Computer Simulation: The Cooperation between Experimenting and Modeling*

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The goal of the present article is to contribute to the epistemology and methodology of computer simulations. The central thesis is that the process of simulation modeling takes the form of an explorative cooperation between experimenting and modeling. This characteristic mode of modeling turns simulations into autonomous mediators in a specific way; namely, it makes it possible for the phenomena and the data to exert a direct influence on the model. The argumentation will be illustrated by a case study of the general circulation models of meteorology, the major simulation models in climate research.

1. Introduction. Although science is strongly shaped by the use of computers, we have only just started to reflect on what this means philosophically. What distinguishes simulations? Opinions in the literature are controversial, ranging from proclamations of a completely new method in science to the view that they contain nothing new philosophically. The goal of the present article is to contribute to the epistemology and methodology of computer simulation by pointing to some novel aspects from the perspective of the philosophy of science.

To start with, simulation models are basically a class of model. This makes recent discussions on models as mediators and their autonomous role highly relevant here. The present article will show that simulation models fulfill this role in a specific way. The central proposition is that the process of simulation modeling takes the form of an explorative cooperation between experimenting and modeling and that it is this characteristic mode of modeling that turns simulations into autonomous me-

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diators in a specific way; namely, it makes it possible for the phenomena and the data to exert a direct influence on the model. At the same time, experimenting acquires a specific meaning.

To clarify this thesis, I shall start by examining the function of numerical experiments in the course of modeling. The material for this comes from a case study of the general circulation models of meteorology, the major simulation models in climate research. The simulation method and these models were developed hand in hand right from the start. The history of the development of these models can also be used to illustrate the transformations characterizing simulation models. It is these transformations that are of interest to the philosophy of science.

I shall show in detail not only that these models are based on a system of partial differential equations (PDEs) representing natural laws *but also* that a modeling process intertwined with experimenting provided the framework in which they were able to work successfully. This detailed argument calls for an analysis of the relation between theoretical models and their so-called discretizations (discrete versions). The discrete model was viewed mainly as a schematic aid for the numerical computation of the solutions to the theoretical model—a very common view. The example of climate simulation points to a rather dramatic quality. This is because a particularly surprising twist is that this approach led climate research into an impasse. The problem of the instability of long-term integrations could only be overcome when the construction of a discrete simulation model was seen as a task in its own right, oriented more at the imitation of phenomena than at solving the equations of the theoretical model. Hence, this example contains crucial and general features of simulation in a nutshell.

The philosophical analysis of simulation modeling has been put forth recently by the work of Evelyn Fox Keller (2003), Eric Winsberg (2003), and Paul Humphreys (2004), to mention some recent ones. These interesting and thoughtful accounts aim at a characterization of simulation by distinguishing and contrasting different types. Winsberg focuses his ideas on "theoretically based models" suggested by a system of PDEs (2003, 107). Based on this type, he demonstrates that simulation provides an excellent view on the balance between theoretical and autonomous aspects in the process of model building: "In the end, the model that is used to run the simulation is an offspring of the theory, but it is a mongrel offspring" (2003, 108). The following argumentation is essentially in line with Winsberg's view but suggests a more general claim; namely, the mentioned cooperation between modeling and experimentation does more than "reconcile" (Winsberg) theory with experiment—it merges them methodologically. This is the key for providing simulations with a much wider range than ordinary mathematical modeling strategies.

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Fox Keller also differentiates between types of simulation modeling. She points to so-called cellular automata (CA) to highlight the power of simulation models to model phenomena directly without drawing upon theory. Fox Keller coins the term "modeling from above" (2003, 209) to characterize this property of CA models, and she identifies it as a significant step in simulation history when CA modeling became established during the 1960s. The case study on meteorology and the atmospheric circulation will exhibit a very strong dependence from theory but, at the same time, show those features of modeling from above Fox Keller ascribes to CA exclusively. Remarkably, the rise of CA modeling Fox Keller investigates occurred at roughly the same time as the mentioned developments in atmospheric simulation. Thus, the argumentation confirms Fox Keller's proposed patterns of history, especially the observation of simulation maturing in the 1960s. The classification scheme according to modeling types, however, gets relativized.

The following analysis aims to highlight the common ground of simulation approaches usually seen as different. In particular, the present article argues that explorative cooperation between experimenting and modeling is indeed a basic characteristic of simulation that applies alike to theoretically based and CA modeling approaches.

