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Teaching the entropy concept by transforming Boltzmann's conjectures into computer experiments

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ABSTRACT. New methods for high school and college Physics instruction engage students in understanding the physical world by constructing and using scientific models to describe, explain, predict and control physical phenomena. Modelling many particle systems involves the need to introduce statistical approaches and to look at reality in a probabilistic way. This paper reports a teaching approach in which the history of Physics is used as a Case Study in order to allow students to assimilate a given sequence of thought long enough to feel that it has a context and a surrounding logic of inquiry and experience. This approach focuses on Boltzmann's conjectures and reasoning aimed at introducing his stochastic models in a mechanist era. The kind of conjectures chosen are described and the structure of our teaching approach is outlined. It will also involve the pedagogical tools prepared in order to make workable the approach even for students not familiar with combinatorial and permutational calculus. Preliminary results of the first pilot test in two Courses for teacher training are also described.

Key words: entropy, history, simulations.

RESUMO. Ensinando o conceito de entropia através de conjecturas transformadas de Boltzmann em experimentos computacionais. Novos métodos para o Ensino Médio e de Graduação levam os estudantes a compreender o mundo físico pela construção e pela utilização de modelos para descrever, explicar, prever e controlar os fenômenos físicos. Modelar um sistema de muitas partículas envolve a necessidade de introduzir aproximações estatísticas e olhar a realidade de uma forma probabilística. O presente artigo expõe um modelo de ensino em que a história da física é utilizada como um "estudo de caso", no sentido de permitir aos alunos conviver com uma seqüência de pensamentos, num contexto e numa lógica de interrogação e experiência. Este modelo focaliza as conjecturas de Boltzmann e o seu raciocínio baseado em modelos estocásticos em uma era mecanicista. São descritos estes tipos de conjecturas escolhidos e a estrutura de nosso modelo aproximativo e ensino é posta junto com ferramentas didáticas preparadas no sentido de familiarizar os estudantes com o cálculo combinatorial e permutacional. São apresentados os resultados preliminares do primeiro teste-piloto em dois cursos de preparação de professores.

Palavras-chave: entropia, história da física, simulações.

The use of history of Physics in high school and in undergraduate education has been widely discussed in papers and conferences: the relevance of the history of science for acquiring proper understanding of scientific concepts and theories, therefore, is beyond any question. Indeed, if we want to convey to students an adequate picture of what science is all about and how its concepts and theories apply to the real world, we must connect it to the historical experiences which constitute the indispensable background for our understanding (Matthews 1994).

It has been pointed out that the history of physics can be used in different ways by Physics teaching (Bevilacqua and Kennedy 1983). Among these, we will point out two approaches that include a proper reflection on the historical evolution of Physics: the first focuses on the epistemological aspects and structure of the discipline in order to guide the students towards the understanding of the role of hypotheses and models, the self consistency of the principles and the growth mechanism of theories; in the second approach, history comes out through the study of paradigmatic cases and thus the systematic teaching of Physics is enriched by knowledge of the emergence of important conceptual schemes, ideas, experiments, etc. In both cases the history of Physics is mainly used to improve knowledge in an internal sense and not merely to introduce students to the importance of science in the development of Western civilisation (Brush 1969): a valuable educational objective relating science with other subjects and/or teaching science from a more humanistic viewpoint. However, our main educational objective is a better understanding of physical theories as they are understood today, by integrating them within the knowledge of what is valid today, how it came about, what were the reasons of the discoveries, what are their conceptual tools, their frames of mind, and how and why all this has changed into the present-day form of knowledge.

Many papers (Brush and King 1972, Bevilacqua and Kennedy 1983) have pointed out that, when history is used not for its own sake, but only as a means to a goal, it can be easily distorted and falsified into what Whittaker (1979) called "quasi-history". It has been stressed that there is a fundamental incompatibility between a logical development of Physics and a realistic, historical development. Very often the way things would logically have happened, was not unfortunately the way that things did happen. There is no doubt on the validity to point out this since the problems come out when we start to define the ways we can realise an historical approach to Physics, given all the constraints of the educational system.

The realisation of an historical laboratory has been pointed out as a possible teaching strategy, useful to illustrate how, in the evolution of physics, the relationships between theoretical accounts and experimental activities have been developed. In this laboratory students should analyse some historical experiments relevant for the introduction of new ideas, for the success of theories or of new experimental procedures. In fact it is an important point to confront antagonist conceptions of a single group or groups of scientists[1].

This paper refers to a more limited case in which history is used as a Case Study in order to allow students to live with a given sequence of thought long enough to feel that it has a context and a surrounding logic of inquiry and experience. In our view this approach workable principally for new teaching approaches, at high school level, stressing pedagogical objectives related to processes of Physics.

New approaches to Physics teaching focus on the process of constructing predictive conceptual models and identify model building as a superordinate process skill (Hestenes 1992, Gilbert 1993). The introduction of modelling activities in Physics courses contributes towards a number of content areas and enables students to see similarities and differences between a wide range of phenomena. Scientific models are usually very different from students' personal views of the world, the spontaneous models (Gentner and Stevens 1983). In order to fill this gap appropriate approaches to scientific models are necessary to perform the "fitting", or rather, to adapt gradually student conceptions to scientific models.

Teaching approaches focusing on the Newtonian modelling of real world phenomena are widely employed. They use various specifically prepared educational tools, software and Microcomputer Based Laboratory (Thornton and Sokoloff 1990, Modeling Group 1999) and have shown their effectiveness for learning (Redish et al.1997, Hake 1998).

