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On the Nature of Theoretical Research*

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The relationship between theoretical and experimental research is discussed. Theoretical research is presented as a process consisting of several stages. The hierarchy of these stages is given and each stage is briefly outlined.

»Nothing is more practical than theory.«

Ludwig Boltzmann

»One good example is worth a ton of theoretical arguments.«

Sir Francis Crick

In this essay we present some ideas about the nature and methodology of theoretical research. But, before we proceed too far, we will first briefly mention the relationship between theoretical and experimental research.

Experimental and theoretical research are equally important parts of pure research. This division is a merely division of labor and personal preferences of researchers. In experimental research the main goal is to measure various natural phenomena (or simulated phenomena), whilst in theoretical research one attempts to capture the processes of Nature and relationships between phenomena in formal mathematical statements.[1]

* This essay is dedicated to the memory of Dr Zvonimir Pučar (1922–1989), the Head of the Physical Chemistry Department at the Rugjer Bošković Institute when I joined the Department and one of the leading experimental physical chemists in Croatia in 60' and 70's who nevertheless supported theoretical chemistry research in his department.

Quantitative measurements are the essence of the experimental research.[2] The most important characteristic of the experimental research is reproducibility. Reproducibility implies that experiments can be repeated by any investigator. Mathematics is essential tool of the theoretical research, because it is much more precise and economical than language. One of the most important characteristics of the theoretical research is predictability. Predictability implies that the theoretical research can lead to a design of new experiments and prediction of the outcome of these experiments. It is important to point out that the experimental research and theoretical research do not compete; they rather cross-fertilize each other and the progress of pure research is related to progress in both fields.[3–5] One should note that theory without experiment is fiction and experiment without theory is merely routine. However, it appears that this is not the generally adopted view. Often amongst the experimental scientists, especially in biology, it is found somebody who ocassionally negates the usefulness of theory in research, *e.g.*[3,6]

Pure research is research for its own sake[7] and is motivated by human curiosity about just everything.[8] To understand the structure of the Universe or the structure of the human mind are equally challenging puzzles that we would like to solve.[9,10] Thus, the aim of pure research is to obtain knowledge which should enable us to understand the Universe and our role in it. There are a number of interesting questions related to that above. Let us mention one of them that we find particularly intriguing. This is what is the limit of knowledge? One way to deal with this question is by means of the second uncertainty principle[11] which may be stated as: *A single human cannot attain absolute knowledge*. Or in other words, one can possess a deep knowledge about a given topic or a smattering knowledge over a wide range of topics.

Pure research is the basis of science. Science is human activity and a scientist is a person who does documented research. Science is one of those elusive concepts that are difficult to define precisely.[12] The characteristic mark of our civilization is the practice of science.[13] History has invariably shown that practically every major scientific advancement had an effect on the development of our civilization.[14] Since there are more scientists now than in the entire history of humankind, it is, therefore, of natural interest of scientists and philosophers of science to venture to define science. Different authors give different definitions of science.[7,15–32] This fact alone suggests that there is no universally accepted view of science. One of the definitions of science offered in the literature that we like is by Dyson:[20] *Science is organized unpredictability.* It is simply a statement that encapsulates that fact that every important discovery in science was unpredicted. The purpose of science is, therefore, to create opportunities for unpredictable things to happen.

Our undestanding of science may be formulated as follows:[32] *Science is an ever-increasing body of accumulated and systematized knowledge and is also an activity by which knowledge is generated.* This is a working definition in which we stressed the generation, accumulation and systematization of knowledge, because it may appear that the knowledge is the only means of human survival in the Universe.[33] We should also mention that science is not the only way to knowledge. For example, art is an equally valid road to knowledge.[19,22,25,34–37] Nevertheless the art and science are very distinct avenues to knowledge which differ in their techniques and methods of attaining knowledge.[38–41] They also differ considerably in presenting knowledge, though both scientists and artists use abstract and complex communication systems.[37,38,42–54] It should be emphasized that the scientific creation is restricted, unlike the artistic achievement, by the necessity of verification.[2,55]

