Thought Experiments and Simulation Experiments:

Exploring Hypothetical Worlds

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1. Introduction

Both thought experiments and simulation experiments apparently belong to the family of experiments, though they are somewhat special members because they work without intervention into the natural world. Instead they explore hypothetical worlds. For this reason many have wondered whether referring to them as "experiments" is justified at all. While most authors are concerned with only one type of "imagined" experiment – either simulation or thought experiment – the present chapter hopes to gain new insight by considering what the two types of experiment share, and what they do not. A close look reveals at least one fundamental methodological difference between thought and simulation experiments: while thought experiments are a cognitive process that employs intuition, simulation experiments rest on automated iterations of formal algorithms. It will be argued that this difference has important epistemological ramifications.

Section two will review positions in the literature that are concerned with the relationship between these types of experiment. The relatively few contributions vary greatly, and the matter is complicated by the fact that neither thought experiments nor simulation experiments have agreed upon definitions. This results in contributions that highlight different similarities and dissimilarities. After this overview, section three will undertake to combine the various insights about similarities and dissimilarities between the two types of experiment. Both thought and simulation experiments explore hypothetical worlds, but via different means – and the main claim is that this matters for epistemology. While thought experiments are – in a sense to be explained later – "epistemically transparent," simulation experiments can be called "epistemically opaque." Consequently, surprises play a more significant role in the latter. If this claim is correct, an immediate question arises: in what sense do simulation experiments create opacity, and how they deal with it? This question will be addressed in section four, where a number of examples are analyzed from the perspective of this question. The concluding fifth section puts forward a consideration about the common ancestral line of thought experiments and simulation experiments, and considers what this says about scientific rationality.

2. **Debates about Taxonomy**

In this section we will try to gain some insight by comparing thought experiments and simulation experiments. This task is complicated by the fact that the status (and closeness) of both as family members is controversial. Let us start therefore with a brief consideration of thought experiments, the older sibling, not with a general discussion, but one oriented at facilitating a comparison to simulation experiments.

2.1 **Thought Experiments**

Obviously thought experiments are extremely economical experiments – intricate conditions can be represented cheaply in thought. It is controversial, however, whether this is an epistemological advantage or disadvantage. Do they play a merely heuristic role, or do they generate trustworthy knowledge? Empirical experiments bring scientific hypotheses and the natural world into contact, which is to say, they integrate them as independent witnesses. Isn't this contact an essential part of the notion of experiment? If so it would be highly problematic to speak of thought "experimentation."[1]

Ian Hacking (1983) is responsible for a famous argument according to which experimental interventions justify a realistic conception of scientific objects. Experiments lead an incorruptible

[1] The experimental character of thought experiments is treated in a separate chapter of this volume. Since the literature on thought experiments is also extensively discussed, I will only reference the contributions on this issue by Jim Brown, David Gooding, John Norton, Nancy Nersessian, and Ian Hacking (all 1993) to a symposium at PSA 1992. These provide a good entry point into the recent discussions in philosophy of science. Hacking as well as Paul Humphreys (1993) favor a more critical outlook on the epistemic virtues of thought experiments.

“life of their own.” This is what Hacking denies for thought experiments (Hacking 1993). What then characterizes thought experiments in a positive way?

One important facet is that they make certain intuitions accessible. Thought experiments have to meet high standards of intelligibility, because the whole process takes place in cognition. If it is ever unclear what happens next, that is, if one cannot comprehend why a certain outcome should happen, the thought experiment fails. It does not fail because of an unwanted outcome, but because it does not work *as a thought experiment*. In this sense, the perceived transparency is a precondition for the feasibility of experimenting in thought.

Is this precondition a strength or a weakness? Jim Brown, among others, advocates the former (see e.g. 1992) and takes intuitive accessibility as indicating credibility, or truth. Brown favours a Platonic account according to which thought experiments allow humans to peek into Plato’s heaven. He focuses on the methods and results of mathematics which are arguably a special case of thought experimentation because of its completely hypothetical form. The context in this case is fixed by definition. Take as an example the often cited checker board problem: First cut out two squares from diagonal corners of a checkerboard. Is it still possible to arrange the board into rectangular pieces, each consisting of one white and one black square? Here, the question defines the problem so that asking whether the problem is adequately posed is missing the point.