The modelling of thermal phenomena in introductory Physics courses shows many difficulties in learning when the empirical approach of thermodynamics and the structural approach of statistical mechanics are used. The primary distinction between the two descriptions is that, whereas thermodynamics deals with measurable parameters, such as pressure and temperature, characterising macroscopic quantities, statistical Physics attempts to go deeper into detail, by modelling the microscopic behaviour of a system. However, owing to the introduction of microscopic arguments the statistical approach deprives thermodynamics of its feature of general theory applicable to all systems and independent from their microscopic structure. On the other hand, thermodynamics shows in this generality the greatest element of difficulty.

It has been pointed out (Alonso and Finn 1995) that many students usually encounter greater difficulties when entropy and the second law of thermodynamics are only presented in the context of a thermodynamic approach, as a state variable without any connection to the internal structure of the system or to what entropy really is. Many teachers and science education researchers think that the statistical approach can overcome some of these difficulties, since it correlates the properties of a

[1] A wide bibliography discusses the educational relevance of this approach, see for example: Conant and Nash 1957, Harvard Project Physics Course 1970, Brush and King 1972, Dhombres 1980, Bevilacqua and Kennedy 1983.

system both with the properties of its constituent units and with their interactions (Baierlein 1994). Moreover, whereas classical thermodynamics is practically restricted to systems in equilibrium or quasi-equilibrium, statistical mechanics does not need the limitation of slow changes in the system, that necessarily eliminates a broad class of important phenomena: the irreversible fast changes. This increased range of phenomena open to statistical physics is purchased at the expense of our needing to built a specific model. This involves many conceptual and mathematical difficulties especially in the case of classical statistics, where the mathematical arguments are particularly abstract. For this reason many textbooks introduce quantum statistics from the start where the less difficult statistical approach of counting states can be applied.

A statistical approach to the entropy concept involves the introduction of mathematical concepts concerning probability and, mainly, the changing of views through which one looks at physical phenomena. Usually students start to study thermodynamics just after Newtonian dynamics, that is, just after having verified that causality and determinism are the categories explaining the observed physical phenomena. Moreover, through the study of the kinetic theory, which gives simple explanations of some thermal phenomena, they can easily be convinced of the possibility to interpret all natural phenomena in terms of motions of the small particles constituting matter, similarly to what Newton in his *Principia* and many physicist of the 19th century did. The requirement to shift from deterministic to probabilistic models involves the ability to modify the way to look at reality and at the relationships among models, theories and empirical phenomena. Looking at the historical evolution of such ideas can be a useful and formative educational approach.

So that such approach may be undertaken, we will focus on Boltzmann's researches, chiefly on his conjectures and reasoning aimed at introducing his stochastic models in a mechanist era. In the next section we will describe the types of conjectures we have chosen for our didactic approach. Later, we will report the structure of our teaching approach and, as a sort of a conclusion, the methods we have followed in order to prepare teachers to put it into practice in the classrooms.

Boltzmann's conjectures for a teaching approach

Boltzmann is the emblematic scientist representing a transition phase: his ideas about the role of models and theories are certainly more advanced than those of his time, although he was enable to overcome the mechanistic and reductionistic aspects of his research:

> *In a very general way, I think that a direct description of many phenomena is not possible, but only a mental representation of them. For this reason, it is not correct to say, as Oswald: "you should not make a representation for yourself," but only: "you must introduce in the representations as less arbitrariness as possible.*
>
> *I would even assert that the process of construction of a mental representation necessarily involves the introduction of some arbitrary characteristics and that each time we infer a new fact, through a deduction from a representation drawn from different experimental facts, we in a strict sense, transcend from experience.* (Boltzmann 1905, p. 141 and p. 57)

> *Certainly, therefore, Hertz is right when he says: "The rigour of science requires that we distinguish well the undraped figure of nature itself from the gay-coloured vesture with which we clothe it at our pleasure." But I think the predilection for nudity would be carried too far if we were to forgo every hypothesis. ... Every hypothesis must derive indubitable results from mechanically well-defined assumptions by mathematically correct methods. If the results agree with a large series of facts, we must be content, even if the true nature of facts is not revealed in every respect. No one hypothesis has hitherto attained this last end, the Theory of Gases not excepted. But this theory agrees in so many respects with the facts, that we can hardly doubt that in gases certain entities, the number and size of which can roughly be determined, fly about pell-mell. Can it be seriously expected that they will behave exactly as aggregates of Newtonian centres of force or as the rigid bodies of our Mechanics? And how awkward is the human mind in divining the nature of things, when forsaken by the analogy of what we see and touch directly?* (Boltzmann 1895, p. 413)

Boltzmann is the best messenger of the methodological renewal of theoretical physics that started in the middle of the last century with Maxwell's work. His interest in epistemological considerations is strictly connected with research problems. He is fully aware of the role of hypotheses and models in the construction of a theory. His conception of this role implies in abandoning the attempt of knowing the real mechanism that regulates phenomena and to consider models as eloquent pictures and analogies able to evidence some aspects of nature, and that are susceptible of being improved in order to give a better description. On the basis of these ideas, he tried to overcome the difficulties concerning the problem of reversibility. He searched (Boltzmann 1905) for analogies among different natural processes, transmission of heat, propagation of electricity in conductors and hydrodynamic processes in order to infer models able to illustrate the general functioning mechanism. He was conscious that

> *[…] these kinds of mechanical models exist only in our spirit.*
>
> *[…] According to me, the aim of a theory is in the construction of a picture of the real world that only exists in our mind and must be the guide for all our thoughts and experiences. […] the main objective of the theory is to continuously improve this picture. Imagination has always been the cradle of theory, the spirit of observation its tutor.* (Boltzmann 1905, p. 76)

Almost at the end of his research he was able to consider also the mechanical descriptions as a useful but not absolute image of nature:

> *[…] No one, so to speak, considers force a reality, and thinks that it is possible to give proof providing that natural phenomena are susceptible of mechanical explanations. I myself have, sometimes, came to universal mechanism's defence, only with the proposal of showing its immense superiority with respect to purely mythical explanations other times received.* (Boltzmann 1905, p. 129)

