INTRODUCTION

William Aspray recorded the first use of computers for scientific usage between 1952 and 1957. By June of 1952, the IAS computer was finished and ready to be tested; although it needed some extra months for repair and general maintenance, the major issue for the team of scientists and engineers was to understand the new instrument. The digital computer, built and designed on solid theoretical foundations, presented a significant challenge; namely, it was necessary to dedicate some extra time to learn the operation of the machine, identify appropriate algorithms, and determine the range of mathematical applications within the computer's capacity (1990, 155). By the time the computer became a more knowledgeable and reliable instrument, scientists and engineers began to use it with great success in specific scientific applications. By 1954, the calculation of the energy band structure of iron that would test the theory of ferromagnetism became the first scientific application to run on a digital computer (1990, 159).

In the years following 1954, the digital computer proved to be a fundamental tool for the development and advancement of scientific understanding. Today, despite their short history, computers are leaving an indelible mark on numerous and disparate scientific disciplines such as particle physics, astronomy, behavioral science, psychology, sociology, and economics. Arguably, there is virtually no scientific discipline that has not been involved, in one way or another, with the digital computer. This durable presence extends widely along the uses and needs of scientific practice. For instance, the numerical experiment of calculating the energy band structure of iron qualifies, in contemporary parlance, as a computer simulation. The main topic of this book is precisely to address the uses of and needs for computer simulations in contemporary scientific practice. In this context, computer simulations are discussed from a philosophical, historical, and scientific point of view.

Nowadays, there is a renewed interest in understanding the role that computer simulations play in scientific practice. Do computer simulations belong with the calculator and the test tube, or do they belong higher in the epistemic hierarchy, closer to theories and experiments? Are they just scientific models implemented on the digital computer, or do they represent a novel way of doing science? Given the centrality of the issue, it is not surprising to find that there have been many attempts to theorize about the nature of computer simulations as experimental devices.

Admittedly, these questions have been around for quite some time. As early as 1967, Naylor, Burdick and Sasser, define a computer simulation as:

> A numerical technique for conducting experiments with certain types of mathematical and logical models describing the behavior of an economic system on a digital computer over extended periods of time (…) The principal difference between a simulation experiment and a 'real world' experiment is that with simulation the experiment is conducted with a model of the economic system rather than with the actual economic system itself (1967, 1316).

It is astonishing to note the similarity of this quotation with more contemporary literature on the topic. Current philosophical inquiry also engages in similar efforts, such as distinguishing between a computer simulation and a 'real world' experiment, or exploring the methodological implications of implementing a scientific model as a computer simulation.

Yet, despite these few similarities, much of the contemporary philosophical investigation is simply not the same as in the late 1960s. From a historical perspective, the introduction of silicon based circuits, and the subsequent standardization of the circuit board significantly helped the industry and the growth in the computational power of computers. Such growth in speed of calculation, size of memory, or the number of programming languages forcefully challenged the established ideas and encouraged the seeking of new questions and answers.

One of the leading questions on this issue has been whether computer simulations stand for a new way of conducting scientific practices, or if they simply represent another computational method subsidiary of experimentation. The work of Rohrlich (1990) sets the grounds in this direction. He argues, computer simulations do provide a qualitatively new methodology for the physical sciences, lying somewhere intermediate between theoretical physics and empirical methods of experimentation.

However, Frigg and Reiss (2009) deliver the most pressing contemporary discussion on the philosophical relevance of computer simulations. The authors understand computer simulations in the context of the philosophy of models and, as such, with no significant distinctions from other uses of modeling in experimental practice. Humphreys (2009) answers their skepticism by indicating that the way the argument is presented is misleading, for it illuminates only computer simulations from the perspective of a philosophy of models. To Humphreys' mind, computer simulations raise questions that cannot be answered by a familiar philosophy, but rather need to be addressed at face value.

