International Studies in the Philosophy of Science

Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/cisp20

How Digital Computer Simulations Explain Real-World Processes

Ulrich Krohs

Version of record first published: 05 Dec 2008

To cite this article: Ulrich Krohs (2008): How Digital Computer Simulations Explain Real-World Processes, International Studies in the Philosophy of Science, 22:3, 277-292

To link to this article: http://dx.doi.org/10.1080/02698590802567324

International Studies in the Philosophy of Science
Vol. 22, No. 3, October 2008, pp. 277–292

How Digital Computer Simulations Explain Real-World Processes

Ulrich Krohs

Scientists of many disciplines use theoretical models to explain and predict the dynamics of the world. They often have to rely on digital computer simulations to draw predictions from the model. But to deliver phenomenologically adequate results, simulations deviate from the assumptions of the theoretical model. Therefore the role of simulations in scientific explanation demands itself an explanation. This paper analyzes the relation between real-world system, theoretical model, and simulation. It is argued that simulations do not explain processes in the real world directly. The way in which simulations help explaining real-world processes is conceived as indirect, mediated by the theoretical model. Simulacra are characterized further, and turn out to be a priori *measurable. This gives a clue to a better understanding of the epistemic role of computer simulations in scientific research.*

1. Introduction

One of the aims of science is to explain the dynamics of the material world, and to predict future states of the world by means of theoretical models. The world, or a world, in this context is to be understood as a system of parts and their relations as it develops in time. Theoretical models need to be further analyzed, or solved, to provide descriptions of and predictions about the dynamics of the world they model. An important tool for analyzing theoretical models is to run computer simulations. However, since simulations are themselves observable processes rather than descriptions of the world, one has to ask in which way such empirically given processes may be used in explaining other empirically given processes. My concern in this paper is to specify what a computer simulation is, and how its use in scientific explanations is to be understood. I argue that the relation between simulation and theoretical model plays a crucial role in how simulations explain real-world phenomena.

Ulrich Krohs is at the Department of Philosophy, University of Hamburg. Correspondence to: Department of Philosophy, University of Hamburg, Von-Melle-Park 6, D-20146 Hamburg, Germany. E-mail: ulrich.krohs@uni-hamburg.de

ISSN 0269–8595 (print)/ISSN 1469–9281 (online)
DOI: 10.1080/02698590802567324

In Section 2, I will specify what theoretical models are, in which sense they are explanatory, how they are used to predict the dynamics of material systems, and where the limits of their predictive power are. I will illustrate this with continuous models of a chemical oscillator, the Belousov-Zhabotinsky (BZ) reaction. Section 3 analyzes how simulations are related to theoretical models, on the one hand, and to the material world, on the other. In Section 4, I address the question what kind of simulacrum is under investigation in a computer simulation. Several candidate *definientes* from the literature are found to cover important aspects of what a computer simulation is, but none accounts for the whole truth. A synthesis is then proposed which is based upon the difference in measurability of real and simulated processes. I shall argue that we know of digital simulacra that their parameters are measurable. We know this from acquaintance with the very concept of a digital simulation, without referring to experience, i.e., we know it *a priori*. Digital simulacra are *a priori* measurable worlds. The argument about measurability will finally be the basis for a discussion of the epistemic role that simulations play in science (Section 5).

2. Theoretical Models

Theoretical models are viewed here as pieces of scientific theory that describe the modelled system, usually in a formalized way. Being a description, a theoretical model can be conceived as a set of assumptions about some object or system (Achinstein 1968). It describes the object or system in a certain state or the dynamics going on in the system. Within the context of simulations, primarily dynamic models are of interest (Hartmann 1996, 82–83), especially those that refer to the internal mechanism bringing about the dynamics. Such models may be regarded as not only describing, but also as explaining, the process under consideration. A fruitful way of conceptualizing mechanisms is conceiving them as being composed of entities and activities (Machamer et al. 2000; Craver 2001; Machamer 2004).[1] Thus a model that states the entities and activities that bring a phenomenon about may be called a mechanistic model. Since discovering the activities involved in a mechanism has to count as the finding of causes (Machamer 2004), an explanation of a phenomenon by a mechanistic model is a certain kind of causal explanation.

I shall discuss different models of the BZ reaction as examples of mechanistic theoretical models. The BZ reaction is famous for displaying chemical oscillations in space and time, which are observable as periodic colour changes of the reaction medium. The overall reaction is an oxidation of malonic acid by bromate, yielding formic acid, carbon dioxide, and bromine. Cerium ions play a catalytic role, and the oscillatory change between two different oxidation states of hydrated Cerium ions causes the colour change. The complicated chemical process can be described by a theoretical model consisting of a system of 14 reaction equations, known as the Field–Körös–Noyes (FKN) mechanism (Field et al. 1972). From this FKN mechanism, a simplified set of only five reactions could be isolated, which was judged to describe the qualitative behaviour of the system satisfactorily. This simplified theoretical model was named the *Oregonator*, after its institution of origin, the University of Oregon (Field and Noyes

1974). Whether the more realistic FKN mechanism, or the simpler Oregonator, is the adequate model to be used in an analysis of the dynamics of the BZ reaction ultimately depends on the epistemic goal that is followed. The quality and usefulness of a particular theoretical model may be judged differently in accordance with aspects of a material system that shall be further explained. I take it that in this instance, the main epistemic goal is to predict the dynamics of the system under certain conditions and to identify qualitatively discernable structures like singularities, limit cycles, or regions of particular dynamical behaviour. Though the FKN model gives a more realistic description of the BZ reaction than the Oregonator, it is too difficult to handle to yield the desired predictions within reasonable time. The Oregonator is much easier to handle, and therefore more useful for an exploration of the behaviour of the reaction system under different conditions. Consequently, theoretical work on the BZ reaction is mainly based on this simpler theoretical model. However, scientists have to be satisfied with a qualitative match of model and modelled system.

