A priori measurable worlds

Ulrich Krohs
Konrad Lorenz Institute for Evolution & Cognition Research,
Adolf-Lorenz-Gasse 2, 3422 Altenberg, Austria
and
Philosophy Department, University of Hamburg,
Von-Melle-Park 6, 20146 Hamburg, Germany
<ulrich.krohs@uni-hamburg.de>

Abstract: Part of the scientific enterprise is to measure the material world and to explain its dynamics by means of models. However, not only is measurability of the world limited, analyzability of models is so, too. Most often, computer simulations offer a way out of this epistemic bottleneck. They instantiate the model and may help to analyze it. In relation to the material world a simulation may be regarded as a kind of a "non-material scale model". Like any other scale model, it does not per se give any scientific explanation but is first in itself an object of scientific enquiry, a world. Since this world is numerical, it is a priori measurable. Its role in scientific explanation will be discussed.

Keywords: chemical oscillator; numerical methods; measurability; model; simulation; virtual world.

1 Introduction

Part of the scientific enterprise is to explain the dynamics of the material world. The world, or a world, in this context may be understood as a system of parts and their relations as it develops in time. For explaining its dynamics, parameters that define the state of the system must be measured. However, not every scientifically interesting feature of the material world turns out to be measurable, be it for principle or for technical reasons. Principle restrictions seem to hold in the cases of quantum indeterminacy. According to quantum mechanics, the state of a system does not uniquely determine a set of values for all its measurable properties, but probability distributions only.[1] Related to this on the level of the measurement of the

[1] A famous thought experiment by Einstein, Podolsky and Rosen was meant to demonstrate that the quantum mechanical description of physical reality is incomplete. The results of the proposed experiment were anticipated to prove that the restrictions on measurability of pairs of non-commuting variables could be

properties of particles is the indeterminacy of position and momentum or any other pair of complementary observable quantities. Such principle constraints on measurability may be regarded as the expectable limits of the mathematization of the world (though the limits of measurability may themselves be described mathematically). They have to be accepted, and they have to be reproduced in "realistic" scientific models and computer simulations of the phenomena. Technical constraints of measurability, in contrast, need not – usually should not – be reproduced by a model. Though it is impossible to overcome in general the limitation of the precision of measuring devices, any particular technical constraint may be overcome with advances in measuring technology. An example of how technical limitations can be misconceived 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 his PhD student Manfred Eigen this was the incentive for his brilliant work on fast kinetics. He comments on this: "I found this quotation in Eucken's Lehrbuch der Chemischen Physik while I was preparing for my doctor's examination. Although as a student of Eucken, 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 then developed relaxation methods, by help of which the kinetics of these reactions became measurable down to the nanosecond scale. For this he was awarded the Nobel price in 1967.

However, with any methodological progress new questions arise and new constraints come up. These may concern not only the question whether the measurement of a certain variable of a particular system is possible with the methods available but also whether it is affordable, reliable, and quick enough; whether the system itself is manipulable in the desired way; and 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 applies in other fields as well. In the sense of all these constraints not reflecting indeterminacy they may be regarded as resembling technical constraints to measurability. So there are many respects in which the measurability of the world can be determined only a

overcome by ruling out the other possible outcome that instantaneous long-range interactions of particles occur (Einstein et al. 1935). When the experiment was carried out, however, it turned out that the seemingly paradoxical results indeed occur, giving strong evidence for the non-locality of quantum states and leaving immeasurability untouched (Aspect et al. 1982). Experiments on the so-called quantum teleportation now take advantage from the non-locality (Bouwmeester et al. 1997).

posteriori, and in which it may fall short from the needs and desires of scientists with respect to observation, experimentation, and theory formation.

There are several ways out of the epistemic bottleneck of limited measurability. In a few cases thought experiments might help, but as the EPR example has already shown (footnote 1) this might not yield reliable results. In other cases, limits of measurability are overcome by the investigation of material systems that are supposed to resemble the system of interest in relevant respects, like the investigation of the hydro- and aerodynamics of scale models instead of real ship bodies and airfoils in water tanks and wind channels. These "naturalistic analog simulations" (Trenholme 1994) or "experimental simulations" (Hartmann 1996) will not be at issue in my paper. I concentrate on the third way, on computer simulations, which are in many cases the way of choice to collect data that cannot be obtained by an investigation of a material system. While they are usually performed on a computer, a human calculator, e.g., is also a possible "device" for running such simulations, though with limited calculating capacity. Consequently, computer techniques applied in simulation are regarded by Paul Humphreys as extensions of our computational abilities, comparable to the technological enhancement of our sensory apparatus by scientific instruments (Humphreys 2004).

