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Juan Manuel Durán

COMPUTER SIMULATIONS IN SCIENCE AND ENGINEERING

Concepts—Practices—Perspectives



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Juan Manuel Durán

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Juan Manuel Durán
Faculty of Technology, Policy and
Management
Delft University of Technology
Delft, The Netherlands

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*To mom, dad, and Jo
For their unconditional support and love.*

*To my Bee
I could have not made this journey without
you.*

*To Mauri
In true friendship.*

*To Manuel
With love and admiration.*

Preface

The ubiquitous presence of computer simulations in all kinds of research areas evidences their role as the new driving force for the advancement of science and engineering research. Nothing seems to escape the image of success that computer simulations project onto the research community and the general public. One simple way to illustrate this consists in asking ourselves how would contemporary science and engineering look without the use of computer simulations. The answer would certainly diverge from the current image we have of scientific and engineering research.

As much as computer simulations are successful, they are also methods that fail in their purpose of inquiring about the world, and as much as researchers make use of them, computer simulations raise important questions that are at the heart of contemporary science and engineering practice. In this respect, computer simulations make a fantastic subject of research for the natural sciences, the social sciences, engineering and, as in our case, also for philosophy. Studies on computer simulations touch upon many different facets of scientific and engineering research and evoke philosophically inclined questions of interpretation with close ties to problems in experimental settings and engineering applications.

This book will introduce the reader, in an accessible and self-contained manner, to these various fascinating aspects of computer simulations. An historical study on the conceptualization of computer simulations throughout the past sixty years opens up the vast world of computer simulations and their implications. The focus then is shifted to the discussion on their methodology, their epistemology, and the possibilities of an ethical framework, among other issues.

The scope of this book is relatively broad in order to familiarize the reader with the many facets of computer simulations. Throughout the book, I have sought to maintain a healthy balance between the conceptual ideas associated with the philosophy of computer simulations on the one hand, and their practice in science and engineering on the other hand. To this end, this book has been conceived for a broad audience, from scientists and engineers, policy makers and academics, to the general public. It welcomes anyone interested in philosophical questions—and conceivable answers—to issues raised by the theory and practice of computer

simulations. It must be mentioned that although the book is written in a philosophical tone, it does not engage in deep philosophical discussions. Rather, it seeks to explore the synergy between technical aspects of computer simulations and the philosophical value there emerging. In this respect, the ideal readers of this book are researchers across disciplines working on computer simulations but holding philosophical inclinations. This is, of course, not to say that professional philosophers would not find in its pages problems and questions for their own research.

One beautiful thing about computer simulations is that they offer a fertile field of research, both for researchers using the simulations as well as those reflecting upon them. In this respect, although the book might have some merits, it also falls short in many respects. For instance, it does not address the work of computer simulations in the social sciences, a very fruitful area of research. It also does not discuss the use of computer simulations in and for policy making, their uses for reporting to the general public, nor their role in a democratic society where science and engineering practice is a common good. This is certainly unfortunate. But there are two reasons that, I hope, excuse these shortcomings. One is that I am not a specialist in any of these fields of research, and therefore, my contribution would have been of little interest. Each of the fields mentioned brings about specific issues in their own right that those involved in their study know best. The second reason stems from the fact that, as all researchers know, time and, also in this case, space are tyrant. It would be an impossible task to even scratch the surface of the many areas where computer simulations are active and thriving.

As a general rule for the book, I present a given topic and discuss problems and potential solutions to it. No topic should be addressed as unrelated to any other topic in the book, nor should a proposed answer be taken as final. In this sense, the book aims at motivating further discussions, rather than providing a closed set of topics and the answers to their core issues. Each chapter should nevertheless present a self-contained discussion of a general theme of computer simulations. I must also mention that each chapter contains profuse references to the specialized literature, giving the reader the opportunity to pursue further his or her own interests on a given subject.