The following chemical equations define the Oregonator:

$$\begin{aligned} A + Y &\leftrightharpoons X \\ X + Y &\leftrightharpoons P \\ B + X &\leftrightharpoons 2X + Z \\ 2X &\leftrightharpoons \mathrm{Q} \\ Z &\leftrightharpoons fY \end{aligned}$$

with A for the concentration of BrO_3^-; B, P and Q having been assigned to the concentrations of various compounds in the exploration of the model; X, Y, and Z being interpreted as the concentrations of the intermediates $HBrO_2$, Br^-, Ce(IV); and *f* being a stoichiometric constant. The overall reaction results in

$$f\mathrm{A} + 2\mathrm{B} \leftrightharpoons f\mathrm{P} + \mathrm{Q}.$$

Reaction constants must be assigned to each direction of each reaction. After their introduction, rate equations can be stated from which ordinary differential equations (ODEs) can be deduced for the change in time of each of the three intermediates of the reaction. For easier numerical handling, Field and Noyes (1974, 1879) transformed their model into a dimensionless form:

$$\begin{aligned} d\alpha / d\tau &= s(\eta - \eta\alpha + \alpha - q\alpha^2), \\ d\eta / d\tau &= s^{-1}(-\eta - \eta\alpha + f\rho), \\ d\rho / d\tau &= w(\alpha - \rho). \end{aligned}$$

This system of three ODEs describes the kinetics of the BZ reaction; it is a dynamic model of the reaction.[2] One can assume from the quadratic term occurring in the first differential equation, or from the autocatalytic third reaction of the mechanism, that within a certain parameter range, the model describes oscillations. This is at least

something one may learn from the model, but scientists aim for a more detailed account of the dynamics of the system over a broad parameter range. Unfortunately, one cannot calculate the state of the system at a given time τ from the initial conditions, since the equation system cannot be solved analytically. In other words, the theoretical description of the BZ reaction by the Oregonator, though it explains the mechanism of the reaction in a simplified way, is almost useless for predicting the dynamics of the system. Many other continuous theoretical models pose such problems for mathematical tractability (Humphreys 1991), and the situation with discrete models is no better (Hughes 1999). This holds true as long as mathematical analysis is regarded as the only means to integrate the equation system: a theoretical model, how powerful it may ever be in explaining the mechanistic basis of the dynamics of a material system, need not provide predictions by analytic methods.

3. Relations of Simulations to Theoretical Models and the Real World

Running simulations allows for predictions of the behaviour of a material system even in cases where no analytical solution can be obtained from a theoretical model. In such a case, a simulation model is implemented on a digital computer and developed in time.[3] The sense in which such an implementation may count as an instantiation of the theoretical model will be discussed below. Anyhow, simulations often yield the desired solutions by numeric integration of the equation system. Thus, *via* simulation, a model may be used as a predictive tool, despite its analytical intractability. It has often been claimed that simulation could therefore be conceived in a way as experimenting with theoretical models, and there is nearly a consensus in regarding simulations as a new kind of scientific method: Rohrlich (1991) conceives computer simulation as a methodology lying somewhere intermediate between traditional theoretical physical science and its empirical methods of experimentation and observation. In his view, simulation allows for 'theoretical model experiments'. Humphreys (1994) regards simulations as 'numerical experimentation', a new kind of method he sees as complementary and intermediate between existing methods of theory and experimentation. Hartmann (1996) agrees when classifying this as one main function of computer simulation. (For a dissenting view see Stöckler 2000, who denies that computer simulation deserves the ascription of a special, intermediate status.)

The methodological aspects that numerical experimentation shares with both sides have been thoroughly analyzed (Winsberg 2003). However, Winsberg objects that it is not clear what is gained by this 'third mode view'. He concludes that it is at best 'a good place to start'. In fact, methodological similarities do not explain how simulations, models, and the material world are related. This is what will be analyzed here.

3.1. Simulations as Related to Theoretical Models

Simulations provide numerical solutions to theoretical models. They are run primarily when theoretical models cannot be integrated analytically (Humphreys 1991) but may, of course, be helpful also in cases where analytical methods are in fact available

(Hartmann 1996, acknowledged by Humphreys 2004, 108). They may, for example, provide an easy way of screening the effects of alterations of some parameter. Simulations are thus a means to analyze theoretical models that turns out to be generally applicable. It is often thought that simulations are faithful instantiations of theoretical models. However, a closer look at the Oregonator example shows that this is not the case, and that the relation between simulation and theoretical model must be construed differently.

