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Tools or Toys?

On Specific Challenges for Modeling and the Epistemology of Models and Computer Simulations in the Social Sciences

Stuttgart, July 12th 2010

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Abstract Mathematical models are a well established tool in most natural sciences. Although models have been neglected by the philosophy of science for a long time, their epistemological status as a link between theory and reality is now fairly well understood. However, regarding the epistemological status of mathematical models in the social sciences, there still exists a considerable unclarity.

In my paper I argue that this results from specific challenges that mathematical models and especially computer simulations face in the social sciences. The most important difference between the social sciences and the natural sciences with respect to modeling is that in the social sciences powerful and well confirmed background theories (like Newtonian mechanics, quantum mechanics or the theory of relativity in physics) do not exist. Therefore, an epistemology of models that is formed on the role model of physics may not be appropriate for the social sciences. I discuss the challenges that modeling faces in the social sciences and point out their epistemological consequences. The most important consequences are that greater emphasis must be placed on empirical validation than on theoretical validation and that the relevance of purely theoretical simulations is strongly limited.

Preprint Series **Issue No. 2010-36**
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1 Introduction

Models play a central role in many sciences. One can safely say that the construction, analysis, discussion and validation of models is the daily bread of most researchers in the natural sciences and engineering. With the development of simulation technology the scope of modeling has vastly increased and it has become even more obvious that models have a "life of their own" independent from theories.

However, there is quite a difference between the extent to which models are used in the natural sciences and in the social social sciences. While in the natural sciences and engineering models are a standard tool and their use is undisputed, it is in the social sciences only economics, where models are the standard form of articulating hypotheses or causal assumptions. In some branches of the social sciences, like history, models are usually not used at all. And in other branches the use of mathematical models depends on the particular school that one adheres to. In sociology and political sciences, for example, it is the rational choice school that makes the strongest use of models.

But even in those parts of the social sciences that use models there exists a considerable unclairity about their epistemic role. It often remains unclear what conclusions can be drawn from models and if and how they can tell us something about the world. The kind of discussion about the role of models in economics that was triggered by Robert Sugden's credible world account (Sugden, 2000) would appear surprising to a natural scientist. And when Robert Sugden wonders that in economics "authors typically say very little about how their models relate to the real world" (Sugden, 2009, p. 25) then he expresses an embarassement that is quite uncommon in the the natural sciences. With the possible exception of economics, it is not only the epistemic status of models that is under discussion in the social sciences, but often it is disputed whether models are of any use at all. The respective discussion blends into the controversies about the usefulness or uselessness of mathematical methods in the social sciences in general (Green and Shapiro, 1994; Shapiro, 2005).

Leaving the ideological question whether everything that happens in this world can meaningfully be rendered in mathematical terms aside, these facts about the social sciences raise the question why there is such an unclarity about the possible role and function of models. In its broadest outline the lesson that I believe can be learned from examining this question, can be summarized in four theses:

1. The possible role and function of models in the social sciences is often unclear, because models in the social sciences face specific challenges which indeed limit the scope of their useful employment.
2. Because of this, the epistemic role of models in the social sciences cannot properly be understood in analogy to the role of models in the natural sciences.
3. An epistemology of models that takes into account these challenges can help us to better understand the possible role and function of models in the social sciences. It might also help us to figure out when and how models and computer simulations can be applied usefully (where "usefully" means: "in such a way that we can learn something about the world from them").

4. As a side effect this may also help us to understand difficulties that models face in the natural sciences in those situations where similar conditions hold as appear to be the standard case in the social sciences (e.g. insufficient background knowledge about the processes involved, strong measurement inaccuracies).

In this article I shall mainly be concerned with the epistemology of models and simulations as traditionally understood and how it relates to the specific challenges that models face in the social sciences. I first state what I consider to be the standard concept of models in the philosophy of science, namely, that models are links between theory and empirical reality (Morgan and Morrison, 1999; Winsberg, 2003). In this context I also discuss the more controversial question what status is to be ascribed to computer simulations. My position is that 1) computer simulations are just models that run on the computer 2) they, therefore, raise more or less the same epistemological questions as models and 3) computer simulations are not experiments, although they may under certain conditions replace experiments. I illustrate this with an example of a computer simulation from chemistry. The example shows that the conception of models as links between theory and reality is by and large appropriate.

After that I go on to review some of the viewpoints on models in the social sciences. These are highly diverse, which emphasizes that there is a considerable unclarity about what role models play in the social sciences. More importantly, the conception of models as a link between theory and empirical phenomena captures at best a rare exceptional case in the social sciences. This naturally raises the question of what distinguishes the social sciences and why models, therefore, play a different and generally much less prominent role in these sciences. I run through a number of distinguishing features which are apt to explain this difference and point out their epistemological consequences. I conclude with some suggestions for adjusting the epistemology of models so as to better capture the role of models in the social sciences.

