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Research Article

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The changing face of scientific practice – seeing things virtually

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Abstract: The purpose of this essay is to summarize and critically evaluate the epistemological and pragmatic questions with regard to computer simulations as a new technological-scientific format as put forth in current philosophical debates. Computer simulation practices are situated in the broader context of model-building practices and experimentation; the scope and limits of knowledge generated by computer simulations are considered.

Keywords: computer simulation; epistemology; philosophy of science; scientific practice.

1 Introduction

Johannes Kepler developed his mechanical theory of light by, among other things, analyzing optical instruments, the camera obscura and the telescope. Studying these man-made instruments provided insight into some fundamental aspects of physics. Paradoxically, it is the technical artifact that provides the means to uncover the mathematical properties of nature. This case shows the importance of understanding the instruments of scientific inquiry in the context of discovery and justification of scientific knowledge, and it is this kind of metascientific navel-gazing that is gaining momentum again in the age of computer simulation-based science.

Computer simulations and the new avenues of research they open have been met with considerable excitement in the community, while at the same time, questions arose concerning the validity and limitations of virtuality in the scientific context. This essay summarizes the most prominent lines of inquiry and issues on computer simulations as scientific tools. A variety of types of simulations has evolved since the early days of computer-based experimentation in the 1940s, such as the Monte-Carlo simulations, equation-based simulations, agent-based simulations, or multiscale simulations [1–3]. At the core of any computer simulation rests a model or representation of a target system under study. This model is formulated by algorithms and equations, which, when implemented in a software, become nominally a computer model. Running the computer program is then an instance of a computer simulation.

As computer simulations are used in such a wide variety of contexts (e.g. simulations in the context of applied sciences vs. natural sciences) and for such a multitude of applications, alongside with differing aims and intentions (simulations can be used solely for the purpose of demonstration or for exploration) that an all-encompassing analysis is hardly achievable. Throughout the paper, therefore, the notion of computer simulation will be used in the broadest possible sense as any type of activity involving the implementation of a model on a digital computer, though most philosophers predominantly consider models from the natural sciences, such as physics or chemistry. Section 2 considers the place of computer simulations among other forms of scientific practice. Section 3 discusses epistemological issues regarding virtual research environments.

2 Situating computer simulations in scientific practice

Numerous authors [4–10] claim that computer simulations represent a radically different way of doing science and should be seen as nothing short of a methodological revolution:

> '[…] computer simulation provides […] a qualitatively new and different methodology for the natural sciences, and […] this methodology lies somewhere intermediate between traditional theoretical science and its empirical methods of experimentation and observation. … Scientific activity has thus reached a new milestone somewhat comparable to the milestones that

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> started the empirical approach (Galileo) and the deterministic mathematical approach to dynamics (the old syntax of Newton and Laplace). Computer simulation is consequently of considerable philosophical interest.' [7, p. 507].

According to this line of thinking, computer simulations additionally open new avenues for scientific inquiry, insofar as they extend our ability to engage with otherwise intractable mathematical problems:

> 'Simulations increase the range of phenomena that are epistemically accessible to us in a way comparable to scientific instruments such as microscopes or telescopes. This is partly due to the fact that most models are specifically tailored to incorporate a particular piece of mathematics that we know how to handle. Computer simulations extend the class of tractable mathematics and thereby broaden the range of modelling tools that we can use. This extension of modelling tools leads to scientific progress because much of the success of modern science is due to [...] "model building", and computers make a huge difference to our ability to build models.' [11, p. 593].

Finally, a lot of the *prima facie* fascination with computer simulation stems from the fact that virtual worlds are created in which, virtually, anything goes.

A simulation is a virtual entity inasmuch as it is a computer-generated representation of a physical system. Its contents depend on the mathematics describing the system, not on the physicality of the system. Being thus removed from the constraints of nature and the limitations of the human observer such as time and scale, computer simulations harbor both advantages and disadvantages. On the one hand, phenomena, which were previously out of the reach of scientific inquiry, became accessible and observable by virtue of being virtually representable; on the other hand, we need to be able to justify whether the results of computer simulations allow us to draw adequate inferences about real-world structures and dynamics.

From the above, we can extract three intuitions about computer simulations and their impact on scientific practice:

(a) Computer simulations represent an entirely new methodological approach to science.
(b) They extend existing practices into otherwise inaccessible domains.
(c) The idea of virtuality requires some careful thinking about the inferential and epistemic properties of computer simulations.