In contrast to logico-mathematical puzzle solving, the question of adequate formulation matters in cases that are related to applications. The wonderful thought experiment with a light-clock in a space ship might serve as an example. This clock consists of two perfect mirrors between which a light pulse “ticks.” The space ship starts from the earth, perpendicular to the clock’s light pulse, and the clock is viewed from two different perspectives: an observer on earth and an astronaut in the ship. Because of the constancy of the speed of light, the clock ticks with the same speed for both observers. Seen from the earthling’s perspective, however, the ship moves, hence the light pulse has to travel a slightly longer way from one mirror to the other. Since it has the same speed but a longer way to travel, time itself has to be stretched accordingly. Now, the formula for time dilatation follows elegantly from the theorem of Pythagoras.[2] The full derivation does not matter here, because my point is a different one.

The thought experiment happens in a setting or scenario that might be misleading. There is no guarantee that this experiment, as elegant as it might be, will lead to the correct formula for time dilatation. Perhaps it is not that the result is justified by the premises, but the other way around. The somewhat exotic setting of the experiment is first accepted, because it gives the right (already known) formula. Afterwards, the argument has sedimented and became a thought experiment. The result of relativity theory, time-dilatation, is not questioned at any time, rather it is ennobled when we show that it is accessible even from a thought experiment.

This role for thought experiments (to only *seem* to establish) is well-known in the literature. For instance, Humphreys assumes it when he highlights the exploratory function of thought experiments that makes clear which assumptions are necessary to obtain a given conclusion (Humphreys 1993, 218). Once an experiment has been worked out – like in the example above – it changes into a rhetorical instrument, targeted rather at an already known formula than establishing something unknown. Ian Hacking also directs attention to the state when a thought experiment has been worked out. At this point, outcome is no longer at stake. For this reason Hacking describes such experiments as “fixed, rather immutable” (Hacking 1993, 307). Finally, Ulrich Kühne, in his monograph on thought experiments (2005), sees their main function in cementing knowledge rather than creating it. However, he urges us to consider more carefully the *evolution* of thought experiments. Only by analyzing the development from exploration toward an accepted, fixed form can we understand their main characteristics.

There is a reason why the activity of performing a thought experiment might lead to further development of the same experiment, and also to its eventual convergence to an “immutable” state. Thought experiments, whatever their aim or function, explore imaginary scenarios that provide a certain setting or context. During the exploratory phase, such a context might be

[2] See Schwinger 1987, chapter 2, for a detailed version of this experiment.

useful, especially in cases when that context is not fully explicated and contains a surplus of possibly relevant material that can be exploited for creating and framing the thought experiment. In situations where complex actions are modeled, such a context might include a rich but implicit reservoir of additional aspects and facts that are also relevant. Nancy Nersessian (1993) stresses this potential when she counts thought experiments as a class of model-based reasoning. Experimenters take the model for granted and let it lead the way.

Certainly the course of the experiment has to fulfill high standards of transparency. Gaps in the argumentation like "the reader might calculate easily" have to be ruled out. Instead, all phases of the experiment have to flow more or less continuously and without creating any gap in the mind. Of course, this need not happen on the first attempt; it might require a couple of iterations. Such iterations, if successful, efface any initial opacity and hopefully make possible free access to a clear intuitive judgement.

It might require some effort to satisfy this condition. Galileo, for example, reckoned it necessary to spend 20 pages in the *Discorsi* for making plausible what happens in the famous thought experiment with two falling and (un-)connected bodies (for more on this thought experiment, see Chapter 5). There is regular dispute about whether certain thought experiments are indeed feasible or have gaps. Bohr and Einstein are a case in point for duels of this kind (see Bishop 1999). Hence thought experiments, or proposals for thought experiments, might be changed or even overthrown during the exploratory phase. Initial opacity about what follows in a given model or scenario requires iteration and critical discussion. One condition, again, is crucial: If the proposal shall eventually be accepted as a thought experiment, iteration has to efface opacity. Only an epistemically transparent process is able to sediment into a thought experiment – maybe with the qualification that a consensus among a group of educated people (and educated intuitions) is sufficient.

