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Science and Computations
(Lecture three of the Course of Theoretical Physics)

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This day, people believe ever more in electronic computation. Electronic means much and fast. Computation means to put together numbers, *i.e.* a succession of something and something not, and reckon, calculate, all these binary digits. This way we estimate chances, *i.e.* if something is that or that, then the other thing is so and so. Some noticed this day that all the science (which I mean physics) is all but digitalized, we put numbers in equations, compute these numbers and get numbers. We get results, and nothing is more satisfactory than getting results. We have then a feeling of achieving something, of going further ahead, of making one step, and another, and so on. We feel then that we move, the faster and the more the better, which is rewarding.

This business of electronically computing everything is successful, so, isn't it boring? The only way to bring excitement in this entertainment is to make mistakes in computation. Then, we are looking for debugging our computing programs, which keeps us busy. Correcting our own mistakes is easy, the computing machinery starts soon to work again, and satisfaction follows. Is not this business boresome, in the end?

"It is not for a man of excellence to waste his precious time in endless computations", used Leibniz to say, approximately. If the computations are for servants, then what are gentlemen good for?

Indeed, this is the question of the science.

Science is precisely to know the result of any computation without doing it really. We have invented calculus and the infinity precisely for being able to know the result of any computation without doing it. Even the result of those computations which cannot possibly be done (because there are, indeed, computations that cannot possibly be done, no matter how fast and big the computer is, and there are uncomputable numbers and undecidable numerical questions. Obviously).

What is science for (and I mean of course the theoretical physics) if not to free us from the burden of computing, measuring or doing experiments in order to know, to live and survive? Science (I mean physics, of course) is "empirical" only in the sense that it refers to this world, not at all that we would derive knowledge from experiments. We are doing experiments only to entertain ourselves with our world, which we are part of, to participate in natural processes, and not to repeat them again, unless a morbid boredom drives us. The role of science is to remove and eliminate the experimental science (I mean, experimental physics) from our endeavours, not less the applied science. Food, transportation, communications will be soon our routinely new scientific experiments, done naturally (or, with an old term, "automatically") by ourselves as part of our world. And this by our being integrated in our world, as its entertaining counterpart. Science (I mean physics) leads us inevitably to this. This is the meaning of science, and the meaning of it all. To be part of our nature, of our world.

This integration is not smooth. Because we are still afraid of being joyful. Computation has rules, and the equations of the theoretical physics are rules. Rules which give us the understanding of us and of our world. Which understanding is joyfulness. Which we are still afraid of. "When we are thinking (*i.e.* let ourselves be conducted by these rules) we are feeling something troubling and worrying us, secretly", noticed Paul Valery, approximately. The joyfulness brought by this understanding is a depersonalization, which we are afraid of, yet, understandably.

"I am not afraid of not knowing the world, I am not freightened of not knowing it", Feynman would have said, reportedly. No, this is no problem at all. Nobody indeed, Feynman included, is ever afraid of not knowing the world. The real fear is precisely of knowing it indeed, and Feynman had a slip of tongue, the saying sounds actually "I am really afraid, I am bone-deeply freightened of knowing our world". This is the meaning Feynman was driving at.

We often prefer instead to send us to the Moon. Then, we need electronic computations in real time to correct the trajectory of the rocket, and we, I mean the computers, are doing that for us. It would not be the same to put the man right on the Moon, or 1700km (Moon's radius) on the right or on the left, when we fly 340 000km distance from the Earth. Here, we ought to be exact.

We often prefer also to build extremely high, extremely lean and fancy, and just on the shore, or on volcanoes. Then, we need the building design be assisted by electronic computations, to ensure, to some extent, the safety construction criteria. Electronic computers do the job, and they do it greatly.

We are much pleased this day to manipulate sound, images, motion, and the electronic computers provide generously for our virtual world of motion pictures, games, for modelling impossible phantesies or simulating meaningless worlds. The fabrication of the integrated electronic chips is simulated and modelled first on computer. Electronic computations generated two new words, electronic simulation and electronic modelling. Others will come, just in order to really circumvent the question, and kick the monotony off.