Beyond the specific contribution that this discussion can offer to the philosophical study of computer simulations, there is general agreement that computer simulations raise important questions for the general philosophy of science. One interesting example is the search for general criteria that distinguish computer simulations from experiments. Such a search has ramifications on studies about the epistemic power of computer simulations, the ontological and epistemological status of simulation data, the importance of new methodologies involved in the design and building of a computer simulation, and similar questions.

From September 21st to September 23rd 2011, the interdisciplinary workshop "Computer Simulations and the Changing Face of Scientific Experimentation," sponsored by the University of Stuttgart and the Stuttgart Research Center for Simulation Technology (SRC SimTech), brought together philosophers, historians, sociologists, and scientists into a common discussion with the purpose of revisiting some of the questions here mentioned, and addressing the new challenges that computer simulations pose to scientific practice.

We have divided this book into three mutually related parts. Part One (Theory) is dedicated to the theoretical understanding of the relation between simulations and experiments in the current philosophy of science. Part Two (Practice) fleshes out some of the theoretical conceptualizations presented in Part One by illustrating case studies from current scientific research on computer simulations. These case studies highlight the shift from experiments to computer simulations that is observed in current scientific practice, and describe the patterns of interaction between simulation methods and experimental methods in current scientific research. Part Three (History) broadens the perspective by offering case studies on the historical development of "computer experiments" as a research method.

The first part of the book is dedicated to the diversity of views among philosophers regarding existing distinctions between computer simulations and experiments, the epistemic power of computer simulations, and the new methodologies that they represent.

In the first contribution ("What Are Data About?"), Paul Humphreys calls our attention to the discussion about the status of data produced by a computer simulation. His paper focuses on the content of data produced, instead of the source that produces such data. According to the author, the origins and modes of production of these data show that the empiricist point of view is no longer an attainable position in the philosophy of science. This argument derives its force from what the author calls 'causal-computational instruments'; that is, an instrument that relies on a causal process that links the data source in nature with the measurement, but that also requires further post-processing for rendering reliable data. In Humphrey's mind, then, such causal-computational instruments cannot be interpreted in the same way as Hacking discusses microscopes, where a realist interpretation of the images is justified by the independent access to the same phenomenon through different observational instruments. The decisive point here is that the data delivered by a causal-computational instrument, like a CT scan, are the result of deliberate engineering. Depending on the particular purpose, say, whether the data is meant to be "read" by a human agent or further processed in the computer, the appearance of the engineered data may differ considerably. In order to determine its representational content, it is therefore central to take into account the origin of the data as well as the engineering steps by which it is formed (and transformed). Causal-computational instruments, then, pose a significant challenge for philosophers interested in traditional problems of empiricism, realism, and the notion of data.

If Humphreys reminds us that there is a considerable amount of engineering involved in the production of the empirical data by causal-computational instruments, Anounk Barberousse and Marion Vorms ("Computer Simulations and Empirical Data") attack the problem from the opposite side; that is, by examining whether the data produced by a genuine computer simulation can, with any good reason, be considered empirical data. Starting from the assumption that empirical data are about physical systems, Barberousse and Vorms challenge the opinion that the data produced by computer simulations cannot be new or surprising. It is frequently assumed that computer simulations, because they rely heavily on pre-existing theoretical background knowledge of the simulated objects, are less capable of producing genuinely novel and surprising insights about their target system than observations or traditional experimentation. The authors support the claim that this assertion is mistaken with the example of computer simulations of deterministic chaos.

While this conclusion emphasizes the capacity of computer simulations to produce empirical data that are as novel and surprising as that of experiments or observations, Eckhart Arnold points out the differences that remain between simulations and experiments as scientific methods ("Experiment and Simulations: Do They Fuse?"). Most notably, he argues that the results produced by computer simulations cannot go beyond what lies in the deductive closure of their premises. According to Arnold, a simulation, unlike a material experiment, cannot be employed as an *experimentum crucis*. The chapter therefore contains an elaborated criticism of some, in Arnold's opinion, misguided philosophical conceptualizations of computer simulations. With respect to the borderline between simulations and experiments, however, one question remains that is not so easily dismissed: How can a measurement that involves the computational refinement of its data properly be distinguished from a computer simulation that makes use of input data of empirical origin? To this question, Arnold gives a tentative answer based on the *measuring a cause by its effect pattern*, a pattern that is typical for many traditional measurement methods already.