My main concern in this paper is to specify what a computer simulation is. After a short sketch on scale models, which will later turn out to show some similarities with computer simulations, I will specify what theoretical models are and how they are used to predict the dynamics of a material system. Next, I will analyze how simulations are related to theoretical models on the one hand and to the material world on the other. As examples I will use continuous models of a chemical oscillator, the Belousov-Zhabotinsky reaction. Next, the question will be addressed what the simulacrum is that is "produced" in a computer simulation. Candidates are, e.g., processes (or systems) that mimic the real world, virtual worlds, and solutions of theoretical models. All these candidate definientes cover important aspects of what a computer simulation is, but none accounts for the whole truth. A synthesis is proposed which will finally give some insight into the epistemic role that simulations play for scientific explanation and into the way how simulations help to overcome some consequences of the technical limitations of measurability.

2 Material scale models

Let me start with a naïve concept of a model: a model is an entity that presents characteristics of something else. A model car displays, to some extent, the shape of a car and the minimal function of turning wheels; a model airplane the aerodynamic characteristics of an airplane

but not its size and carrying capacity; the model of the body of a ship in a water tank the hydrodynamic properties of the ship; the model of an aircraft wing in the wind channel aerodynamic properties of the wing, which holds also for the wing in a water tank if some theoretical effort is made to account for the different Reynold's numbers of the media. These concrete *scale models* are obviously *not* theoretical models, to which simulations shall be related below, but they show some characteristics that will be relevant with respect to simulations themselves. A conceptual link is that, if a concrete scale model represents the mechanism of the modeled system, it can be regarded as simulating its dynamics by providing an analog system (Trenholme 1994).[2]

Several things can be learned from scale models about the relation to the entity they are a model of. First, that they depict aspects of the modeled entity: what a Ferrari looks like, how a wing behaves in laminar and in turbulent flow, which forces water flow exerts on the hull of a ship. Second, representation is restricted to selected characteristics of the entity, e.g., not on the size, not on being able to drive by own force (in the case of a matchbox car), and it may represent them in a simplified way. Third, the entity that is "represented" might not or not yet exist. The latter is usually the case when engineers are testing a model to learn for constructing an airplane or a ship, and models of spaceships like the Enterprise represent something that most probably will never be built in reality. The fourth thing we can learn from the example of concrete models is that they may in fact fail to represent the characteristics to the desired precision they are meant to represent. A model car may badly represent the shape of the modeled car; a model wing that has for example not an adequate surface may not represent the aerodynamic properties of the real wing.

Having the examples in mind, we must specify the naïve concept of a model even with respect to material models: the representation relation need not hold in a way of a strict mapping, there need not hold a homomorphism (or even an isomorphism) between model and modeled entity. The model is *conceived as* representing particular characteristics of the modeled entity, and it is the matter of the *quality* of the model whether or not it represents adequately what it is meant to represent. There are good and bad models (and everything in between), and there might not be an absolute quality scale: a model may be good in one respect and a bad one in another. It is perhaps most useful in overemphasizing (and thus badly representing) a certain trait of the depicted entity.

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[2] There might be a problem using this term with respect to so-called model organisms in biology, like the mouse being used as a "model" for the immune system of humans. "Scale model", I admit, would be a strange label. However, it needed a longer argument to decide whether or not the use of "model" in this case must be reconstructed differently anyway (Keller 2000).

3 Theoretical models

Theoretical models is cartegorically different from a scale model. It is a piece of scientific theory and does not *depict* and mimic the modeled system, as a scale model does, but *describes* it, usually in a formalized way. A theoretical model is a set of assumptions about some object or system (Achinstein 1968). Such a model may describe the entity or system in a certain state or the dynamics going on in the system, it may be static or dynamic. In the context of simulations, we are interested mainly in dynamic models (Hartmann 1996, 82-83), especially in those that refer to the internal mechanism that brings the dynamics about. Such models may be regarded as not only describing but also as *explaining* the process under consideration. "Dynamic" here does *not* mean that the model itself has any kinetic properties but only that it describes the dynamics of a material system. Regarding computer simulations as simulations of the model's behavior (Hughes 1999) therefore misconceives the relation between models and simulations.