The introduction of the concept of probability modifies the nature of the physical quantities involved:

> *[…] I have underlined that my H-theorem as well as the second law of thermodynamics are only theorems of probability. The second law of thermodynamics cannot be mathematically demonstrated only on the basis of dynamical equations […].*
>
> *[…] Only on the basis of the equations of motion, it is not possible to demonstrate that the H-function has to decrease in a constant way. It is only deducible from the probability laws that, if the initial state is not specifically set out for a given objective, but chance reigns at discretion, the probability that H decreases is in all occasions greater than that with which it increases.* (Boltzmann 1895, p. 414)

These sentences empty the mechanistic paradigm of all meanings. However, he was unable to abandon completely his starting idea in search for a dynamical and evolutive description of the universe that explains each phenomenon on the basis of interactions among the particles that constitute matter.

The kinetic theory of gases developed in the 19th century was very successful, but brought about many difficulties concerning its foundations and, in particular, the hypothesis of molecular chaos. All scientists studying this theory, including Boltzmann, started with a strictly mechanistic program: in his 1866 paper Boltzmann wrote that his objective was to provide a general and purely analytical demonstration of the second law of thermodynamics and to find the corresponding mechanical theorem. When he started to consider the kinetic viewpoint, that is, the distribution function instead of the individual kinetic variables of the molecules, he found Boltzmann's equation and the H-theorem that gave the first explanation of irreversibility of natural processes. However, in all his papers written before 1872, Boltzmann's ideas were developed in a mechanistic context and he seemed firmly convinced that his results derived directly from the application of the mechanical laws. This approach resulted in many conceptual difficulties, leading to a wide dispute among physicists. Consequently Boltzmann began to re-analyse the foundations of his theory until he reached the fundamental conclusion that the nature of its theory is basically probabilistic: he introduces the concept of probability as a foundation of physical laws.

Brush (1976) pointed out that Maxwell's 1860 arguments for the derivation of the velocity distribution of gases included probabilistic arguments for the first time, without any considerations on peculiar molecular processes. However, the viewpoint was considered inadequate at that time and it had to be justified by calculations based on special molecular models as in Boltzmann's paper of 1872 having their acme in the H-theorem. In a few sentences Boltzmann's transition from a stochastic past to a statistical approach is positioned:

> *If one does not merely wish to guess a few occasional values of the quantities that occur in gas theory, but rather desires to work with an exact theory, then one must first of all determine the probabilities of the various states which a given molecule will have during a very long time or which different molecules will have at the same time. In other words, one must find the number of molecules out of the total number whose states lie between any given limits.* (Boltzmann 1872, Brush 1966 p. 90)

In all the paper, one can find sentences which almost postulate that molecular motions are at random and argue that irregular events, occurring in the same proportions, give the same average values and explain the "completely definite laws of behaviour of warm bodies" (Boltzmann 1872). However, in proceeding to mathematical derivations, he clearly refers to the distribution function f as to the "number" of molecules having some specified velocity or other characteristic quantity. In this paper he gave the H-theorem using a functional called E, equivalent to the H-function, written in terms of energy x rather than velocity.

$$E = \int_0^\infty f(x,t)\left\{\log\left[f(x,t)/\sqrt{x}\right]\right\}dx$$

Boltzmann's 1872 paper introduces too the descriptions of particle energies in discrete values:

> *We wish to replace the continuous variable* x *by a series of discrete values* ε, 2ε, 3ε,... pε. *Hence we must assume that our molecules are not able to take up a continuous series of kinetic energy values, but rather only values that are multiples of a certain quantity ε. Otherwise we shall treat exactly the same problem as before. We have many gas molecules in a space* R.. *They are able to have only the following kinetic energies:*

ε, 2ε, 3ε,... pε.

> *No molecule may have an intermediate or a greater kinetic energy. When two molecules collide, they can change their kinetic energies in many different ways. However, after the collision, the kinetic energy of each molecule must always be a multiple of* ε. *I certainly do not need to remark that for the moment we are not concerned with a real physical problem. It would be difficult to imagine an apparatus that could regulate the collision of two bodies in such a way that their kinetic energies after a collision are always multiples of* ε. *That is not the question here. In any case we are free to study the mathematical consequences of this assumption, which is nothing more than an artifice to help us to calculate physical processes. For at the end we shall make* ε *infinitely small and* pε *infinitely large, so that the series of kinetic energies will become a continuous one, and our mathematical fiction will be reduced to the physical problem treated earlier.*
>
> *We now assume that at time* t *there are* w_1 *molecules with kinetic energy* ε, w_2 *with kinetic energy* 2ε, ... *and* w_p, *with kinetic energy* pε, *in unit volume.* (Boltzmann 1872, Brush 1966 p.119)

In its paper of 1877, in order to answer to the reversibility paradox, Boltzmann argued that it is possible:

> *to calculate, from the relative numbers of the different state distributions, their probabilities, which might lead to an interesting method for the calculation of thermal equilibrium.* (Boltzmann 1877, Brush 1976 p. 606)

In this way he developed his statistical method for calculating equilibrium properties, based on the relation between entropy and probability and concluded that:

> *if perhaps the reduction of the second law to the realm of probability makes its application to the entire universe dubious, yet the laws of probability theory are confirmed by all experiments carried out in the laboratory.* (Boltzmann 1877, Brush 1976 p. 607)

He reached his conclusion by reasoning from what he calls "probability theory", while assuming that exact deterministic laws still apply to molecular motion and collisions.

