or wave function to a particle, as in quantum mechanics, can also affect how the thermodynamics subsequently work.

### *6.2. Comparing the microscopic and macroscopic levels and increasing the number of particles in the macroscopic system*

The above-mentioned approach of gradually varying the number  $N$  of microscopic particles make it possible to move closer to an in-depth understanding of macroscopic concept formation (this consists of more than just identifying the concepts at both levels). At the level

of what we call mechanics, or a form of mechanics, we manipulate material points, forces, energy, work, etc. At the higher level, we start to consider ensembles of large numbers of these points. The two levels are linked because the goal is to treat macroscopic ensembles as types of new material points, using the same concepts (energy, movement, forces, work, etc.) as for microscopic points. The theory at the second level defines a specific system of thermodynamics. Looping energy conservation implies introducing additional energy or energy transfers: internal energy, or transfer of a quantity of heat. You also bring into play a new quantity for evolving macroscopic systems: entropy, for which the maximum determines the end. At the macroscopic level, this quantity takes on a meaning that is linked to heat transfer. At the microscopic level, it takes on a statistical meaning. When taking large systems into account, it is no longer possible to control the individual trajectories of particles, so reasoning must be based on changes that correspond to the most probable situations. This is how practical irreversibility appears. It is linked to the effect of minor uncertainties in calculating the positions of the different particles, such as can be observed in molecular simulations.

In short, the concepts of heat, internal energy, entropy and preferred direction of evolution (as well as the entire resulting construct, i.e. a system of thermodynamics) appear each time that, for a mechanical system, you set up a divide between two scales and share your knowledge (and ignorance) between these two scales. The separation can be made wherever you want (you can build more than one system of thermodynamics as a function of the location of the divide between the two scales). You can decide to observe the overall movement of a mountain, compared to which small local movements (even macroscopic at the human scale!) are “heat exchanges”, and define thermodynamic quantities for the entire mountain. However, it is important to remember that if you consider only a small number of particles, the new quantities no longer mean anything; specifically, there will no longer be any difference between heat and work, and the thermodynamic concepts disappear. All new thermodynamic concepts must be considered in the context of this transition from microscopic to macroscopic as you increase the number  $N$  of particles: the notion of a system with its interior and exterior, its opening or closing; and notions of equilibrium or disequilibrium. If  $N$  is not too large, writing such transitions is key to rethinking the theory’s entire line of reasoning and operation, and to writing one that is adapted to the chosen scale. This can be the case, for example, when studying nanosystems.

A comparison of the microscopic and macroscopic levels, which we seek to do by identifying or describing new concepts, is not made based on the ultimate reality of either of the two levels. As mentioned before, smaller microscopic levels can be considered (physicists are discovering that the behavior itself of some particles in some conditions resembles that of large systems). You can also imagine new quantities at higher, coarser levels to be linked to others using new statistical hypotheses.

### *6.3. Discussion of the constraints at the macroscopic level*

The concepts chosen at the macroscopic level that happen to be identical to those at the microscopic level, e.g. time or space, can be discussed in the same way as at the microscopic level. For the concepts and laws that are specific to the macroscopic level, there are two possible approaches: if the objective is to establish identifications between the concepts from both levels, in principle you can make changes to those at the macroscopic level separately. If the objective is instead to use a bottom-up approach to build a theory at the macroscopic level, there is nothing to be changed at this last level insofar as it is assumed that nothing is to be posited there. What is just as essential if not more so for the macroscopic level are the global quantities for the system being considered, which will determine the values for the averages calculated at the microscopic level. There is no latitude in that respect, except perhaps for the method used to measure macroscopic quantities (which could possibly have an effect on their definition?).

### *6.4. Discussion of the rules for changing from microscopic to macroscopic level*

How could some of the above-mentioned rules be changed?

If the extensivity property is not used, the way the statistical and entropy laws are formulated will change. This is the case for systems with long-range interactions.

The statistical assumptions themselves are subject to discussion. It is clear that their validity is linked to the value of  $N$ : the smaller the value of  $N$ , the less statistical are the assumptions. So these must be scrutinized at the same time as the value of  $N$  and the issues around comparing

the microscopic and macroscopic levels (Section 6.2). When  $N$  decreases, the particles become more and more “detectable”; you reach situations where the systems cannot be simplified through averaging. In that frame of reference, you can discuss whether or not to take into account the ergodic postulate or the postulate of equiprobability of microstates as a function of how the states are defined (particles detectable or not, degeneracy, ways to name or rank the particles, etc.).

