SCIENCE IN THE AGE OF COMPUTER SIMULATION

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Abstract:

Computer simulation was pioneered as a scientific tool in meteorology and nuclear physics in the period directly following World War II, and since then has become indispensable in a growing number of disciplines. The list of sciences that make extensive use of computer simulation has grown to include astrophysics, particle physics, materials science, engineering, fluid mechanics, climate science, evolutionary biology, ecology, economics, decision theory, medicine, sociology, epidemiology, and many others. There are even a few disciplines, such as chaos theory and complexity theory, whose very existence has emerged alongside the development of the computational models they study. In Others word, Computer simulations have become a major source of information all over the scientific landscape, often used instead of experimentation to investigate phenomena. Until recently, however, they have received very little attention from philosophers of science.

After a slow start, philosophers of science have begun to devote more attention to the role of computer simulation in science. Several areas of philosophical interest in computer simulation have emerged: What is the structure of the epistemology of computer simulation? What is the relationship between computer simulation and experiment? Does computer simulation raise issues for the philosophy of science that are not fully covered by recent work on models more generally?

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1. What is Computer Simulation?

Computer simulations have become a major source of information all over the scientific landscape, often used instead of experimentation to investigate phenomena. Until recently, however, they have received very little attention from philosophers of science.

No single definition of computer simulation is appropriate. In the first place, the term is used in both a narrow and a broad sense. In the second place, one might want to understand the term from more than one point of view.

1.1 A Narrow definition

In its narrowest sense, a computer simulation is a program that is run on a computer and that uses step-by-step methods to explore the approximate behavior of a mathematical model. Usually this is a model of a real-world system (although the system in question might be an imaginary or hypothetical one). Such a computer program is a *computer simulation model*. One run of the program on the computer is a computer simulation of the system. The algorithm takes as its input a specification of the system's state (the value of all of its variables) at some time t. It then calculates the system's state at time t+1. From the values characterizing that second state, it then calculates the system's state at time t+2, and so on. When run on a computer, the algorithm thus produces a numerical picture of the evolution of the system's state, as it is conceptualized in the model.

This sequence of values for the model variables can be saved as a large collection of "data" and is often viewed on a computer screen using methods of visualization. Often, but certainly not always, the methods of visualization are designed to *mimic* the output of some scientific instrument—so that the simulation appears to be measuring a system of interest.

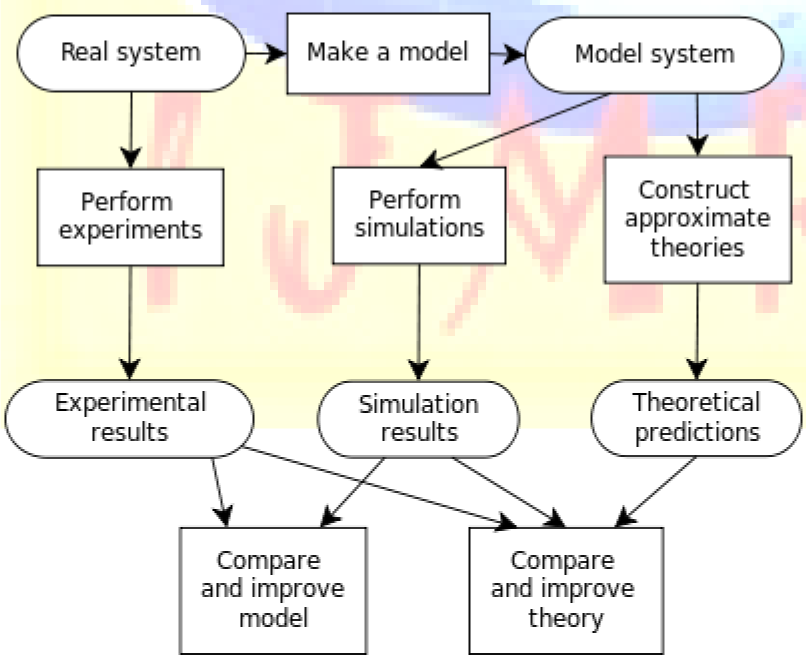
Sometimes the step-by-step methods of computer simulation are used because the model of interest contains continuous (differential) equations (which specify continuous rates of change in time) that cannot be solved analytically—either in principle or perhaps only in practice. But even as a narrow definition, this one should be read carefully, and not be taken to suggest that simulations are only used when there are analytically unsolvable equations in the model. Computer simulations are often used either because the original model itself contains discrete equations—which can be directly implemented in an algorithm suitable for simulation—or because the original model consists of something better described as *rules of evolution* than as *equations*.