An example of an explanatory dynamic model is the *Oregonator*, a model of the Belousov-Zhabotinsky reaction (BZ reaction). This reaction is famous for displaying chemical oscillations in space and time, which are observable as periodic color 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 of the different colors of Cerium ions in two different oxidation states accounts for the color changes. The complicated chemical reaction can be described by a system of 14 reactions, known as the FKN (Field-Körös-Noyes) mechanism (Field et al. 1972). A simplified set of only 5 reactions could be isolated from this FKN mechanism that is sufficient to describe the behavior of the system. It was named the *Oregonator*, after its institution of origin, the University of Oregon (Field and Noyes 1974). These systems are two theoretical models, the more detailed FKN model, and the more easily tractable Oregonator. The following chemical equations define the Oregonator:

$$A + Y \Leftrightarrow X$$
$$X + Y \Leftrightarrow P$$
$$B + X \Leftrightarrow 2X + Z$$
$$2X \Leftrightarrow Q$$
$$Z \Leftrightarrow fY$$

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. Reaction constants must be assigned to each direction of each reaction.[3]

After introducing the reaction constants, 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 transformed their model into a dimensionless form:[4]

$$d\alpha/d\tau = 0\ s(\eta - \eta\alpha + \alpha - q\alpha^2),$$
$$d\eta/d\tau = s^{-1}(-\eta - \eta\alpha + f\rho),$$
$$d\rho/d\tau = w(\alpha - \rho).$$

This system of three ODEs describes the kinetics of the BZ reaction; it is a dynamic model of the reaction.[5] Unfortunately one cannot calculate the state of the system at 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 is almost useless for predicting the dynamics of the system – as long as mathematical analysis is regarded as the only means to integrate the equation system (see, e.g., (Humphreys 1991) for a discussion of the mathematical intractability of many continuous theoretical models, and (Hughes 1999) for an account of this problem in a discrete model). At least, one can assume from the first differential equation or from the autocatalytic third reaction of the mechanism that the model yields oscillations within a certain parameter range. This is something, but desired is more, and more is achieved by means of numerical integration in computer simulations. I will come back to this in the following sections on simulation.

The quality and usefulness of a particular theoretical model may be judged differently in dependence from the aspects of a material system that shall be explained. I take it here that an epistemic goal that is followed with theoretical dynamic models is to predict the dynamics under certain conditions and to identify qualitatively discernable structures like singularities, limit cycles, or regions of particular dynamical behavior. Though the FKN model gives a more realistic description of the BZ reaction than the Oregonator, the Oregonator is much better to handle and therefore more useful for an exploration of the behavior of the reaction

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[3] The overall reaction results to: $f\mathrm{A} + 2\mathrm{B} \Leftrightarrow f\mathrm{P} + \mathrm{Q}$.

[4] For the values assumed for the constants and for the initial conditions as well as and for the definition of the dimensionless variables and constants see Fields and Noyes (1974, 1879).

[5] It should be noticed that, in contrast to what model theory calls a model, a scientific model is not just a mathematical structure, which is a set of objects and a set of relations defined on the object set (Balzer et al. 1987). It includes what in the structuralist jargon is called an 'intended application', by providing an interpretation of the variables (Krohs 2004).

system under different conditions. One may have to be satisfied with a qualitative match of model and modeled system if otherwise the predictive power would be lost.

4 Relations of simulations

A way that allows for predictions even in cases where no analytical solution can be obtained from a theoretical model is running simulations. In such a case, the model is instantiated on a computer and developed in time, which may 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 put forward that simulation could therefore be conceived in a way as experimenting with theoretical models and there is a near consensus in regarding simulations as "numerical experiments", a new kind of scientific method that lies somewhere in between theory and experiment (Rohrlich 1991; Humphreys 1994; Hartmann 1996; Winsberg 2003; Peck 2004). The methodological aspects that numerical experimentation shares with one and the other method were thoroughly analyzed (Winsberg 2003). This, however, does not explain the structural aspect of this relation.

4.1 Simulations as related to theoretical models

Simulations provide numerical solutions to theoretical models and are run primarily when theoretical models cannot be integrated analytically (Humphreys 1991). They may, of course, be helpful also in cases where analytical methods are available (Hartmann 1996, acknowledged by Humphreys 2004, 108). Simulations are thus a means of analyzing theoretical models. It will shed light on the relationship to look at the Oregonator example, which shows that this relationship is not to be described as a faithful instantiation of the model by a simulation.

