The Computation of Nature, Or: Does the Computer Drive Science and Technology?

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It has often been claimed that the computer has not only revolutionized everyday life but has also affected the sciences in a fundamental manner. Even in national systems of innovation which had initially reacted with a fair amount of reserve to the computer as a new scientific instrument (such as Germany and France; cf., e.g., [33,18]), it is today a commonplace to speak about the "computer revolution" in the sciences [27]. In his path breaking book *Revolution in Science*, Cohen diagnoses that a general revolutionary change in the sciences had followed from the invention of the computer. While he asserts that the scientific revolution in astronomy in the 17th century was not based on the newly invented telescope but on the intellect of Galileo Galilei, he maintains in contrast that the "case is different for the computer, which [...] has affected the thinking of scientists and the formulation of theories in a fundamental way, as in the case of the new computer models for world meteorology" [10, pp. 9-10 & 20-22].

The modern electronic digital computer had originally been invented as an extremely fast and programmable calculator to solve mathematical problems in the sciences and in technology in the 1940s. Although the use of the computer as a new form of a scientific instrument became more and more widespread in the sciences from the 1960s onwards, historians of science and technology did not pay much attention to this important development. Although history of computing has been established as a sub-discipline of the history of technology during the last decades and contributed to a better understanding of the development of hardware and software as well as of the advent of the information age,[1] there are still large gaps in our knowledge on the history of "scientific computing". There are only a few studies that have contributed to our understanding of the use of computers in the many fields of science and/or research institutions. Research to date has largely focused on the development of supercomputing at the large national research laboratories in the United States [30,38], the use of the computer in high-energy physics [39] and in Roentgen crystallography [12], as well as to the efforts to computerize bio-medical research in the 1950s and 1960s [34].

A second related problem is that we know only a little about the different new computer based methods which became established in the various national innovation systems in the second half of the 20th century. The, admittedly, very

[1] For an overview on the history of computing, cf. [8,9,17].

P. Bonizzoni, V. Brattka, and B. Löwe (Eds.): CiE 2013, LNCS 7921, pp. 263–270, 2013.

small number of historians and philosophers researching on these subjects have for the most part concentrated on just one phenomenon: computer simulation (cf., e.g., [37,24]). Computer simulation, such is the basic assumption, has opened a third way of doing science besides experiment and theory. And this is said to have caused the revolutionary change by computers (cf., e.g., [21,28,44]) There are a number of issues in this field on which a detailed historical analysis would be useful, and it is doubtful whether "simulation" was really invented with the digital computer—instead it should be accepted that there are several classes of "simulations" with different epistemological qualities.

In general, the question of whether the computer changed scientific practice and the setting of the agenda in various scientific disciplines has not found much attention in the history of science. In his pioneering study on *John von Neumann and the Origins of Modern Computing*, William Aspray has shown how a noted mathematician "invented" the computer as a mathematical machine and how the computer decisively transformed numerical mathematics as a field of study [3,2]. Secondly, the introduction of numerical methods to weather forecasting and the change of meteorological practice by using computers has been analyzed in a few studies on the development of "scientific computing" in meteorology (cf., e.g., [11,29,16]). Finally, the British historian of computing, Jon Agar, has made an attempt to analyze the changes in various disciplines triggered by the advent of the computer. According to Agar, "computerization" of a discipline in the 1950s only occurred if "material practices of computation" had already existed beforehand [1]. In support of this assessment, historical studies show that (social) networks between the objects of research (or artifacts), the computing machines, the computer-staff, and the scientists and engineers, as well as the formation of formalized working structures and working routines, did have great importance for the "computerization" of a field or discipline.

