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Nanoscience and the Janus-Faced Character of Simulations

Johannes LENHARD
Institute for Science and Technology Studies, University of Bielefeld
johannes.lenhard@uni-bielefeld.de

Abstract. In nanoscience, simulations (partly) take the place of "real" experiments. For example: in a simulation, well-known physical laws can produce surprising behaviors. It is argued that simulations are both part of experimental practice and form a theoretical instrument, inducing a methodological shift in scientific practice: if one desires a "quantitative understanding" of matter at the nanoscale, one must rest content with the ability of simulations to imitate systems and cannot ask for more direct means of validation.

1. Illustration: Simulation in Nanoscience

At the beginning, I would like to discuss two examples of simulations in nanoscience. There is, of course, a wide variety of simulations used in nanoscience as well as in other branches of science. The following examples are by no means exhaustive, rather they illustrate some typical properties of simulations and give a glimpse of some problems connected with them.

Both examples stem from Uzi Landman, director of Georgia Tech's Center for Computational Materials Science. In a landmark 1990 *Science* paper, Landman and his coworkers employed large-scale molecular dynamics simulations. They showed that when a nickel tip was brought into close proximity to a sheet of gold, gold atoms would jump from the sheet to the probe (Landman 1990).

Figure 1 consists of six (simulated) snapshots. On the upper left, a nickel tip has crushed into a gold surface. On the following slides, the tip is removed slowly and a thin wire of gold atoms is generated. The coloring is added to make the visualization more convenient. The atomic layers in figure 1 are marked with different shades of gray, the original images used artificial coloring which is here adapted to black-and-white print. Hence, unfortunately, the images loose a great deal of what F. Rohrlich (1991) has called the character of simulations as "dynamically anschaulich". Landman describes his situation as being very similar to that of an experimenter who is watching the outcome of a complicated experimental setup. I quote Landman from an interview:

> To our amazement, we found the gold atoms jumping to contact the nickel probe at short distances. Then we did simulations in which we withdrew the tip after contact and found that a nanometer-sized wire made of gold was created. That gold would deform in this manner amazed us, because gold is not supposed to do this.

Their "amazement" is also theoretically amazing, because well-known physical laws at the atomic level served as the basis of the simulation that, in turn, showed unexpected behavior at the nanoscale. The formation of a nanowire was, at that time, a prediction. It was confirmed by experiment with AFM some years later.

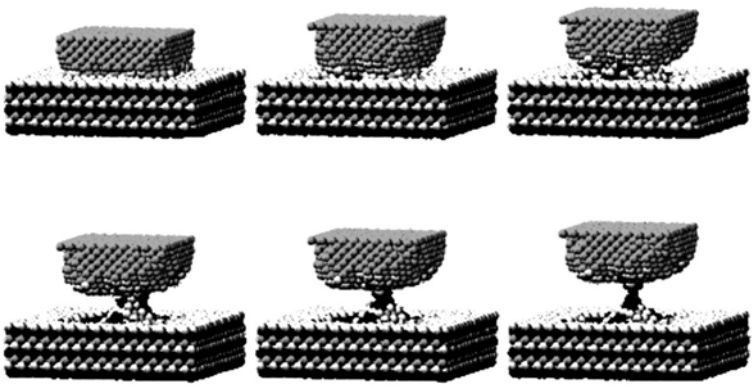

Figure 1. A nanowire of gold atoms emerges between a nickel tip and a sheet of gold (from Landman 1990).

The second example is concerned with lubrication and the properties of lubricants that are confined to very small, that is, nanoscaled spaces. When confined to tight spaces, long-chain lubricant molecules seem to act more like "soft solids" than like fluids.