The Oregonator is a simplified theoretical model of the BZ reaction with only three intermediates. Three is already too much for an analytic treatment: there are no known methods to analytically obtain quantitative, and even many of the desired qualitative, results from such a system of ODEs. So the integration of the system had to be performed purely numerically (Field and Noyes 1974, 1882). This was done using the established Runge–Kutta method. This method reconstructs a trajectory in the phase space as described by a set of ODEs by a stepwise integration of the system developed in discrete time. Roughly, the method may be described as estimating the slope of the trajectory in the middle of an interval, and stepping forward one interval Δt on a straight line defined by the starting point and the estimated slope. The end point of the line segment is taken as the starting point of the next interval, where the procedure starts again, and so forth. The resulting traverse will follow more or less closely the trajectory of the system, but always shows some deviation. This error is smaller in the actual Runge–Kutta method than it appears from the sketch given, since, e.g., not only the slope in the middle of an interval is used but the average of the slopes at its beginning, in the middle, and at the end. A deviation is nevertheless present (Hairer et al. 1993). The deviation has two sources: the local discretization error and the numerical error. The local discretization error depends on the increment Δt and can be minimized, though never completely eliminated, by decreasing the increment. Unfortunately, this leads to an increase of the number of steps that must be performed to simulate a certain interval of the trajectory, which results in two restrictions to such a decrease of the increment. First, more steps lead to an increase of the required computation time, so there are limits of feasibility. Second, and even worse, it results in an increase of the second kind of error, the numerical error. Every computation is done with a limited number of digits, and therefore gives rise to a rounding error. This numerical error increases with the number of steps, so a decrease of the increment Δt, while decreasing the discretization error, leads not only to an increase of required computing time, but also to an increase of the numerical error (Hairer et al. 1993).

This sketch of the integration procedure already shows that, while the results obtained from the simulated system may come close to those expected from the system described by the theoretical model, the simulation model itself differs from the theoretical model. But the simulation of the Oregonator had to face another problem. The system of ODEs turned out to be *stiff*, i.e., to show quick relaxation of one variable as compared with the others. In order not to end up with qualitatively erroneous results, the integration of stiff systems requires special methods (Hairer and Wanner 1996). Field and Noyes were aware of this. Mentioning that even with small increments

'the computed values … oscillate wildly about their asymptotic values' (Field and Noyes 1994, 1880), they modified the system on integration. The problem of irregular values was overcome by setting one differential quotient equal to 0 whenever these wild oscillations began during the integration of the system, i.e., by making a severe change to the system. This modification is not represented in the integrated equations, but applied on occasion of certain results that were judged as erroneous by independent methods. The results obtained with the modified system were double-checked, using a different integration method, and judged to be reliable (Field and Noyes 1994, 1880).

From this description of the simulation, we learn that the simulated system differs from the theoretical model at least in the following three aspects: (i) it has a discrete rather than a continuous time scale; (ii) its results deviate from those to be expected from the theoretical model by the sum of discretization and numerical errors; and (iii) it deviates by ad-hoc changes that had to be made in order to overcome the problems that the stiffness of the theoretical model poses on numerical integration. While (i) and (ii) may perhaps be seen as being just some imprecision, the modifications (iii) show that the model that constitutes the basis of the simulation is not identical to the theoretical model. The simulation does not strictly rely on the mechanism described by the theoretical model. It refers to an ad hoc modified mechanism, which is not supposed to occur in the real-world system. The justification for this intervention is that the dynamics of the modified system, in contrast to the simulation of the unaltered Oregonator, is similar to the dynamics of the physical system.

It might be conjectured that the theoretical model could then simply be replaced with the model that is the basis of simulation. Such a replacement, however, is no way out, since the simulation model does not provide an acceptable explanation of the material system, due to the alterations mentioned. For the sake of the phenomenological adequacy of the results, the simulation model involves assumptions that plainly contradict empirical knowledge about the reaction mechanism acknowledged in the theoretical model.

It is helpful to regard the relation between theoretical and simulated model from the opposite side, and to ask how the theoretical model relates to the simulation: Regarding the simulation as an empirically given and empirically investigated 'numerical phenomenon', the theoretical model can be regarded as a simplified (in the present case nevertheless non-computable) description of the simulation. From Section 2 this relationship is already known to hold also between theoretical model and material world: the theoretical model is a simplified, but often not computable description of a real-world phenomenon. Yet, while the theoretical model states the mechanism of the BZ reaction, it does not do so with respect to the simulation. The simulation relies on a 'mechanism' that deviates by systematic and ad-hoc modifications from the mechanism described by the theoretical model. It is therefore not explained by the latter. Only in the weak sense of being described by a theoretical model a simulation may be regarded as its—not fully faithful—instantiation.

The case is similar with simulations run on electronic analog computers, though there is not necessarily a discretization error, and though the theoretical model can in many cases simply be 'plugged together' without modifying the mathematical structure

(Mead 1989). In these respects, an analog simulation is set up more directly from the set of ODEs than a digital one. However, being a physical device, the setup analog computer neither *is* nor approximates the theoretical model. It is set up so that its dynamics falls under the description given by the theoretical model, like the dynamics of a digital simulation.