2.2 **Simulation experiments**

Simulation experiments are a newborn sibling in the family of experiments. Their epistemic status is arguably the most debated topic in the growing literature on computer simulation. The general strategy is to discuss the status of simulation experiments by locating them in an established coordinate system, i.e., by stressing certain similarities and dissimilarities to other methods. A most striking feature is that these experiments do not intervene in the natural world. This makes them similar to thought experiments, and inspires the hope that a comparative epistemological study will bear fruit.

Simulation experiments seem to be a special kind of experiment. They investigate the behaviour of simulation models by computer methods and have been analyzed as experiments with models, virtual experiments, or experiments without materiality (respectively by Deborah Dowling 1999, Eric Winsberg 2003, and Mary Morgan 2003, to name just a small sample of the growing philosophical literature). Although simulation experiments appear to be at least partially experimental, it is controversial in the philosophical literature whether this justifies speaking of them as experiments. Depending on what we take to be essential for being an "experiment," simulation experiments are advocated as a new kind of experiment, or not as experiments at all. To different degrees, Francesco Guala (2002), Morgan (2003, 2005), and Anouk Barberousse et al. (2009) argue for the latter standpoint, while Winsberg (2003, 2009) and Wendy Parker (2009) want to include simulation experiments into the esteemed family of experiments. However, I do not intend to enter the taxonomical debate on the status of simulations, rather I will focus on the comparison between simulation experiments and thought experiments.

Only a relatively small number of contributions exist that tackle the relationship between these two types of experiments. Some of them come from researchers working with simulation experiments, notably in the field of social simulations. While many or most scientific fields with well-established experimental traditions, like physics or mechanical engineering, have added simulation experiments to their repertoires, the problem of categorizing the experimental practices comes up in social simulation in a particular way. The whole field came into existence with simulation methods, so there is no methodological tradition of manipulating models or doing experiments *apart* from simulation. Thus it seems plausible that the question for scientists who reflect about their own practice is especially pressing. It seems, at least, that there is no direct interrelationship possible between simulation experiments and experiments that would intervene into the natural world to check whether the former got it right. Hence scientists like di Paolo et al. (2000) take thought experiments as point of comparison, exactly because thought experiments have an independent history as method and also do not intervene.[3]

Di Paolo et al. (2000) categorize simulation experiments as “opaque thought experiments,” meaning that they explore the interplay of hypothetical assumptions, but in a computational way that human beings could not follow. Di Paolo and his colleagues touch upon a most important point when they bring opacity into play. This notion will play a major role in the following discussion. However, from a logical point of view, it seems a bit misleading to subsume simulation experiments under thought experiments. It has been argued above that epistemic transparency is an essential precondition for thought experiments; hence, speaking of opaque thought experiments seems questionable or even inconsistent.

Aside from social scientists, there are also philosophers of science who have asked whether simulation experiments should be counted as a sort of thought experiment. The fact that interventions are missing from both is the genus proximum, but then opinions diverge. Claus Beisbart and John D. Norton (2012) argue that thought and simulation experiments only logically analyze some set of starting assumptions. Hence they both do not belong to the family of experiments, but to that of arguments – a position that Norton has earlier advocated with regard to thought experiments.

Sanjay Chandrasekharan et al. (2012) also analyze the way both experiment types deal with their assumptions, but arrive at a different conclusion. They stress that a thought experiment starts

[3] In general, it is a widely distributed opinion in the field of social simulation and artificial societies that thought experiments are the adequate benchmark for simulation experiments. Michael Weisberg (2013) analyzes how thought experiments and simulations both represent target systems, though he admittedly does not discuss further aspects of their relationship.

rather with a mental model than with a set of logical assumptions, and proceeds by analyzing this model in intuition – also a standpoint earlier advocated by the co-authoring Nersessian (see Chapter 18). Simulation experiments are similar to thought experiments, since both are a sort of model-based reasoning. However, simulation experiments, unlike thought experiments, are not tied to intuition, but can utilize a range of algorithmic procedures. Therefore, Chandrasekharan et al. conclude that simulations will likely outpace (and eventually *re*place) thought experiments.