The contribution by Juan M. Durán ("The Use of the 'Materiality Argument' in the Literature on Computer Simulations") continues the discussion on the differences between computer simulations and experiments, but this time from a meta-critical point of view. Durán's main concern is to unpack the underlying rationale that has been guiding the argumentation in current literature. By addressing the so-called "materiality argument" present in three different conceptualizations, the author shows that there is a common argumentative structure that inevitably shapes the final epistemological evaluation of computer simulations. Specifically, Durán presents what he calls 'the materiality aftermath,' a meta-criticism that exposes the rationale underlying the arguments in the current literature on simulations. In the author's mind, 'the materiality aftermath' is the result of the philosopher's ontological commitment to computer simulations, from which epistemological consequences are drawn. The author believes that adapting the philosophical investigation to this rationale leads to a conceptual corset in the inquiry of the epistemology of computer simulations. Durán's conclusion is sober, and aims at endorsing the philosophical investigation on computer simulations as neither restricted by, nor limited to, ontological commitments, but rather addressed at face value.

The contribution by Pío García and Marisa Velasco ("Exploratory Strategies: Experiments and Simulations") turns the discussion to a notion of 'exploratory strategy' applicable to computer simulations. Particularly, the authors analyze exploratory strategies in experiments and computer simulations, and elucidate the methodological and epistemological role in both domains. Their proposal, then, consists first in drawing some distinctions between computer simulations and experiments. Second, the authors make explicit the concept of 'exploratory strategy,' establishing a further distinction between exploratory experiments and other types of experiments. This second step allows them to present their own proposal as a different way to approach the epistemic and methodological aspects of scientific practices, particularly, computer simulations. Some relevant cases of experimental and simulation activity are considered in the context of 'exploratory strategies.'

In the second part of the book, the focus is shifted from the abstract and theoretical philosophical discussion to the analysis of concrete examples. The first of these papers is the study of simulations of cardiac electro-physiology by Annamaria Carusi, Blanca Rodriguez and Kevin Burrage ("Model Systems in Computational System Biology"). Their case study concerns multi-scale models of cardiac electro-physiology. These models represent a challenge from a technical as well as a philosophical point of view. Defying any sharp distinction between simulations and experiments, the authors claim that "the basic unit of analysis when considering questions of the validation and epistemic warrant of computational methods in systems biology" is the model-simulation-experiment-system (MSE). In particular, the target system cannot be understood simply as a given reality, rather it is co-constructed with the MSE system. The construction of the target domain is inevitable because the validation data need to be comparable to the MSE system. However, the term 'construction' must not be misunderstood as implying a relativistic understanding of science in this context. The validation experiments remain independent in the sense that they do not make use of any data that have been used for model construction.

Anne Marcovich and Terry Shinn's contribution ("Computer Simulation and the Growth of Nanoscale Research in Biology") explores three links between computer simulations and nanobiology research. First, they show that there is a correlation between nano-related biology publications in the early 1990s and the introduction of computer simulations in scientific practice. Second, computer based research contributes to the cognition of nanobiology through the creation, organization, and consultation of databases. Finally, the authors show that "simulation molecular graphics generate images that are informationally and analytically rich, and that offer a fundamental input into novel forms of epistemology." Their contribution shows not only how the academic agenda is strongly driven by the introduction of new technologies, but also how computer simulations can provide a genuine understanding of their simulated target system, requiring a novel form of epistemology.