We preferred once to explode an atomic bomb, and spent time in computing exactly whether the explosion will equal 10 kilotons of conventional chemical explosive, or 20 kilo. That is, whether we would be going to kill with that bomb 100 thousands people, or 200 thousands. Electro-mechanical computation in its infancy at that time helped us a lot to be very exact on that issue. It turned out that we killed 150 000 and the power was about 15 kilotons of the most powerful chemical explosive at the time. Was it any worth of? I mean, to do all those computations?

Electronic computers had been finally invented around 1940 by von Neumann who laid down definitely the principle, the means and the architecture. It was a wonderful adventure, even more pleasant when the electronic circuits became integrated, and we were able to see that the world may go fast and for long on calculating digits, without getting tired. Our inclination of being exact was satisfied then, like starting suddenly to write with sharp pencils instead of the blunt ones. Now, we have all these sharp pencils, and they may get ever sharper with this nanoelectronics. We have them already, wouldn't be the time to look for something else? Is it any sense in doing computations without telling anything, in transcribing old books with sharper and sharper pencils? Isn't it a little boresome? Is it any pleasure in being very exact without being a little more accurate? Yet, with electronic computations we are always exact and never accurate.

Science is not about being exact, it is about being accurate. Accuracy is harmony and equilibrium, and it solely gives pleasure and happiness. Our soul is then taken by angels and lift to the feet of God. "Our Sun will get exhausted of its nuclear fuel in about 5 billions years, and extinction of life will then follow", says the speaker. "You said billions? OK, that's great", says the old man up at the bottom of the auditorium, back in the audience, "I thought you said millions, and was quite worried about myself". This is the difference between exactness and accuracy. "We are in theoretical physics where the mathematical rigour is not only impossible, but it is not even desirable", Landau was saying, approximately. It is rigour mortis in science, and better a vigorous mathematics than a rigorous one.

There is nothing mysterious or mystic in theoretical physics, there is only a mysterium in the old sense of the word, *i.e.* an immense joyfulness arising from shutting down the mouth and the eyes. It teaches precisely how to compute the result without actually computing it. Then, why computing exactly, when we already have science that takes us, if not to the ethernal life, at least to the difference between our world and a foreign world? For practical reasons? What are practical reasons, and what is praxis? Isn't it exactly anti-science? A famous Romanian practical joke is to gather together all the hand's fingers as in a small pocket, and turn them quickly about the hand axis, in a short, swirling motion. The meaning is to show how to steal something (money from a pocket, a chicken from the household backyard, etc). It is practical, since it works if you are not caught. And it is only a joke, if you get caught. So, it is a practical joke. This is praxis, and of such kind are the practical reasons.

Let's see the anti-science at practical works.

Since 1930s there has been much effort in computing chemical bonding, matter aggregation and atomic cohesion. First for molecules, latter on, under the impulse of the electronic computers, for larger aggregates. With little progress. This day, atomic nano-aggregates still wait to be computed. The corresponding computation programs (or codes, more fancy, which means that everything in there is coded, *i.e.* secret, and only those who know the code can decode them and use them) fail in being stable, producing meaningful results, or just working at all. The reason for such a failure resides obviously in the fact that we compute what we do not yet know, or understand. That is, equations governing the atomic aggregation are not yet understood. These pseudo-scientific procedures start either *ab initio*, *i.e.* with the wavefunctions of the atomic orbitals, or with a so-called functional of electronic density, and just the difference between the two shows their precarity.

Energy bands in solids wasted much electronic computation during decades. Without any useful result, the relevant numbers having been computed by hand by Bethe since 1930. Everything we know about solids the energy bands are relevant for has also been thoroughly electronically computed, without any new result, except for the computation errors. There is an enormous number of so-called procedures for computing energy bands in solids, with an impressively large number of acronyms, or just arbitrary letter notations (for instance, the so-called GW technique), which only proves how indefinite this activity is.

Nuclear structure and nuclear reactions have their own enormous share in electronic computations. As for solids, these computations, when correct, proved nothing but the correctness of the quantal mechanics. As if we may ever doubt it! High energy physics and elementary particles exhibit truly an enormous volume of electronic computations, just to justify the grandeur of their large colliding experiments. Scattering cross-sections are known already from theory, or are measured, and all these big computations bring nothing new, except for an enthusiastic excitement.