The really new method for determining the state of thermal equilibrium of a system is described in his paper of 1877. The method is applicable to any system, not only to that of gases, and consists in enumerating all the ways in which a given total amount of energy can be distributed among a specified number of molecules, *complexions*, by assuming that the probability of a macroscopic state is proportional to the number of corresponding molecular complexions and that each complexion is assigned equal probability. He evaded the problem of counting a continuum of microstates by assuming the same discrete distribution of energy among the particles, described in the 1872 paper and, consequently, that each molecule can have only a finite value of energy values.

To look at the ensemble of microscopic configurations compatible with a given macrostate of the system is a relevant change of point of view with respect to methods used until that time to study the gas laws (Cercignani 1998). The focus was a single system following the time evolution of its macroscopic state, without any direct interest in the actual microscopic configurations. In order to study the microscopic configurations in all, compatible with a given macroscopic state, in his 1877 paper Boltzmann considers not merely a single system, but a purely conceptual ensemble constituted by a great number of identical systems (intended as mathematical models and/or ideal copies), all in the same macroscopic state, but each one having a different microscopic configuration. Each microscopic configuration is then represented by an ideal copy of the given system and the macroscopic configuration is intended as the ensemble of its microscopic configuration.

The modelling of a system through an ensemble of microstates is a consequence of the need to define the probability of a given macrostate. This important aspect of theoretical physics at the end of the 19th century pointed out the relationships between models and abstract theories. The scientists desire to abandon the need of a mechanistic description of reality: the concept of mean system property, intended as an average over a large time of its evolution, is now replaced by the new concept of mean behaviour of an ensemble constituted by identical systems. The identity of the two definitions has been taken for granted (Cercignani 1998). This approach to the description of thermal properties of a physical system has also been used in an independent way by Maxwell. However, only through the Gibbs and Einstein's work it had its definitive formulation in Statistical Mechanics.

Boltzmann's problem was to calculate the number of ways in which a macroscopic state can be realised: as a consequence, a state corresponding to a greater number of ways will be more probable. Thermodynamic evolution will bring the system in its more probable macrostate: since entropy has its maximum, a link must exist between entropy and probability of its macroscopic state. This is an important conjecture drawn from Boltzmann's lectures on the Gas Theory of 1896 (translated in English in 1964):

> *To begin, we will make some preliminary observations concerning the principles of the calculus of probability. From a vessel, where we have a large number of black spheres and an equal number of white spheres, for the rest identical, randomly pick 20 spheres. The chance that we pick only black spheres is not at all less probable that the chance that the first sphere we pick is black, the second white, the third black, etc.... The fact that it is more probable to obtain 10 white spheres in 20 choices than 20 black spheres is due to the fact that the first event can be realised in much more ways than the second. The relative probability of the first event with respect to the second is the number 20!/(10! 10!) which indicates how many permutations can be made of the terms of the series of 10 white spheres and 10 black spheres, considering that the black spheres as well as the white spheres are identical. Each one of these permutations represents an event that has the same probability of the event of all black spheres. If in the vessel we have a great number of black spheres, a greater number of blue spheres, a great number of red spheres and so on... , the probability to choose* a *white spheres,* b *black,* c *blue, etc.... is:*

$$\frac{(a+b+c+...)!}{a!b!c!...}$$

> *times greater than the probability of having spheres of the same colour.*
>
> *As in this simple example, the event that all the molecules of a gas have exactly the same velocity in the same direction is not at all less probable of the event that each molecule has exactly the same velocity and motion direction that it actually has at a given instant. However, if we compare the first event with the event that in the gas the molecule velocities are in concordance with Maxwell' distribution law, we find a much greater number of equi-probable configurations corresponding to the second event.*
> (Boltzmann 1964, pp. 55 and 443)

The focal point is in the consideration that all the microscopic configurations have the same probability, but the different macroscopic configurations can be realised in a different number of microscopic configurations.

Boltzmann's operation of considering discrete values of energy is equivalent to consider the portion of velocity and position space μ, limited by the dimension and the total energy of the system, divided into cells of equal volume $\delta\upsilon_\mu = \delta r \delta v$ (a six-dimensional space). If the number of particles n_i occupying the cell *i-th* is assigned, the distribution functions $f(r,v,t)$ in this cell is defined as:

$$f(r,v,t) = n_i \delta\upsilon_\mu \qquad \sum^K n_i = N$$

and the set of occupation number is called a partition $\{n_i\}$. Each partition corresponds to a macroscopic state, since it defines the distribution function f.

> *Instead of white spheres we have a number* n_1 *of molecules in the first cell, a number* n_2 *of molecules in the second cell, and so on....... Consequently we have:*

$$W = N!/(n_1!\, n_2! \dots n_K!)$$

> *for the relative probability that* n_1 *molecules occupy the first cell, and so on.*
> *(Boltzmann 1964, p. 56)*

Following Boltzmann's reasoning we can define the quantity *logW* and, through simple calculations, show the following relation for Boltzmann's *H-function*:

$$H = \int f \log f \,\mathrm{drdv} = -\log W + \mathrm{cost}$$

Therefore, the *H*-value for a given macrostate, corresponding to a given distribution $f(r,v,t)$, is connected to the probability to realise the macrostate, i. e., to the number of different and equi-probable microstates.

From the previous expression we can find the partition $\{n_i\}$ that corresponds to the maximum of probability and consequently to the equilibrium distribution $f(r,v,t)$, Maxwell's distribution.

The reported approach does not makes any reference to collisions or time evolution of a particle system, but the distribution function f is analysed in terms of probability to find a given number of particles in a given volume of the space μ.

Teaching approach and computer simulations

Boltzmann's conjectures that we have considered relevant in helping students to understand some main points of Thermodynamics as well as of the Physics process of modelling involve: i) his ideas about physics models and their relationships with theories; ii) the probabilistic approach to model phenomena involving many particle systems. They resemble thought-experiments, that is, reasoning on quasi-empirical models, on analogies and/or similarities. It has been shown that thought-experiments have been powerful means of tackling conceptual problems during the historical evolution of Physics (Kuhn 1962). Thought-experiments have also been considered as good educational tools for physics and mathematical education (Stinner 1990, Glas 1997). Results of thought-experiments may be achieved through logical deductions from starting hypotheses and mathematical calculations and both involve many difficulties for the students of introductory Physics courses.

