From Science to Computational Sciences

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From Science to Computational Sciences

Studies in the History of Computing and
its Influence on Today's Sciences

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Foreword

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The volume emphasizes the history of computing as well as its influence on today's science and society, focusing on the humanities' and philosophy's point of view of computing. Therefore two additional papers were included: Thomas Langes' historical research on "Computer Simulation in the V2 Rocket Development" and a reprint of Peter Galison's seminal paper "Computer Simulations and the Trading Zone".

Gabriele Gramelsberger, Berlin 2011

I. Introduction

Gabriele Gramelsberger

A Brief Introduction to the Volume

1 The Culture of Computation

In September 2007, the Blankensee-Colloquium invited researchers from science and the humanities to discuss the scientific and societal influence of computing, in particular that of the field of computer-based simulation.[1] Seventy years after the first automatic computing machines were built, these devices have changed science and society to a tremendous extent. While in the 1930s the final decision between analogue and digital computers had yet to be taken, the preference for digital computing based on electronic circuits seems to be facing new challenges today. Because circuits have become too fast, they are beginning to reach their physical limits. The imminent approach of this boundary is stimulating debates about massive parallel computing, new kinds of computers like quantum computers, and even about computing itself. The challenging question (besides faster or new forms of computers) is: Do we face the end of number-based computing as it was originally developed several thousand years ago?[2]

The Colloquium did not enter much into these debates of new computers and computing itself, but tried instead to understand the consequences of the current situation in which science and society are inevitably depending on numerical computation—more than ever before in their history. Assuming that computers still can reach slightly higher speeds, this dependency was best articulated when Henry Markram, participant of the Colloquium and Director of the Center for Neuroscience and Technology at Lausanne University (the Blue Brain project), called out after his talk to Alan Gara, also a participant and Chief Developer of IBMs BlueGene/L Supercomputer: "If you do not build this new chip, we can't go on with our research!" This statement is striking because it shows that progress in some fields of science depends entirely on numerical computation and that some areas have been completely transformed into computational sciences. Hence it is no surprise that Thomas Lippert, another participant of the Colloquium and Director of the Institute of Applied Mathematics at the German Research Center Jülich, was about to establish the world's first Institute of

1. The volume presents a selection of papers from the Colloquium. The Blankensee-Colloquium took place at the Berlin-Brandenburg Academy of Science and Humanities from 20 to 22 September 2007. It was funded by an award from the presidents and chancellors of the Berlin universities and academies (Kooperationsfonds Berlin). The annual award of the Blankensee-Colloquium honours promising research in the fields of social sciences and the humanities and is coordinated by the Wissenschaftskolleg, Institute for Advanced Study Berlin.
2. The development of numbers and counting dates back more than 5,000 years and is documented in Mesopotamian and Egyptian texts. Counting, and the calculations it made possible, are powerful and successful cultural techniques. Cf. Howard Eves: *An Introduction to the History of Mathematics*, (6th ed.) Saunders: Brooks Cole 1990.

Advanced Simulation.[3] Opened in January 2008, this institute supports research whose progress is exclusively based on computing. In his presentation Thomas Lippert asserted that scientific theories and models which are not conceivable as computable from the outset will become decreasingly successful. As the physical limits of computing are reached, massive parallel computing will result on the petabyte scale; accordingly, he concluded, scientific practices are about to change. The practices at present, based on the subsequent creation of computable forms of theories and models by algorithms, interfere with the requirements of parallelized representations of these theories and models. Therefore theories and models have to be conceived from their very inception as computable, like ab-initio methods in material sciences or molecular modelling.

If the transformation from science to computational sciences is taken seriously, the described impact on theorizing and modelling unveils an ongoing revolution in science. The mathematician James Glimm calls it the second half of the scientific revolution, which started back when "John von Neumann foresaw that the equations describing scientific phenomena, once expressed in mathematical terms, could be solved numerically, without recourse to routine or repetitive experiment. This vision is nothing less than the second half of the scientific revolution. Throughout four centuries we have expected that a successful scientific theory would have its major concepts expressed quantitatively as numbers and its major relationships expressed as mathematical equations; the truth of this theory was settled by experimental tests and hand calculations, often in idealized situations. The second half of the scientific revolution is no less sweeping in its goals. The solutions of the equations are also to be obtained on mathematical grounds, by numerical computation, without restriction to idealized cases."[4]

Massive parallelization, petabyte-scale performance, and grid computing as experienced today, intensify the revolutionary changes in science. A new form of theories and models will arise from these changes, but also new insights into nature. These new theories and models will reverse-engineer and resolve natural phenomena to an unknown degree. The Blue Brain project that computes the interaction in and between several neocortical columns, each consisting of about 10,000 highly connected 'in-silico' neurons, is a good example of this new style of science. "The Blue Brain Project is an attempt to reverse engineer the brain, to explore how it functions and to serve as a tool for neuroscientists and medical researchers. It is not an attempt to create a brain. It is not an artificial intelligence project. Although we may one day achieve insights into the basic nature

3. Two days after the Blankensee-Colloquium JUBL, a BlueGene/L IBM computer based on 64,000 CPUs was put into operation at the Institute of Applied Mathematics at the German Research Center Jülich. This supercomputer was expanded to up to 256,000 CPUs and should perform one 10^{15} floating point operations per second (petaFLOP) at the end of 2009—in words: one quadrillion operations per second.