3.2. Simulations as Related to the Material World

To further explicate the concept of a simulation, the relationship between simulations and the material world must be investigated. As Hartmann points out, 'the most significant feature of a simulation is that it allows scientists to *imitate one process by another process*' (Hartmann 1996, 77). A confirmation of this view can be found in the Oregonator example, where the simulation is meant to mimic the behaviour of a material system, namely the BZ reaction system. The 'imitation' usually relies on approximations and idealizations but may include even 'self-conscious falsifications' (Winsberg 2003), which is nicely illustrated in the Oregonator example by the intervention of setting one differential quotient equal to zero whenever a certain behaviour occurs. This is not only a deviation from the theoretical model, but also contradictory of the testable expectation that the concentrations of the intermediates in the chemical reaction are not constant for longer time intervals. So there is a discrepancy between the simulation and the chemical reaction, a deviation from the goal to imitate the chemical system, which is accepted to avoid obviously strongly erroneous results of the numerical integration of the equations. 'Imitation', in science as in other fields, is never perfect, and its quality comes in degrees.

But how shall an imitation of a process be understood that relies crucially on deviations with respect to the mechanism that brings the phenomenon about? We can reconstruct the imitation relation that holds between a simulation and a process in the material world as an indirect one. It is mediated by the theoretical model, which describes both the simulation and the material system. The theoretical model may not fit any of its applications in a perfect way, and the imperfections with respect to the real-world process may be different from the imperfections with respect to the simulation. Nevertheless, the theoretical model describes the material system and explains its dynamics mechanistically, and it also describes the dynamics of the simulation. So the theoretical model mediates between simulation and material system.[4] Such a relation was also described by Peter Achinstein. According to him, one characteristic of a theoretical model may be the 'analogy between the object or system described in the model and some different object or system' (Achinstein 1968, 216). This is exactly what the theoretical model does with respect to simulation and material world: it displays their analogy by describing uniformly the dynamics of both.

This way the simulation may be regarded as an analogue of the modelled system with respect to its dynamics (that any such analogy is restricted to certain respects was stressed by Bunge 1969). However, displaying aspects of a process is not yet explanation. Explanation in science, as it is conceived here, refers to an account of the *basis* of the dynamics of a system, in particular of the mechanism which brings about this

dynamics. The mechanism which underlies the phenomenon in question is described in the theoretical model. However, in Section 3.1 it was argued that one should conceive the theoretical model not only as stating the mechanism of the simulation but also as a phenomenological description of its dynamics. The explanatory relation holding between simulation and real world is therefore an indirect one. In the triangle of real-world process, theoretical model, and simulation, explanation of the real-world process by simulation involves a detour via the theoretical model. Only considering this detour is it possible to understand why simulations as 'experiments in theory' (Keller 2003) and as 'virtual experiments' (Morgan 2003) may nevertheless help to explain phenomena in the real world.

3.3. Simulations without a Correlate in the Real World

In contrast to the examples used until now, a simulation need not always imitate a *given* material system. There are many cases in which there is no material correlate to a simulation. What is depicted by the image need not be present in reality: in engineering, e.g., simulations are usually run already before a system is realized, for the sake of testing and improving the design of the system before money and work are devoted to building a prototype. But even being aware of such 'pre-imitation' is not sufficient to do justice to the varieties of simulation. Simulations may also be used to investigate the dynamics of non-realizable, fictitious systems. This can be witnessed when considering the predecessors of the Oregonator. Scientists had been thinking about theoretical possibilities of realizing chemical oscillations long before the establishment of the FKN reaction scheme of the BZ reaction on which the Oregonator is based. Two famous models were developed to prove the possibility of sustained chemical oscillations in reaction systems far from chemical equilibrium: Alfred Lotka's model of 1920, and the Brusselator, developed and analyzed by Ilya Prigogine and his group in Brussels from 1968 on.

Lotka (1920) developed a set of three hypothetical chemical reactions. The system generates sustained oscillations, but does not return to or approach its previous state after perturbation. It has no limit cycle, but when disturbed it resumes a new cycle with the same frequency and different amplitudes. The Brusselator, in contrast, has a limit cycle, and thus produces not only sustained, but also stable oscillations. It uses a scheme of four chemical reactions, one of which involves an autocatalytic step similar to the one in the Oregonator. In contrast to the latter, only two, and not three, chemical intermediates are postulated (Lefever 1968; Prigogine and Lefever 1968). Two-dimensionality allows to get at least some qualitative results on the behaviour of the model by analytical methods. Nevertheless, simulations were used extensively in the analysis of the theoretical model.

It is noteworthy that there is no real process known of which simulations of the Brusselator may be regarded as imitations. The correlate of the simulations is fictitious. While a reframed version of Lotka's model was applied later on to the development of populations of predator and of prey, and became famous as the Lotka–Volterra model in ecology (see Krohs 2004, 167), the Brusselator still lacks application to any material system. One reason for this is that it assumes a third-order chemical reaction. Such a

reaction is highly unlikely to occur because of the improbability of an encounter of three molecules in a diluted homogeneous solution. Hence, the Brusselator was often accused of being an unrealistic model (see Fields and Noyes 1974), and it might well be that no realization of its dynamics by any chemical system will ever be accomplished. Considering this, we should either not count numerical integrations of the Brusselator as computer simulations—but rather as pure numerical analysis—or admit that the characteristic of simulations to imitate one process by another allows for exceptions, and that the reality of the imitated process is not a necessary condition for regarding a numerical integration as a simulation.