The Oregonator as described above is a simplified model of the BZ reaction with only three intermediates. But three is already too much for an analytic treatment. There are no known methods to analytically obtain quantitative and even many qualitative results from such a system of ODEs, so Field and Noyes's integration of the system had to be performed purely numerically (Field and Noyes 1974, 1882). This was done by way of stepwise integration, using the established Runge-Kutta method. Roughly and simplified, this method may be described as reconstructing a trajectory in the phase space as described by a set of ODEs by estimating its slope at the beginning of an interval and stepping forward one interval Δt on a straight line defined by the starting point and estimated slope. The endpoint 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. The discretization error is smaller in the actual Runge-Kutta method than it appears from this sketch, but it is nevertheless present (Hairer et al. 1993).[6] The error per step, the local discretization error, depends on the increment Δt. It can be minimized, though never completely eliminated, by decreasing Δt. Unfortunately, there are two restrictions to decreasing Δt, since this leads to an increase of the number of steps that must be performed to simulate a certain interval of the trajectory. First, more steps lead to an increase of the required computation time. Second, and even worse, it results in an increase of another kind of error: every computation is done with a limited number of digits and therefore leads 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 power but to an increase of the numerical error. This already shows that the simulated system may come close to the system described by the theoretical model but nevertheless differs from it. This might be regarded as merely a lack of precision of the simulation with respect to the model. The simulation of the Oregonator, however, 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 to the others. For not ending 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). The problem was overcome by setting one differential quotient = 0 when these wild oscillations began during the integration of the system, i.e. by making changes to the system.[7]

From this description of the simulation we learn that the simulated system differs from the system described by the model at least in the following three respects: (i) is 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 changes that had to be made on the descriptive level in order to overcome the problems that the stiffness of the theoretical model poses on numerical integration. While (ii) can be seen as being just some imprecision, the theoretical modifications (i) and (iii) show that the model

[6] The method uses, e.g., not the slope at the beginning of an interval but the average of the slopes at the beginning, in the middle, and at the end of an interval

[7] The results were double-checked, using a different integration method, and turned out to be reliable (Field & Noyes 1994, 1880).

that is the basis of the simulation is *not* identical with the theoretical model.[8] The simulation does *not* strictly show the dynamics of the theoretical model. It shows the dynamics of another system, but this dynamics is similar to the dynamics of the model. The theoretical model may thus be regarded as a simplified and in the present case non-computable description of the simulated model. Seen the other way around, the simulation is an instantiation of the theoretical model. From Section 3 this relationship is already known to hold as well between theoretical model and material world: the theoretical model is a simplified but often not computable description of the world. Since the model explains the dynamics of both, the material world processes and the simulation, both are to be regarded as instantiations or intended applications of the same model.

The case is similar for simulations run on an analog computer, though there is no discretization error, and though the theoretical model can in many cases simply be "plugged together", without modifying the mathematical structure. The simulation is set up more directly from the set of ODEs than in the digital case. However, in this analog case the physical system, the analogue computer, introduces deviations from the theoretical model. They may be negligibly small in many cases, but the electronic circuit elements are subject to limited stability and they introduce systematic errors due to unavoidable nonlinearities, in addition to the generally limited precision (Smith and Wood 1959; Mead 1989). Being a physical device, the setup analog computer *is* not and even does not approximate the theoretical model but is its –often faithful – instantiation.

4.2 Simulations as related to the material world

Before being able to define the concept of a simulation, the other relationship must be inquired that holds between simulations and the material world. As Stephan Hartmann pointed to, "the most significant feature of a simulation is that it allows scientists to *imitate one process by another process*" (Hartmann 1996, 77). We find this confirmed in the Oregonator example, where the simulation is meant to describe and to predict the behavior of a material dynamic 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 = 0 for certain intervals of a simulation. This is not only a deviation from the theoretical model but also contradicts the testable expectation that the

[8] Nevertheless, the theoretical model cannot be replaced by the model that is the basis of simulation, since there is no reason to assume that the latter describes the world as good as the further. Besides, the latter is the more complicated – though better computable – model.

concentrations of the intermediates in the chemical reaction are not constant for longer time intervals. It is an accepted misfit between the simulation and the chemical reaction, a deviation of the goal to imitate the chemical system, which is accepted in order to avoid obviously erroneous results by the numerical integration of the equations. But "imitation" comes in degrees anyway.