In view of contemporary science journals and books, it becomes clear that the "picture" of a uniform, omnipotent and omnipresent computer revolution in all disciplines and in every nation does not correspond to the facts. There was rather a plurality of processes of computerization with different repercussions on the different disciplines. Examples are: Firstly, it is quite clear that the development of high-performance computation was of enormous importance in many fields of science and technology. This holds for all fields in which ordinary and/or partial differential equations and integral equations are used in mathematical modeling of natural phenomena, as for instance in fluid dynamics, reactor design, chemical reactions, astrophysics, crystallography, DNA-sequencing, and geophysics (cf., e.g., [13,36]). These fields are, secondly, closely connected to the phenomenon of computer simulation being used for pure research in the sciences as well as for the design of technical artifacts. Thirdly, the practice of computer based instrumentation and computer based experiments became all-important in many fields of the sciences and medicine, as the computer was more and more needed to control the ever more complicated experiments. Fourthly, in some fields methods of information retrieval were of utmost significance (cf., e.g., [6]). The upshot of all this is that in almost all cases it was one thing that was fundamentally changed by the computer: the time-economy of science. (Today, scientists and engineers take it for granted that the electronic computer and appropriate software systems that deliver rapid and reliable data for most of their scientific problems, but this has been only the case since the late 20th century. The case of the British *Nautical Almanac and Astronomical Ephemeris*—an annual publication describing the positions of the moon and other celestial bodies for the purpose navigation at sea which has been published by *HM Nautical Almanac Office* since 1767—serves to illustrate how time-consuming, laborious and tedious the work of the human computers for rather easy scientific problems has been until the first half of the 20th century [43].

The above-cited metaphor of the computer as a revolutionary artifact implies—as the recently deceased American historian of science Michael S. Mahoney aptly remarked some years ago—the image of a revolutionary technology changing all parts overnight and splitting all societal groups in two separate parties: either one jumps on the continuously accelerating bandwagon or one comes to a standstill as a "dinosaur" at the platform [32]. It seems quite easy to identify candidates for the "jumping-on-the-bandwagon". Dorothy Crowfoot Hodgkin's discovery of the structure of the vitamin B_{12}, for which she was awarded the Nobel Prize, was essentially based on the use of one of the first available electronic computers in Britain [1]. Or: the design of the hydrogen bomb was essentially based on the use of novel mathematical models and methods computed with the then new electronic computers [14]. Or, to put it another way, one could examine an important question of the history of technology in an new way: Does technology drive science? (Cf. [40].)

At the same time the computer-based "knowledge-revolution" in the sciences seems strongly connected with a "qualitative decline" in the falsification of scientific theories or models. It would appear, therefore, that a digital "Pandora's Box" had been opened and that the scientists are no longer masters of the situation, since the verification or validation of computer-based models does not seem to be justified from a philosophical point of view. Naomi Oreskes, in her article about Verification, Validation, and Confirmation of Numerical Models in the Earth Sciences (published together with philosopher Kristin Shrader-Frechette and geologist Kenneth Belitz) in *Science*, raised fundamental doubts about the common practice of numerical modeling in the sciences. The authors stated that "verification and validation of numerical models of natural systems is impossible", since "natural systems are never closed and because model results are always non-unique". They eventually came to the conclusion that the "primary value of models is heuristic" [2].

To better understand the development that led to this situation, as described in [35], we shall briefly analyze the development of computational fluid dynamics as it was one of the most important origins for the development of computational

[2] Cf. [35]. This article met with very positive responses in the sciences as well as in the history of science and in science studies. It became the starting point for a series of articles on the use of computer simulations in geoscience and in climate science. Cf., e.g., [20].

physics in general. Today, this field is "by far the largest user of high performance computing in engineering" [7] and at the same time is of enormous significance in pure research in physics (cf., e.g., [5]).

In the 17th century, scientist had begun to describe natural phenomena in the exact sciences (astronomy, physics, ...) by physical models which in turn were described in mathematical structures. As a result—to portray it in simplified terms—the "Galilei Principle" (physical phenomena can be described by mathematical models) and the "Newton Principle" (physical phenomena can be described mathematically by differential equations) became crucial for the further development of the exact sciences. This made the theoretical physicist and Nobel laureate, Eugene Wigner, wonder about the miracle of the *Unreasonable Effectiveness of Mathematics in the Natural Sciences* [42]. Since the existence and uniqueness of a solution of an ordinary differential equation (initial value problem) can be proven under certain (quite general) conditions, the Newton principle served as a basis for a deterministic conception of the world of the exact sciences until the end of the 19th century. On the other hand it became apparent to scientists during the 19th century that it was by no means possible to predict and/or to compute all physical phenomena. The history of the three-body problem in celestial mechanics is the most striking example yet of a quite simple physical problem which proved to be extremely difficult to handle. After more than two hundred years of research by outstanding mathematicians and astronomers concentrating all energies on finding an analytical solution of the nonlinear differential equation problem in the 18th and 19th century, it was proven that the three-body problem has no analytical solution in terms of algebraic integrals (cf., e.g., [4]). Even if it is known since the early 20th century that the three-body problem could be solved in quite general cases through a convergent power series which unfortunately converges extremely slowly and is therefore futile for all practical purposes. As the solution of the three body problem was not only of theoretical interest but had also important applications in practical astronomy such as navigation, since the 18th century astronomers "simulated" the solution of the three body problem by developing complicated numerical approximation methods and by using teams of human computers for the tedious work of calculation (cf., e.g., [19]).