### *Entropy*

Without going into the details of the formulations again, it is possible to conclude from these considerations that entropy does not appear to be an intrinsic quantity for a material particle of any size, any more than are other quantities in thermodynamics. It is a macroscopic quantity connected to the organization of a system of a large number of particles. The second principle itself is not a universal law of nature, it is a law that is valid for the most probable macroscopic systems; it can be transgressed, as some numerical (molecular simulation) and practical experiments show. The familiar notion of probability of states is also linked to that of the probability of the trajectories that lead to these states, i.e. considerations of the end of equilibrium changes are linked to consideration of the changes themselves. The mathematical expression for entropy depends on a certain number of hypotheses, at the very least the one on whether or not the systems have extensive properties.

## **7. Conclusion – The architecture of thermodynamics**

To close, we must examine our understanding of the architecture of thermodynamics. The freer approach here has been to discuss the potential choice of hypotheses at two levels simultaneously (microscopic and macroscopic) instead of a single one. This can be a problem. A correct scientific approach would have required hypothesizing at a single level and comparing the conceivable predictions with the experimental results. The two architectures shown in Figures 1 and 2 are the product of the latter approach, whether you make the hypotheses at the microscopic level (and from which will result what concerns the macroscopic level) or you make general hypotheses independently of scale (see the Keenan school of thought). If you make hypotheses simultaneously and independently at two levels as shown in Figure 3, how can they be reconciled? Is there not a risk of contradictions? How is it even possible to establish four groups of hypotheses independently (by adding the statistical

assumptions to the hypotheses made at the microscopic level and the choice of N number of particles in the system to those made at the macroscopic level)?

There are several different explanatory modes for answering these questions, and determining the extent to which each participates is worth some additional research.

- 1) You can say that the hypotheses made at the microscopic and macroscopic levels are not independent, i.e. they are to a certain extent equivalent as, for example, are local and global formulations in mechanics.
- 2) You can say that the two groups of hypotheses are distinct but complementary. They do not concern the same degrees of liberty in systems and are not competing.
- 3) Another point of view combines the first two: different hypotheses go together (in a certain way, this makes them equivalent) insofar as they are posited in opposition to each other in recursive relationships. This concerns the general process of thought in a very fundamental way and is not specific to thermodynamics. It is expressed in terms of relation-based thinking: whatever it is you are defining is placed in reference to everything else that you are setting apart; as a result, you cannot make independent choices at the microscopic and macroscopic levels, since each is defined by the other. It is impossible to avoid such loops between the macroscopic and microscopic when discussing energy, for example, because the energy is what is being conserved in a transformation (macroscopic aspect), but the transformation itself is defined by reference to individual entities to which essential properties appear to be attributed. This type of recursive process is inevitable because the values of the quantities to attach to the particles are known only through the global transformations. Also, the value of the mass of a particle in general relativity does not just concern the particle, it expresses the interactions with all the masses in the universe. There is also the definition of wave functions for microscopic particles, which has a macroscopic aspect to it. These recursive features bring about a certain latitude, or uncertainty, in the definition of the concepts (which is linked to the uncertainty on the measuring results), and this is expressed by degrees of liberty that could be termed “epistemological”. In order to stop a process that would lead to an infinite regression, you show what your basis is without claiming to define it (as Poincaré said, rather than the choices themselves, it is the relationships between choices that are opposed to reality, which is where the degrees of liberty internal to the approach come in).

- 4) You can assume that the internal degrees of liberty for statistical and other assumptions (also linked to the number  $N$ ) can accommodate the choices made on both sides at the microscopic and macroscopic level.
- 5) Finally, you can state, and this case can't be rejected out of hand, that the chosen hypotheses are incompatible. Specifically, between the way the entropy function is constructed at the macroscopic level based on the quantity of heat and the temperature, and the way it is constructed based on the statistical assumptions about the probabilities for the different states.