The book is organized as follows. In Chap. 1, I address the question ‘what are computer simulations?’ by giving an historical overview of the concept. Tracking back the concept of computer simulation to the early 1960s, we will soon realize that many contemporary definitions owe much to these early attempts. A proper grasp of the history of the concept will turn out to be very important for the development of a solid understanding of computer simulations. In particular, I identify two traditions, one that puts the emphasis on implementing mathematical models on the computer, and another for which the prominent feature is the representational capacity of the computer simulation. Depending on which tradition researchers choose to follow, the assumptions and implications to be drawn from computer simulations will differ. The chapter ends with a discussion on the now standard classification of computer simulations.

The core of Chap. 2 is to introduce and discuss in detail the constituents of *simulation models*—that is, the models at the basis of computer simulations. To this end, I discuss diverse approaches to scientific and engineering models with the purpose of entrenching simulation models as a rather different kind. Once this is accomplished, the chapter goes on presenting and discussing three units of analysis constitutive of computer simulations, namely the specification, the algorithm, and the computer process. This chapter is the most technical of the book, as it draws extensively from studies on software engineering and computer science. In order to balance this with some philosophy, it also presents several problems related to these units of analysis—both individually and in relation to each other.

The sole purpose of Chap. 3 is to present the discussion on whether computer simulations are epistemologically equivalent to laboratory experimentation. The importance of establishing such equivalence has its roots in a tradition that takes experimentation as the solid foundation for our insight into the world. Since much of the work demanded of computer simulations is to provide knowledge and understanding of real-world phenomena that would otherwise not be possible, the question of their epistemological power in comparison with laboratory experimentation naturally occurs. Following the philosophical tradition of discussing these issues, I focus on the now time-honored problem of the ‘materiality’ of computer simulations.

Although Chaps. 4 and 5 are independent of each other, they do share the interest of establishing the epistemological power of computer simulations. While Chap. 4 does so by discussing the many ways in which computer simulations are reliable, Chap. 5 does it by showing the many epistemic functions attached to computer simulations. These two chapters, then, represent my contribution to the many attempts to ground the epistemic power of computer simulations. Let us note that these chapters are, at their basis, an answer to Chap. 2 which discusses computer simulations *vis à vis* laboratory experimentation.

Next, Chap. 6 addresses issues that are arguably less visible in the literature on computer simulations. The core question here is whether computer simulations should be understood as a third paradigm of scientific and engineering research—theory, experimentation, and Big Data being the first, second, and fourth paradigm respectively. To this end, I first discuss the use of Big Data in scientific and engineering practice, and what it means to be a paradigm. With these elements in mind, I begin a discussion on the possibilities of holding causal relations in Big Data science as well as computer simulations, and what this means for the establishment of these methodologies as paradigms of research. I finish the chapter with a comparison between computer simulations and Big Data with a special emphasis on what sets them apart.

The last chapter of the book, Chap. 7, addresses an issue that has been virtually unexplored in the literature on ethics of technology, that is, the prospect of an ethics exclusively for computer simulations. Admittedly, the literature on computer

simulations is more interested in their methodology and epistemology and much less on the ethical implications that come with designing, implementing, and using computer simulations. In response to this lack of attention, I approach this chapter as an overview of the ethical problems addressed in the specialized literature.

Stuttgart, Germany
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Juan Manuel Durán

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Finally, in times where science and technology are undoubtedly a fundamental tool for the progress of society, it is heartbreaking to see how the current government of Argentina—and in many other places in Latin-America as well—are cutting funding in science and technology research, humanities, and the social sciences. I observe with equal horror the political decisions explicitly targeted to the destruction of the educational system. I then dedicate this book to the Argentinean

scientific and technological community, for they have shown time and time again their greatness and brilliance despite unfavorable conditions.

This book owes Kassandra too much. She left her impression when correcting my English, when suggesting me to re-write a whole paragraph, and when she let go a planned appointment that I forgot while finishing a section. For this, and for thousands of other reasons, this book is entirely dedicated to her.