Many teaching approaches use computers for simulations, enabling students to analyse Physics models and overcoming many of the mathematical difficulties involved. In this paper we will focus on one aspect of simulations that we call "Experimenting with models". We use a procedure very similar to that used in a laboratory experiment, wherein a conceptual model or idea is being tested within the framework of existing physical laws. The terminology "computer experiment" is intended to emphasise that this kind of simulation shares some of the features of ordinary experimental work, in that it is susceptible to statistical and systematic errors.

The models of our simulations are representations of microscopic evolution of particle systems modelling matter. Their behaviour will be analysed and their validity verified by comparing simulation results with experimental results and/or with theoretical accounts.

The conventional analytical treatment of microscopic models is not straightforward. The formalism of combinatorial and permutational calculus and the representational problems connected with the geometry of a discrete system make the analytical approach very difficult for many undergraduate students, even in the case of simple systems, such as dilute gases. In order to overcome mathematical difficulties, many computer simulations of models of dilute gases have been published for teaching purposes: some analyse particle systems evolving toward Maxwell-Boltzmann velocity distribution (Sauer 1981, Eger and Kress 1982, Ftacnik et al 1983, Aiello-Nicosia and Sperandeo-Mineo 1985), others focus on the entropy definition (Black et al 1971, Bellomonte and Sperandeo-Mineo 1997) and calculations (Moore &. Schroeder 1997). All use a statistical approach based either on the Molecular Dynamics or on the Monte Carlo methods. In both methods the elementary physical events are well defined and easily comprehensible by students. Mathematical problems emerge when the synthesis of these elementary events is attempted. In a computer experiment synthesis is realised implicitly in the logical design of the fundamental, branching, computational flow sequence used to define the conceptual model being studied. Physical values are obtained by taking a simple average over the set of values occurring in each of a very large number of particular computational sequences. Consequently simulations can allow high school and undergraduate students to compare experimental data with theoretical curves in detail and gain an exhaustive view of the logical consequences evolving from the assumptions defining a physical model.

Our educational approach uses simulations in order to visualise analogies, detect model behaviours and count the number of microstates associated with different macrostates of simple models. We have used two different computational environments: the spreadsheet Microsoft EXCEL and stand-alone programs written for the purpose[2]. Educational uses of the two environments are different: the first allows students an easy modification of model properties and, consequently, the evaluation of their influence; the second visualises possible model evolutions and the influence of some relevant parameters. The Appendix reports the results of some performed simulations and the concepts and/or process they are supposed to focus.

The first simulation introduces the concept of equi-probable configurations: we simulate Boltzmann's vessel containing a large number of little spheres all equal except for the colour (half of them are white and the other half black) and perform M random picks of N spheres. The program calculates the frequencies of different events $\{n_b,n_w\}$ ($n_{black} = 0.....N$ and $n_{white} = N...0$, with $n_b+n_w = N$) and plots their distributions for various values of the number of picks M. The frequencies are also confronted with the probabilities of all the possible events $\{n_b,n_w\}$. Students initially use the simulation for small values of N and M, observing the different configurations

[2] Programs are written in Visual Basic and their transformation in Activix for the Internet network is in progress.

displayed by the program, then analyse what happens for large values of N and/or M (see simulation n° 1 in the Appendix).

The second simulation reports in how many different ways N spheres of different colour can be apportioned in two halves of a box (the position within each half box does not matter). The program performs M different apportionments of N spheres and calculates the occurrence of each apportionment $\{n_l, n_r\}$ ($n_{left} = 0.....N$; $n_{right} = N...0$) plotting the frequency distribution. Analogously to first simulation, an analysis for low and high values of M and N is possible. Simulations in which the box is divided into parts of different volumes and, consequently, particles have different probabilities to occupy the various parts, can also be performed.

On the basis of the two reported computer simulations, students are supposed to have gained a clear understanding of the concepts of random events, equi-probable events, distributions, macrostates and microstates.

The third simulation introduces students to the concept of energy distribution and microstates associated to a given distribution. We use the term energy without any specification; later, we will specify if we intend kinetic energy of ideal gas molecules or energy of oscillators modelling the Einstein's solid or other.

By recalling Boltzmann's idea, we consider N particles having discrete values of energy:

$0, \varepsilon, 2\varepsilon, 3\varepsilon, \ldots\ldots k\varepsilon.$

We define a system macrostate by determining its partition $\{n_i\}$, i. e. the numbers $n_0, n_1, n_2, \ldots. n_k$ of particles having the energies $0, \varepsilon, 2\varepsilon, 3\varepsilon, \ldots\ldots, k\varepsilon$, respectively. The values of n_i are subjected to the two conditions:

$$0n_0 + 1n_1\varepsilon + 2n_2\varepsilon + 3\, n_3\varepsilon + \ldots + k\, n_k\varepsilon = E$$

$$n_0 + n_1 + n_2 + n_3 + \ldots\ldots n_k = N$$

where N is the total number of particles and E the total energy of the system.

The program visualises and calculates, for small values of N and E, the number of ways W we can put N distinguishable particles into k boxes (schematising the different energy values) so that there are $n_0, n_1, n_2, \ldots, n_k$ particles in each box:

$W = N!/(n_1!\, n_2! \ldots . n_k!)$,

This is the value of Boltzmann's number of *"complexions"*, i.e. the number of microstates W associated with a given macrostate (defined by its partition $\{n_i\}$) and, consequently, the relative probability of the macrostate.