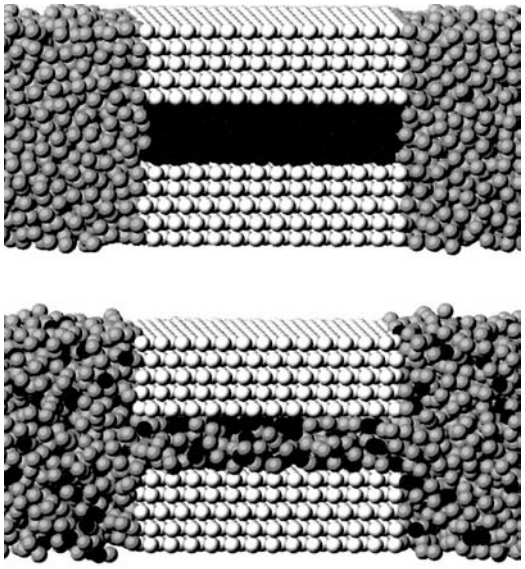

Figure 2. Ordered high friction state (upper image) and oscillation-induced disordered low friction state (from Landman 2001)

The result of a numerical experiment with two sliding surfaces is shown in figure 2. Two surfaces (light-colored, originally yellow) are sliding one against the other. Lubricant molecules are in the small, nanosized, gap between the surfaces, as well as in the bulk outside. The upper part of the picture again shows a simulated snapshot: the molecules of the lubricant are forming *ordered* layers that significantly influence the movement of sliding surfaces as friction increases. The molecules that are confined between the surfaces are colored dark. (The coloring of the original visualization on the computer screen is much more vivid.) Landman also tried to "overcome the problem" of high friction in a simulation

study. Carrying forward the molecular dynamics simulations, he manipulated the movement of the slides. The simulation shows how oscillating the gap between the two sliding surfaces reduces the order of thin-film lubricant molecules (thereby lowering the friction). In the lower part of the image, molecules that had been confined within the surface, and which where marked red after the first snapshot, have moved out into the bulk lubricant unconfined, and molecules from the bulk areas have moved into the gap. (Admittedly, that is hard to recognize without colors.) These "soft-solid"-properties are unexpected from the normal behavior of fluids. Again quoting Landman:

> We are accumulating more and more evidence that such confined fluids behave in ways that are very different from bulk ones, and there is no way to extrapolate the behavior from the large scale to the very small. (Landman 2001)

Again one is confronted with really surprising behavior, even though the theoretical ingredients of the simulation are well-known. (To be sure, it is very demanding to implement a simulation model in a parallel computing environment.)

For his achievements, Landman has received several prizes, *e.g.* the Feynman prize in theoretical nanotechnology (2000), and the Materials Research Society Award (2002) for "the development and implementation of research methodologies that use molecular dynamics simulations to predict the often-surprising behavior that occurs at the nanoscale when surfaces of solid and liquid materials meet" (press statement, see Landman 2002).

The examples should illustrate that using simulations is an important part of nanoscience. Furthermore, the cases exhibited some intriguing properties that shape the practice of nanoscience. I will argue that this gives reason, in turn, to revise some central concepts in the philosophy of science.

2. The Epistemic Status of Simulations

2.1 Simulations as Models of Second Order

Recall the statement of Landman about accumulating evidence for unexpected behavior. By what means is this new evidence obtained? And in what sense is it unexpected? To tackle these questions, it is necessary to consider the epistemic status of simulations.

Traditionally, mathematical modeling is oriented to the paradigm of partial differential equations (PDE) that model the propagation of a system governed by natural laws. One can say that PDE and the analytical tools of the differential calculus fit like gloves. (And do so since the days of Leibniz, Newton, and the Bernouillis.)

But in complex systems this approach encounters severe difficulties. H. Poincaré was among the first to experience this when he was conducting equally ingenious and tedious calculations to solve the so-called three-body-problem. At last, he had to acknowledge the insolubility of this problem. Even seemingly simple questions about highly idealized systems with only a very limited number of particles can be very difficult to treat. The question whether our solar system is stable, is of that kind. This observation applies even more so to systems with many interacting particles, like the cases from nanoscience that were considered above. With mathematical-analytical means it is nearly hopeless to achieve interesting results. As Dirac, for instance, had observed, although the basic quantum laws governing large parts of physics and chemistry are known, progress will still be obstructed by the fact that the pertinent equations are too difficult to solve. In particular, this observation applies to the laws governing the nanoscale. You have a mathematical model, but it doesn't help you. In a certain sense, simulations help to circumvent this problem. They are a kind of imitation in the computer of mathematical models. In other words, simulations build a *model* of the mathematical model, namely of the system of equations.