2. Computer Simulation: A New Instrument and the "First Experiment." While much of science, especially physics, has long depended on differential equations to describe phenomena, in fact many phenomena are too complex to be handled in this way. Prominently among them ranks the main example of the present article: the global circulation of the atmosphere. Whereas the weather, for example, follows a chaotic dynamic rendering long-term prediction impossible, climate concerns something like "average weather." It addresses very stable phenomena such as the so-called surface westerlies, the band of steady west winds (the trade winds) north of the equator.

The relevant laws of hydrodynamics were well understood theoretically and generally recognized prior to the advent of the computer. The observable atmospheric dynamics, however, emerges from the interaction of basic equations and assumptions and hence lay beyond the reach of the mathematical instruments available at that time. As a result, the dominant opinion was "that a consistent theory of the general circulation is out of reach" (Lewis 1998, 42). This skeptical outlook was to change fundamentally when a new mathematical instrument became available: computer simulation.[1]

1. This can serve as an illustration of P. Humphreys's (2004) principal point that we are "extending ourselves" by new instruments.

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The work of John von Neumann is of particular interest here. His cooperation with Stanislaw Ulam in the context of the Manhattan Project led to fundamental ideas on computer simulation.[2] Whereas Ulam thought that a simulation-based experimental approach provided an inspirational element in mathematics (see Ulam 1952), von Neumann was less enthusiastic. He viewed the "experimental" approach as a kind of stopgap measure: basically inappropriate for mathematical problems but offering the only way forward at the time.[3] Nevertheless, von Neumann was convinced that considerable progress could be made and organized the establishment of a meteorological workgroup at the Institute for Advanced Studies (IAS) at Princeton. This group was headed by Jule Charney and later turned into the Geophysical Fluid Dynamics Laboratory (GFDL), which was founded in 1960. The goal of that working group was to model the flow processes in the atmosphere with the help of hydrodynamics and to solve the corresponding differential equations with the computer. Arakawa (2000, 5) cites Charney as stating, "To von Neumann, meteorology was par excellence the applied branch of mathematics and physics that stood the most to gain from high-speed computation."

For the reasons mentioned above, prevailing opinion was skeptical regarding the chances of modeling the global atmosphere, and one can view those working at the IAS as a group of outsiders. A major breakthrough changed this fundamentally. In 1955, Norman Phillips, who was working at the IAS, managed in his so-called first experiment to simulate the dynamics of the atmosphere; that is, he managed to reproduce atmospheric wind and pressure relations in a computer model.[4]

The simulation model used in the "first experiment" worked with a very rough spatial discretization of the atmosphere. The physical principles of atmospheric dynamics were then adjusted to fit the discrete grid. This means that the global equations of hydrodynamics that are continuous in space and time had to be reformulated to "fit" the mathematical instrument: computer simulation—a conceptually new type of task.

2. Von Neumann and Richtmyer (1947) and the work of Metropolis and Ulam (1949) are viewed as the fundamental documents for the Monte Carlo method. See also the collection of Ulam's essays (Ulam, Bednarek, and Ulam 1990) and the reports in Galison (1996) and Fox Keller (2003).

3. The term "experiment" is initially used here in an unusual and highly innovative sense, although, in some ways, it concerns experiments with mathematical entities. This usage has now become common practice. It has even finally influenced the meaning of "experiment" (see subsequent discussion in this article).

4. "First Experiment" is the title of the article in which Phillips (1956) described his experiment. For a discussion, see Lewis (1998); for a more detailed history of ideas on modeling the general circulation of the atmosphere, see Lorenz (1967) and Dahan (2001).

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The next step in the simulation experiment was to add the dynamics, that is, the radiation of the sun and the rotation of the earth. The atmosphere left its state of rest and settled into a so-called steady state corresponding to a stable flow pattern.[5] This is a process that occurs during the running time of the computer simulation. The decisive question was whether the model would adequately reflect the patterns observed in the real atmosphere, such as the steady westerlies mentioned above. The outcome was positive. Everybody agreed that the model reproduced the known phenomena.

This successful simulation experiment generated a "realistic" atmospheric dynamics with a system of only six partial differential equations forming the core of the theoretical model. The "experiment," the quasi-empirical proof that these six equations sufficed, granted them the immediate recognition as "the primitive equations," which they still possess to this day, raising them from a speculative model assumption to the rank of a causal description of the basic features of atmospheric dynamics. It should be noted that none of the single equations were "speculative"; they all were, and continue to be, very well confirmed and in no doubt. The speculative question had been: Which arrangement of equations would lead to an adequate model? The construction of a theoretical model was confronted with the fact that the hypothetical-deductive testing of the model assumptions seemed hopeless. Numerical experiments then made this possible, leading surprisingly quickly to a generally accepted theoretical model. Within a short time, the simulation-based approach of such "general circulation models" (GCMs) became the royal path of climate research and exerted a decisive and formative influence on the developing discipline.