Beside all these exercises in futility, the big electronic computations have even a worse side. We claim to simulate, or to model by them large ensembles of interacting particles, looking for statistical correlations, inter-dependencies, or whatever, or complex phenomena, like turbulence. We do not know the laws of such processes, yet hope to understand them by such computations. How is it ever possible to understand something, without not knowing it? Non-linear equations are solved plentifully in this respect, without even knowing whether there are solutions in there.

Electronic computers are a very good market this day. Everything bigger, faster, or, in general, exceeding limits attracts much interest. By associating science with computers some hope to attract an interest for science also, or, at least, for the scientific research. Computers' manufacturers are pleased to see their stuff associated with science, and sponsor research gladly. However, science is precisely the opposite, knowing without computing, and accurately designing limits under conditions. Dealing with computers we move pretty away from science.

Let me give an example of the difference between science and computation.

Suppose that we are interested in the motion of a body along an x-axis, say, like in the free fall, for instance. We may imagine the trajectory of the particle as a succession x_n of positions labelled by some integer n, with the initial position x_0 equal to, say, the height h where the body starts to fall freely from. Then, we notice that every position x_{n+1} is the previous one x_n plus something, which can be smaller or greater according to the time τ elapsed between the two. Then, we take a serious step by assuming that if these bits τ of time are small enough then something which adds to positions is $v_n\tau$, where we call v_n velocity, so that we get

$$x_{n+1} = x_n + v_n\tau \ \ . \tag{1}$$

The existence of this velocity is not at all obvious, and it may not exist at all, in fact. The positions do not exist by necessity too, though we see the trajectory and assume they exist. As we see, at least two serious assumptions are made in deriving (1), granted by nothing. In addition, velocity v_n is not known, in the sense that we may, supposedly, measure positions x_n and x_{n+1} and time τ, and get the velocity by subtracting them and divide the result by time, $v_n = (x_{n+1} - x_n)/\tau$, but this would not get us much further. Up to now, we just made two assumptions (at least), for deriving (1), and we may even put numbers in (1) and get numbers, and do computations, and what? What are we more advanced in describing motion by, by doing all this? By nothing, of course. Moreover, we do not even know at this stage what, in fact, we want, what we wish. As a matter of fact, what we really aim at? We do not yet know. We just made some observations and some assumptions about motion, and put them in a little mathematics with a few notations.

Next step is decisive. We notice that if all else remain the same and equal, *i.e.* if nothing special happens to space, time and particle, *i.e.* if space and time are absolute and uniform and the particle is free, then the motion proceeds by equal spaces in equal times, *i.e.* $\Delta x_n = x_{n+1} - x_n$ are the same at every step n. Consequently, a free particle moves along a straight line with a constant velocity. We call this the principle of inertia. We may write it down as $v_{n+1} = v_n = v$. We may write then equation (1) as

$$x_{n+1} = x_n + v\tau = x_{n-1} + 2v\tau = ... = x_0 + (n+1)v\tau \ \ , \tag{2}$$

or, noticing that $(n+1)\tau$ is the time t elapsed from the beginning of the motion, and denoting by x the position at that time,

$$x = x_0 + vt \ \ . \tag{3}$$

We say that we solved the equation of motion (1), in the sense that we know the position x at time t, provided we know the velocity v and the initial position x_0. Thereby we learned what to ask from our description of motion, like being given something, for instance the initial position and velocity, to find out something else, like the position x at any subsequent time t. We can put numbers again in (1) and compute numbers, do all the computations, but it is again useless: we already know by (3) what to ask and how to find it. The principle of inertia is an assumption, but of such a generality that it is truly a principle. It organizes our searches, teaches us what to ask, and gives answers in describing motion. The principle of inertia is both obvious and not obvious. Obviously it holds for such assumptions like free particle, space and time absolute and uniform, and obviously such assumptions are quite natural. Yet, obviously, it is seriously at odds with our daily, practical observations. Physics is so special because it hurts our intuition just from the beginning.