One should be aware of the fact that simulations are not mere calculations in the sense that they would provide just a numerical solution of the original equations that are analytically unsolvable. Surely, there are important differences between an analytical solution and a numerical one. The former typically provides information about what will happen when some initial conditions are altered, while a numerical solution provides nothing of that kind. If anything is altered, everything has to be computed again. While this might not be a serious constraint, because computational time is cheap, it constitutes a fundamental difference between analytical and numerical solutions. I want to stress, however, that this difference does not concern the essential point here.

Often simulations do not intend to *solve* a system of continuous non-linear partial differential equations at all. Instead, such a system is replaced by a discrete model, that is, the mathematical model is modeled again. Simulations work with a discrete version of the mathematical equations and it is a rather difficult task to construct a simulation model that is at once computationally treatable and sufficiently similar to the original system. This, one could say, is the generic problem of modeling – to find a tractable and at the same time adequate analogue. P. Humphreys (1991) has remarked that the approach of computer simulations broadens the realm of tractable mathematics enormously. Much in the same way as PDE and the differential calculus fit to each other, simulation models and the computer fit. (I use simulation and computer simulation equivocally.) Mathematically intractable models become computationally tractable models. Thereby, the art of modeling changes.

I propose that simulations involve a specific kind of modeling that can be called 'modeling of the 2nd order'. For example, the problem of finding an adequate discretization is typical for simulation modeling. At the same time this problem is an instance of a more general type of problem: the adequacy of a certain model always needs to be considered in scientific, or mathematical, modeling. Thus, firstly, there are specific problems connected with simulations, and secondly, these problems are of a type generally found in modeling. For this reason, I prefer to speak of *simulation modeling* to indicate that the core of simulation consists of a special kind of modeling. Another was of putting this: simulations are second order models (see Küppers & Lenhard 2003, 2004). Admittedly, in fields like mathematics or physics, models of models are common – as indicated by the verdict of the mathematician Stefan Banach that good mathematician see analogies between models and theories, while the best see analogies between analogies. So, what is peculiar about simulations? It is how the modeling is carried out and which new possibilities open up. A decisive point is that simulation modeling borrows from experimental practices.

The concept of experiment is itself a much debated topic in philosophy and history of science (see, for example, Radder 2003), thus one would not be well advised to use this concept as a fixed basis of philosophical analysis. To me, it seems promising to argue along empirical case studies, so to say a methodologically mixed approach. A heuristic use of 'experiment' appears admissible, even if the concept is not well defined. Anyway, simulation experiments are part of scientific practice and I will argue that a philosophical account of what an experiment is can learn from that.

2.2 Experimental Practice with a New Theoretical Instrument

Having implemented such a simulation model, one is able to *observe* what happens when the system evolves in time and what surprises it may offer. Taking into account the enormous capacity for visualization that is provided by the computer, the use of the term "observation" appears well justified.

Admittedly, one can think of the behavior of such a system as guided by natural laws, for example by the Schrödinger-equation, and indeed this was the starting point of our ex-

amples. But this is, as Dirac had observed, only a consideration "in principle". In fact one is simply not able to derive the observed properties from general theory.

Simulations of the kind performed by Landman therefore look like experiments in the computer. This experimental aspect of simulations has attracted some attention of philosophers and has occasioned a series of perspicacious investigations. However, there is no consensus on how the experimental aspects should be grasped conceptually (see Humphreys 1995/96, Hughes 1999, Fox Keller 2003, or Winsberg 2003.) I like to point to the stance of the scientists: The examples have highlighted how even a computer scientist's behavior resembles that of an experimenter. One can be amazed or even surprised by unexpected observations. Simulations are thus part of the experimental practice of, for example, nanoscience.