In their contribution, Lucía Ayala and Jaime Forero-Romero ("Computer Simulations in a Cosmological Context") discuss the case of testing hypotheses in cosmology. Physical cosmology represents a special case in the natural sciences with regard to the available methods for testing a hypothesis. Since direct experiments are excluded, observations and simulations must carry out this testing function. In their contribution, the authors discuss the special case of numerical simulations as an essential tool for understanding the observed large-scale structures in the Universe. This discussion is followed by a description of the limitations of simulations in understanding such large-scale structures. For instance, the physical nature of computer simulations becomes a limitation. As the authors point out, time, data storage, and data transfer rates are restricted. Ultimately, theory, observations, and simulations work together and, with their different potentials and limitations, mutually complement each other in contemporary astronomy.

Muniza Rehman traces the latest developments in the use of simulations and experiments in the pharmaceutical industry ("Experimentation and Simulations in the Pharmaceutical Industry"). Rehman places simulations between traditional experimentation and theoretical accounts. To the author's mind, two kinds of simulation studies are common in the pharmaceutical industry: Computer-assisted trial designs (CATD) and computer-simulated clinical trials (CSCT). The former are employed to study the experimental design of clinical studies, before they are conducted. The latter are used to estimate the outcome of clinical trials, potentially rendering some of these trials unnecessary and thus reducing the number of clinical trials that actually have to be conducted. Some philosophers have disputed that simulations provide a true novelty over traditional modes of modeling and theoretical exploration. Nevertheless, given how strongly the use of computer simulations has affected the practice of drug testing in the pharmaceutical industry, Rehman concludes that from this perspective simulations are indeed a *sui generis* activity in a Humphreyan sense.

The third and last part completes the book with historical case studies. Wolfgang Brand ("Designing the Membrane Roof of the Munich Olympic Stadium using Supercomputers") presents a historical case study of the deployment of the first supercomputers in architecture and civil engineering. The events around the design of the tent-shaped membrane roof of the Munich Olympic Stadium for the 1972 Olympic Games demonstrates how physical models of constructions enable technologies for the construction of naturally shaped buildings. It is argued that the 1960s mark the period in which the usage of high performance computers triggered the change toward architectural design processes. The technology available had already reached a state where model building was no longer necessary. It is shown how two groups using different methods on the same computing infrastructure designed the roofs inspired by the ideas of Frei Otto. They developed wide-spanning lightweight structures consisting of pre-stressed cable nets covered by transparent tiles. The group of John H. Argyris relied on the Finite Element Method, which he co-invented. While another group headed by Klaus Linkwitz used least-square fitting and developed the new Force Density Method, all influenced by geodesic methods. Both attempts were successful and led to the landmark Olympic Stadium in Munich, as we know it today.

A somewhat different perspective on simulations is introduced by Michael Resch ("What's the Result? Thoughts of a Center Director on Simulations"). As head of the high-performance computing center in Stuttgart, Resch addresses the technological procedures (and their limitations) by which simulations are implemented and executed on the computer. In this respect, Resch proposes an addition to Winsberg's (2010) layered model of simulations, which also includes numerical schemes, program structures, programming models, and hardware architectures. All of these influence the capabilities as well as the limitations of the simulation approach. Resch, then, embeds his 'prototypical workflow' into a broad philosophical perspective, covering the question of verification and validation, as well as the need for rendering simulation results comprehensible to human beings. The latter issue does not only concern the specialist user of simulations, but also is of interest for society –as the example of climate simulations may illustrate.

We hope that readers from different humanistic and scientific fields that concern themselves with computer simulations find the broad perspective of our book useful. The editors would like to thank the University of Stuttgart and the SRC SimTech for financial support that made the workshop possible. This book is a publication of the papers presented at that workshop. We are in debt to the participants for making the workshop a successful event. Most of all, we would also like to thank all the authors that, with their excellent contributions, made this book possible.

Juan M. Durán and Eckhart Arnold

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