As a criterion for classifying the numerical integration of a dynamical system as a simulation may count whether it is an application of numerical methods to a scientific rather than to a mathematical problem (Humphreys 1991, 502). In the case of the Brusselator, this criterion holds: the model refers to physical chemistry and in particular to non-equilibrium thermodynamics. At least some variables of the system are interpreted as entities and relations of kinds investigated in the field: they are interpreted as concentrations of different molecule species, rate constants, or stoichiometric factors. Humphrey's criterion does not require that any variable refer to an actual parameter of the real world, as long as the variables are understandable in terms of the theoretical framing of the field. So numerical integrations of the Brusselator may count as simulations of the dynamics of a material system—though not of a real one, but only of one fictitious or imagined. The Brusselator was developed to demonstrate the in-principle possibility of a certain dynamics within a chemical system, disregarding contingencies of a real-world system. If 'possibility' is interpreted as 'thermodynamic soundness', this goal was achieved.

4. Simulacra of Computer Simulations

In the preceding section, the role computer simulations play in science was characterized by their relations to theoretical models and, insofar as it applies, to the material world. This, however, does not sufficiently characterize what the simulation itself is, or is about. The simulation constructs a simulacrum, something that imitates a real or a conceivable world. The simulacrum has to be characterized in addition to the mention of these relations in order to understand what computer simulations are. A simulacrum is something that appears *like* something else (be it real or imagined) in particular respects, without having its (real or insinuated) substance, or proper qualities.[5] Nevertheless, it is something. So we must ask what the simulacra of computer simulations are. We have seen above, in Section 3.2, that Hartmann's view of simulations as processes that imitate other processes matched the examples in cases where real processes are at all simulated. These processes are 'worlds' in the non-ambitious sense of the term introduced in the first paragraph of this paper. The processes that are subjects of scientific enquiry are *material* worlds, so the simulacra may be classified as *virtual* ones. And, in fact, talk of systems investigated by means of simulation, as well as talk of simulacra, quite commonly refers to worlds in this sense: the simulacrum is conceived as mimicking the real world (Winsberg 2001; Peck 2004); it is said that it

may also give us information about non-real, possible, or even impossible worlds (Hughes 1999, 142), and simulations are regarded as belonging to a virtual world (Winsberg 2003) or being created as a 'computer world' (Peck 2004). Other authors characterize computer simulacra similarly as mimicking the world, though without classifying the simulacra explicitly as worlds. Instead, they are conceived as objects copying a given system in some respect (Bunge 1969) or processes used to mimic or imitate other processes (Hartmann 1996).

4.1. Measurability of Real-World and Simulated Processes

How can simulated worlds be further, and positively, characterized, besides as being non-real? Sometimes they are regarded as nearly perfect representations of real systems (Peck 2004). I dare claim that in many cases the degree of accuracy of representation is fairly low and that accuracy is not the most relevant criterion. The primary question with respect to models, as well as with respect to simulations, is whether they are adequate, not whether they are accurate. Adequacy, as pointed out above, is to be judged relative to the epistemic goals for which simulations are used. Even a non-accurate simulation can be of great epistemic value if it sheds light on mechanisms, on qualitative peculiarities, on quantitative behaviour within a certain parameter range, on the realizability of a certain dynamics within a system of a particular kind, etc. It does so by enabling scientists to instantiate a theoretical model—in the weak sense of 'instantiation' introduced above—and to observe its dynamics, as was shown in Section 3.

However, the relation to the material world does not suffice to characterize simulacra. A better clue to what simulacra are can be gained from the following characteristic of digital computer simulations: all their variables and constants are given numerically, in any state the system may ever assume. The numerical values can in principle be read out, for each variable at any time of the development of the system. Reading out the variables of the virtual systems is equivalent to what measurement is with respect to a real-world system: it ascertains the parameters. So if computer simulacra are regarded as worlds, they are *measurable* worlds.[6]

Measurability of simulacra is not limited by any technical restriction. Though the precision of the calculations performed on numerical integration is limited, any actual result of the calculations can be read out with full precision. This contrasts sharply with the situation regarding the processes in the real world, where measurability may be severely restricted. The most striking limitations to the measurability of material systems are due to the limited resolution of any measuring device. It is impossible to overcome *all* limitations of the precision of measuring devices imposed, e.g., by thermal noise, or the finite duration of a single measurement. Nevertheless, any particular technical constraint may be overcome to some degree with advances in measuring technology. An example of one's misconceiving a technical limitation as provably insurmountable is the following statement, which Arnold Eucken made in the 1949 edition of his textbook on chemical physics: 'The rate of true neutralization reactions has proved to be immeasurably fast'. For Eucken's PhD student Manfred Eigen, this was the incentive for his brilliant work on fast kinetics: 'I found this quotation in

Eucken's *Lehrbuch der Chemischen Physik* while I was preparing for my doctor's examination. Although … this book was for me the "bible of physical chemistry", I was then at the age when one accepts practically nothing unquestioned, and so I started to reflect on just how fast an "immeasurably fast" reaction might be' (Eigen 1972). Eigen, in collaboration with Leo de Maeyer, then developed relaxation methods, through which the kinetics of these reactions became measurable down to the nanosecond scale. For this achievement, he was awarded the Nobel Prize in 1967.