3. Explorative Cooperation. Phillips's simulation experiment was based on two successful stages of modeling: formulating the right fundamental equations (continuous PDEs) for the theoretical model and successfully constructing a discrete model (of difference equations), that is, a simulation model of this theoretical model that then made the numerical treatment possible. Each of the two stages was necessary, and the successful outcome of the experiment simultaneously confirmed both. The decisive criterion was the successful imitation of the phenomena, that is, the flow patterns in the atmosphere. However, what is so special about the sim-

5. The analysis of the generated (simulated) data already has to specify when one can talk about such a steady state and when it should not just be regarded as a transitional stage in the simulation model. In fact, Phillips went wildly astray in his estimates. A follow-up study showed that his model required far more time to settle down than he had assumed (Wiin-Nielsen 1991).

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ulation method compared with theoretical modeling? At this point, we should examine this issue very carefully; otherwise, the special characteristics of simulation modeling will be lost. Taken precisely, the fundamental equations of the atmosphere were not solved numerically. Instead, a simulation model was added, and its difference equations were integrated numerically. It was the generative mechanism of the difference equations that then imitated the atmospheric phenomena so astonishingly well. How should one assess this transition to a discrete simulation model? One central argument will be that simulation models can profit from theoretical models, and they will often be impossible to construct without them. Nonetheless, simulation models are not derived in a strict sense from the theoretical models. This argument is very much in line with Winsberg's account (1999, 2003). Furthermore, simulation models are also determined decisively by the phenomena or the data. This fact will prove crucial for a characterization of simulation not restricted to particular techniques like finite differences, cellular automata, or neural networks. The argument will be presented below, and a consideration of the further progress of the circulation model will illustrate it well.

However, before doing this, I should like to take a look at the close relation between experimenting and modeling that characterizes simulation. It was Phillips's numerical experiment, and not their derivation from physical theories, that granted the primitive equations their status. Strictly speaking, the result was also not justified theoretically, because it was not derived from the primitive equations. Instead, the first stage was the observed agreement between the simulated and the real patterns. If the experiment had produced only confused and chaotic patterns or—perhaps even worse—ones that were stable but dissimilar to the observed ones, this would have influenced a number of assumptions on various levels. Perhaps the formulation of the PDEs had been inadequate, and further processes needed to be added. However, perhaps the finite difference equations did not fit the continuous model well enough. Finally, the implementation of the algorithm may have been incorrect, and so forth.[6]

Before the experiment, Phillips did not know whether his GCM worked with a suitable theoretical basis or whether he had an appropriate discretization of the theoretical model. It was the exploration of the simulation model in a quasi-empirical way that first made it possible to make a theoretical model the object of research. One can then say that experiments are set up exploratively to sound out the consequences of the model.

6. Winsberg (2003) talks about the task of error management that is typical of the experiment. And Hon (1998) even goes so far as to pursue some sort of fundamental recognition of errors.

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Simulation modeling makes it necessary to run through a process of repeated reciprocal comparisons between experiment and model.[7] Humphreys (1991, 497) writes that simulation modeling "requires a new conception of the relation between theoretical models and their applications." And he maintained and strengthened his view recently (2004). I wish to emphasize the function of the numerical experiments in the modeling process. I shall call this "explorative cooperation." In my opinion, this cooperation is essential for the "new conception" claimed by Humphreys, and it is based on the new types of experiment labeled in the literature (from slightly varying perspectives) as numerical, computational, or even theoretical-model experiments (see Humphreys 1991, 1994; Rohrlich 1991; Dowling 1999; Hughes 1999; or Fox Keller 2003). They are an indispensable component in the construction of a simulation model that takes the form of a process of iterated experimental sounding out and model testing. One could say that the traditional hypothetical-deductive testing of model assumptions is transformed into a quasi-empirical process. Hence, simulation introduces a new methodology of modeling that opens up a specific perspective on *how* models manage to be both autonomous and mediators. Explorative cooperation leads to an enormous extension in the scope of the models—the modeling of the global dynamics of the atmosphere is only one example among many.