1.2 A Broad Definition

More broadly, we can think of computer simulation as a comprehensive method for studying systems. In this broader sense of the term, it refers to an entire process. This process includes choosing a model; finding a way of implementing that model in a form that can be run on a computer; calculating the output of the algorithm; and visualizing and studying the resultant data. Simulations make creative use of calculational techniques that can only be motivated extra-mathematically and extra-theoretically. As such, unlike simple computations that can be carried out on a computer, the results of simulations are not automatically reliable. Much effort and expertise goes into deciding which simulation results are reliable and which are not."

1.3 An Alternative point of view

Both of the above definitions take computer simulation to be fundamentally about using a computer to solve, or to approximately solve, the mathematical equations of a model that is meant to represent some system—either real or hypothetical. Another approach is to try to define "simulation" independently of the notion of computer simulation, and then to define "computer simulation" compositionally: as a simulation that is carried out by a programmed digital computer. On this approach, a simulation is any system that is believed, or hoped, to have dynamical behavior that is similar enough to some other system.



2. Types of Computer Simulations

Two types of computer simulation are often distinguished: *equation-based simulations* and *agent-based* (or *individual-based*) *simulations*.

Computer Simulations of both types are used for three different general sorts of purposes: prediction (both pointwise and global/qualitative), understanding, and exploratory or heuristic purposes.

2.1 Equation-based Simulations

Equation-based simulations are most commonly used in the physical sciences and other sciences where there is governing theory that can guide the construction of mathematical models based on differential equations. Equation based simulations can either be particle-based, where there are n many discrete bodies and a set of differential equations governing their interaction, or they can be field-based, where there is a set of equations governing the time evolution of a continuous medium or field.

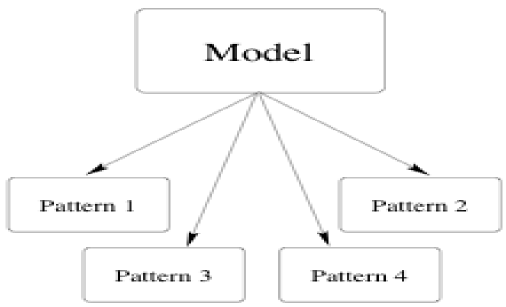
2.2 Agent-based simulations

Agent-based simulations are most common in the social and behavioral sciences, though we also find them in such disciplines as artificial life, epidemiology, ecology, and any discipline in which the networked interaction of many individuals is being studied. Agent-based simulations are similar to particle-based simulations in that they represent the behavior of n-many discrete individuals. But unlike equation-particle-based simulations, there are no global differential equations that govern the motions of the individuals. Rather, in agent-based simulations, the behavior of the individuals is dictated by their own local rules.

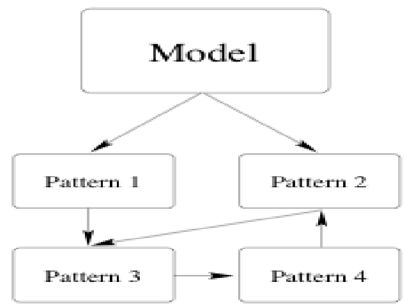
2.3 Monte Carlo Simulations

In the scientific literature, there is another large class of computer simulations called Monte Carlo (MC) Simulations. MC simulations are computer algorithms that use randomness to calculate the properties of a mathematical model and where the randomness of the algorithm is not a feature of the target model.

A nice example is the use of a random algorithm to calculate the value of π. If you draw a unit square on a piece of paper and inscribe a circle in it, and then randomly drop a collection of objects inside the square, the proportion of objects that land in the circle would be roughly equal to π/4. A computer simulation that simulated a procedure like that would be called a MC simulation for calculating π.



Observation



Explanation

3. Purposes of Simulation

1. Many situations are difficult to be modeled into conventional mathematical models such as linear programming, integer programming, etc. Sometimes, the approximation of real life parameters may not be desirable. In these cases, simulation is an effective way to model and analyze the situation.
2. Simulation may be cost effective as compared to real experimentation.
3. Sometimes, the observation of real system is impossible, as it is not yet implemented. The analysis of a manufacturing-system design through simulation is widely used before implementing the actual system.
4. Simulation provides modeling flexibility. Various parameters may be changed and various combinations of parameters may be evaluated.
5. Simulation provides the ease in modeling the system.
6. Simulation provides a faster way of evaluating the system. Many computer-based simulation models can evaluate the performance of the system in few hours. For the real life observations, many years are needed.
7. Simulation may be designed to have the graphic capability and on-screen display potential. For example, in few simulation packages of manufacturing system such as QUEST, WITNESS, etc., the color of a machine changes as soon as there is a failure of machines. This gives an immediate indication to the observer regarding the status of the system.
8. Simulation is normally associated with large observations over a period of time. Many inputs the system may contain a statistical distribution. For example, arrival of parts to a machine may be treated as coming from a normal distribution.
9. Simulation may have the capability to analyze the results in the statistical terms.