4.2. A Posteriori *and* a Priori *Measurability*

While the example of Eigen's work shows how particular technical constraints may be overcome successfully, new questions arise, and new constraints come up with any methodological progress. These questions and constraints may concern not only the issue whether the measurement of a certain variable of a particular system is technically possible, but also whether it is affordable, reliable, and quick enough; whether the system itself is manipulable in the desired way; whether it is available or producible in the required quantity (Humphreys 1991); whether the relevant time scale is neither too large nor too small (Hartmann 1996); and whether there are ethical constraints (Peck 2004), which is most obviously an issue in the biological sciences, but applicable to other fields as well. There are many respects in which the measurability of the world may fall short from the needs and desires of scientists with respect to observation, experimentation, and theory formation. These limits of measurability need to be learned from experience and are subjected to change. They can be determined only *a posteriori*.[7]

Measurability is a property that distinguishes simulations, not only from material systems, but also from the systems defined by theoretical models. If a theoretical model is not analytically integrable, the system it defines is not measurable. And since simulations are based on systems that deviate more or less from the ones defined by the theoretical models, the latter systems are not themselves made measurable by the simulations, but merely supplemented my measurable ones.

However, there are also theoretical models that *can* be integrated by analytic methods. For example, the dynamics of various physical systems is modelled as a harmonic oscillation, and the harmonic oscillator can be integrated by the sine function. These theoretical models define measurable worlds as well. Nevertheless, there is an important difference with respect to the measurability of simulations. This difference can be used to delineate simulations: the analytic solvability of a theoretical model depends in part on the state of the art in mathematics, and it does so in a different way than simulations do. One needs first to state the theoretical model before being able to decide whether or not it can be integrated analytically. In particular, one cannot read from the system to be modelled whether the model will be analytically integrable—at least as long as no preconception with respect to the complexity of the model is accepted.[8] This turns out only *a posteriori* and is, as already noticed, subject to change according to the development of analytic methods. With simulations the situation is different: again, the availability of adequate mathematical tools is highly dependent on the state of the art.

Moreover, one cannot say once and for all what a simulation of a system will look like, and which parameter space can be covered by running the simulation. So the set of states that can be accessed by a simulation may be highly dependent on the state of the art in mathematics and computer science, and be much smaller than the set of possible states of a system. But in advance of any experience and consequently before starting any simulation, we already know that any tool that may be used to integrate a model numerically will yield only numerical, i.e., measurable states. Digital computer simulacra are *a priori* measurable worlds.[9]

Though I have demonstrated this for the case of discrete simulations of continuous models only, the argument holds for discrete simulation of discrete models as well (e.g., the Ising model as discussed by Hughes 1999). It is arguable whether it may hold even for simulations that are run on an electronic analog computer. In such a machine, all variables are represented by electric potentials within an easily measurable range on a device that provides in itself the capacity of tracking the potentials. The precision of the simulation is more restricted than in the digital case due to the noise level, and depends on factors like the constancy of temperature, speed of simulation, etc. (Smith and Wood 1959; Mead 1989), but the potentials can be measured. Nevertheless, regarding an analog simulation as being *a priori* measurable would be misleading: the limited precision and speed of all measuring devices given, it becomes clear that the measurement need not necessarily follow all changes in the state of the computer, and therefore need not necessarily track the variables. Measurement of analog simulations is a physical process. Consequently, despite the fact that analog computers might be constructed and set up to allow for best possible measurability, the simulacrum world of an analog simulation is not *a priori* measurable. Measurability in this case is limited by the measuring devices, and the limits turn out *a posteriori* only. Other analog computer simulations, e.g., mechanical ones, lack *a prioricity* of measurability for related reasons.[10] Only digital simulacra are measurable *a priori*.

5. Conclusion: Epistemic Virtues of Measurable Simulacra

I have characterized the relation between computer simulation and imitated system and the way in which simulations explain processes in the material world as indirect, mediated by theoretical models. Digital simulations were then characterized by *a priori* measurability of the simulacra. These considerations referred to models and their relations and properties. Finally, something needs to be said about the use scientist can make of the data gathered by means of simulation. It must be discussed how such data can play a role in predicting material-world processes and testing theoretical models.

Let me assume counterfactually that in the BZ reaction the kinetics of some intermediate, say, $HBrO_2$, was not measurable in the 1970s for technical reasons, though the intermediate itself was chemically identified. This intermediate is represented by X, one of the intermediates of the theoretical model of the Oregonator. The kinetics of X is supposed to be analog to the kinetics of $HBrO_2$ in the BZ reaction. But the Oregonator

is not integrable by analytic means. Consequently, it neither leads to the particular predictions about the behaviour of $HBrO_2$ scientists may aim at nor is testable in this respect when the assumed technical limitations of measurability of the kinetics of $HBrO_2$ cease to apply. Both epistemic restrictions can be overcome to a certain extent by running simulations, since the *a priori* given measurability of the simulation helps collect the missing data.

First, *predictions* about the dynamics of the intermediate can be derived from the readout of the *a priori* measurable parameters of the simulacrum, under the assumption that the theoretical model is an adequate description of the reaction as well as of the simulation, so that the latter is analog to the reaction with respect to its dynamics. This, of course, does not guarantee the validity of the predictions. *A prioricity* holds for knowledge of the measurability of the simulacra, but not for knowledge of the adequacy of the simulation and the reliability of the predictions which may be based upon it. Reliability needs to be judged independently. In this respect, limitations arise that are related to the second epistemic restriction. They will be discussed after presenting this restriction.