Does this way of talking about experiments overextend the term? Is it only being used metaphorically? After all, no intervention is being made in the domain of the modeled phenomena, as M. Morgan has pointed out (2003). It has to be accepted as an empirical fact that this usage is common practice. What was, for Ulam, still an unconventional use of the term "statistical experiment" has asserted itself on a broad front in the domain of computer simulation. I personally consider its use to be completely legitimate, even when it occupies a still unclear field between theoretical and empirical experiments. After all, the experiment concept is also, strictly speaking, far from being clearly delineated or unproblematic (see, e.g., Gooding, Pinch, and Schaffer 1989; Radder 2003).

The quasi-empirical experiments accompanying simulations may contribute to the discussion on the experiment in the theory of science. For example, the function of numerical experiments in the explorative cooperation within the framework of simulation modeling cannot be distinguished clearly into separate explorative parts and testing parts. There are close links here to the discussion on the discrimination between the context of discovery and the context of justification. F. Steinle (2002) has pointed to the problems with this distinction when referring to the fre-

7. Similar ideas are to be found in Humphreys (1994, 2004) and Winsberg (2003).

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quently neglected explorative function of experiments. According to my thesis of explorative cooperation, this is a central component of the methodology of simulations.

Hence, the philosophical analysis is in some sense underdetermined—simulation rests on experimentation, and to determine the former seems to be as contentious as to explicate the latter. In this situation it seems favorable to me to base the analysis on cases from scientific practice. In my view, simulation modeling introduces and gradually forms a new conception of modeling—taking up established concepts like experiment and exploiting its vagueness to build new practices.

4. Instability and Arakawa's Trick. Despite its great success, Phillips's simulation experiment revealed one serious deficit: the dynamics of his atmosphere did not remain stable. After approximately 4 weeks, there was a build up of internal energy and the system "exploded"; that is, the stable flow patterns dissolved into chaos. As Phillips (1956, 145) himself remarked laconically: "After 26 days, the field . . . became very irregular owing to large truncation errors, and is therefore not shown." Phillips was well aware of the crucial significance of the stability issue, and he suspected that truncation errors were responsible for the instability of his procedure. Computers present numbers with only a fixed number of decimal places, and the recursive determination of system states means that even the smallest error can lead to major errors over the course of millions of iterations.

Nonetheless, the experiments were considered to be a general success. No doubt was cast on the possibility of simulating atmospheric dynamics in general. Instead, making the simulation model stable was simply considered to be an additional challenge for future work. This was important for not only climate research, with its interest in the goal of predicting long-term phenomena, but also simulation methods in general. This is because the problem of successfully and, above all, stably substituting the "natural" dynamics found in hydrodynamic PDEs with the "artificial" dynamics of a discrete simulation model is one of the core tasks of the simulation method.

Once again, it was von Neumann who, following Phillips's experiments but before the publication of his findings, called a conference on the "Application of Numerical Integration Techniques to the Problem of the General Circulation" in 1955 (Pfeffer 1960). The main topic was how to handle truncation errors, the suspected cause of the instabilities.

This was followed by years of intensive research, and it was Phillips (1959) himself who discovered that a "nonlinear computational instability" was responsible for even very small errors leading to major deviations. Researchers, including Phillips himself, tried to solve the problem

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with truncation procedures designed to effectively average out errors before they can build up. This strategy was clearly oriented toward the ideal of the most correct computation possible—instabilities being conceived as a consequence of a lack of precision when deriving the discrete simulation model from the continuous PDEs of the theoretical model. It would later become apparent that this perspective leads to an impasse. In actual fact, this provides the main motivation for pursuing this case study further in the present article. It can be used to present my argument that simulations, even when they have a very strong orientation toward theoretical models, rest on methodological approaches motivated by imitating phenomena, independently from theory.

The decisive breakthrough for a simulation of the atmosphere with long-term stability came from a completely different approach. This was pursued by Akio Arakawa, a Japanese meteorologist who was exceptionally well versed in mathematics and developed a GCM at the University of California, Los Angeles (UCLA). However, from the very start, he was more interested in imitating the dynamics rather than seeking the most precise possible computation of solutions. Basically, Arakawa recognized that one could, and, indeed, that one should, dispense completely with any search for a true solution to the primitive equations. If the temporal development of the simulation provides a good reproduction of relations in the atmosphere and manages to do this in a stable way, then it does not need to be a solution of the primitive equations—not even in the limit. One could summarize this approach by stating that imitating the phenomena of the atmosphere is more important than solving the primitive equations.