The above statement is clearly a one-sided account of simulations since simulations are also theoretical instruments. Obviously, simulations are based on highly theoretical efforts of applied mathematics and computer science. Without recent progress in applied mathematics one would not be able to tackle most of the problems actually investigated by simulation methods. Again, Landman's efforts provide a good example: what is implemented are models, guided by general laws of interaction between atoms (the Schrödinger equation).

2.3 Simulation as a New Method?

In philosophical literature, one can find claims about the hybrid status of simulations. For example, "their use requires a new conception of the relation between theoretical models and their applications" (Humphreys 1991, p. 497). And Peter Galison speaks of simulations as a "Tertium Quid" between experiments and theory (Galison 1996). I find it very attractive to think of simulations as crossing the boundaries of experiment and theory. As the last two concepts are not understood very consistently, the considered cases can provide reason to doubt the existence of a clear-cut boundary between experiment and theory in the first place.

The main line of philosophical debate is whether simulations present an entirely new method of science or not. I find the claim of novelty rather convincing. While the computational powers of the electronic computer are necessary, they by no means determine the whole picture. Simulation is faster than computation. The methodological ingredients, so to say, are standard – extensive experimentation and model building. But their combination seems to be very specific, constituting a new methodological approach.

I have argued for both points: Simulations are part of experimental practice and simulations are theoretical instruments – new instruments that bring with them a new practice that is still in flux in many scientific fields. It appears astonishing how components as divergent as experiment and theory can merge in such an effective way. What traditionally counts as a problem or even a painful insight in the philosophy of science, namely that observation is always theoretically "contaminated", now seems to be part and parcel of the method itself. This may be seen as a change of the very conception of experimentation, one that transposes *explanans* and *explanandum*: Instead of explaining simulation as a hybrid, constituted from experiments (and other ingredients), one could take the practice of simulation as a starting point, contributing to the question of what is meant by "experiment". As Alfred Nordmann has pointed out in discussion, the concept of experiment causes constantly philosophical troubles, so it could be fortunate not to take it as a basis.

3. Back to Nanoscience

In May 2002, a DOE-Workshop on "Theory and Modeling in Nanoscience" took place. The report formulates the *Central Challenge*: "Because of the rapid advance of experimental investigations in this area, the need for quantitative understanding of matter at the nanoscale is becoming more urgent, and its absence is increasingly a barrier to progress in the field quite generally" (DOE 2002, p. 5).

Let us assume that the report is right in stating that the missing quantitative understanding is one of the central problems of nanoscience. This raises the question whether simulations are part of the problem or part of the solution?

On the one hand, simulation is an experimental practice that requires theoretical understanding. In the case of the golden nanowire, created by withdrawing a nickel tip, the amazing behavior could be observed, and even validated independently, but the simulation does not offer an explanation in the usual sense. Clearly, the laws that are implemented in the simulation model produce the behavior – somehow. The simulation, mediating between the general Schrödinger-equation and a concrete wire, has rendered the phenomenon somewhat opaque. Despite being obviously theory-based, the simulation does not offer something like a theory-based insight! In this respect and emphasizing the term "understanding", simulation does not provide "quantitative understanding of matter" and is therefore part of the problem.

On the other hand, simulations are quantitative and present an opportunity to explore the field where no general and accepted theoretical basis exists, or at least, where it is not applicable. Dirac's verdict that the knowledge of the guiding laws does not lead to an understanding of behavior in complex situations, expresses a rather general fact. Mathematical insights into computational complexity indicate that this situation will persist: general laws are often useless in concrete situation of applied problems. One has to look after instruments that scientists can work with and that allow for a kind of understanding so that manipulation becomes possible. What is at stake is thus the potential for intervention. In *this* respect and emphasizing the term "quantitative" in "quantitative understanding of matter", simulations seem to provide a solution. In the case of the moving slides, for instance, the manipulation of the movement, from a flat to a slightly oscillating one, restored the desired properties of the lubricant. Therefore, too, simulations can be seen to be part of the solution.

I do not intend to give an unequivocal answer to the question whether simulations are part of the problem or of the solution. The adequate court to address this question would be the future development of nanoscience.