If $v_{n+1} = v_n$ for a free particle, then what if it would not be free, but subject to a force ? Then, of course, v_{n+1} would be equal to the previous v_n plus something, which again can be written as $(f_n/m)\tau$, for small τ, where f_n is the force and m belongs to the particle, and we call it mass. Therefore,

$$v_{n+1} = v_n + (f_n/m)\tau \ . \tag{4}$$

Now, we know what to do. Give forces, compute velocities from (4), and use (1) to compute positions. We notice that we also do need only the initial position and the initial velocity to know definitely everything. We can put numbers, compute, and get numbers. But is already useless to do all these computations. We know everything with respect to the description of motion given above. Particular instances of forces are only exercises. Some are amusing, like Kepler's problem was. Or the free fall of a body, subjected to a uniform force $f_n = mg$, where g is called the gravitational acceleration. Indeed, from (4) we get straightforwardly

$$v_{n+1} = v_n + g\tau = v_{n-1} + 2g\tau = ... = (n+1)g\tau \ , \tag{5}$$

or $v = gt$, the velocity law in the free fall. Similarly, from (1) we get

$$\begin{aligned} x_{n+1} &= x_n + v_n\tau = x_{n-1} + (v_{n-1} + v_n)\tau = ... = h + (v_1 + v_2 + ...v_n)\tau \\ &= h - (1 + 2 + ...n)g\tau^2 = h - \tfrac{1}{2}n(n+1)g\tau^2 \ , \end{aligned} \tag{6}$$

or, in the limit $\tau \rightarrow 0$, the space law in the free fall $x = h - gt^2/2$. We can put numbers in the equations of motion (1) and (4), compute them, do all the computations and get numbers. It is, however, useless. Differential equations

$$dx/dt = v \ , \ \ mdv/dt = f \tag{7}$$

have been invented precisely for getting the result without doing computations, and calculus as well. Of course, we know solutions for a very few particular forces, and we can have results for other forces only by electronic computations. The question is, however, why? Nothing new will be obtained, except trajectories. Do we expect something new? Yes, it may be, and may be welcome, but first we need to know what is it? and only thereafter do the computations. Otherwise, doing computations without knowing what we are computing will never tell what all the numerical results of these computations are about.

The principles of mechanics have been described above, equation (4) is Newton's law, of course. There is much more knowledge in mechanics, beside the principles, like prime integrals, constants of motion, conservation laws, collisions, oscillations, the motion of the rigid body, the principle of least action, the hamiltonian motion, Jacobi integration of motion, etc. None was ever derived from computations, all was derived by descriptions, observations, assumptions like those sketched above. By a similar method has beeen constructed all the physics, the fields, quantal mechanics, statistical phyiscs, etc. Science, as a whole, is assumption (a "hypothesis", as Poincare used to say), an assumption, however, which works, *i.e.* teaches us what to ask, how to find the result (actually it first gets the result, and afterwards tells what to ask). It is not much knowledge in the universal law of attraction that goes like the inverse square of the distance, but there is a wealth of knowledge in the fact that it does indeed exist a force which keeps the planets in motion around the Sun, on elliptical orbites, whose semi-axis cubed goes like the squared period, *i.e.* Kepler's laws of the celestial motion are indeed derived from the same doctrine which describes the fall of a body at the surface of the Earth, and a wealth indeed of knowledge in these laws which tell us where and what can we interfere in the motion to change it according to our needs, desires, caprices, etc. It is the universality of mechanics, and especially of its scientific method, that makes it valuable. There are also many things in mechanics, as well in the whole of the already established body of science that are not yet made explicit, and many expect surprisingly new things therein. Like, for instance in the three-body problem, where instabilities, chaos and particular patterns of motion are suspected. Non-integrability word has been coined for such a situation, which means that we are not able to solve for the motion of N interacting bodies, in the sense that we are not able to write down all the constants of motion, and then, of course, we may resort to electronic computing for getting the trajectories, only that as small errors as ever in the initial conditions may result in indefinitely large trajectories after a sufficiently long time, which means indeed that we are not able to solve for the motion even by computers. Interaction has ever produced troubles, indeed. Surely, one sure way to see all this (if it does exist indeed) is to compute electronically all the possible trajectories, as far as possible, and as exact as possible, and analyze them, and classify, etc, in order to be able to see a new world perhaps by means of the computer. Which becomes thereby another tool of looking at the world, joining the usual, pretty sophisticated tools of the experimental physics. All this is, however, not enough. After doing all the highly complicated and minute computations we may end with an immense pile of numbers, and see nothing therein. Either because there is nothing to see, or because we are not able to see, we do not yet know what to look for. More, even if we have seen something there deeply inside we still have to know what it might ever be, and make assumptions about it that may work. That is, we need science, and should do science in order the electronic computations have any meaning, get any sense, and be of any use ever. This is the difference between science and computations.