Admittedly, this does not imply that it is possible to simulate a given complex dynamics with completely arbitrary mechanisms. Even Arakawa stuck closely to the primitive equations. However, his stability-bringing approach permitted a degree of contradiction in the equations. The primitive equations define a generative mechanism whose temporal development is described in formal terms through the (continuous) Jacobi operator. Arakawa did not follow the common practice of replacing the Jacobi operator with the discrete Jacobi operator but used his own specially constructed Arakawa operator. The derivation of the Arakawa operator is full of extremely refined mathematical arguments, the details of which need not be discussed here (see Arakawa [1966] and the later reconstruction in Arakawa [2000]). What is decisive is that the Arakawa operator overcame the nonlinear instability and permitted a long-term stable integration. Arakawa was able to prove this property mathematically.

To achieve the stabilization of the simulation procedure, Arakawa nonetheless had to introduce additional assumptions, some of which ran directly counter to experience and to the laws underlying the theoretical

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model. Hence, as well as retaining vorticity (a variable in turbulent currents), he also assumed the conservation of kinetic energy in the atmosphere, although it was well-known that this energy is transformed into heat through friction; in other words, it is definitely not conserved. Arakawa's conservation assumptions obviously seemed unacceptable. In terms of physics, one can say that Arakawa artificially limited the growth of instability by conserving kinetic energy.

The use of conservation measures that obviously contradict both theory and experience triggered a skeptical response in the research community. As Arakawa (2000, 16) later recalled, the basic criticism was: "Why require conservation while nature does not conserve?" Most modelers applied their skills to seek the most precise approximation to the solution of the primitive equations (which, naturally, did *not* contain these conservation assumptions). In contrast, Arakawa went one stage further in his modeling that was not derived from the physical basis but could only be justified afterward when the results of the simulation experiments produced a successful imitation.[8] It was success that finally justified Arakawa's approach, and the initial controversy soon gave way to the broadest recognition among professionals. What was initially a dubious new concept has now become established as "Arakawa's computational trick" (see Weart 2003).

Initially, Arakawa's approach was rivaled by the various independently pursued truncation methods that also sought to master the instability problem. Once again, it was finally a simulation experiment that delivered the decisive outcome. In 1978, Jule Charney performed an experiment comparing GCMs that ran parallel starting with the same initial conditions. He compared three models: those of Leith (Lawrence Livermore Laboratory), Smagorinsky (GFDL Princeton), and Arakawa (UCLA). The first two implemented truncation methods, whereas the UCLA model was based on the Arakawa operator. Phillips describes what happened: "three general circulation models . . . were used for parallel integrations of several weeks to determine the growth of small initial errors. Only Arakawa's model had the aperiodic behavior typical of the real atmosphere in extratropical latitudes, and his results were therefore used as a guide to predictability of the real atmosphere. This aperiodic behavior was possible because Arakawa's numerical system did not require the significant smoothing required by the other models, and it realistically represented the nonlinear transport of kinetic energy and vorticity in wave number space" (2000, xxix).

This once again strengthens the argument that the traditional perspec-

8. This is also revealed by the fact that Arakawa, one of the leading theoreticians, initially implemented his approach in a GCM, which led to a delay of several years before he set about publishing it.

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tive of simulation as a numerical computation of a mathematical or physical system had reached an impasse. It had to apply smoothing methods to attain the desired stability. However, in the long run, these led to unrealistically smooth behavior in the model. Arakawa's approach, in contrast, produced a "more realistic" picture of atmospheric dynamics by drawing completely contra-intuitively on artificial assumptions that could not be justified theoretically. Their legitimacy came from the stability and the experimentally confirmed high agreement with the phenomena being modeled. Arakawa did not view the formulation of finite difference equations as a mere derivation from the continuous system of physical primitive equations but as a (partially) autonomous construction task. This gives the discussion on the autonomy of models (Morrison 1999) its specific meaning in the context of simulations: the study, modification, and adjustment of a discrete simulation model is partially disengaged from the theoretical model.

Arakawa exploited the autonomy of simulation modeling.[9] Phillips (2000, xxviii) describes this in retrospective as "the formulation of a *physically meaningful* finite-difference scheme that will simulate the nonlinear process in the equations of motion." And a major lesson of simulation modeling is that something "physically meaningful" need not be constructed "from below" out of the analysis of basic physical laws but can be obtained "from above" by adjusting it to fit the phenomena.

5. Simulation and Modeling. The present example of the general circulation of the atmosphere was able to draw on an established physical theory. The laws of hydro- and thermodynamics form the theoretical basis for the primitive equations, a system of continuous PDEs. Theoretical models based on mathematically formulated physical laws of nature are typically continuous in space and time and are described through continuous functional relations. The concept of the continuous mathematical function has been of eminent importance for the revolutions in mathematics and the natural sciences since the seventeenth century. This type of theoretical model, as formed by the primitive equations in the case of atmospheric circulation, will be labeled C (for continuous).