These intuitions are reflected, though, perhaps, not exposed as such, in a prominent philosophical debate on whether computer simulations are experiments. In this debate, the intuition that virtuality poses a barrier to gaining information about reality plays against the intuition of computer simulations as extensions of already established practices such as model building. The proponents of the 'materiality thesis' (e.g. Morgan [12], Guala [13, 14]) claim that simulations are not experiments in that experiments bear greater epistemic weight by being by default closer to the reality of a (physical) system. Inferences about the real world are, thus, better justified when they are drawn on the basis of experiments. Francesco Guala writes:

> 'The difference lies in the kind of relationship existing between, on the one hand, an experiment and its target system, and on the other, a simulation and its target. In the former case, the correspondence holds at a "deep," "material" level, whereas in the latter, the similarity is admittedly only abstract and formal. ...In a genuine experiment, the same material causes as those in the target system are at work; in a simulation, they are not, and the correspondence relation (of similarity or analogy) is purely formal in character.' [13, p. 214–215].

The argument, thus, points to the fact that virtuality pushes the observer one step back from the world in comparison to laboratory experimentation where the 'natural' system is at least partly present in its physical form.

However, as has been pointed out by Winsberg [9] and also Parker [15], both experimentation and simulation are heavily dependent on the use of models, and experimentation these days is not simply a form of intervention on a physical target system any more. The epistemic strength or weakness depends, thus, in both cases on the representational properties of the model of the target system:

> 'Strictly speaking the model is what is being investigated and manipulated in a simulation. However, that model functions as a representation of a physical system via its relationship to the mathematical model of the target, so to that extent the system itself is also the object of inquiry. ... this type of model/system relation is not simply a peculiarity of computer simulations but is also present in more traditional forms of experimentation. Consequently it does not provide a basis for epistemic differences between the two.' [16, p. 44].

From a more pragmatic point of view, the philosophical debate on whether computer simulations are kinds of experiments appears misguided, as in practice, computer simulations come to bear when laboratory experimentation is impossible, too expensive, or obsolete, as the defining parameters of the real-world system are sufficiently known. The design-exercise of creating a computer simulation involves similar pitfalls as in designing experiments – thus far, these two forms of scientific practice are comparable and on a methodological par. When the context of application is incomparable, however, it is also beyond comparison whether experiments and computer simulations have the same epistemic power or whether one is superior to the other.

Any kind of scientific activity, be it classical experimentation or computer simulation or even measurement [16], requires a strategy to implement one's background assumptions (models) into a methodologically controlled setting. This strategy takes different forms in each setting: within an experimental context, models and assumptions can be hypothetical to a much higher degree, as the experiment will provide falsifying or non-falsifying (non-falsified does not mean that the hypothesis is confirmed) results, whereas in computer simulations, the output is, to a much higher degree, if not entirely, dependent on the input, given that the environment executes the simulation correctly and as intended (below, I will come back to the issue of errors).

If we want to know whether and how computer simulations represent a new way of doing science, we first need to charter the territory of scientific practices. Along a fictional dimension of empiricality, we can place mere observation on one end, and computer simulations on the other with laboratory experimentation in between. However, it raises the question whether our characterization of scientific practice is fully developed when we only take into account how much or how little manipulation of, and control over, a real-world system can be exerted. Along more abstract dimensions, such as theory ladenness or model involvement, the picture might get less clear. A commonly stated position in the philosophy of computer simulation is that simulating lies on a kind of continuum between theorizing and experimenting. If experiments are a form of intervention on a real-world target system and if a theory is a mathematical formulation of a system's dynamic behavior, then, simulating draws from both. A computer simulation is an implementation of a model in its mathematical formulation in computer environment, which can be manipulated beyond the physical constraints imposed on a real-world target by virtue of our ability to vary the parameters.

Computer simulations can, therefore, be defined as technology-driven science or a 'techno-scientific format'. The semi-natural components of classical laboratory experimentation were replaced by virtual components within a digital/virtual environment, but experimentation also relies on partial 'technification' of its targets, by making them measurable. In a sense, simulations are only possible as, or because, natural laws as correlations between parameters have already been encoded in technological formats such as instruments and mathematical models, and thus, simulations can be seen as a more radical form of this already existing trend in modern natural science [17].