10. Simulation is a useful way to draw customer attention about the system performance. It also provides customer support.
11. Sometimes, the operation and observation of the system in a particular situation may be too dangerous or disruptive. In these cases, simulation is a good way to analyze the system's behavior.
12. Many times, simulation may be the only way to solve. In such situations, use of mathematical model of real life system is just impossible.
13. Simulation is useful to judge the system's behavior in a controlled environment. This is important when effect of changes in few parameters needs to observed.
14. Simulation provides a better understanding of the system.
15. Simulation is a useful teaching tool when there is a time limitation for working on a real system for many years and cost of procuring and handling the real system is too high.
16. Simulation is helpful in giving new insights of a complex system with facility to undertake wide experimentation in relatively lesser time. Wide experience may be developed in a lab setting.

4. The Epistemology of Computer Simulations

As computer simulation methods have gained importance in more and more disciplines, the issue of their trustworthiness for generating new knowledge has grown, especially when simulations are expected to be counted as epistemic peers with experiments and traditional analytic theoretical methods. The relevant question is always whether or not the results of a particular computer simulation are accurate enough for their intended purpose. If a simulation is being used to *forecast* weather, does it predict the variables we are interested in to a degree of accuracy that is sufficient to meet the needs of its consumers? If a simulation of the atmosphere above a Midwestern plain is being used to *understand* the structure of a severe thunderstorm, do we have confidence that the structures in the flow—the ones that will play an explanatory role in our account of why the storm sometimes splits in two, or why it sometimes forms tornados—are being depicted accurately enough to support our confidence in the explanation? If a simulation is being used in engineering and design, are the predictions made by the simulation reliable enough to sanction a particular choice of design parameters, or to sanction our belief that a particular design of airplane wing will function? Assuming that the answer to these questions is sometimes "yes", i.e. that these kinds of inferences are at least sometimes justified, the central philosophical question is: what justifies them? More generally, how can the claim that a simulation is good enough for its intended purpose be evaluated? These are the central questions of the epistemology of computer simulation (EOCS).

4.1 Novel features of EOCS

The epistemological issues that take center stage in traditional confirmation theory, an adequate EOCS must meet three conditions. In particular it must take account of the fact that the knowledge produced by computer simulations is the result of inferences that are *downward*, *motley*, and *autonomous*.

Downward. EOCS must reflect the fact that in a large number of cases, accepted scientific theories are the starting point for the construction of computer simulation models and play an important role in the justification of inferences from simulation results to conclusions about real-world target systems. The word "downward" was meant to signal the fact that, unlike most scientific inferences that have traditionally interested philosophers, which move *up* from observation instances to theories, here we have inferences that are drawn (in part) from high theory, *down* to particular features of phenomena.

Motley. EOCS must take into account that simulation results nevertheless typically depend not just on theory but on many other model ingredients and resources as well, including parameterizations (discussed above), numerical solution methods, mathematical tricks, approximations and idealizations, outright fictions, ad hoc assumptions, function libraries, compilers and computer hardware, and perhaps most importantly, the blood, sweat, and tears of much trial and error.

Autonomous. EOCS must take into account the autonomy of the knowledge produced by simulation in the sense that the knowledge produced by simulation cannot be sanctioned entirely by comparison with observation. Simulations are usually employed to study phenomena where data are sparse. In these circumstances, simulations are meant to replace experiments and observations as sources of data about the world because the relevant experiments or observations are out of reach, for principled, practical, or ethical reasons.

Parker (forthcoming) has made the point that the usefulness of these conditions is somewhat compromised by the fact that it is overly focused on simulation in the physical sciences, and other disciplines where simulation is theory-driven and equation-based.

4.2 Verification and Validation

Practitioners of simulation, particularly in engineering contexts, in weapons testing, and in climate science, tend to conceptualize the EOCS in terms of *verification and validation*. *Verification* is said to be the process of determining whether the output of the simulation approximates the true solutions to the differential equations of the original model. *Validation*, on the other hand, is said to be the process of determining whether the chosen model is a good enough representation of the real-world system for the purpose of the simulation. The literature on verification and validation from engineers and scientists is enormous and it is beginning to receive some attention from philosophers.