4. James Glimm: "Scientific Computing: Von Neumann's Vision, Today's Realities, and the Promise of the Future," in: James Glimm; J. Impagliazzo; I. Singer (eds.): *The Legacy of John von Neumann*, Proceedings of Symposia in Pure Mathematics 1988, Providence Rhode Island: American Mathematical Society 1990, pp. 185–195, here p. 185.

of intelligence and consciousness using this tool, the Blue Brain itself is simply a representation of a biological system and thus would never be considered conscious itself."[5] In the petabyte-scale period of science, the reverse-engineering of nature seems to become a synonym for modelling and simulation insofar as the computer is used as a tool for equation-based reconstructions of phenomena at a previously unknown degree of resolution. The mathematical reverse-engineering of nature is replacing research on natural phenomena, in particular when empirical experiments are substituted by computer-based ones. A multitude of examples and disciplines using the computer as a reverse-engineering tool can be identified, including climate modelling, cell biology, material sciences, chemistry, particle physics, fluid dynamics, and others.

The computer as a reverse engineering tool extends our insight as the microscope has done for centuries. Corresponding to the scientific revolution in the 17th century, which extended the natural senses of man through instrumental observation and detection, the computer is extending our senses in a new way today. The interesting question from the point of view of philosophy and the humanities is: What kind of insight is created by this new form of 'empirical extension'?[6] This question opens up a plenitude of other questions: What kind of science arises based on this new form of empirical extension? Where do the roots of these developments lie? What are the consequences for science and society? What will happen to science when even parallel computing reaches its limits? Is the dissolving of law-driven processes into numbers the future way of science?[7]

These questions were addressed in the seven panels of the Blankensee-Colloquium which reconstructed the storyline of the increasing computation of science: the rationality of quantification; the infrastructure of a culture of computing; the shaping of reality with algorithms; the artificial nature of a technoscientific world; loops between methods; rational prognosis, the management of uncertainties, and future II; and the societal and cultural influence of calculation.

5. Blue Brain Project: *Project Description*, 2007, cf. http://bluebrain.epfl.ch. Cf. Henry Markram: "The Blue Brain Project," in: *Nature Reviews Neuroscience*, 7, 2006, pp. 153–160.

6. Paul Humphreys calls computer-based simulation "the third type of empirical extension," which is "giving us instrumental access to new forms of mathematics that are beyond the reach of traditional mathematics. Here the question naturally arises: Could instrumentally enhanced mathematics allow an investigation of new areas of mathematics to which our only mode of access is the instrument itself?" Humphreys, Paul: *Extending Ourselves. Computational Sciences, Empiricism, and Scientific Method*, Oxford: Oxford University Press 2004, p. 5.

7. The extensification of numerical computation has also been criticized as "the old vocabulary of sequential equations and numbers." James Bailey: *After Thought. The Computer Challenge to Human Intelligence*, New York: Basic Books 1996, p. 4. James Bailey, a former Senior Manager at Thinking Machines Corporation, criticizes the traditional use of computers solely as number crunchers. He argues that "symbolic numbers, equations, and the formulation of universal laws are what people and thought are good at. Electronic circuits are good at different things [..., e.g.] at letting higher level behavior emerge from the interplay of millions of tiny operations, all interacting with each other in parallel, handing on each its own little bit of understanding. [...] As a result, a whole new set of parallel intermaths is coming to the fore to challenge the sequential maths of the Industrial Age, which had only humans to carry them out." James Bailey: *After Thought*, op. cit., p. 4.

The following introductory paper "From Science to Computational Sciences" outlines this storyline in detail.

2 Studies in the History of Computing and its Influence on Today's Science and Society

The volume presents a selection of papers from the Blankensee-Colloquium and focuses on the humanities' and philosophy's point of view of computing. It emphasises the history of computing as well as its influence on today's science and society. Therefore two additional papers were included: A reprint of Peter Galison's seminal paper "Computer Simulations and the Trading Zone" and Thomas Langes' primary historical research on "Computer Simulation in the V2 Rocket Development".

Origins of Simulation and Rational Prognosis
The chapter "Origins of Simulation and Rational Prognosis" illustrates that computer based simulations are rooted in the operational use of symbols, based in particular on the invention of the calculus in the 17th century. Simulation can be traced back to the 18th century as manually computed integrations of calculus for astronomical purposes, but also to the 19th-century 'mimetic experiments'—precursory simulation techniques for laboratory research on dynamic processes. The semiotic and the experimental uses merged in the 1940s, in the general context of World War II, when the transition from mechanical simulators to electronic analogue-computer-based simulation took place, followed later by electronic digital-computer-based simulation.

The chapter opens with remarks on quantification in early European modernity by Sybille Krämer. Her paper "Roots and Media of Computational Power" argues that quantification is unavoidably based on an operational use of symbols. This use allows the invisible to be visualized and the immaterial to be materialized by means of perceptible and palpable systems of symbols. An outstanding example of the cultural technique of quantification through visualization is given by the development of calculus during the 17th century. Yet the cultural technique of quantification goes beyond the use of calculus. This can be demonstrated by investigating other media relevant for the rise of modernity, such as money and maps.

David A. Grier explores the roots of simulations in his paper "The Early Progress of Scientific Simulation". He argues that the mathematical simulation of physical phenomena is far older than the electronic computer. It can be traced as far back as the 18th–century astronomers who used calculus to trace planets and comets to their origins. An example is the manually-calculated simulation of the return of Halley's Comet in 1757.

The grasp on the infinite through symbols (calculus) and the actual performance of calculus by simulation illustrates the need for dynamic knowledge tools in modern science and engineering. As long as calculus had to be tediously