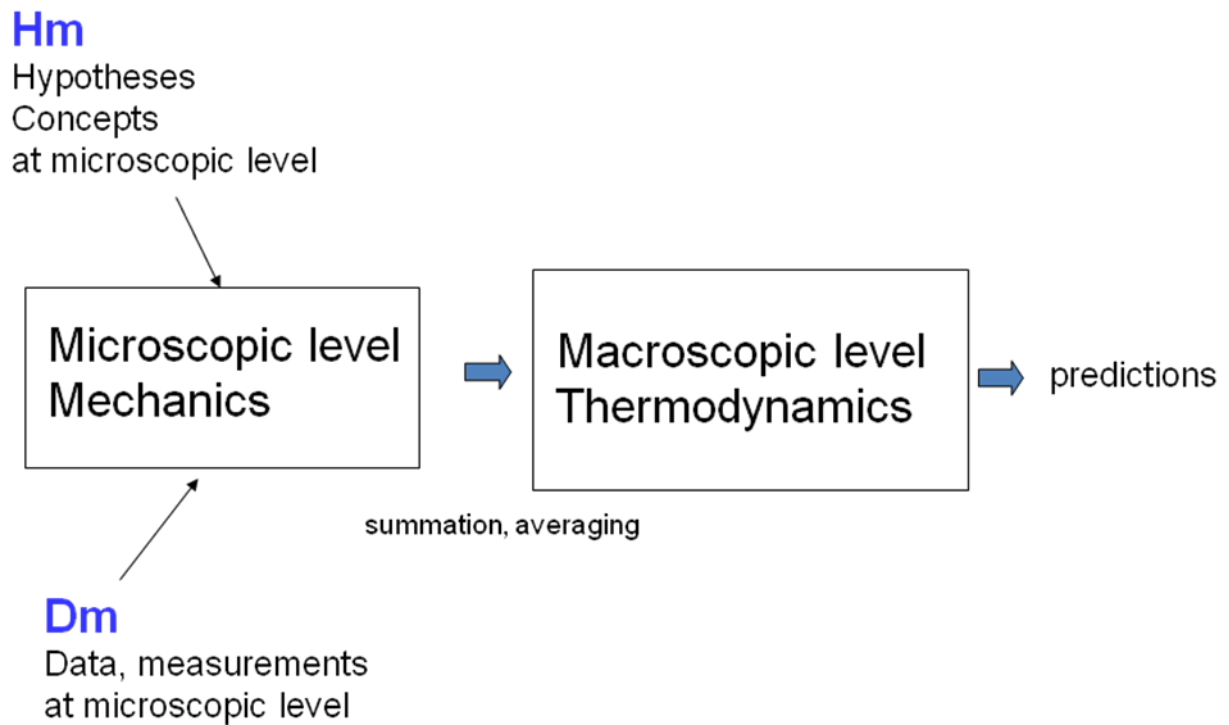
In the end, as elsewhere in science, a theoretical pluralism is possible. Reality and experience do not strictly “impose” thermodynamic quantities and laws any more than in any other science. There are necessarily arbitrary choices; you then accommodate in different ways, by showing (with uncertainty), and through the internal degrees of liberty and the many different modes of what we call “interpretation”.

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## **References:**

No detailed bibliography is given in this initial version of the present text. The bibliography will eventually include references to the following authors: Andresen, Bedeaux, Beretta, Boltzmann, Dujardin and Guy, Gibbs, Guy (works on the concepts of time, space and the theory of relativity; epistemological reflections on the way we express the laws on reality – notions of theoretical pluralism, recursivity, relation-based thinking, contradiction, etc.), Guyot, Hoffmann, Jou, Keenan, Kjelstrup, Lecoze, Maxwell, Mizony, Muschik, Poincaré, Richet, and Rubi, among others.



**Figure 1**

An architecture of thermodynamics (Architecture 1) in which it is assumed that everything is given at the microscopic level only.

**Caption for all three figures:**

**Hm** = hypotheses, concepts, laws... at microscopic level

= { space, time, mass, position, velocity, momentum, kinetic/potential energy, Newtonian laws... }

**Dm** = data, measurements on individual particles

**HM** = hypotheses, concepts, laws... at macroscopic level

= { heat, internal energy, entropy... }

**DM** = measurements on macroscopic systems

**HS** = hypotheses, rules... to go from microscopic to macroscopic level

= { extensivity property; ergodic postulate; definition of microscopic state and numbering of particles: degeneracy of states, discernable/ non-discernable character; equiprobability of microscopic states ... }