Yet, it would be wrong to conclude that simulating does not introduce novel elements into scientific inquiry, if only in form and not in kind. The advantages of simulations in the broader context of scientific practice consist in an impressive number of powerfully combined features: visualization, limitless repeatability, time-scale independence, vast computing power and speed, management of massive data sets, and the at least approximate solvability of otherwise untractable equations are just a few heavy weight factors that define and expose computer simulations as outstanding tools. The fact that computer simulation results are, nevertheless, often not self-explanatory has its root in the technological complexity that supersedes and underlies the simulation environment, which can contain very different sources of errors than laboratory environments and which have direct consequences on the justification and inferential value of computer simulations results.

3 The epistemology of computer simulation: the scope and limits of simulation-generated knowledge

From the vantage point of philosophy of science, the focus of investigation is traditionally on fundamental aspects of science. When it comes to the knowledge-generating potential of computer simulations, philosophers are at odds about their importance for epistemology. In a famous exchange of arguments, Winsberg [9, 10], on one side, and Frigg and Reiss [11], on the other, debate whether the scientific novelty and specifics of computer simulations warrant the demand for a 'new' epistemology.

Epistemology in philosophy is the study of knowledge. The standard definition states that knowledge is 'justified true belief'. To explain: a proposition *that p* needs to be internalized by a subject (hence, be a belief), the proposition *that p* needs to adhere to certain truth conditions, such as being factually realized in a real-world system or to adhere to a set of formal rules, and last, the subject needs to be able to point to reasons why he believes *p* to be true, i.e. some form of evidence. It is this context of justification that becomes interesting with regard to computer simulations as scientific instruments. What is the evidential basis for claiming that computer simulation results provide *correct* insights into the real behavior of real-world target systems when the truth conditions lie solely within the virtual environment of the simulation? Are we not dealing here with a closed-off parallel world that does not warrant inferences on systems outside of this environment? This is the so-called validation problem.

Norton and Suppe [6] claim that a simulation is validated when the relation between the so-called base model, the modeled physical system, and the computer environment on which the algorithm is run, is somehow 'optimal', i.e. to the best of our knowledge, error-free and the best fit between technology (e.g. software) and epistemic target. Under these optimal 'realization' conditions, we can say that beliefs about the real-world system that have been derived from the computer simulation are warranted.

Such a concession, however, brings us to a related, though distinct epistemological issue, namely, to the question whether the insights we arrive at by a computer simulation exceed the knowledge that was loaded into the simulation (e.g. in the form of a model) or whether the output just represents a detailed formulation of the in-principle predicted outcome. In other words, does the knowledge output exceed the knowledge input, quantitatively and qualitatively? Do computer simulations yield *novel* insights?

Winsberg wants to affirm that they do:

> '[…] simulation modeling, when successful, does reveal novel aspects of nature. Often simulation will enable us to produce a representation of a certain aspect of nature that is extremely difficult to observe. Even if the system in question can be observed in detail, often the simulation will bring a level of mathematical order where before there was only seemingly random detail.' [8, p. 286].

However, this brings us back to the issue of validation: we still need to be able to justify that the simulation has the potential to let us make inferences back to the world.

Given the wide variety of contexts and intentions in which, and with which, scientists pursue their epistemic goals with the help of computer simulations, these issues probably address only a very minor portion of instances, but the issues of verification and validation are not trivial (for more details, see Refs. [18, 19, 3]).

The pragmatic solution to both lies in what I want to capture here as 'transparency' and 'skill'.

Transparency relates to uncovering and taking into account the sources of the hypothetical character of computer simulation results, i.e. the potential sources of errors.

Computer simulations often produce only approximate solutions due to the analytically unsolvability of certain equation types; moreover, limitations in basic computing lead to round-off and truncation errors, which introduce a certain degree of imprecision into the solution. In general, computer simulations require a heightened awareness for potential error sources. Parker [20] exemplifies seven distinct types of errors, all of which ought to be accounted for when verifying computer simulation results (see Box 1).

Scientists are, thus, responsible for explicating why their results are *close enough* to the correct solution of the equations underlying the model assumptions to be reliable, by excluding, addressing, or qualifying potential errors. This process of making the potential imprecision transparent can serve as a quasi-form of formal verification.