From the pioneering work of, for example, Maxwell or Hertz up to

9. This implied validation problems, particularly when empirical values were not available, because of the need to predict future developments. This is precisely the problem with climate simulation in the political discourse on climate policy, in which recourse to the theoretical model plays a major role in the justification. For a critical stance, see Oreskes, Shrader-Frechette, and Belitz (1994) and the reply from Norton and Suppe (2001). The validation problem is, in general, a central problem in the epistemology of simulations (see also Winsberg 1999).

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the most recent debates on models as mediators, the focus has always been on the insight that general theories cannot be applied without the mediation of models. Suppes already drew attention to this in 1961. In recent times, the publications of Hacking, Cartwright, Giere, Morgan, and Morrison have become standard references regarding such insights into the significance, locality, and autonomy of models.

In the case of computer simulation, the situation becomes a bit more complex. There is another characteristic type of model as well as C—a discrete model D that is often called a "discretization of C." In the general circulation example, this consists of a system of differential equations describing the evolution of the system at the grid points in discrete time steps. As a rule, little fuss is made about D. Practitioners are only too aware that a computer can only handle discrete objects, and the D type of model is omnipresent. In philosophy, however, D generally appears as a rather unimportant intermediate step; the true modeling and mediation effort, it is claimed, has already been made for C. This becomes clear in the tendency to view D as an auxiliary construction derived from C that by and large mechanically obtains a numerical solution.[10] This perspective may be tempting, but the Arakawa example nonetheless showed that one should have emphasized the difference between D and C rather than playing it down.

Simulation models do not just apply the brute force of the computer in order to squeeze results out of C. Instead, they require their own new kind of modeling that is characterized by type-D models. This type of discrete model defines the spectrum of potential models anew, motivated by the specific requirements of the computer. The reason for this is that the generative mechanism selected to imitate a certain dynamic has to "run" on the computer; that is, it must not require excessive computing capacity and must, above all, not become unstable, because, for example, discretization or truncation errors will build up. In principle, this applies to all types of generative mechanisms such as systems of finite difference equations, cellular automata, or neural networks. Paul Humphreys (2004) emphasizes that one essential characteristic of simulations is to redefine the domain of tractable mathematics, and he underlines effective implementation as a characteristic of a simulation that goes beyond a mathematical algorithm.

It is certainly the case that the study of simulation models raises general questions regarding modeling. The insights from recent debates on models,

10. See, e.g., Hartmann's (1996, 83) otherwise so accurate presentation, which makes no difference between the two types: "Simulations are closely related to dynamic models. More concretely, a simulation results when the equations of the underlying dynamic model are solved."

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on their autonomous and mediating character, are highly relevant here, as Winsberg (2003) points out. The argument so far reveals that, in the case of GCMs, which certainly belong to the class of theoretically based models, aspects of their autonomy play an important role. Models are not derived—and certainly not deductively—from the general theory. Nonetheless, the link between the simulation model and the theoretical model plays a key role. This leads me to accept the characterization of simulation models as "semiautonomous," as in Winsberg's (2003) modification of Morrison's (1999) claim that models are "autonomous agents." This leaves the question regarding the specific characteristics of simulation models completely open: Are they a special kind of modeling? If so, which aspects make them special?

The philosophical debates on the specifics of simulations focus on their status between experiment and theory. It was particularly numerical experiments that led to the emphasis on the idiosyncrasy of simulations. In my opinion, there are two approaches in the literature, although they are admittedly not completely disjunct. One stresses a new kind of experiment (Fox Keller, Humphreys, Hughes, Winsberg, etc.); the other emphasizes the status of simulations between theory and experiment (Galison, Humphreys, etc.). Of course, there is also the completely opposing point of view that simulations have nothing new to offer in philosophical terms. This common stance is taken by, for example, Stöckler: "Computer simulations enable tremendous progress on a pragmatic level, as a matter of degree in terms of speed and quantity, but not a revolution in the principles of methodology" (2000, 356).