Finally, Rawad El Skaf and Cyrille Imbert (2013) take an ecumenic stance and re-conceptualize the genus proximum. They underline that thought experiments as well as simulation experiments proceed by allowing us to see how a scenario unfolds. According to this view, the initial assumptions or hypotheses from which one starts somehow entail what will happen in the experiment and hence determine its outcome. The outcome is not initially known. Instead, it takes the unfolding as part of an experimental process that brings to light what was actually included already in the hypotheses. This viewpoint seems to be compatible with Nersessian's as well as with Norton's, at the cost of accepting a broad spectrum of what "unfolding a scenario" means.

There is of course a counterpart in the literature that also stresses the dissimilarities between thought and simulation experiments, especially with respect to their "unfolding" processes. Humphreys (1993), for instance, rightly points out that algorithmic processes are very different from the processes of intuition. From this perspective, thought and simulation experiments take place in very different realms. Let us turn therefore to the compatibility of the two kinds of experiment in more detail.

3. Experimenting, Iteration, and Opacity

A most important difference between thought and simulation experiments is that normally, simulations are epistemically opaque. This opacity deserves further attention. At first sight, it appears paradoxical since compiled computer programs are arguably the most explicit of all descriptions in scientific use. Executable software cannot tolerate any vagueness because at each step of the program the next step has to be specified precisely, else the compiler would not accept it. However, this condition does not guarantee transparency. Simulations are not opaque because it would be unclear how one step follows from its predecessors. On the contrary, it is the multitude of interrelated steps that can render the overall process opaque. Humphreys characterizes this problem in the following way:

> This opacity can result in a loss of understanding because in most traditional static models our understanding is based upon the ability to decompose the process between model inputs and outputs into modular steps, each of which is methodologically acceptable both individually and in combination with the others. (2004, 148)

Of course, there can be simulation models that are not opaque at all. Opacity is a feature of complex models, though the use of such models is widespread. Even if interactions in a simple target system were modeled in a simple way, a great number of them could lead to very complex model dynamics; especially when the simple events of the target system are highly related. The analysis of such real-world systems is therefore too complicated for analytical mathematical treatment and so testing the dynamics of the system has to proceed via simulation experiments. In brief, *algorithmic* transparency is a condition for executable programs, which however is consistent with the creation of epistemic opacity.

Despite the important separation in terms of epistemic transparency and opacity, there is an important methodological similarity: the use of iteration. It will be useful to discern two types of iteration for the following discussion. Iteration is not a standard topic in philosophy and there are only few recent attempts to give iteration a standing in the epistemology of science (see Hasok Chang 2007, who examines "epistemic iteration" in the development of scientific concepts).

I would like to discern two types of iterations pragmatically, namely the "convergence" and the "atlas" type. The first is involved in cases like exploring a new pathway that eventually becomes your routine way. At the beginning, there is much uncertainty and back-and-forth, but after a couple of repetitions the pathway begins to stabilize. After many iterations, it sediments to become a routine path that you inattentively take. Repeating exercises in music or sports is often of this kind. A violinist uses his bow intuitively, as does a bowman. In this way, iterations create 'convergence,' which can influence and educate intuition. Such iteration can generate high levels of certainty, but is usually bound to a fixed context. If the violinist plays a piano, or the bowman uses a pistol, the question of how to maintain intuitive mastership becomes legitimate.

The second type of iteration works rather by exhausting the possibilities and thereby creating a compendium, or atlas. It functions on a more abstract level. Iteration here is used for exploring a set of options under controlled variations, gathering the results and thus obtaining an overview. Such iterations, again, are very common in science as well as in everyday life. My children, for instance, are quick in scanning each piece of a cake to find out which one is the biggest (and most attractive) one. If the number of possibilities is high, however, one will have to resort to automated iterations, which is exactly what computers are good at.