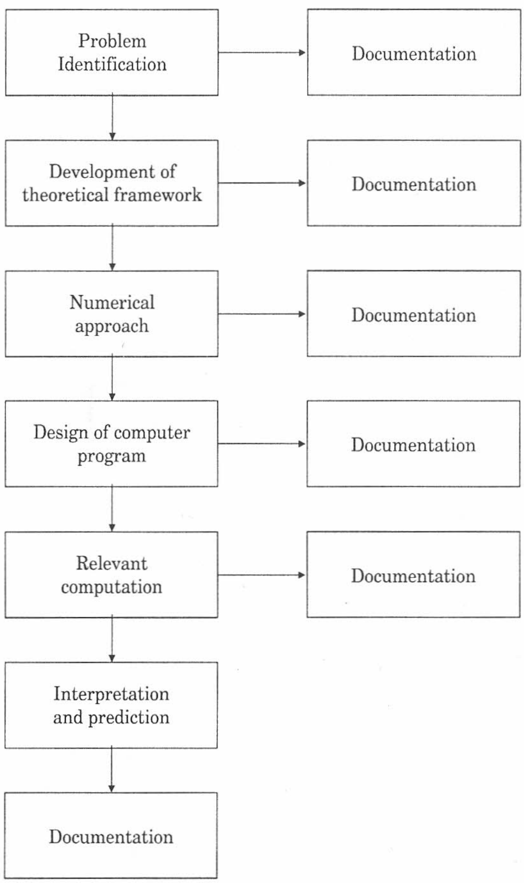

Figure 1. The structure of theoretical research.

The development of science strongly depends on the educational system of a country. Education has a unique place in culture.[36] It provides links with the past, enables us to understand the present and to face the future and to participate in its creation. A good educational system is one which is based on liberal teaching, that is, teaching without indoctrinating and/or manipulating students. A better educational system produces better scientists and they in turn create science of higher level. Therefore, the investment in the educational system is always profitable.[56]

Let us now turn to the nature and methodology of theoretical research. Theoretical research may be partitioned into several stages (see Figure 1) that may be characterized as follows:[57] (1) Problem identification; (2) Development of the theoretical framework; (3) Numerical approach; (4) Design of computer program; (5) Relevant computations, (6) Interpretation and prediction; and (7) Documentation.

There are no strict boundaries between these stages; they merge naturally one into other. However, many results obtained at a certain stage may be documented separately.

Problem identification

The problem identification is a starting point of any research. There may be many ways from which the problem can originate. The problems may be less or more challenging. The challenging problems may be classified as difficult, very difficult, deep or grand, but well-understood and well-defined problem will make a search for the solution a lot easier and will minimize unproductive straying. One should work on a range of problems because the cross-fertilization between different problems is often of value. Credit should be given to those rare individuals with a gift to state a problem in a clear and simple way. It should be emphasized here that it is often more difficult to state the problem unambiguously than to find its solution. It may be even appropriate for a problem to be published as it is often done in the mathematical literature.

Development of the theoretical framework

This stage consists of looking for the fitting theoretical framework for a given problem. In order to do that satisfactorily, knowledge, erudition and experience is required. However, there may not be any usable theory available. In such a case one has to develop, if she or he can, a new theoretical framework. This often occurs in connection with deep problems. To reach a novel or new theoretical approach usually a creative leap over the boundaries of the known is required. The scientific discoveries are not always a result of a sequence of logical steps, but are often achieved in a random way.

The same may be said for theoretical work. The discovery of a new theory is often a result of an accidental stumbling upon the sought-after result.

Since there cannot be progress of science without the conflict of ideas, one has to select among several offered theoretical frameworks. If there are several possibilities, the simplest of competing theoretical frameworks should be selected, because more complex theories may not necessary bring new (or novel) insights into the treatment of a problem. Actually we consider the search for the truly simple solution of the problem as a major intellectual challenge in theoretical research. However, the selection, shall we say, of the simplest theory can be helped by the Ockham's razor criterion: »*Pluralitatis non est ponenda sine necessitate*«, whose literal translation »*Plurality must not be posited without necessity*« is less usable for the present purpose than the more liberal translation: »*An explanation of the facts should not be more complicated than necessary*«.[58] Ockham's razor is known in philosophy as the principle of parsimony. This principle is attributed to William of Ockham (ca 1285–ca 1349) who was born in the village of Ockham in Surrey near London and was a member of the Franciscan order and philosopher. However, the principle of parsimony, that is popularly called Ockham's razor, is not original of William of Ockham. Versions of this principle are to be found, for example, in Aristotle and were used by many scholastic philosophers.[59] Besides the above formulation is only one of four ways in which Ockham has stated the principle of parsimony in his writings.