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Introduction

In 2009, a debate erupted around the question of whether computer simulations introduce novel *philosophical* problems or if they are merely a *scientific* novelty. Roman Frigg and Julian Reiss, two prominent philosophers that ignited the debate, noted that philosophers have largely assumed some form of philosophical novelty of computer simulations without actually engaging the question of its possibility. Such an assumption rested on one simple confusion: Philosophers were thinking that scientific novelty licenses philosophical novelty. This gave course to issuing a warning over the growth of overemphasized and generally unwarranted claims about the philosophical importance of computer simulations. This growth, according to the authors, was reflected in the increasing number of philosophers convinced that the philosophy of science, nourished by computer simulations, required an entirely new epistemology, a revised ontology, and novel semantics.

It is important to point out that Frigg and Reiss are not objecting to the novelty of computer simulations in scientific and engineering practice, nor their importance in the advancement of science, but rather that simulations raise few, if any, new philosophical question. In their own words, '[t]he philosophical problems that do come up in connection with simulations are not specific to simulations and most of them are variants of problems that have been discussed in other contexts before. This is not to say that simulations do not raise new problems of their own. These specific problems are, however, mostly of a mathematical or psychological, not philosophical nature' (Frigg and Reiss 2009, 595).

I share Frigg and Reiss' puzzlement on this issue. It is hard to believe that a *new* scientific method—instrument, mechanism, etc.—however powerful as it might be, could all by itself imperil current philosophy of science and technology to the point that they need to be rewritten. But this is only true if we accept the claim that computer simulations come to *rewrite* long-standing disciplines, which I do not think is the case. To me, if we are able to reconstruct and give new meaning to old philosophical problems in light of computer simulations, then we are basically establishing their philosophical *novelty*.

Let us now ask the question in what sense are computer simulations a philosophical novelty? There are two ways to unpack the problem. Either computer simulations pose a series of philosophical questions that escape standard philosophical treatment, in which case they can be added to our philosophical corpus; or they challenge established philosophical ideas, in which case the current corpus expands standard debates into new domains. The first case has been proposed by (Humphreys 2009), whereas the second case has been argued by myself (Durán, under review). Let me now briefly discuss why computer simulations represent, in many respects, a scientific and philosophical novelty.

The core of Humphreys' argument is to recognize that we could either understand computer simulations by focusing on how traditional philosophy illuminates their study (e.g., through a philosophy of models, or a philosophy of experiment), or by focusing exclusively on aspects about computer simulations that constitute, in and by themselves, genuine philosophical challenges. It is this second way of looking at the questions about their novelty that grants philosophical importance to computer simulations.

The chief claim here is that computer simulations can solve otherwise intractable models and thus amplify our cognitive abilities. But such amplification comes with a price 'for an increasing number of fields in science, an exclusively anthropocentric epistemology is no longer appropriate because there now exist superior, non-human, epistemic authorities' (Humphreys 2009, 617). Humphreys calls this the *anthropocentric predicament* as a way to illustrate current trends in science and engineering where computer simulations are moving humans away from the center of production of knowledge. According to him, a brief overview on the history of philosophy of science shows that humans have always been at the center of production of knowledge. This conclusion includes the period of the logical and empirical positivism, where the human senses were the ultimate authority (Humphreys 2009, 616). A similar conclusion follows from the analysis of alternatives to the empiricist, such as Quine's and Kuhn's epistemologies.

When confronted with claims about the philosophical novelty of computer simulations, Humphreys points out that the standard empiricist viewpoint has prevented a complete separation between humans and their capacity to evaluate and produce scientific knowledge. The anthropocentric predicament, then, comes to highlight precisely this separation: It is the claim that humans have lost their privileged position as the ultimate epistemic authority.¹ The claim finally gets its support from the view that scientific practice only progresses because new methods are available for handling large amounts of information. Handling information, according to Humphreys, is the key for the progress of science today, which can only be attainable if humans are removed from the center of the epistemic activity (Humphreys 2004, 8).

¹ Humphreys makes a further distinction between scientific practice completely carried out by computers—one that he calls *the automated scenario*—and one in which computers only partially fulfill scientific activity—that is, the *hybrid scenario*. He restricts his analysis, however, to the hybrid scenario (Humphreys 2009, 616–617).