Thought experiments are tied to the convergence-type of iteration. When you perform a thought experiment, repeated execution eliminates initial intransparency or ambiguity. Simulation experiments, on the other hand, involve the atlas type of iteration. Repeated, and slightly varied, model runs do not eliminate opacity, but rather explore the space of possible model behaviour. Thus the dynamics can be understood like an atlas that compiles many single maps. In sum, thought experiments have to conform to a condition of epistemic transparency, which accords to the convergence-type of iteration. Simulation experiments, in contrast, are part of simulation modeling because epistemic transparency about model behaviour is not attainable. The computer as an instrument, in particular one with an ability to automate iterations, offers an instrumental compensation for lack of transparency. The set of gathered results then substitutes for intuitive certainty.

While thought experiments and simulation experiments are similar in that they exploit the facts contained in assumptions or modeled situations, they are dissimilar regarding the types of methods they use. Processing in intuition requires transparency, which computer-automated iterations often cannot provide. However the insights simulations gain from collecting many results is something thought experiments do not provide.

4. Dealing with Opacity

How can one work with epistemically opaque systems? And how can epistemically opaque models play an epistemically fruitful role? This section will briefly discuss a number of typical examples with increasing degrees of complication that illustrate how simulation experiments deal with opacity.

4.1 **Social Segregation**

The first example is the well-known model for urban social segregation introduced by economist Thomas Schelling (1978). An idealized simple town map is represented by a grid of neighbouring cells, like a checkerboard. Each cell has inhabitants of a certain type (like skin color) and with certain preferences, for instance, not having a majority of neighbours of type different from their own. Inhabitants will move to an available cell so that their preference is respected.

It is obvious that such preference, if strong enough, will lead to segregation. In the extreme case, when everybody would insist on a homogeneous neighbourhood, segregation would happen immediately. The model gets interesting with weaker preferences. The surprising result of Schelling's is that even under conditions of great tolerance, i.e., when inhabitants welcome a mixed neighbourhood, but not one too dominated by the other type, complete segregation obtains. What does "too dominated" mean? Reasoning does not help here, one needs to try out and actually perform a great number of iterations. In the model, one cell is inspected after the other and it is determined whether inhabitants want to move. After all cells have been checked, the process starts over. After many iterations, an equilibrium will occur and then one can see whether segregation has happened or not. The intriguing question is how weak preferences have to be to prevent segregation. This question can be answered only by exploratory trials with varying parameter values.

The simulation looks like a thought experiment, but the role of iteration is importantly different. There is no way to determine the segregating behaviour of the simulated inhabitants under varying parameter values, except by iterated trials. Schelling started with a checkerboard and some coins and attempted to find a feasible specification of the model. The decisive point is how robust the phenomenon of segregation is. That segregation can occur in particular models is trivial. A model that shows how weak assumptions can be that nevertheless lead to segregation is an interesting model since it indicates how generic the phenomenon is. Therefore, everything depends on the actual range of parameters that generate segregation. This range can be determined only by a great number of iterations. Consequently, Schelling had to give up the checkerboard and employ a computer, i.e., run a simulation experiment, to process a sufficient number of iterations. This experiment produced a great number of single results that allowed him to compile a sort of atlas of model behaviour. If instead he had dispensed with simulation experiments he could not have gained insight about the likelihood of segregation via various degrees of bias; no thought experiment could possibly sediment from the simulation runs to produce an epistemically transparent intuition of comparable import.

4.2 **Phase Transition**

The next example, the Ising-model of physics, predates the computer and its architecture which served as the blueprint for Schelling's model. It works again on a regular grid. Each grid point (or cell) can take on one of two states (spin up – spin down) and neighbouring cells influence each other, for example by the tendency to take on the state of their neighbour. There is also a thermic parameter that controls the strength of influence. The higher the temperature, the higher the tendency to flip to an arbitrary state, i.e., the lower the influence of neighboring-states. The Ising-model is famous because it can exhibit phase transitions. In other words, there is a critical value of the thermic parameter above which sudden dramatic fluctuations occur, and below which widely mixed states grow into homogeneous clusters. This behaviour makes it a model for magnetization, a similar phenomenon.