The second restriction is that of the *testability* of a model. Even if empirical data on the dynamics of a real-world system are available, a theoretical model which is not integrable analytically cannot be tested straightforwardly since it simply does not provide data for comparison. Such a theoretical model becomes testable only by numerical integration, i.e., by generating the required data by measuring a simulacrum. In the case of the BZ reaction, the Oregonator becomes testable as soon as the kinetics of the intermediate becomes measurable, but only with the help of simulations: experimental data may then be compared with data obtained from the simulation, which again are assumed to give a reliable picture of what the model describes. A model like the Oregonator, which is not solvable analytically, can be used as a predictive tool, and tested adequately only if it is instantiated by a system allowing for the numerical output of all parameters. Computer simulations allow for exactly this. Yet it remains a problematic issue to check the reliability assumption. Whether it can be satisfactorily justified depends on the bits of knowledge about the theoretical model that can be obtained independently, for example by analytic methods. Scientists succeeded in this respect in the case of the Oregonator. In less favourable cases, simulations have to be interpreted with more caution.

As with any prediction of scientific results, correctness of the predictions by means of simulations cannot be guaranteed, but needs to be established empirically. This is problematic in cases where simulations are used to predict the future development of a system that cannot be subjected to experimental manipulation, e.g., in the investigation of probable future climate changes. Here, measurability of the simulation allows for an extrapolation of the observed time series of climate parameters into the immeasurable space of future development. Simulations may also allow checking the robustness of the model and by this show the reliability of the explanation it gives, but they cannot fully substitute for the limitations in experimental cross-checking. Bunge's insight that 'nothing can replace the study of the real thing' (Bunge 1969), taken in the strict sense, cannot be overcome by any method. However, if one is aware of the

limitations of simulation, an *a priori* measurable world may at least help explaining the real thing.

Acknowledgements

The work presented here was carried out at the Konrad Lorenz Institute for Evolution and Cognition Research, Altenberg, Austria. Support by the institute is gratefully acknowledged. An earlier version of this paper was presented at the workshop *Models and Simulations*, Paris, June 2006. I would like to thank the discussants for their helpful comments. I also owe thanks to the two anonymous referees of this journal for valuable hints that helped further to improve the paper.

Notes

[1] See Glennan (1996, 2002) for an account of mechanisms that does not include activities. I stick with the account of Machamer et al. (2000), which fits better to the scientific models in question.

[2] It should be noticed that a scientific model is not just a mathematical structure (in contrast to the use of the term 'model' in model theory: Balzer et al. 1987), but includes what in the structuralist jargon is called an 'intended application' (Sneed 1971) by providing an interpretation of the variables (Krohs 2004).

[3] While digital simulations are usually performed on a computer, a human calculator, for example, is also a possible 'device' for running such simulations, though with limited calculating capacity. Consequently, computer techniques applied in simulation are regarded by Humphreys (2004) as extensions of our computational abilities, comparable to the technological enhancement of our sensory apparatus by scientific instruments.

[4] Construed like this, it turns out that models may mediate between two phenomena (processes), allowing for understanding one as an imitation of the other. This is an additional kind of mediation by models, supplementing that between phenomena and theory (Morgan and Morrison 1999).

[5] This is the sense in which also Nancy Cartwright uses the term 'simulacrum', though with respect to theoretical models, not to simulations (Cartwright 1983, 152–153). Applied to simulations only, my use of the term does not commit one to a Cartwrightian anti-realistic account of scientific explanation but remains neutral in this respect. See Stöckler (2000) for a defence of the view that the use of simplified models and simulations could be reconciled even with a full-fledged realism.

[6] The numerical values are definite even if they are not read out, so one might be tempted to speak of *measured* worlds instead. However, to count as measured, the values had to be not only definite but also recorded, by an observer or by the computer. Since this need not happen, no more than *measurability* can be claimed.

[7] I am not concerned with the issue of the indeterminacy of certain parameters, which may not be overcome by any advance in measuring technology. Indeterminacy of this kind has to be regarded as a feature of the real world and therefore needs to be reproduced in some way in a simulation of a process, where it is relevant.

[8] In many cases it may be possible for an experienced modeller to 'see' this 'immediately', but this means nothing more than that one is able to conceive the model or central features of it without writing down the equations.

[9] This general claim holds *a fortiori* with respect to any particular parameter of the simulation. We know, in advance of any experience, that the parameter is measurable without restrictions.

[10] Several kinds of mechanical calculating machines, in particular pinwheel machines (Martin 1992), seem to be an exception, but these have to be properly classified as mechanically working digital machines, not as analog ones.

References

Achinstein, P. 1968. *Concepts of science: A philosophical analysis.* Baltimore, MD: Johns Hopkins University Press.

Balzer, W., C. U. Moulines, and J. D. Sneed. 1987. *An architectonic for science: The structuralist program.* Dordrecht: D. Reidel.

Bunge, M. 1969. Analogy, simulation, representation. *Revue Internationale de Philosophie* 23: 16–33.

Cartwright, N. 1983. *How the laws of physics lie.* Oxford: Clarendon Press.