The anthropocentric predicament, as philosophically relevant as it is in itself, also brings about four extra novelties unanalyzed by the traditional philosophy of science. Those are *epistemic opacity*, *the temporal dynamics of simulations*, *semantics*, and the *in practice/in principle* distinction. All four are novel philosophical issues brought up by computer simulations; all four have no answer in traditional philosophical accounts of models and experimentation; and all four represent a challenge for the philosophy of science.

The first novelty is *epistemic opacity*, a topic that is currently attracting much attention from philosophers. Although I discuss this issue in some detail in Sect. 4.3.2, briefly mentioning the basic assumptions behind epistemic opacity will shed some light on the novelty of computer simulations. Epistemic opacity, then, is the philosophical position that takes that it is impossible for any human to know all the epistemically relevant elements of a computer simulation. Humphreys presents this point in the following way: “A process is essentially epistemically opaque to [a cognitive agent] X if and only if it is impossible, given the nature of X, for X to know all of the epistemically relevant elements of the process” (Humphreys 2009, 618). To put the same idea in a different form, if a cognitive agent could stop the computer simulation and take a look inside, she would not be able to know the previous states of the process, reconstruct the simulation up to the point of stop, or predict future states given previous states. Being epistemically opaque means that, due to the complexity and speed of the computational process, no cognitive agent could know what makes a simulation an epistemically relevant process.

A second novelty that is related to epistemic opacity is the ‘temporal dynamics’ of computer simulations. This concept has two possible interpretations. Either it refers to the necessary computer time to solve the simulation model, or it stands for the temporal development of the target system as represented in the simulation model. A good example that merges these two ideas is a simulation of the atmosphere: The simulation model represents the dynamics of the atmosphere, for a year and it takes, say, ten days to compute.

These two novelties nicely illustrate what is typical of computer simulations, namely the inherent complexity of simulations in themselves, as is the case of epistemic opacity and the first interpretation of temporal dynamics; and the inherent complexity of the target systems that computer simulations usually represent, as is the case of the second interpretation of temporal dynamics. What is common between these two novelties is that they both entrench computers as the epistemic authority since they are able to produce reliable results that no human or group of humans could produce by themselves. Either because the process of computing is too complex to follow or because the target system is too complex to comprehend, computers become the exclusive source for obtaining information about the world.

The second interpretation of temporal dynamics is tailored to the novelty of the *semantics*, which asks the question of how theories and models represent the world, now adjusting the picture to fit a computer algorithm. Thus, the chief issue here is how the syntax of a computer algorithm maps onto the world, and how a given theory is actually brought into contact with data.

Finally, the distinction in *principle/in practice* is intended to sort out what is applicable in practice and what is applicable only in principle. To Humphreys, it is a philosophical fantasy to say that, in principle, all mathematical models find a solution within computer simulations (Humphreys 2009, 623). It is a fantasy because it is clearly false, although philosophers have claimed its possibility—hence, in principle. Humphreys suggests, instead, that in approaching computers, philosophers must keep a more down-to-earth attitude, limited to the technical and empirical constraints that simulations can offer.

My position is complementary to Humphreys' in the sense that it shows how computer simulations challenge established ideas in the philosophy of science. To this end, I begin by arguing for a specific way of understanding simulation models, the kind of model at the basis of computer simulations. To me, a simulation model recasts a multiplicity of models into one 'super-model.' That is to say, simulation models are an amalgam of different sorts of computer models, all having their own scales, input parameters, and protocols. In this context, I claim for three novelties in philosophy, namely *representation*, *abstraction*, and *explanation*.

About the first novelty, I claim that the multiplicity of models implies that *representation* of a target system is more holistic in the sense that it encompasses all and every model implemented in the simulation model. To put the same idea in a rather different form, the representation of the simulation model is not given by any individual implemented model but rather by the combination of all of them.