My personal position supports the claim that simulations are something new. They launch a new conception of modeling, as has been highlighted by Humphreys (1991), Schweber and Waechter (2000), or Fox Keller (2003). Usually the case of finite difference methods is treated as a kind of theory-biased exception. I shall argue, however, that model-D simulation models represent a new species of model that is very characteristic for simulations in general. They lead to a decisive change in the process of model formulation: the way in which the simulation model is *formulated* is of major importance for its philosophical characterization. As a direct result, it is inappropriate to take a position that already proceeds from the assumption of a prior model and only sees the simulation as a "realization" of that model (see the approaches from Neelamkavil [1987] or Stöckler [2000]). Simulation modeling depends on the potentials and on the use of numerical experiments, as described in the previous section. It pursues a new mode of cooperation with experiments and can in this way give its own specific meaning to the discussion on the autonomy of models.

6. Two Types of Model. The difference between the theoretical model C

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and the discrete simulation model D emphasized in the case study is highly significant for the simulation method in general.[11] When modeling general circulation, the continuous primitive equations, the core of the theoretical model C, were replaced by a system of finite difference equations. One can conceive of a coarser resolution if D were to be constructed in such a way that it complies with the following approximation property (*), in which x represents a parameter for the mesh size of the spatiotemporal grid:

$$\lim \mathrm{D}_\Delta = \mathrm{C} \text{ for } \Delta \to 0; \qquad (*)$$

that is, for increasingly fine grids, D will finally turn into C. So far, so good. This relation gave rise to the misunderstanding that the results of D are "numerical solutions" of C or would, in any case, correspond to these with an arbitrary precision. However, this is in no way the case. In the circulation models, it was precisely the deviation from the schematic approximation that brought the breakthrough. However, let us simply try proceeding from (*). In practice, one is never confronted with an infinitely fine grid. Moreover, it is generally impossible to derive any quantitative statement on the "distance" from D_Δ to C with a $\Delta > 0$. This means that the properties of model C, let us call them prop(C), can, at times, differ greatly from prop(D_Δ) for a small but finite Δ.

This can be expressed quite clearly in formal notation. The vertical lines $|\cdot|$ should represent an appropriate measure whose selection is a matter of pragmatic judgment. They will depend on the purposes and goals of the model and its application—for example, the agreement between statistical variables and the pattern of circulation zones in the atmosphere, such as the above-mentioned surface westerlies. Although, because of (*), we can anticipate the relation $|\mathrm{Prop(C)}, \mathrm{Prop}(\mathrm{D}_\Delta)| \to 0$ for $\Delta \to 0$, there is generally no estimation of $|\mathrm{Prop(C)}, \mathrm{Prop}(\mathrm{D}_\Delta)|$ for $\Delta > 0$. And, even worse, there is no guarantee that the properties will approach one another monotonously as the grid becomes finer. The path on which D_Δ approaches C, that is, prop(D_Δ) conceived as a function of Δ, is, in general, simply unknown. Hence, one is faced with a very open situation: D is not determined by (*), how Δ becomes smaller is not determined unequivocally, and prop(D_Δ) is not known for any concrete D_Δ. Increasing

11. Winsberg (1999) distinguishes a complete hierarchy of models that play a role in relation to simulations, including types C and D. That these two types are different is common knowledge, and Winsberg does not claim any discovery in that respect (nor do I, of course). In the present context, I am interested in the *implications* of the differentiation between types C and D and hence restrict my argument to that.

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the resolution of the grid could, in some circumstances, also lead to a less adequate approximation.[12]

These mathematical facts are basically well-known. If one knows something about the solutions for C and D, one can often derive certain statements on the approximation properties, such as an estimate of the speed with which the models will approach each other (as the grid becomes finer). However, in complex cases, which tend to be the rule in simulation modeling, no statements of such a type exist, because, right from the start, no solution to C can be obtained with which one can compare it. Hence, D is in no way a schematic approximation to C or a numerical solution of C.[13]

This confronts simulation modeling with a dilemma. The justification of the simulation refers back to the physical basis of the theoretical model, that is, in the case of the climate, on the scientific status of the laws of hydro- and thermodynamics. The solutions of D are viewed as approximate solutions of C. However, strictly speaking, this is not the case, because D approximates C at best in only a weak sense, as we have seen. This somewhat complicated situation in which the relation seems to be "approximated" in two different ways has already been analyzed by M. Redhead (1987) in another context. He distinguishes between two types of approximation, or, better put, two perspectives on the term "approximates." The concern is to approximate equations that Redhead (1987) summarizes as theory T (in our case, one can think of the primitive equations in the theoretical model C). We can consider approximations to a theory T from two points of view:

> (*a*) We can look for approximate solutions of the exact equations employed in the theory.
> (*b*) We can look for exact solutions to approximate equations; that is, we can simplify our equation before we start to solve it (Redhead 1987, 150).