Craver, C. F. 2001. Role functions, mechanisms, and hierarchy. *Philosophy of Science* 68: 53–74.

Eigen, M. 1972. Immeasurably fast reactions. In *Nobel Lectures in Chemistry* 1963–1970. Vol. 4: 170–203. Amsterdam: Elsevier.

Field, R. J., and R. M. Noyes. 1974. Oscillations in chemical systems IV: Limit cycle behavior in a model of a chemical reaction. *Journal of Chemical Physics* 60: 1877–1884.

Field, R. J., E. Körös, and R. M. Noyes. 1972. Oscillations in chemical systems II: Thorough analysis of temporal oscillation in the Bromate–Cerium–Malonic acid system. *Journal of the American Chemical Society* 94: 8649–8664.

Glennan, S. 1996. Mechanisms and the nature of causation. *Erkenntnis* 44: 50–71.

———. 2002. Rethinking mechanistic explanation. *Philosophy of Science* 69 (Proceedings): S342–S353.

Hairer, E., S. P. Nørsett, and G. Wanner. 1993. *Solving ordinary differential equations 1: Nonstiff problems.* 2nd ed. Berlin: Springer.

Hairer, E., and G. Wanner. 1996. *Solving ordinary differential equations 2: Stiff and differential-algebraic problems.* 2nd ed. Berlin: Springer.

Hartmann, S. 1996. The world as a process: Simulations in the natural and social sciences. In *Modelling and simulation in the social sciences from the philosophical point of view,* edited by R. Hegselmann, 77–100. Dordrecht: Kluwer.

Hughes, R. I. G. 1999. The Ising model, computer simulation, and universal physics. In *Models as mediators: Perspectives on natural and social science,* edited by M. S. Morgan and M. Morrison, 97–145. Cambridge: Cambridge University Press.

Humphreys, P. 1991. Computer simulations. In *PSA 1990: Proceedings of the 1990 Biennial Meeting of the Philosophy of Science Association,* edited by A. Fine, M. Forbes, and L. Wessels, 2: 497–505. East Lansing, MI: Philosophy of Science Association.

———. 1994. Numerical experimentation. In *Patrick Suppes: Scientific philosopher,* edited by P. Humphreys, 2: 103–121. Dordrecht: Kluwer.

———. 2004. *Extending ourselves: Computational science, empiricism, and scientific method.* Oxford: Oxford University Press.

Keller, E. F. 2003. Models, simulations, and 'computer experiments'. In *The philosophy of scientific experimentation,* edited by H. Radder, 198–215. Pittsburgh, PA: University of Pittsburgh Press.

Krohs, U. 2004. *Eine Theorie biologischer Theorien: Status und Gehalt von Funktionsaussagen und informationstheoretischen Modellen.* Berlin: Springer.

Lefever, R. 1968. Dissipative structures in chemical systems. *Journal of Chemical Physics* 49: 4977–4978.

Lotka, A. J. 1920. Undamped oscillations derived from the laws of mass action. *Journal of the American Chemical Society* 42: 1595–1599.

Machamer, P. 2004. Activities and causation: The metaphysics and epistemology of mechanisms. *International Studies in the Philosophy of Science* 18: 27–39.

Machamer, P., L. Darden, and C. F. Craver. 2000. Thinking about mechanisms. *Philosophy of Science* 67: 1–25.

Martin, E. 1992. *The calculating machines.* Cambridge: Cambridge University Press.

Mead, C. 1989. *Analog VLSI and neural systems.* Reading, MA: Addison-Wesley.

Morgan, M. S. 2003. Experiments without material intervention: Model experiments, virtual experiments, and virtually experiments. In *The philosophy of scientific experimentation,* edited by H. Radder, 216–235. Pittsburgh, PA: University of Pittsburgh Press.

Morgan, M. S., and M. Morrison, eds. 1999. *Models as mediators: Perspectives on natural and social science.* Cambridge: Cambridge University Press.

Peck, S. L. 2004. Simulation as experiment: A philosophical reassessment for biological modeling. *Trends in Ecology and Evolution* 19: 530–534.

Prigogine, I., and R. Lefever. 1968. Symmetry breaking instabilities in dissipative systems II. *Journal of Chemical Physics* 48: 1695–1700.

Rohrlich, F. 1991. Computer simulation in the physical sciences. In *PSA 1990: Proceedings of the 1990 Biennial Meeting of the Philosophy of Science Association,* edited by A. Fine, M. Forbes, and L. Wessels, 2: 507–518. East Lansing, MI: Philosophy of Science Association.

Smith, G. W., and R. C. Wood. 1959. *Principles of analog computation.* New York: McGraw-Hill.

Sneed, J. D. 1971. *The logical structure of mathematical physics.* Dordrecht: D. Reidel.

Stöckler, M. 2000. On modeling and simulations as instruments for the study of complex systems. In *Science at century's end: Philosophical questions on the progress and limits of science,* edited by M. Carrier, G. J. Massey, and L. Ruetsche, 355–373. Pittsburgh, PA: University of Pittsburgh Press.

Winsberg, E. 2001. Simulations, models, and theories: Complex physical systems and their representations. *Philosophy of Science* (Proceedings) 68: S442–S454.

———. 2003. Simulated experiments: Methodology for a virtual world. *Philosophy of Science* 70: 105–125.