In order to find the equilibrium partition, Boltzmann calculates the maximum of the function $\ln W$, obtaining Maxwell's velocity distribution. Instead of using analytical arguments, we perform an experiment with our model in order to construct an ensemble of systems, all equally probable, representing the different microstates of our system. The model simulates those substances whose internal energy can be written as a sum of single-particle energies. Einstein's model of solid and a model of dilute gas are two examples: the first considers particles as oscillators, all fixed in place, storing energy in units of the same size; the second model assigns to particles discrete values of kinetic energy as follows: to all n_0 particles having values of energy between 0 and $\Delta\varepsilon$ is assigned an energy equal to 0, to all n_1 particles having values of energy between $\Delta\varepsilon$ and $2\Delta\varepsilon$ is assigned an energy equal to ε, and so on, until $k\varepsilon$, assigned to the n_k particles whose energies are between $k\Delta\varepsilon$ and $(k+1)\,\Delta\varepsilon$, under the condition that:

$$n_1\varepsilon + 2n_2\varepsilon + 3\, n_3\varepsilon + \ldots + k\, n_k\varepsilon = E$$

The introduction of discrete values for the allowed particle energies can be considered, in line with student knowledge, as a natural assumption descending either from quantum mechanics or from a first approximation aimed to simplify calculations.

The program uses the Monte Carlo random sampling method (Binder 1986, Whitney 1990): each microstate of the physical system under consideration is determined by chance. It allows us to look for small samples that are able to approximately represent the whole ensemble under consideration. As a consequence, if we can manage to construct a small sample representing adequately the ensemble of microstates of the analysed systems, then the conceptual difficulty of classical statistical mechanics will be reduced by a large extent.

The program starts with an arbitrary energy distribution and generates successive microstates through a shuffling generator of energy exchanges simulating random binary interactions among particles, in which two identifiable particles exchange energy according to energy conservation law. Microstates successively generated are different only from the energies of the two interacting particles. A large number of repetitions of these procedures results in a large number of microscopically different configurations adopted by the system and the initial distribution will tend to the distribution having the maximum of multiplicity: the equilibrium distribution corresponding to the maximum of possible microstates.

The analysis of the sequence of model macrostates is performed in terms of their relative probabilities W. Entropy S is calculated according to:

$S \propto \log(W)$

The results show that the two analysed systems evolve towards states characterised by values of *S* which never decrease (except for fluctuations due to the low number of system particles) and equilibrium energy distributions are exponential for Einstein's model and Maxwell's distribution for the dilute gas model.

While the operations of the energy shuffling generator give a concrete representation of the Boltzmann statistical ensemble associated with each macroscopic system, the method of counting system multiplicity gives an understandable description of the meaning of equilibrium. The logarithmic quantity called entropy has a perfectly clear meaning in terms of the fundamental notion of the 'multiplicity of a macrostate'. This notion can be easily related to the qualitative terms 'order' and 'disorder' that are usually related in introductory textbooks to the entropy (entropy as 'a measure of disorder'). The relationship with multiplicity becomes clear if we use the notion of 'correlation' as a conceptual intermediary (Baierlein 1994). In fact the notion of order implies that of strong correlation and consequently small multiplicity; that of disorder implies the notion of an absence of correlation and hence a large multiplicity. It follows that although the usual way of considering entropy as a measure of disorder is correct, this does not take one very far since a quantitative description of entropy from a statistical point of view can be gained only by connecting disorder with the 'absence of correlation' and then with multiplicity.

Different simulated experiments can be performed using two systems **A** and **B**, having energies E_A and E_B and entropies S_A and S_B respectively, that are allowed to interact in different irreversible ways. The simulated experiments show that entropy is an extensive non-conserved quantity since the final entropy of system **A+B** is greater than the sum of initial entropies of the two systems **A** and **B** (for further details see Bellomonte and Sperandeo-Mineo 1997). Looking quantitatively to interactions of systems with different initial energies and analysing the direction of the energy flows, statistical entropy can be connected with temperature and with energy input by heating and, consequently, to its thermodynamical definition (Bairlein 1994, Moore and Schroeder 1997).

Discussion and conclusion

The described approach has been tried out in two university courses for teacher training: a pre-service teacher training course and an in-service teacher training course. Approximately thirty people attended each course. They had graduated in mathematics and had already frequented two Physics courses. Their university curriculum only included a thermodynamic introduction of entropy concept.

After a lecture recalling fundamental aspects of the thermodynamic definition of entropy, in both courses teachers (and future teachers) attended to a Seminar[3] aimed to introduce the main aspects of Boltzmann's work, including his role in the development of Physics. They investigated the subject by using some chapters of two books (Brush 1976, Cercignani 1998) and some chosen pages of Boltzmann's papers. Successively, they worked in small groups using the prepared software: simulations visualising system evolutions as well as spreadsheets (allowing easy modifications of model features). At the end of the course, they were requested to prepare a small project of experimentation aimed at the introduction of the subject in high school classrooms. The project was supposed to describe the chosen teaching approach and materials: conceptual maps of the subject, Students Sheets to guide students in using computer simulations and bibliographic references reporting the historical elements considered relevant for student understanding.

Twenty teachers experimented the approach in their classrooms and evaluated learning and interest of their students. The analysis of the evaluation materials is in progress. Nevertheless, some preliminary results can be drawn:

- The students' interest for original historical materials was unfailing. Students evidenced that it was really stimulating to follow the conjectures of the scientist who discovered a fact and/or invented a model. They reported that "since Boltzmann's paper was the first one describing the topic, inevitably it must contain the clearest explanation, since he had the privilege of convincing people to accept his ideas".
- Students have shown a clear understanding of the equilibrium concept as well as of the second law of Thermodynamics. The meaning of irreversibility and heat flow has been well understood.
- Many students revealed a strong interest for paradoxes and scientific controversies and some teachers decided to amplify this aspect in successive classroom experimentation.