While it seems to be adequate to conceive of simulations as a quantitative approach, the question is whether it can provide genuine understanding. I have argued that simulations involve a second order modeling and this causes serious problems of validation. Simply put, simulation results have to face the objection that they are "only imitating" the real system.

In the case of nanoscience, however, it seems to be questionable whether another approach that provides genuine understanding and thereby overcomes the barrier diagnosed in the DOE-workshop, is possible at all. In this field, there is perhaps simply no alternative to simulation.

Let me consider as a further case so-called density functional theory (DFT), a fundamental theory in computational chemistry. It is especially useful for dealing with the properties of larger molecules that have many interacting electrons. The situation is quite similar to Dirac's problem, that is, the properties should in principle follow from the Schrödinger-equations, but the number of involved electrons makes a solution unachievable. The point of DFT is to replace the many interacting electrons by an electron density function.

The DFT was essentially developed by W. Kohn in the late 1960s. Since it offers a strict simplification, theoreticians question the justification of its use, but it turned out to be an effective approach in computational chemistry. However, the application of DFT is far from trivial. In fact, only with the availability of simulation programs has DFT become applicable in a wider range of quantum chemistry problems. Again, the mediating simulation models make the relation between theory and phenomena opaque. The DFT is used to obtain quantitative rules and its success is unquestioned. Consequently, in 1998 the Nobel Prize in chemistry went to W. Kohn and A. Pople to equal parts. The latter had written extensive simulation programs that ensured DFT's widespread use.

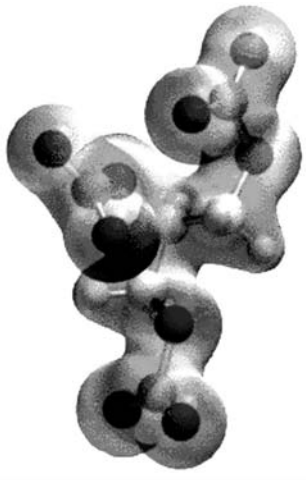

Figure 3: Electron density of nitroglycerine, The Coloring is altered to fit black-and-white print (from the Nobel e-Museum, http://www.nobel.se/chemistry/laureates/1998/illpres/density.html).

That simulations have become eligible for a Nobel Prize underlines their status as theoretical instruments. This leads us directly back to the report on "Theory and Modeling in Nanoscience" and its call for more quantitative understanding. The report mentions a paradigmatic example for the success of nanotechnology. It is the so-called Giant Magnetoresistance (GMR) that has led to miniaturized hard-disks only a few years after the discovery of this rather obscure effect. The key for this extraordinary quick development from an obscure effect to a reliable product of nanotechnology was just the "quantitative understanding" that could be provided by DFT. The report itself thus provides an instance for the desired kind of "quantitative understanding", namely the DFT-account of the GMR which is essentially a simulation-based approach.

The goal is not theory-based insight as it is elaborated in the philosophical literature about scientific explanation. Rather, the goal is to find stable design-rules, rules that might even be sufficient to build a reliable nano-device.[1] Thus, clearly, simulation does not meet the high standards of theoretical explanation, nevertheless, it offers potential for intervention. This challenges the received criteria for what may count as adequate quantitative understanding.

We have observed that simulations have a Janus-faced character which reveals properties of both experiment and theory. Yet, the hybrid epistemological status of simulations is precisely what undermines the alternative assumed in the question. Thus, I conclude that simulations are both part of the problem *and* the solution. The judgment depends on how the problem is formulated and "understanding" is conceived. From the perspective of theory-based explanations, simulations are part of the problem. But they answer the needs of applied science to work with stable design-rules. From this perspective, therefore, simulations also offer the solution.

The simulation method is continuing its triumphal march through large parts of the sciences, observable particularly in nanoscience. The methodological shift connected with simulations seems to indicate that the role of design-rules becomes more important at the expense of theories. And this, in turn, has the potential to change the very conception of scientific understanding.

Acknowledgment

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Notes

[1] See Roukes 2001 for a consideration of rules versus laws. The claim that theory leaves centre stage is not uncommon in current science studies, see, for example, Hessenbruch 2003.

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