The original theory or the original extension of the known theory may always be published. However, we should remember that there are several requirements for the theory to be applicable; the most important being a good agreement between the theory and experiment (this is a necessary but not sufficient condition for the validity of the theory), elegance and beauty, internal consistency, evidence of the adjustable parameters and a high level of predictivity is also relevant. The main purpose of any theoretical framework is to explain and to systematize the experimental observations by a few unifying concepts. It is also important to stress the role of mathematics in formalizing the theoretical framework,[60] since the most economical language of science is mathematics.

There is a simple rule of thumb to judge the value of a given theoretical framework: *The value of theoretical framework depends on its usefulness*.

Numerical approach

After a theoretical framework is established, numerical work is almost always necessary task. The numerical approach is required to prepare the theory for computations that are relevant for the problem under consideration. And again known numerical approaches are reviewed and if these are not satisfactory, new (or novel) numerical methods and techniques need to be introduced. The theory is then transformed into a numerical algorithm which provides a framework for the computer program design and computation. Original work in this area also warrants publication.

Design of computer program

In this stage the logic and structure of the software is designed.[61–63] The process of designing computer algorithms and programs is not simple by any means and it requires much work and creative leaps before it is successfully accomplished. It is a notable achievement to truly master the art of computer program design. Creative work in this area is being published in many journals which report the achievements and advances in the field of computer science. In addition, the introduction of supercomputers to science placed a heavy task on computer scientists to design a special and efficient software for often lengthy and time-consuming theoretical computations. This stage in theoretical research may also be expensive, especially if outside help is required. One of the masters in software design Dijkstra[64] tried to explain in an interesting essay why software is sometimes very expensive. It is as simple as that: *There is a great lack of creative computer program designers*. Or in other words, the incompetent programming increases the cost of computer program design.

The additional important point to mention is that reliable computer programs are characterized by simplicity and clarity. Complicated programs are usually overly complex and, consequently, almost always full of bugs and patches.

Relevant computation

Computations are nowadays exclusively carried out by means of electronic computers which are readily available in the range from personal computers to supercomputers. The use of supercomputers entirely altered the strategy of doing computations.[65–68]

Today computations are ordinarily based on the computer algorithms which represent translations from numerical algorithms. The computer programs based on these algorithms are often developed in codes which depend on the problem and hardware at hand.

The role of computation is to quantify theoretical research and offer a possibility for experimental testing of computed quantities. The great value of theoretical research is that through the computation one can make predictions that can be used by experimentalists to facilitate their research. For example, it is advisable to run a computation on a novel molecular system before it is made in order to obtain computed characteristics of it such as geometry, stability, spectra of various kinds, ionization potentials, heats of atomization, reactivity predictions, *etc*. The experimental chemists supplied with all these data about the prospective molecule may now devise a better strategy for its preparation than otherwise. This approach, that is, the computationally-guided experimental work, is a rational way which can make the preparation of a certain molecule or elucidation of a certain reaction mechanism a lot easier. In this respect we may consider the computation as a powerful experimental tool too.

Interpretation and prediction

Because the language of theory and computation is symbolic and very different than the one used by experimentalists, the interpretation is a stage which serves as translator between the theoretical level and the level of experiment. In other words, this stage in the methodology of theoretical research is assigned to making physical, chemical or biological interpretation of the theoretical framework. It may also serve for the derivation of general principles from the theoretical and computational work. An important aspect of this stage is also the prediction of the outcome of the not yet performed experiments as well as the design of new experiments.

Documentation

Since there cannot be science without communication, results of the research must be written up, preferably in a clear well-motivated manner and offered to scientific community at large in the form of some open document.[69] The type of documents we have in mind are research papers, reports, reviews, tables, monographs, handbooks, computer files, *etc*. We do not believe in knowledge floating around without being recorded, because people are very unreliable knowledge-deposits. People generate knowledge, use knowledge, but easily lose knowledge. Or as the Croatian poet Dobriša Cesarić said in his poem »The Return«:[70] *Fragile is knowledge*!

In conclusion, many aspects or stages of theoretical research can be seen all of which are important. But throughout all of these stages a most crucial underlying feature is the creative intelligent thought. The driving force behind theoretical research is the urge of a theoretician to produce theories that rationalize experimental facts in a simple unambiguous way and suggest new experiments to the experimentalist.

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SAŽETAK

O naravi teorijskog istraživanja

Nenad Trinajstić

Razmotren je odnos između teorijskoga i eksperimentalnoga istraživanja. Teorijsko je istraživanje prikazano kao proces koji se sastoji od nekoliko etapa. Dana je hijerarhija tih etapa, a svaka je etapa ukratko opisana.