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[3] The seminar has been conducted by a professor of the History of Physics.

- Some students met with difficulties when statistical concepts were connected with thermodynamic concepts: qualitative relationships appeared easily understandable but quantitative correlations needed more accurate calculations. Further spreadsheet calculations are in preparations in order to clarify this aspect.

Our experience shows that, even if the introduction of statistical analysis of thermal phenomena may appear a bit difficult and sophisticated to many experienced teachers, the use of appropriate educational methods and tools makes this workable. Students show a much better understanding of thermal phenomena than when they are exposed only to empirical Thermodynamics and computer experiments. Moreover, historical accounts have a significant role in helping understanding and in stimulating interest.

Appendix

Experiments with models

1. Boltzmann's vessel. A very large number[4] of little spheres, all equal except for the colour, since half of them are white and the other half black, are contained in a big vessel. A player picks from vessel *N* spheres *M* times. The program enumerates the various events $\{n_b, n_w\}$, calculates their frequencies and compares these with their probabilities for different values of *N* and *M* (see Figure 1).

2. Shuffling of energy among particles. We consider an isolated system of *N* particles having a total energy $E = \Sigma\varepsilon_i$: where ε_i indicates the energy of particle *i*, $\varepsilon_i = k\varepsilon$ (with *k* an integer ranging $0 \div K = E/\varepsilon$)and ε is an arbitrary energy unit.

Assigned the initial energy values ε_{oi} ($E = \Sigma\varepsilon_{oi}$), different system microstates are generated by random exchanges of energy among particles. This shuffling procedure generates successive microstates according to the following rules of generalised binary interactions:

a) two identifiable, randomly selected particles *i* and *j* are chosen and are supposed to interact with each other;
b) the interaction produces a random change in particle energies from ε_i and ε_j to ε_i' and ε_j' subjected to energy conservation law:

$$\varepsilon_i + \varepsilon_j = (k_i + k_j)\,\varepsilon = k_{ij}\varepsilon = (k'_i + k'_j)\,\varepsilon \qquad (1)$$

[4] The number of balls contained in the box must be much greater than the number of the drawn balls in order to make all the drawings equivalent.

Initial and final values of energies are related to each other by:

$$k_i' = \text{int}(r\,k_{ij}), \quad k_j' = k_{ij} - k_i' \qquad (2)$$

where *r* is a random variable (in the range $0 \div 1$), with a proper probability distribution, and k_i' and k_j' are the numbers of energy units assigned to particles *i*, and *j* respectively, as a consequence of interaction.

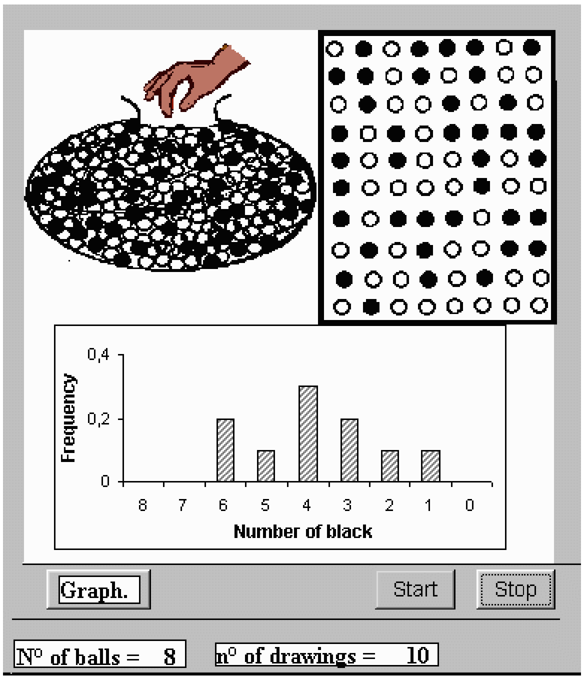

Figure 1a. Video-display of the vessel program: for low values of the number of spheres *N* and of picks *M*, the program displays the result of each pick and the event frequencies. The figure shows the result of 10 picks of 8 spheres

In order to determine the variable *r*, we need more information about particles, in particular about their degrees of freedom. In this way the program differentiates Einstein's solid model *(I Case)* and dilute gas model *(II Case)*.

I Case- modelling an Einstein's solid. The first pioneering educational simulation of *N* Einstein's oscillators has been performed in the Nuffield Project Unit "Change and Chance" (1972). Our simulation is in the same direction and shows that uniform random interchanges of energy among distinguishable elements give rise to an exponential distribution. The system starts with an arbitrary distribution of energy units and successive system microstates are generated according to equation (2), where *r* indicates a random number uniformly distributed in the range $0 \div 1$.

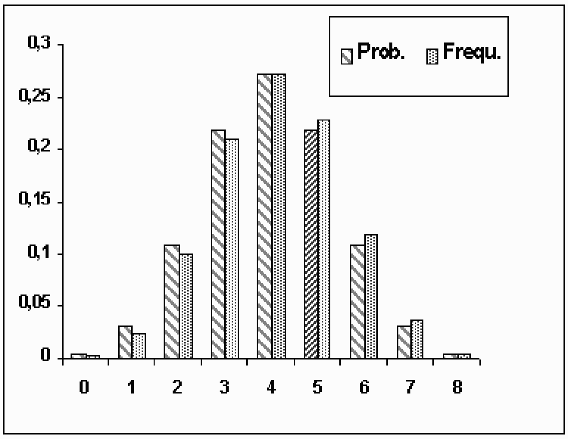

Figure 1b. Plots of the frequencies of occurrence of the various events $\{n_b, n_w\}$ (n_{black} = 0…..8; n_{white} =8…0) and of their probabilities in 10,000 picks

Figure 2 shows the mean energy distribution for a sample of 1,000 oscillators, after 10,000 interactions. For each partition $\{n_i\}$, the program calculates its multiplicity and the related entropy S according to:

$$S \propto \log(W) = \log[N!/(n_1!n_2!.....n_k!)]. \qquad (3)$$

The program allows a qualitative as well a quantitative analysis of the results and, in this last case, the system temperature can be calculated and related to system energy and entropy.