We can reconstruct the imitation relation that holds between a simulation and a process in the material world as an indirect one, mediated by the theoretical model of which both, the simulation and the material system, are instantiations. The theoretical model describes a material system and explains its dynamics. It describes as well the dynamics of the simulation. According to Peter Achinstein, one important trait of a model is that it "may display an analogy between the object or system described and some other object or system" (Achinstein 1968). This is exactly what the theoretical model does with respect to simulation and material world. The structural similarity of both systems, of course, is present independently of the unifying description by a theoretical model. So the simulation may be regarded as a scale model of the modeled system, though an abstract one, that *depicts* the system. But it is not in itself an explanation of any process, as, e.g., the structure of a car of a particular brand is not in itself an explanation of the structure of another sort of car, though both will be similar in many respects. The explanatory relation that holds between simulation and real world involves the detour via the theoretical model.

However, there are many cases in which there is no material correlate to a simulation; it need not be present in reality what is depicted by the image: in engineering at least, and we should not exclude simulation in this field from our considerations, the theoretical model is often built and simulations run already before the system is constructed. But even being aware of such "pre-imitation" is not sufficient to do justice to simulation, it may be used for tackling more principle questions. Let me have a look at the predecessors of the Oregonator. Scientists had been thinking about theoretical possibilities of realizing chemical oscillations long before the FKN reaction scheme of the BZ reaction was established. Two famous models were developed to prove the possibility of sustained chemical oscillations in reaction systems far from chemical equilibrium, Alfred Lotka's model from 1920 and the Brusselator, developed and analyzed by Ilya Prigogine and his group in Brussels from 1968 on.

Lotka (1920) develops a set of three hypothetical chemical reactions. The system generates sustained oscillation if undisturbed but does not return into or approach its previous state after perturbation. It has no limit cycle but assumes on disturbance 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 is 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 for getting at least some qualitative results on the behavior of the model. Nevertheless, simulations had to be used extensively in the analysis of the theoretical model. It is noteworthy that there is no real process known of which these simulations may be regarded as imitations. While a reframed version of Lotka's model was applied to the development of populations of predator and of prey and became famous as the Lotke-Volterra model in ecology, 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 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 the dynamics of the Brusselator will be possible by any chemical system. So we either should not count numerical integrations of the Brusselator as computer simulations but, e.g., as pure numerical analysis, or have to admit that the characteristics of simulations to imitate one process by another process allows for exceptions and is not a necessary condition for a numerical integration being a simulation. The latter seems to be more plausible. The variables of the Brusselator are interpreted as concentrations of different molecule species; some constants as rate constants, others as stoichiometric factors. The Brusselator was developed to demonstrate the possibility of a certain dynamics within a chemical system. If "possibility" is interpreted as "thermodynamic possibility", this goal was achieved, though the result might be judged differently with respect to the steric possibility of a third order reaction mechanism. At any rate, the numerical integration of the Brusselator is an application of numerical methods not to a mathematical problem but to a specific scientific problem. This may count as a criterion for judging it as simulation (Humphreys 1991, 502). It is the simulation of the dynamics of a material system, though not of a real but only of an imagined one (which might hardly count as an instance of imitation).

5 The simulacrum of computer simulations

A simulation is not completely characterized by its relations to theoretical models and, if it applies, to the material world. It shows us a simulacrum and this has to be characterized as well. The simulacrum is something that appears *like* something else in particular respects,

without having its substance or proper qualities.[9] Nevertheless, it is *something*. So we must ask what the simulacra of computer simulations are. We have seen above, in section 4.2, that Hartmann's view of simulations as processes that imitate other processes was matching the examples in cases where real processes are 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 subject of scientific enquiry are material worlds, the simulacra may be classified as virtual ones. And, in fact, talk about systems that are investigated by means of simulation as well as talk about 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 give us also information about non-real, possible or even impossible worlds (Hughes 1999, 142), and simulations themselves are regarded as belonging to a virtual world (Winsberg 2003; Peck 2004).