Today one can conveniently simulate and experiment with the Ising-model on a computer screen, and again, this model presents great difficulties for a mathematical-analytical treatment. By analytical I mean that one can hardly show more than the existence of phase transitions, i.e., the critical parameters. This has made the model famous among philosophers for combining conceptual simplicity with computational complexity. The latter arises from the high level of interdependence, i.e., from the fact that the state at one grid point depends on that of its neighbours, which in turn depend on others, etc.

An iterative algorithm can simulate the model in a straightforward way, much like in the first example. Then, in a second layer of iterations, the temperature can be varied to sound out what the critical value is and how clusters form near this value. These iterations are not compressible, i.e., they have to be actually performed – which is feasible only by using a machine. However, this strategy brings even modern computers quickly to their limits. The number of necessary computational steps increases exponentially with the number of cells, and in cases of computational complexity like this, brute force strategies regularly fail.

At this point the Ising-model ceases to be parallel to the social segregation model. Only a second layer of simulation experiments has led to a methodological breakthrough, namely the use of so-called Monte-Carlo Marko-chains. The trick is to replace the unfeasibly large iteration problem by iterations on a different layer, namely by iterations of a random process.[4] This process is

[4] This does not seem to be an advantage, because the random process takes place in a logical space that is too big to analyze. The advantage lies in the mathematical fact that Markov processes converge surprisingly quickly. A Markov process in stationary distribution indicates the typical territory, so the reasoning goes, even if much is left out. In this way, the complexity barrier is circumvented by the random process approach – with the caveat that there are no results concerning the actual speed of convergence of the Markov-process. The high speed of convergence, though often observed, remains a kind of mystery, hence the adequate number of iterations depends on the feeling of the simulation modelers. R.I.G. Hughes (1999) discusses

locally defined, i.e., for each state of the process the transition probabilities to other states are given. Iteration of this random process approximates the long-term behaviour of the process. In a sense, the simulated Markov-chain explores the territory that is otherwise unknown. By compiling the results of the much-iterated simulation experiments (runs of the random process) one eventually gets the desired atlas of the space that was originally "too big."

4.3 **Chaos**

The third example is iconic of complexity theory, as it connects to computational models. It illustrates how simulation experiments are employed to circumvent opacity. A famous instance of a complex system was identified early on by the meteorologist Edward Lorenz. Using partial differential equations, he investigated a dynamic meteorological system, and found it to display some alarming behaviour. A marginal change in the initial conditions could lead to a severe alteration of the overall behaviour. This system property has been aptly named "deterministic chaos" (cf. Lorenz 1967, 1993). In deterministic systems, the initial conditions completely determine the future development. At the same time, this system is unpredictable in the sense that even the slightest uncertainty about initial conditions, which is unavoidable in any practical application, could potentially change the long-term behaviour entirely. Such systems are called "chaotic." The term "nonlinear behaviour" refers to more or less the same thing: the long-term behaviour of the model does not depend in any linear way on the initial conditions, in other words, closely neighboured initial conditions can lead to widely differing final states.

Lorenz's example is famous, and has become a paradigm of chaos theory, or the theory of complex dynamical systems. His model, however, was not deliberately constructed for its mathematical properties, but emerged from his work in meteorology. And the results were relevant for that subject. The so-called "butterfly-effect" conceptualizes nonlinearity in a picture: Even small events can have great effects; a butterfly can change the weather – at least in principle. All these considerations concern dynamical systems theory, a field expressed in the

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Ising model simulations, and the mathematician Persi Diaconis (2008) appreciates the revolutionary character of Markov-chain Monte-Carlo methods.

mathematical language of differential equations. The point is that analytical methods could discover how strange the behaviour can be, but they are not sufficient to give insight into what happens in these systems. How should one conceptualize a system that would be attracted to very different states depending on an initial waggle?

The mysteriousness vanished only when the computer-generated image of the Lorenz attractor displayed the intricate trajectories of the system, making sense of their strange behaviour. Such visualizations were based on simulation experiments that were iterated many times. For each grid point (or pixel), the system's behaviour is computed. In a way, the computer scans or sounds out the system for systematically varying initial conditions, and afterwards the isolated results are put together into one image. Only then a picture of the overall dynamics emerges that suggests continuity and gives a vivid impression, though it is based on a great number of single results, comparable to pointillism in art. In this way, visualizations can provide insights into complex dynamics, although it is often not well understood how the assumptions that are used interact with each other in detail while bringing about the dynamics. The enormous computational capacity of computers renders possible the exploration of phase space and, inversely, visualizations render complex behaviour cognitively graspable. In this way, the epistemic opacity due to computational and target system complexity gets circumvented.