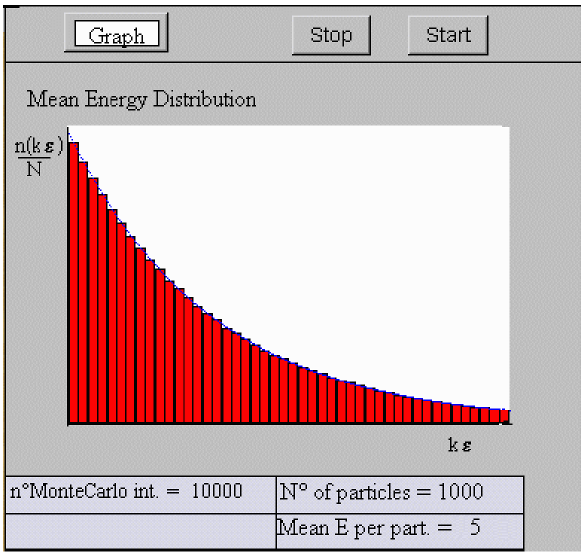

Figure 2. Histogram of the mean energy distribution for a system of 1,000 Einstein oscillators: the mean energy per oscillator is 5 (in arbitrary units). Averages are calculated upon 10,000 partitions. The curve plots the theoretical exponential distribution

II Case: modelling a diluted gas. A microstate of a system of *N* particles, simulating a diluted gas, is determined when the positions and velocities of all particles are known. Let us limit ourselves to kinetic energy. In order to visualise our discrete modelling of particle energies we divide the three-dimension velocity space into shells of thickness $\Delta v = \sqrt{(\Delta v_x^2 + \Delta v_y^2 + \Delta v_z^2)}$ in a such way that two adjacent shells include velocity vectors of particles whose energy values are different only for one energy unit ε: i. e., two particles (of unitary mass), whose velocity vectors are proper to two adjacent shells, have an energy difference given by:

$$1/2\,[(v+\Delta v)^2 - v^2] = \varepsilon \qquad v\Delta v = \varepsilon \qquad (4)$$

by disregarding the Δv^2 term.

The volume of the k^{th} shell is:

$$\Delta V = 4\pi v^2 \Delta v = 4\pi \sqrt{(2k\varepsilon)}\, \varepsilon = 4\pi \varepsilon \sqrt{(2k)} \quad (5)$$

where $v=\sqrt{(2k\varepsilon)}$.

According to basic assumption that equal *a priori* probabilities are assigned to equal volumes in velocity space[5], each particle *i* has a probability of having an energy $k\varepsilon$ proportional to $(\sqrt{k})$:

$$P(k\varepsilon) \propto \sqrt{k} \qquad (6)$$

The shuffling generator will assign to interacting particles *i* and *j* the new energies $\varepsilon_i' = k_i'\varepsilon$ and $\varepsilon_j' = k_j'\varepsilon$ according to the composed probability:

$$P(\varepsilon_i, \varepsilon_j \Rightarrow \varepsilon_i'\varepsilon_j') \propto \sqrt{(\varepsilon_i')}\sqrt{(\varepsilon_j')} = \varepsilon\sqrt{(k_i'(k_{ij} - k_i'))} \quad (7)$$

where k_{ij} is the constant defined in (1).

It turns out that, for each interaction, we have to generate a random number *r* in the interval $0 \div k_{ij}$ with the probability distribution given by (7). We used the "rejection method" (Wong 1992). For further information see Bellomonte and Sperandeo-Mineo (1997).

Figure 3 reports the results obtained in the simulation of a system consisting of 1,000 particles. The initial conditions assign to all the particles the same energy $\varepsilon_0 = 15$ (in arbitrary units). The calculated entropy values show that approximately after 1.5 ÷ 2 mean interactions per particle the system is already in equilibrium and *ln(W)* approaches its maximum value. It can be also

[5] This assumption is easily understandable on the base of previous simulations analysing the diffusion of particles in boxes of different volumes.

observed that the energy distribution becomes almost constant, except for fluctuations due to the small number of particles. It is well fitted by Maxwell's energy distribution. The plotting of velocity distribution is straightforward.

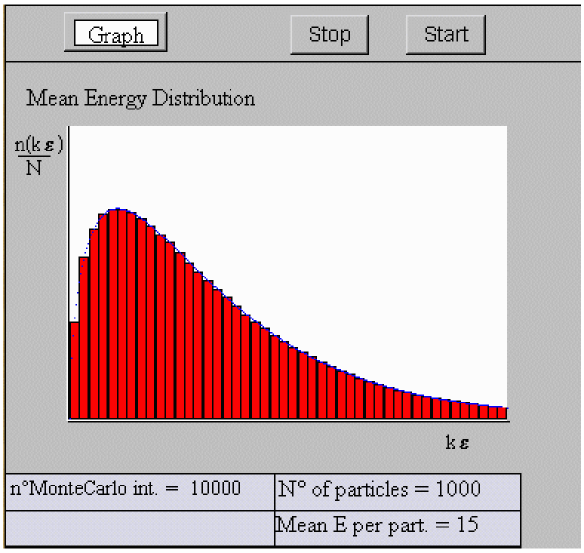

Figure 3. Histogram of the mean energy distribution for a system of 1,000 particles modelling a diluted gas: the mean energy per oscillator is 15 (in arbitrary units). Averages are calculated upon 10,000 partitions. The curve plots the theoretical Maxwell distribution

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