How can simulacrum worlds be further characterized, besides being non-real or virtual? First, they need not even represent real worlds. This was the case with the examples of the Lotka oscillator and the Brusselator where there are no known chemical systems to which these models and the respective simulations apply (there may be ecological systems in the case of the Lotka model). The simulacrum of the Lotka model is at least a chemically possible world, while the one of the Brusselator might even be an impossible world because of the involvement of a third order chemical reaction. Some of the simulacra, however, fit well to processes in the material world, as is the case with the Oregonator simulations. Such simulacra are good abstract scale models. Sometimes they are regarded as accurate representations of real systems (Peck 2004), but I dare claim that accuracy of representation is for sure not the most relevant criterion and usually does not apply. 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 is to be judged relative to the epistemic goals for which simulations are used. A non-accurate simulation – this seems to be the standard case – can be of great epistemic value if it sheds light on mechanisms, on qualitative peculiarities, on quantitative behavior within a certain parameter space, on the realizability of a certain dynamics with a system of a particular sort, etc.

The relation to the material world therefore does not suffice to characterize the simulacra. Referring to one of the rationales for the employment of simulations gives a better clue to what the simulacra are. Simulations are run mainly in cases in which models do not yield

[9] This is the sense in which also Nancy Cartwright uses the term, 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 to a Cartwrightian anti-realistic account of scientific explanation but remains neutral in this respect.

analytic results that describe interesting states of the modeled system, so that numerical solutions were searched for. A characteristic of all computer simulations is thus that all their variables and constants are given numerically, in any state the system may assume. The numerical values can in principle be read out, for any of the variables. This is equivalent to a measurement of the state of the system; so all these simulacra are *measurable* worlds.[10]

Measurability is a property that distinguishes simulations not only from material systems but also from many theoretical models. Models that are not analytically integrable are not measurable, and since simulations are based on systems that are more or less deviating from the theoretical models they are not themselves made measurable by the simulations. But there are also theoretical models that can be integrated by analytic methods. For example, the dynamics of many different physical systems is modeled as a harmonic oscillation, and the harmonic oscillator can be integrated by the sinus function. These theoretical models define measurable worlds as well. But there is an important difference with respect to the measurability of simulations: the analytic solvability of a theoretical model depends in part on the state of the art in mathematics. And, more important, one needs first to state the model before one can decide whether or not it can be integrated analytically.[11] Especially, one cannot read from the system that shall be modeled – as long as no preconception with respect to the complexity of the dynamics allowed for the model is accepted – whether the model will be analytically integrable. This turns out only a posteriori. With simulations the situation is different: again, the available tools are highly dependent on the state of the art. One cannot say for once and ever what a simulation of a system will look like. But we know even before starting any simulation that any tool that may be used to integrate a model numerically will yield only numerical, i.e., measurable states. Simulations are a priori measurable worlds. Though I have developed this for the case of discrete simulation of continuous models only, this holds for discrete models as well and even for simulations that are run on an electronic analog computer. There, 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 with the given precision and reliability all

[10] The numerical values are defined even if they are not read out, so one might tend to speak of *measured* worlds instead. However, for counting as measured the values had to be not only defined but recorded, by an observer or by the computer, which need not be the case, so *measurability* is all that can be claimed.

[11] In many cases it may be possible for an experienced modeler to "see" this "immediately", but this means nothing more than that one is able to conceive the model without writing it down.

parameters are measurable, and non measurable parameters of the machine the simulation is run on do by definition not belong to the simulation.

Initially, I have discerned principle and technical restrictions to the measurability of the material world. We now may relate the measurability of simulations to these two kinds of restrictions. We have seen that there is no principle restriction to the measurability of simulations (while there are restrictions to setting up simulations with respect to the available numeric tools). Therefore, some principle restrictions to measurability of the material world may be overcome with simulations. This, of course, makes a particular simulation not realistic in this very aspect. It depends on the rationale of the research whether this may be aimed for, e.g., in investigating how the material world would behave if physics would be different. Of more general interest in using simulations is that they overcome technical limitations to measurability, which does not make the simulation unrealistic. It helps, in contrast, to collect information about the material system that could not be acquired experimentally.