4.4 **Electron Density**

The fourth and last example comes from the interface of computational chemistry and computational physics. The Schrödinger-equation of quantum theory describes the electronic structure of atoms and molecules. This is true only in principle, however, since even the simplest cases involving molecules are already at the limit of mathematical tractability. For all application-oriented problems, the Schrödinger-equation is too complex to be solvable. Again, this complexity arises from interdependence, namely the interdependence of the energy potentials of interacting electrons. The so-called "density functional theory" (DFT) offered a ground-breaking simplification. It is based on the fact that the many interacting energy potentials can be replaced by one single density function. The fundamental work was done by Walter Kohn and his co-workers Pierre Hohenberg and Liu Sham in the mid-1960s. This work on DFT won

Kohn the Noble Prize in chemistry in 1998. He shared the prize with John Pople who received it for his development of computational methods. Today, DFT is widely used in computational quantum chemistry, at least partially because it is included in software packages that are convenient to use, for instance the package "Gaussian," that Pople helped to create.[5]

A Noble Prize for computer methods is remarkable; it makes plain the growing role of computational methods in supporting scientific theory. Again, the success of DFT in chemistry depended on the availability of the software. From a theoretical perspective, DFT is implemented in a computer program. And DFT doesn't just exist in *one* program; there are dozens of programs and packages, many of them available online, that feature the theory. Typically, such software comes with a blurb indicating the sets of situations, materials and mixtures with which it performs well. Hence DFT is not simply implemented, but splits into many different variants. Why is this a significant observation?

The answer is closely related to the iterative character of simulation modeling. The step from a theoretical model to a computer model involves a separate, partly autonomous construction task. This task must bridge the gap between the continuous formalism of traditional mathematics in which theories are formulated, and the discrete operations digital machines can perform. Of course, one can reason with limiting cases, for instance the limit of an infinitely fine-grained grid, but one must always compute in finite steps. Therefore, theoretical laws and models, like Schrödinger's wave-equation, have to be fit into a Procrustean bed. Discretization, the name for this step, inevitably distorts. Each simulation model therefore requires some way to compensate for the distortions in the simulation model so that it remains relevant to the theoretical model or target system. Normally it is hard to discern whether such measures really re-establish the quality of the original theoretical model, or whether they merely compensate for some of its imperfection.

[5] For more details on density functional theory in the context of quantum chemistry and computer methods, see Lenhard 2014.

These compensation measures are a regular part of simulation models that we expect to increase their theoretical impact. Whether and how they do this can be guided by mathematical formalism only to a very rudimentary degree. Therefore simulation experiments are necessary to check and balance the compensating measures, and to adapt the simulation model accordingly.[6]

Given these considerations, the multitude of DFT methods looks less surprising. They differ essentially in the compensating strategies they implement. Since these are based on instrumental reasons rather than theoretical ones, they have to be judged according to the net-effect they produce on the dynamics of the model system. In other words, assessing and modifying DFT methods depends heavily on our knowledge of the applications for which they will be used. Over the course of such modifications, which take the form of stepwise iterated software developments, a particular instantiation of DFT will be formed by the applications for which it has been prepared, and in view of which it will be developed.

Experiments therefore take a central position in simulation modeling and help to make usable simulations as an instrument, especially at first. Instead of eliminating opacity, however, they work around it, replacing epistemic transparency with stepwise exploration. For this, a single simulation experiment does not suffice. Rather, one needs a whole series of experiments for charting model behaviour. A series of experiments like this utilizes iterations which we have called atlas-type. To sum up: simulation modeling regularly resorts to artificial (compensating) measures that are motivated by the performance of a simulation model, not by theoretical reasoning. Such measures have to be coordinated according to their interactions in the embedding model. They have to be tried out in an iterative and exploratory mode; hence the atlas-type of iteration is part-and-parcel of simulation modeling.