The challenge that computer simulations bring to the notion of *abstraction* and idealization is that, typically, the latter presupposes some form of *neglecting* stance. Thus, *abstraction* aims at ignoring concrete features that the target system possesses in order to focus on their formal setup; *idealizations*, on the other hand, come in two flavors: While Aristotelian idealizations consist in 'stripping away' properties that we believe not to be relevant for our purposes, Galilean idealizations involve deliberate distortions. Now, in order to implement the required variety of models into a single simulation model, it is important to count on techniques by which information is hidden from the users, but not neglected from the models (Colburn and Shute 2007). This is to say that the properties, structures, operations, relations, and the like present in each mathematical model can be effectively implemented into the simulation model without stating explicitly how such implementation is carried out.

Finally, *scientific explanation* is a time-honored philosophical topic where much has been said. When it comes to explanation in computer simulations, however, I propose a rather different look at the issue than the standard treatment offers. One interesting point here is that, in the classic idea that explanation is of a real-world phenomenon I oppose the claim that explanation is, first and foremost, of the results of computer simulations. In this context, many new questions emerge seeking an answer. I discuss scientific explanation in more detail in Sect. 5.1.1.

As I have mentioned before, I do believe that computer simulations raise novel questions for the philosophy of science. This book is living proof of that belief. But even if we do not believe in their philosophical novelty, we still need to understand

computer simulations as scientific novelties with a critical and philosophical eye. To these ends, this book presents and discusses several theoretical and philosophical issues at the heart of computer simulations. Having said all of this, we may now submerge ourselves into their pages.

Chapter 1

The Universe of Computer Simulations



The universe of computer simulations is vast, flourishing in almost every scientific discipline, and still resisting a general conceptualization. From the early computations of the Moon's orbit carried out by punched card machines, to the most recent attempts to simulate quantum states, computer simulations have a uniquely short but very rich history.

We can situate the first use of a machine for scientific purposes in England at the end of the 1920s. More precisely, it was in 1928 when the young astronomer and pioneer in the use of machines Leslie J. Comrie predicted the motion of the Moon for the years 1935–2000. During that year, Comrie made intensive use of a Herman Hollerith punched card machine to compute the summation of harmonic terms in predicting the Moon's orbit. Such groundbreaking work would not stay in the shadows, and by the mid 1930s it had crossed the ocean to Columbia University in New York City. It was there that Wallace Eckert founded a laboratory that made use of punched card tabulating machines—now built by IBM—to perform calculations related to astronomical research, including of course an extensive study of the motion of the Moon.

Both Comrie's and Eckert's uses of punched card machines share a few commonalities with today's use of simulations. Most prominently, both implement a special kind of model that describes the behavior of a target system, and which can be interpreted and computed by a machine. While Comrie's computing rendered data about the motions of the Moon, Eckert's simulation described planetary movement.

These methods certainly pioneered and revolutionized their respective fields, as well as many other branches of the natural and social sciences. However, Comrie's and Eckert's simulations significantly differ from today's *computer simulations*. Upon closer inspection, differences can be found everywhere. The introduction of silicon based circuits, as well as the subsequent standardization of the circuit board, made a significant contribution to the growth of computational power. The increase in the speed of calculation, size of memory, and expressive power of programming language forcefully challenged the established ideas on the nature of computation

and of its domain of application. Punched card machines rapidly became obsolete as they are slow in speed, unreliable in their results, limited in their programming, and based on stiff technology (e.g., there were very few exchangeable modules). In fact, a major disadvantage of the punched card over modern computers is that they are error-prone and time-consuming machines, and therefore the reliability of their results as well as their representational accuracy is difficult to ground. However, perhaps the most radical difference between Comrie's and Eckert's simulations, on the one hand, and modern computer simulations on the other, is the automation process that characterizes the latter. In today's computer simulations, researchers are losing ground on their influence and power to interfere in the process of computing, and this will become more prominent as complexity and computational power increases.

Modern computers come to amend many aspects of scientific and engineering practice with more precise computations, and more accurate representations. Accuracy, computational power, and reduction of errors are, as we will see, the main keys of computer simulations that unlock the world.