In order computations have ever any meaning we need to have a definite problem: either an exercise, or an application, or an "idea" to hunt it for by computers. Definite means accurate, consistent, *i.e* scientific. Otherwise, we have only an exact computational non-science.

There are a few "hot" subjects this day in scientific research, of which I give here some examples. One is nanostructures, another is spintronics, other is organic electronics, and a fourth one is ferroelectricity. They are widely debated everywhere. These subjects are "hot", *i.e.* there is a great deal of interest in them, because we hope to make a greatly profitable use of advancing the knowledge in these directions. It is not very clear, however, in what sense specifically we will be able to use such a scientific advance, and not what sort of advance is expected. The prevalent opinion is however that *ab-intio* computations in these areas will make real breakthroughs in bringing science to society, if not society to science. Yet, all such endeavours, briefly described below, are ultimately both non-scientific and non-societal. They fail to achieve what they claim.

One of the hottest topic in nanostructures is to compute their excited states (especially in nanotubes, nanowires and molecular structures), in order to obtain information about their transport and spectroscopical properties. The transport in nanostructures (*i.e.* the motion of heat, electric charge, mass, energy, spin, etc in atomic aggregates smaller than 10^3Å in linear size) may range from quantal, both coherent and incoherent, to diffusive. According to the present knowledge, the main characteristics of such types of transport are known, and they do not depend critically on the particulars of the excited states, at least as far as the nature of these excited states is so as this transport assumes it to be. It is true that there exist, occasionally, conflicting interpretations of experimental data in so-called non-equilibrium transport in such nano-aggregates, but it is not obvious that the resolution may reside in knowing exactly the excited states. The usual spectroscopies on nanostructures are Raman scattering, infrared scattering, electron scattering or nuclear magnetic resonance. All are affected by the electron-atoms excited states, specifically by the density of states. Beside the resonance, these spectroscopies produce spectral intensities, and getting these intensities requires the knowledge of as many excited states as possible. As long as we are interested in many excited states, a serious problem appears, according to the actual wisdom, because their interaction is no more ineffective; so, we have to resort to solving the Bethe-Salpeter equation (for electron-hole interaction, for instance), which is the usual standard approach. However, we should notice that with many excitations we have another many-particle interacting ensemble besides the original one, which takes the problem no further but to itself, only more complicated this time. Obviously, this cannot be the way to the problem. Similar questions may be raised for the time-dependent density functional theory currently employed for excited states. In addition, apart from being a difficult computational problem, there is no further point in getting these intensities. There is, however, a special, very interesting question regarding the excited states of the nanostructures, which is usually overlooked. Indeed, it is well-known that the nanostructures have many isomeric, dense states, *i.e.* atomic structural states whose energy are slightly above the energy of the ground state, and which differ by slight differences in the atomic arrangement. The difference in energy between such isomeric states is small, so they can easily be strongly coupled to the electronic excitations of the nanostructures. This coupling may result in qualitative distinct behaviour of the electrons in nanostructures, and a qualitatively different response to external probes. The statistical ensemble of the isomeric states may be of such a nature as to give rise to localization of the charge carriers, for instance, with obvious implications on transport as well, though such differences may weaken for open nanostructures. This may be a particularity of the nanostructures, qualitatively distinct from bulk behaviour, or from molecular structures, that might be worth looking at. So, the question is why to compute the excited states of the nanostructures, and what sort of new information is expected thereby in transport and spectroscopical properties? Would it be there a new type of transport, a new type of response, do we have any inkling about something new, peculiar in there?