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[6] For a discussion of particular cases, c.f. Winsberg (2003) about “artificial viscosity,” and Lenhard (2007) about the “Arakawa-Operator,” a feat of atmospheric modeling.

5. **Conclusion: The Common Root of Thought Experiments and Simulation**

Thought experiments and simulation experiments are similar in that both make use of iterations. However, they differ fundamentally in the types of iterations they use, and in the functions those iterations fulfill. In thought experiments, the iterations of the convergence-type eventually produce a cognitive tool that is sufficiently transparent to run in human intuition. Simulation experiments, on the other hand, do not remove, but rather circumvent or compensate opacity with the help of atlas-type iterations. Iterative algorithms utilize computational power and can work where thought experiments cannot. In particular, if iterations are incompressible, there is hardly a chance to render the results epistemically transparent.

Thought experiments entail the possibility of an aha-effect that is arguably tied to epistemic transparency. Converging iterations then can bring about new aha-effects. In contrast to this, simulation experiments result in an instrument-based collection of single calculations. Such collection lacks the intimacy of intuition, and therefore creates a certain cognitive distance, even if visualizations occasionally help to negate this distance.

Hence the essential difference is: The iterative mode in thought experiments eventually makes iterations superfluous by crystalizing the most intuitive approach. In simulation experiments, in contrast, the iterations remain structurally necessary. They do not crystalize a cognitive pathway to an intuition; instead, the extensive set of iterations are preserved. Of course, there must be some way to make the output of the set of iterations comprehensible, as the atlas-type of iteration is suitable only under this condition. But this is not at all the same thing.

Let me conclude by presenting a perspective that puts thought and simulation experiments under the same historical framework. Here is some uncontroversial common ground shared by the different viewpoints discussed in this chapter: The thought-experimenter immerses him or herself into a hypothetical world, a world explored in intuition. This exercise of creating and exploring hypothetical worlds has been part of the arsenal of modern science since its inception. This indicates how closely related the (philosophical) formation of human epistemological subjects and the emergence of modern science are. Kant's classic formulation of this relationship can be found in his *Critique of Pure Reason*: that human epistemology depends on the constructive activity of epistemic subjects. He was motivated by Newton, whose theory of gravity can be seen as the paradigm of a mathematized science. From an epistemological viewpoint, it intertwined the construction of a mathematical model with scientific – or more generally, *human* – rationality and epistemology. The way simulation experiments differ from thought experiments tells us something about the evolution of mathematical modeling, and our relationship to it.

Mathematization proved to be an essential element of what are now called the "hard" sciences. Ongoing formalization and, in particular, algebraization since the 17th century went hand in hand with ever more elaborate algorithms and mathematical constructions. However, human tractability has been a limitation that prevented constructions from becoming too complicated or lengthy. There were several phases in history at which the development of mathematics was thought to be at an end, because it reached the limits of tractability and transparency. Generalization proved to be the way forward for mathematization in the attempt to provide or re-establish epistemic transparency, arguably culminating in 20th century axiomatic thinking.

The pivotal impact of constructive activity for human culture reached a new level with the industrial revolution. Automation was an integral part of this revolution, and it has continued to gain importance in ever more areas of society and culture. This is the point where we re-enter our discussion. Simulation experiments, like thought experiments, are a method of exploring hypothetical models. Simulation experiments, however, make this possible using automated iterations.[7] In this sense, simulation experiments can be seen as transformed thought experiments. They present a new and surprising methodological twist to find out or determine the conclusions that follow from our assumptions. The surprising fact is that we have to encounter our own epistemological inventions as complex and foreign objects and employ

[7] This perspective is in line with Humphreys' concluding verdict that humans are driven out of the center of epistemology (2004).

machines to help us deal with them. This is hardly compatible with the classical paradigm of mathematical construction and epistemology.

Thought experiments are meant to help us gain insight into a complicated world. Simulation experiments explore new possibilities that automated calculations open up. The intricate relationship between thought and simulation experiments is a product of, and perhaps the key to understanding, the position of human subjects in a culture increasingly suffused with computer models and algorithms.

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