6 Conclusion: epistemic virtues of measurable simulacra

Let me conclude with some considerations on the benefits that science draws from the a priori measurability of simulations or, more precise, of the a priori measurability of the simulacra. It was already mentioned that the main benefit can be seen in overcoming technical restrictions to measurability, but it must be discussed how the measurements taken from a simulation can help to explain material world processes. Let me assume contrafactually 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 one of the intermediates in the theoretical model of the Oregonator, X. The Oregonator describes the kinetics of the intermediate X which is supposed to be analog to the kinetics of $HbrO_2$ in the chemical oscillator of the BZ reaction. But since the Oregonator is not integrable by analytic means, this leads neither to predictions about the behavior of $HbrO_2$, nor is the theoretical model 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 by means of simulation, since the a priory given measurability of the simulation helps to collect the missing data. First, predictions about the dynamics of the intermediate can be derived from measurements of the parameter in the simulacrum, under the assumption that the theoretical model is an adequate description of the reaction and the simulacrum an adequate instantiation of the theoretical model. Secondly, the theoretical model becomes testable by relying on simulations as soon as the

kinetics of the intermediate is measurable: 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 that allows for numerical output. Computer simulations allow exactly for this, due to the measurability of the simulacra.

References

Achinstein, P. (1968). *Concepts of science: a philosophical analysis*. (Baltimore: John's Hopkins Press)

Aspect, A., Gragnier, P. & Roger, G. (1982). Experimental realization of Einstein-Podolsky-Rosen-Bohm *Gedankenexperiment*: a new violation of Bell's inequalities. *Physical Review Letters, 49*, 91-94

Balzer, W., Moulines, C. U. & Sneed, J. D. (1987). *An architectonic for science: the structuralist program*. (Dordrecht: D. Reidel)

Bouwmeester, D., Pan, J.-W., Mattle, K., Eibl, M., Weinfurter, H. & Zeilinger, A. (1997). Experimental quantum teleportation. *Nature, 390*, 575-579

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

Eigen, M.(1972). Immeasurably fast reactions.(In *Nobel Lectures, Chemistry 1963-1970* (pp. 170-203). Amsterdam: Elsevier.)

Einstein, A., Podolsky, B. & Rosen, N. (1935). Can quantum-mechanical description of physical reality be considered complete? *Physical Review, 47*, 777-780

Field, R. J., Körös, E. & Noyes, R. M. (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

Field, R. J. &. Noyes, R. M. (1974). Oscillations in chemical systems. IV. Limit cycle behavior in a model of a chemical reaction. *Journal of Chemical Physics, 60*,1877-1884

Hairer,E., Nørsett, S. P. & Wanner G (1993). *Solving ordinary differential equations I: Nonstiff problems*. (2nd ed., Berlin: Springer)

Hairer, E. & Wanner, G. (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 R. Hegselmann (Ed.), *Modelling and simulation in the social sciences from the philosophical point of view* (pp. 77-100). Dordrecht: Kluwer.)

Hughes, R. I. G. (1999). The Ising model, computer simulation, and universal physics. (In M. S. Morgan & M. Morrison (Eds.), *Models as mediators: Perspectives on natural and social science* (pp. 97-145). Cambridge: Cambridge University Press.)

Humphreys, P. (1991). Computer simulations. (In A. Fine, M. Forbes & L. Wessels (Eds.), *PSA 1990, Vol. 2* (pp. 497-505). East Lansing: Philosophy of Science Association.)

Humphreys, P. (1994). Numerical experimentation. (In P. Humphreys (Ed.), *Patrick Suppes: Scientific philosopher, Vol. 2* (pp. 103-121). Dordrecht: Kluwer.)

Humphreys, P. (2004). *Extending ourselves: computational science, empiricism, and scientific method*. (Oxford: Oxford University Press)

Keller, E. F. (2000). Models of and models for: Theory and practice in contemporary biology. *Philosophy of Science, 67 (Proceedings)*, S72-S86

Krohs, U. (2004). *Eine Theorie biologischer Theorien. Status und Gehalt vonFunktionsaussagen und informationstheoretischen Modellen*. (Berlin: Springer)

Levever 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

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

Prigogine, I. & Lefever, R. (1968). Symmetry breaking instabilities in dissipative systems. II. *Journal of Chemical Physics, 48*, 1695-1700

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

Rohrlich, F. (1991). Computer simulation in the physical sciences. (In A. Fine, M. Forbes & L. Wessels (Eds.), *PSA 1990, Vol. 2* (pp. 507-518). East Lansing: Philosophy of Science Association.)

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

Trenholme, R. (1994). Analog simulation. *Philosophy of Science, 61*, 115-131

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

Winsberg, E. (2003). Simulated experiments: Methodology for a virtual world. *Philosophy of Science, 70*, 105-125