Instead of answering such questions we prefer to assemble enormous computing codes in order to do all these computations, which, it is claimed, would be going to be used by non-experts for getting results about transport and spectroscopical response in nanostructures. But we are not sure whether there would be any non-expert interested in using such a computing code, so it is not obvious what the societal needs are in this respect.

Another point is to address the question of computing *ab-initio* the electronic structure of nano-electronics, spintronics and magnetoelectronics devices materials, in order to provide data for the search of optimized materials, processes and devices in this area. In nano-electronics the transport pertains to the electronic charge. In spintronics, spin-polarized currents may hopefully control the electric conductivity or the magnetization state of the nanostructures. The magnetronics hopes to control the electric conductivity or the magnetization through a magnetic field. The discovery of the giant magneto-resistance in 1988 in metallic ferromagnets, *i.e.* the drastic drop in electrical resistivity in the presence of the magnetic field, is widely used in hard disc memories, and it brought hopes for magnetic random access memories in computers, especially through the magnetic tunneling. They consist basically of a magnetic tunnel junction, but, unfortunately, the magnetic field required to operate them, or the electric current are too high. It is hoped to get diminished for dilute magnetic semiconductors, where the magnetization might be conveniently controlled by low spin-polarized currents. Such proofs have been actually already produced, but another difficulty arised: the operating time turned out to be very long, so it precludes an efficient use (Nature **427** 821 (2004); **428** 539 (2004)). Magnetic semiconductors have to operate at room temperature, and in magnetic junctions of utmost importance is the quality of the magnetic/non-magnetic interface. It is hoped that electronic-structure computations may guide efforts in finding out those semiconductors with a high ferromagnetic transition temperature, and those binary combinations of materials that may ensure a high-quality magnetic/non-magnetic interface. However, there is no indication as to why such hopes are to be entertained.

On the other hand, basic questions arise in the field of spintronics and magnetoelectronics, especially in nanostructures or dilute magnetic semiconductors, which usually are overlooked. For instance, one of the main questions in this respect is the basic interaction, and its effects, between an electric current, polarized or not, and the magnetization. Such a curent plays the role of a control parameter for magnetization, and the dynamics of the latter could be extremely rich, from spin waves to spin-density waves to soliton domains, with their own dynamics, etc (Phys. Rev. Lett **92** 086601-1 (2004); arXiv:cond-mat/0407116 v1, July (2004)). Non-linear equations govern such a dynamics, which is still poorly understood.

An important issue is that of organic polymers, which are highly active electro-optical materials, with a high versatility and a low cost. The main problem with such materials is their reliability and lifetime, so that, their efficient use, from the molecular transistor, to functional self-assembled and supra-molecular stacks (like liquid crystals, for instance) to charge and energy transport in disordered mesoscopic units (like light-harvesting chromophores in proteins) to large-area optical displays, is probably limited to a niche market. Usually, we focus on modelling and simulating the function of such materials, processes and devices. The most common process in such π-electron conjugated materials is the electroluminiscence, derived from the exciton des-excitation, such excitons being created by injection of electrons and donors (as in light-emitting diodes). The reverse phenomenon of photoelectricity (photovoltaics) is obtained by creating electric charges under the action of the light, as in photocells. Similar processes are present in the field-effect transistor. It is hoped that atomic-like structural parameters which govern the chemical bonding are relevant for the electro-optical functionalities of such materials, processes and devices, to such a degree that the latter depend critically on the former. However, such an extreme position is not obviously justified. In fact, one of the basic issues in this area is the apparently erratic changes in working parameters in time, which leads to degradation. There is no obvious indication that we would ever get aware of the cause and origins of such phenomena by electronic computations.