In light of contemporary computers, then, it is not correct to maintain that Comrie's prediction of the motion of the Moon and Eckert's solution of planetary equations are computer simulations. This is, of course, not to say that they are not simulations at all. But in order to accommodate to the way scientists and engineers use the term today, it is not sufficient to be able to compute a special model or to produce certain kinds of results about a target system. Speed, storage, language expressiveness, and the capacity to be (re)programmed are chief concepts for the modern notion of computer simulation.

What are computer simulations then? This is a philosophically motivated question that has found different answers from scientists, engineers, and philosophers. The heterogeneity of their answers makes explicit how differently each researcher conceives computer simulations, how their definitions vary from one generation to another, and how difficult it is to come up with a unified notion. It is important, however, to have a good sense of their nature. Let us discuss this in more extent.

1.1 What Are Computer Simulations?

Recent philosophical literature takes computer simulations as aids for overcoming imperfections and limitations of human cognition. Such imperfections and limitations are tailored to the natural human constraints of computing, processing and classifying large amounts of data. Paul Humphreys, one of the first contemporary philosophers to address computer simulations from a purely philosophical viewpoint, takes them as an 'amplification instrument,' that is, one that speeds up what the unaided human could not do by herself (Humphreys 2004, 110). In a similar sense, Margaret Morrison, yet another central figure in philosophical studies on computer simulations, considers that although they are another form of modeling, "given the various functions of simulation [...] one could certainly characterize it as a type of 'enhanced' modelling" (Morrison 2009, 47).

Both claims are fundamentally correct. Computer simulations compute, analyze, render, and visualize data in many ways that are unattainable for any group of humans. Contrast, for instance, the time required for a human to identify potential antibiotics for infectious diseases such as anthrax, with a simulation of the ribosome in motion at atomic detail (Laboratory 2015). Or, if preferred, compare any set of human computational capabilities with the supercomputers used at the High Performance Computing Center Stuttgart, home of the Cray XC40 Hazel Hen with a peak performance of 7.42 Petaflops and a memory capacity of 128 GB per node.¹

As pointed out by Humphreys and Morrison, there are different senses in which computer simulations enhance our capacities. This could be by amplifying our calculation skills, as Humphreys suggests, or it could be by enhancing our modeling abilities, as Morrison suggests.

One would be naturally inclined to think that computer simulations amplify our computational capability as well as enhance our modeling abilities. However, a quick look at the history of the concept shows otherwise. To some authors, a proper definition must highlight the importance of finding solutions to a model. To others, the right definition centers the attention to describing patterns of behavior of a target system. Under the first interpretation, the computational power of the machine allows us to solve models that, otherwise, would be analytically intractable. In that respect, a computer simulation ‘amplifies’ or ‘enhances’ our cognitive capacities by providing computational power to what is beyond our cognitive reach. The notion of computer simulation is then dependent on the physics of the computer and furnishes the idea that technological change expands the boundaries of scientific and engineering research. Such a claim is also historically grounded. From Hollerith’s punched card machines to the silicon-based computer, the increment of the physical power of computers has enabled scientists and engineers to find different solutions to a variety of models. Let me call this first interpretation *the problem-solving viewpoint* on computer simulations.

Under the second interpretation, the emphasis is on the capacity of the simulation to describe a target system. For this, we have a powerful language that represents, to certain acceptable degrees of detail, several levels of description. In that respect, a computer simulation ‘amplifies’ or ‘enhances’ our modeling abilities by providing more accurate representation of a target system. Thus understood, the notion of computer simulation is tailored to the way in which they describe a target system, and thus on the computer language used, modularization methods, software engineering techniques, etc. I call this second interpretation *the description of patterns of behavior viewpoint* on computer simulations.

Because both viewpoints emphasize different—although not necessarily incompatible—interpretations of computer simulations as enhancers, some distinc-

¹It is worth noting that our neuronal network activity is, in some specific cases, faster than any supercomputer. According to relatively recent publication, Japan’s *Fujitsu K* computer, consisting of 82,944 processors, takes about 40 min to simulate one second of neuronal network activity in real, biological time. In order to partially simulate the human neural activity, researchers create about 1.73 billion virtual nerve cells that were connected to 10.4 trillion virtual synapses (Himeno 2013).