**DS** = proportion between sizes of microscopic and macroscopic systems

= **N** number of microscopic particles in the macroscopic system

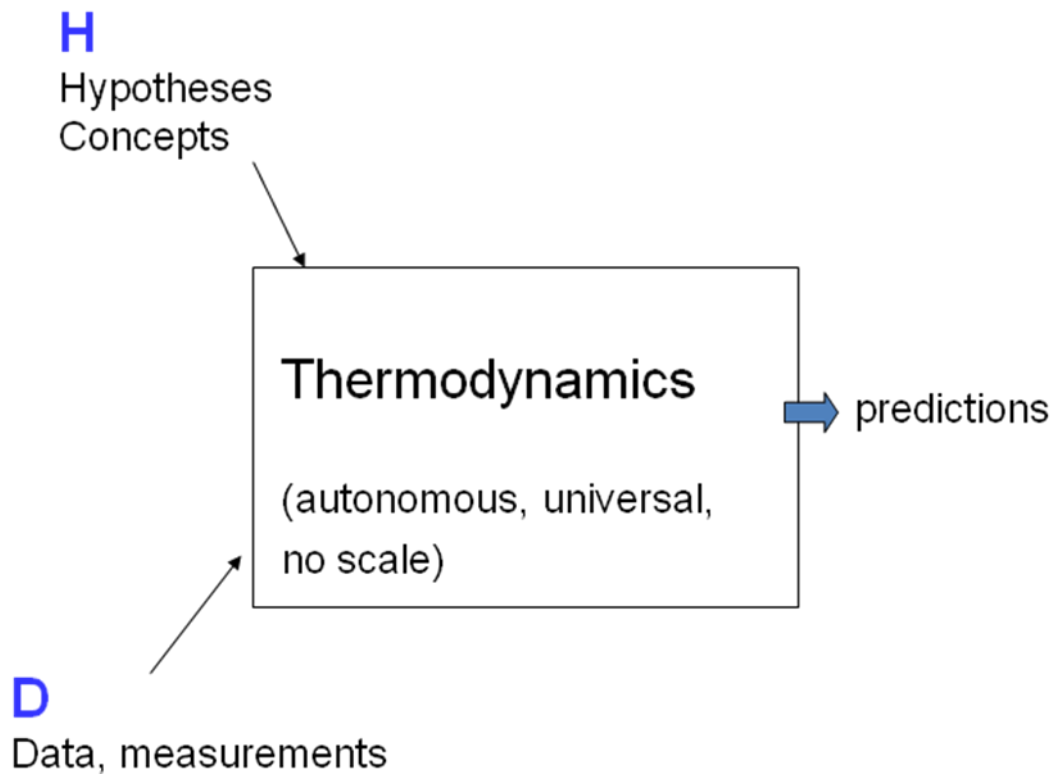
**H** = hypotheses, concepts, laws... on systems, whatever their size

= { mass, position, velocity, momentum, kinetic/potential energy...; heat, temperature, entropy... }

**D** = data, measurements on systems, whatever their size

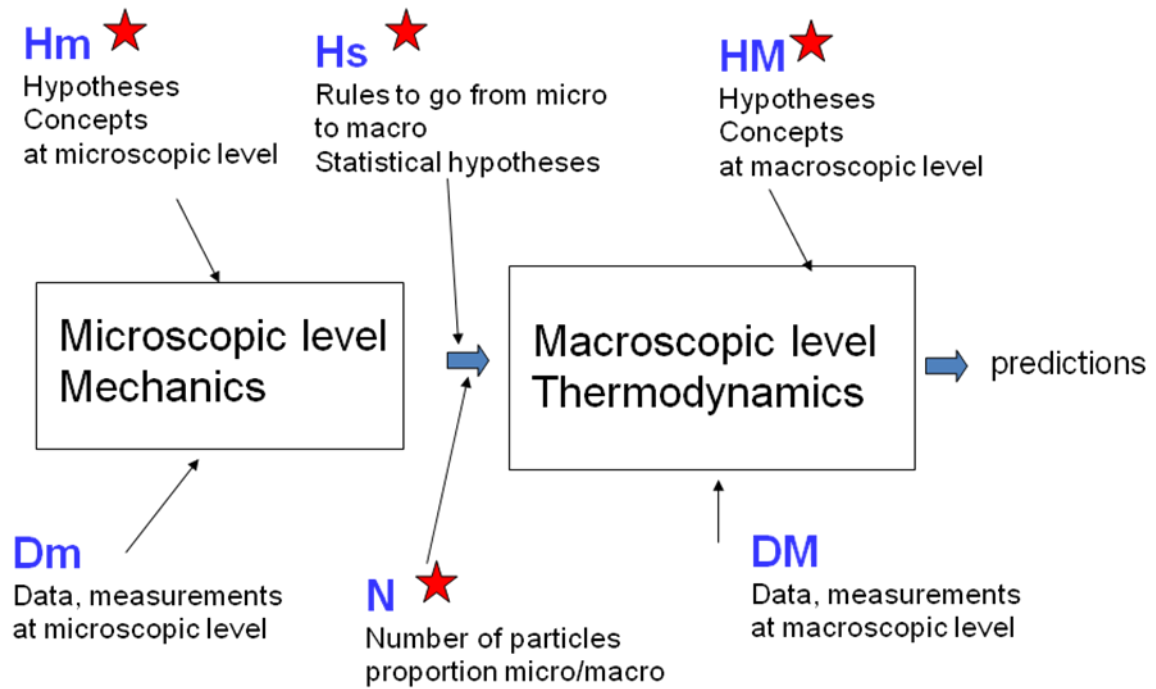


## Architecture n°2



**Figure 2**

Another architecture (Architecture 2) in which thermodynamics is considered autonomously and universally, with no considerations of scale.



★ Places with degrees of freedom to change the theory

**Figure 3**

Architecture 3 (there could be other sub-variants, see Guy JETC XI), in which all hypotheses at different levels and scales are considered.