Parker (forthcoming), claims that "Current practice in verification and validation fits Winsberg's vision of a motley epistemology of computer simulation: practitioners employ a wide-ranging toolkit of methods, which they continue to expand and improve, but there are no simple recipes."

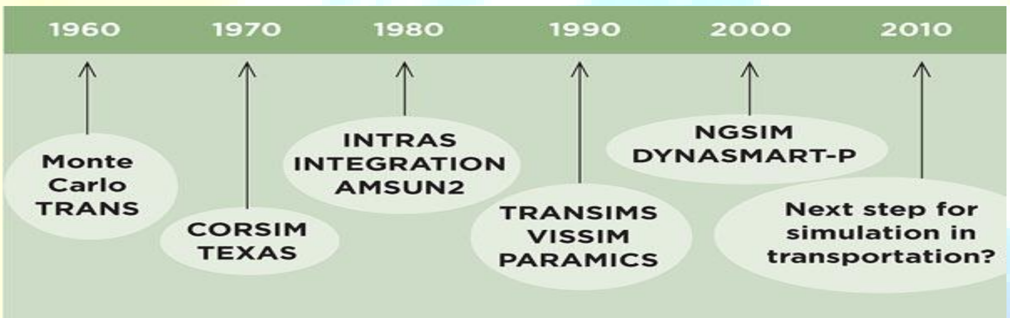
Verification can be divided into solution verification and code verification. The former verifies that the output of the *intended algorithm* approximates the true solutions to the differential equations of the original model. The latter verifies that the code, as written, carries out the intended algorithm. Code verification has been mostly ignored by philosophers of science; probably because it has been seen as more of a problem in computer science than in empirical science—perhaps a mistake. Part of solution verification consists in comparing computed output with analytic solutions (so called "benchmark solutions"). Though this method can of course help to make case for the results of a computer simulation, it is *by itself inadequate*, since simulations are often used precisely because analytic solution is unavailable for regions of solution space that are of interest. Other indirect techniques are available: the most important of which is probably checking to see whether and at what rate computed output converges to a stable solution as the time and spatial resolution of the discretization grid gets finer.

The principal strategy of validation involves comparing model output with observable data. Again, of course, this strategy is limited in most cases, where simulations are being run because observable data are sparse. But complex strategies can be employed, including comparing the output of subsystems of a simulation to relevant experiments

5. Simulation and Experiment

Working scientists sometimes describe simulation studies in experimental terms. The connection between simulation and experiment probably goes back as far as von Neumann, who, when advocating very early on for the use of computers in physics, noted that many difficult experiments had to be conducted merely to determine facts that ought, in principle, to be derivable from theory. Once von Neumann's vision became a reality, and some of these experiments began to be replaced by simulations, it became somewhat natural to view them as versions of experiment.

A simulation that accurately mimics a complex phenomenon contains a wealth of information about that phenomenon. Variables such as temperature, pressure, humidity, and wind velocity are evaluated at thousands of points by the supercomputer as it simulates the development of a storm, for example. Such data, which far exceed anything that could be gained from launching a fleet of weather balloons, reveals intimate details of what is going on in the storm cloud.



6. Emergence

The connection between emergence and simulation was perhaps best articulated. Conception of emergence must meet the twin hallmarks of explaining how the whole depends on its parts and how the whole is independent of its parts. Philosophers often focus on what he calls “strong” emergence, which posits brute downward causation that is irreducible in principle. But he argues that this is a mistake. Focuses instead on what he calls “weak” emergence, which *allows* for reducibility of wholes to parts *in principle* but not *in practice*. Systems that produce emergent properties are mere mechanisms, but the mechanisms are very complex . As a result, there is no way to figure out exactly what will happen given a specific set of initial and boundary conditions, except to “crawl the causal web”. It is here that the connection to computer simulation arises.

7. Fictions

Models of course involve idealizations. But it has been argued that some kinds of idealization, which play an especially prominent role in the kinds of modeling involved in computer simulation, are special—to the point that they deserve the title of "fiction." This section will discuss attempts to define fictions and explore their role in computer simulation.

There are two different lines of thinking about the role of fictions in science. According to one, all models are fictions. This line of thinking is motivated by considering the role, for example, of "the ideal pendulum" in science(e.g., "the ideal pendulum has a period proportional to the square-root of its length").

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