Skill relates to a number of capacities involved in designing and implementing computer simulations. As such, simulating as a practice requires model constructions, thorough knowledge of how to build the simulation package and the simulation environment (i.e. the specifics of the device and software), and a knack for asking the relevant question that shall yield scientifically relevant results. It is this advanced interaction with

Box 1: Error sources according to Ref. [20].

1. Study design error
    a. Error due to limited number of simulation runs/trials
    b. Inadequate sampling method
2. Substantive modeling Error
    a. Error in equations for modeled processes (form, parameter values)
    b. No representation of relevant processes
    c. Overly simplified/erroneous initial and/or boundary conditions
3. Data processing error
    a. Error introduced by processing of raw simulation results
4. Solution algorithm error
    a. Inapplicable solution algorithm
    b. Unstable solution algorithm
5. Numerical error
    a. Discretization error
    b. Iterative convergence error
    c. Truncation error
6. Programming error
    a. Inadequate/faulty program design
    b. Coding typo/mistake
7. Hardware-related error
    a. Round-off error
    b. Internal malfunction
    c. External interference

theory and models that represents the true virtual aspect of computer simulations, insofar as the real world can give little feedback in the process (it gives data as input and computer simulation results as outputs, which can be compared with real-world data, but not in the course of the simulation). Winsberg speaks in this respect of the ‘techniques of simulations’ and off-loads the weight of validation onto them:

> ‘By the “techniques” of simulation, I am here referring to the whole host of activities, practices, and assumptions that go into carrying out a simulation. This includes assumptions about what parameters to include or neglect, rules of thumb about how to overcome computational difficulties – what model assumptions to use, what differencing sceme [sic] to employ, what symmetries to exploit – graphical techniques for visualizing data, and techniques for comparing and calibrating simulation results to known experimental and observational data. Whenever these techniques and assumptions are employed successfully, that is, whenever they produce results that fit well into the web of our previously accepted data, our observations, the results of our paper and pencil analyses, and our physical intuitions, whenever they make successful predictions or produce engineering accomplishments, their credibility as reliable techniques or reasonable assumptions grows.’ [9, pp. 121–122].

To close this section, let us return to the question whether computer simulation as scientific practice demands or warrants a new epistemology. The short answer is ‘no’. The basic principles of scientific inquiry are not overturned; if anything, they are more clearly exposed by computer simulations. According to Parker [20], computer simulations serve at least two epistemic functions: they might be used as heuristic tools wherein ‘the interaction with computer simulation models might help scientists to arrive at novel hypotheses to be subjected to further investigation via observation and experiment’ [20, p. 371], or they might be evidential resources, providing ‘good evidence for hypotheses about real-world target systems’ [20, p. 371], where good evidence might be not ‘exact’, but ‘good-enough’. In addition, as the practices involved in creating computer simulations are not exclusive to them, the philosophical implications are less accentuated: the ubiquitous use of models in simulation as well as in experimentation calls into question whether there are fundamental differences in the way scientists form new beliefs. Methodologically, simulation and experimentation share forms of abstraction that create more overlap than distinction, and in this context as well, the reliance on models renders the materiality/virtuality distinction obsolete. If there is work for the philosopher, it is to uncover the relation of models to theory and to nature [21], and to use computer simulation practices as further cornerstones of investigation.

4 Conclusion

The philosopher Humphreys [4] claimed that computer simulations allow scientists to ‘extend’ themselves, just like the telescope or the microscope extends our visual capacities. Computer simulations in this sense broaden our faculties, but exactly which faculties these are remain to be specified.

As an in-between thing, computer simulations also share a few features with thought experiments and mental imagination, especially with regard to the visualization aspect of simulations (on the heuristic value of visualizations in science, see Ref. [22]).

Even if computer simulations might not demand a new epistemology or a new philosophy of science, their cognitive merits are indisputable. Not only do they represent a highly demanding, knowledge-rich exercise but also a new class of interactive devices, which enhance scientific modeling practices and demand a new awareness of error sources. Moreover, they, like probably no other scientific instrument before, have the capacity to mimic features of the human mind, such as imagination and mental simulation. By visualizing and materializing abstract data, computer simulations help us to intuitively grasp the abstract while making it mathematically explicit at the same time.

In fact, while looking at the proposed merits of computer simulations, we can learn a lot about our own mental needs when we want to understand the world. However, this is a topic for a yet to be devised psychology of computer simulations.

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