If one views the formulation of a discrete model D as an approximation to C, then Redhead's distinction deals with the problems occurring in simulation models. Redhead (1987) also advises caution: "Of course we must be careful in talking about approximate equations. They may have

12. It was Arakawa's basic insight that the theoretically valid discretization methods lead to a D_x that approaches C over a path on which its properties (the instability of the flow pattern) greatly differ from prop(C). The statistics of that path are the relevant measures in practical applications. They build a complex function that can be determined only by numerical experiment.

13. Rather, D can be viewed as a model of C; see Küppers and Lenhard (2005), who characterize simulations as "models of second order."

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quite different solutions from the original equations due to instability effects. Conversely, quite different equations may have approximately (or even exactly) the same particular solutions" (1987, 151).

Redhead's description of the problem applies to models completely in general: D finally models C, and how well it does this seems to be a general problem of successful modeling. How can one obtain a D with the desired properties? What characterizes *simulation* models is their specific *way of dealing* with this problem. Simulations give a special answer that I wish to call modeling from above. Moreover, this justifies the status that turns simulations into autonomous (or semiautonomous) mediators: the concern is in no way to solve C using D but to go for prop(D) *directly*.

The transition from C to D is a decisive and characteristic step in the construction of a simulation model. Whereas N. Cartwright's verdict that models cannot be pulled out of theories like candy out of a vending machine is generally accepted in the philosophy of science, there are often gray areas regarding the relation between the two types of model. Therefore, it is perhaps no exaggeration to point out once again that D proceeds from C just as little as C proceeds from the theory. This point is of utmost importance: in general, D does not present a solution to C. In order to imitate a process, D does not have to solve the equations of C—and it also did not do this in the case example of the GCMs! The key point is that the consequences of a model, its properties, can be observed in experiments, and through this, by implementing different discretization schemes or by introducing, tuning, and adjusting parameters, one can obtain, in turn, a further change in the model that is driven directly by the phenomena or the data. The model becomes the object of a recursive process that runs repeatedly through numerical experiments, observations, and parameter adjustments.

Almost every model contains a number of parameters. Simulations are special here, because the specification of parameters does not belong to the initial or boundary conditions; in other words, it is not the adaptation to a special applied situation. The parameters that we are talking about here are not specified "from outside" by, for example, an initial velocity, but "from inside" by adjusting them in light of the results of numerical experiments. Often a kind of black-boxed parameters without interpretation in theoretical terms is very successful. A key methodological point of simulation modeling is to turn the coordination of the phenomena (or data) and the model itself into components of model construction.

Let us look at this process in a strongly idealized form: let us take a complete host of parameters $p := \{p_1, p_2, \cdots\}$, so to say adjustors for the discrete model $\mathrm{D} : \mathrm{D} = \mathrm{D}(p)$. $\mathrm{Prop}(\mathrm{D}(p))$ is conceived as a function of $p = \{p_1, p_2, \cdots\}$. The goal is to vary p so that the observed behavior

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(in the numerical experiment) approaches the phenomenon to be modeled (Ph). The task is:

Find p so that $|\text{Prop}(\text{D}(p)), \text{Prop}(\text{Ph})|$ is small.

The formal notation of the goals suggests a more quantitative solution here than is generally possible. However, even a more qualitative judgment by experts does not demolish the argument. This is because the appropriate model specification, that is, concrete parameter values p, is found in an iterative process of explorative cooperation between modeling and experimenting. What traditionally had to be attained "from below" by applying the most precise possible approximations to the theoretically valid model assumptions can now be achieved "from above" by comparing the model characteristics with the phenomena. Neural networks, for instance, can achieve good imitations of phenomena whose theoretical structure they virtually ignore.

Fox Keller (2003) has highlighted the far-ranging consequences of "modeling from above." She coined that term to describe the features of cellular automata (CA) in particular, letting a new epoch of simulation start with them.[14] In contrast, I wish to defend the claim that modeling from above actually represents a more general characteristic of computer simulations. The case study on climate research can confirm this. It is a classic case of a theoretically based simulation model that, nonetheless, relied on modeling from above at a decisive point, namely, the modeling step from C to D. Hence, I maintain that the different simulation modeling approaches, like cellular automata or finite differences, have more in common than is usually acknowledged. The process of model formation is an essential and quite general characteristic of simulation modeling: it occurs in the mode of explorative cooperation between experimenting and modeling that seems to form an important component of a new conception of modeling.

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14. Likewise Rohrlich (1991, 516), who emphasizes the "new syntax" to characterize simulations "in the narrow sense."

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