Another case of a non-linear problem, Navier-Stokes equations (non-linear partial differential equations) in hydrodynamics, became the starting point of modern computer-based methods of "scientific computing" and sounded the bell for a new round in the relation between theory, experiment and computation in the exact sciences. At the outset of this "science as software"[3] were the ideas of the Hungarian mathematician John von Neumann, who was confronted with the problem to solve hydrodynamic problems for the Manhattan Project in the second world war. Von Neumann failed miserably in his attempts to solve non-linear partial differential equations of hydrodynamics with the traditional methods of analysis. This led him to the conclusion that these difficult problems could only

[3] Cf. [31]. My argumentation in this paragraph partly follows the same line as in Mahoney's article.

be addressed if one would divorce the close marriage of physics and the classical methods of analysis: "Our present analytical methods seem unsuitable for the solution of the important problems arising in connection with non-linear partial differential equations and, in fact, with virtually all types of non-linear problems in pure mathematics [15]". Since, in the case of the non-linear partial differential equations of hydrodynamics, the strategy of using teams of human computers for the tedious work of calculation was also a hopeless undertaking, von Neumann in 1946 suggested to use numerical methods and new nonexistent "Large Scale Computing Machines" instead. From there, von Neumann ultimately arrived at a fundamentally new philosophical position on the relationship between natural phenomena, physical models, and mathematical models; and he proposed to discard the "Galilei Principle". Instead of describing natural phenomena in the exact sciences by physical models which in turn were described in mathematical structures, von Neumann suggested to describe natural phenomena only with a mathematical model, which was characterized by him as a "mathematical construct which, with the addition of certain verbal interpretations, describes observed phenomena [41]".

This method had instantaneous consequences for the scientific understanding of physical processes, as the solution was no longer a scientific theory "explaining" nature, but only a numerical result. Numerical solutions did obviously not provide for similar insights into physical processes as analytical solutions had done. Moreover, it became much more difficult to "explain" the discrepancies ("errors") between the numerical solutions and the results of experiments. Also, from a philosophical point of view, it became difficult to compare *Theory-1* with *Theory-2* with regard to experimental results when the model of constructive falsifiability (Lakatos) was applied [25]. This, of course, leads to the logical conclusion that the door was opened to a variety of potential new mistakes, ignorance and contingency. Furthermore, it became soon apparent that the "generation" of numerical solutions in computational fluid dynamics led mathematicians, physicists, and engineers to fundamentally new mathematical problems. Apart from the general problem of rounding errors in the field of numerical mathematics being newly defined by digital computers, it turned out that the numerical solution of partial differential equations was a tricky mathematical problem, since the vividness (Anschaulichkeit) of mathematical approaches to numerical solutions could easily result in false mathematical models. Moreover, over the last few decades the rise of computational science and the widespread use of large software tools in various fields of science and engineering has made the reproducibility of results principally more and more uncertain, if the source code of the used software is inaccessible [22].

The development set in motion by von Neumann had far-reaching consequences for the evolution of science and technology in the late 20th century. On the one hand the new field of computational fluid dynamics developed into a design tool for engineers, and on the other hand computational fluid dynamics made novel "mathematical experiments" in hydrodynamics possible. This, in turn, made it something like the model for the development of the methods of computational science in other fields [26]. At the end of the 20th century, computational fluid dynamics seems to have developed into what Terry Shinn has called research technology being characterized by its “pragmatic universality” and by its “robustness” in dealing with mistakes, ignorance, contingency and errors [23]. This process can be further analyzed by asking: How did physicists and engineers succeed in handling problems of errors, ignorance and contingency in computational fluid dynamics despite the fundamental philosophical problems of computer-based models in the sciences and in engineering? In the end a careful historical analysis of this questions will hopefully help historians of science and technology as well as scientists and engineers in their understanding of Cohen’s assertion: By what means and to what extent does the computer change science and technology?

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