Many think that it is desirable to integrating the knowledge from the atomic and molecular level, to intermediate scale length up to the macroscopic level for piezoelectric and ferroelectric ceramic materials (like PZT, lead-zirconate-titanate). These materials are of wide use as sensors, actuators, noise-adaptors, etc. Their main drawback is the fiability, reliability, lifetime, which are presumtively assigned to grain boundaries, vacancies, cracks, etc. It is often undertaken to compute such issues, though the knowledge gained is of rather incremental nature, and it is not obvious if not such computations will just confirm what we already know from practice. Probabilistic studies of material failure are also, wisely, envisaged sometimes in this respect. One of the basic problem in these materials and processes is the long range of the Coulomb interaction, of which we ought to have an understanding first, and then compute its possible effects. Such a point is currently overlooked.

All such examples share a fundamental philosophy, that of computing everything from "first principles" (*ab-initio*) with the hope of advancing thereby the knowledge, and, with it, the technology of materials, processes and devices from the nanoscale to the macroscopic scale. Such a philosophy is inconsistent, *i.e.* non-scientific (and even anti-scientific). Because we can only compute what we know already, in order to be exact. Computing does not advance knowledge, just made its results more exact. Suppose that we measure positions x_n in the example given above about the free fall of a body, or give them some way, or hypothesize their existence, then we can compute their differences $\Delta x_n = x_{n+1} - x_n$, even the velocities $v_n = \Delta x_n/\tau$, or whatever else. We never would get this way the principle of inertia, or Newton's law. We never have any science by computing, because science is hypothesis, and only with accurate, consistent hypotheses we may go into the unknown, and gain new knowledge, while computation is only exactness about knowledge. "First principles" and *ab-initio* in the examples described above mean atomic structure, which we yet know pretty qualitatively, so from the beginning our computations are plagued with uncertainties. Thereafter, by doing such computations we would get a wealth of numbers regarding all the known properties of those materials, which we already know qualitatively. Knowing them more and more exact will never get us into a qualitatively new knowledge. Designing materials, processes and devices by employing and manipulating quickly such a large number of "exact" constitutive parameters will certainly help. But this is only an incremental advance, we should know in advance that design, which we are going only to make it more exact by such large computational codes, but never new, or different. Technology will make a profitable use of such "deliverables", but they won't make a breakthrough, nor even a scientific advance. With such projects our society will never be more "knowledge-based", on the contrary, promoting such enterprises we may induce the impression this is science, which is not, it is precisely the contrary of science, it is non-, anti- and pseudo-science. Because it computes exactly what we already known, and don't take us any further into the unknown.

How science may help industry, economy, technology, etc, is of course a basic question. Because we know that science is at the origin of the wide use of constructions, themal machines, electricity, materials, transportation, communications, etc, so we would like to know how this process might be controlled, harnessed, accelerated, developed on a larger scale, put at work for the societal benefit. This is a legitimate question, indeed. The answer is actually simple, and it is furnished precisely by the history of science and technology. Technological matters are applications of science, and they were brought to the use of the society by the enterpreneurial spirit. It is the latter which must be emphasized and improved, in its relationship with science. Of utmost importance, indeed, is this relationship, which, this day, is weakening considerably, and this is, in fact, the ultimate cause that produces all this stir, commotion, about the necessity of a deeper involvement of the science in society and technology, economy, industry, etc. Strenghtening of this relationship should be our main concern in this respect, truthfully. How should we do that? In my opinion by meetings, close relationships, betwen scientists and "applicationists", high-tech enterpreneurs, whereby the scientific culture is transferred to the latter, and the applied science to the former. There would be a great benefit for each side, making the effort of trying to familiarize an "applicationist" with the basics of the physical phenomena, as difficult as it may be it is very rewarding, as well as the opposite, trying, as a "theorist" to get familiar with technogical problems is really fascinating. The applied science is a special world, with its own rules, questions, guide marks, and it is completely surprising to discover that indeed all these particulars have in fact a serious connection to the basic physical phenomena and nature laws. Actually, the greatest challenge for a "theorist" is to decipher at least once in life a technological problem. The main problems in nanostructures transport, nanoelectronics, spintronics, molecular electronics or ferroelectrics are not what the scientists know to do, but they are precisely those raised by "aplicationists". Whom we ought to listen to, and try to understand, and to differentiate what is scientific from what is not. This way, "theorists" must invade the realm of technology, applied science, experimental science, and remove thereby, eliminate, send them into non-existence, and replace their scope with us and our science.