2 The role of models in science

2.1 The nature of models

In the recent philosophy of science literature it has become popular to conceive models as "mediators" between theory and empirical reality (Morgan and Morrison, 1999) or, what amounts to more or less the same, as a link between theory and reality (Winsberg, 2001). I take this notion to imply three core aspects about models:

1. *Theoretical foundation*: Models are at least partially derived from theories. They contain "laws of nature" that are taken from one or more background theories.
2. *Semi-autonomy*: Models are not just logical consequences from theories and facts. The construction of models involves model building techniques like simplification and approximation, the inclusion of auxiliary assumptions or other "tricks of trade". In extreme cases a model may even contain assumptions that contradict the theory (Küppers and Lenhard, 2005, 2.14).
3. *Relation to a target system*: Models are related to target systems in the real world. The relation between model and target system is at least one of similarity.

I do not claim that this concept of a model covers all types of models that occur in science, but only that it describes the most commen kinds of models. In fact, by dropping any of these requirements meaningful boundary cases can be derived: If a model does not have a theoretical foundation, it is either a purely phenomenological model or a model of data. If a model is not partially independent from its background theories, i.e. if it can logically be derived from the theory and known facts, then it is not a model any more but simply the application of the theory to a particular instance of the laws of the theory. Finally, if the model is not related to a particular target system then it is a purely theoretical model or a "speculative model" or a "toy model".

Saying that a model provides a link between theory and reality is not meant to imply that models are the only possible way how theory can be linked to reality. A theory can also be linked to reality via intermediate theories or by simple "application of the theory" in the just mentioned sense. It is true that very often theories cannot be applied in a simple straight-forward manner but still sometimes some theories can.

2.2 Where models get their credentials from

If models are mediators between theory and reality in the just described sense, then the next question would be what gives models their credibility or how they can be validated. Obviously, if models are partially independent from theory, we cannot rely on the credibility of the background theory alone. Instead, models draw their credibility from three different sources:

1. *Credible background theory and background knowledge*: In so far as it makes use of background theories, the models' credibility depends on the credibility of the background theory. And the validity of the model depends on how faithful it is to the background theories (where it makes use of them). The same holds for any factual background knowledge that is incorporated into a model.
2. *Well approved modeling techniques*: A model furthermore draws credibility from the credibility of modeling techniques that have been employed in its construction (Winsberg, 2006). These techniques in turn are credible either because they can be analyzed or tested with regards to their reliability or simply because they have been successfully employed in the past.[1] In order to validate this aspect of the model one would have to inquire into the reliability of the modeling techniques used and also check whether they have been employed correctly.
3. *Successful empirical tests*: Finally, a model derives credibility from being in accordance with the target system as assessed by empirical tests. The direct validation through empirical testing may not always be possible, though. In fact, one of the most important uses of computer simulations is as substitutes for experiments in cases where experiments are costly or impossible.

If these are the sources of credibility for models, then the question arises if and how they are be related to each other. The following two conjectures about the mutual relation of these sources seem reasonable:

1. *Precedence of empirical validation*: If reliable empirical tests of a model are available, then empirical validation takes precedence over the other validation paths. This means: If a model does not seem to be valid in terms its theoretical assumptions or the employed modeling techniques but withstands empirical testing nonetheless then the model is still acceptable if only as a phenomenological model. The precedence of empirical testing as a validation criterion reflects the epistemic primacy of empirical facts in science.
2. *Synergy of credibility sources*: The less one can rely on a particular one of the three above mentioned sources of credibility, the more strain is put on the remaining sources. E.g. if empirical testing of the model is not possible then the more important it becomes to be able to rely on a well confirmed background theory or on well-proven and reliable modeling techniques.

It seems reasonable to distinguish the models that derive their credibility primarily from the reliance on background theories, background knowledge and modeling techniques from those that are validated by direct empirical testing. The former could be termed "*input-controlled*" models and the latter "*output-controlled*"

[1] In the latter case, however, their success must at least at some point in the past have been assessed by more direct means.

models. The distinction is of course one of “more or less”. Some models may be both input and output controlled. This distinction is meaningful, because with these two ideal types of models are associated quite different modes of validation. With this terminological convention no general assumption is made about the relatively greater or smaller reliability of the one or the other. But it stands to reason that different levels of credibility or reliability might be associated with input or output-controlled models in specific contexts.

There is not much more that can be said about the credibility of models on this very general level. Further below a case study will be discussed in order to show how these three sources of credibility come into play in a simulation model. But before, a few things need to be said to justify why the terms “model” and “computer simulations” are used more or less interchangeably in this paper.

3 Why computer simulations are merely models and not experiments

With regards to the nature and epistemic role of computer simulations, a definite consensus has not yet been reached by philosophers of science. I do not intend to enter into all the philosophical disputes about computer simulations. But I’d merely like to defend two positions that are important in the context of my article:

1. Computer simulations are models. Therefore, computer simulations do not raise any other epistemological questions than models. In particular, the burden of validation is exactly the same for models and simulations.
2. Computer simulations are not experiments. There is a sharp distinction between computer simulations and models on the one hand side and experiments on the other hand side. Just like models and theories, computer simulations belong to the theoretical side of science as opposed to the empirical side which encompasses experiments, observations and experiences.[2]

3.1 Computer simulations are just elaborate models

Quite a few authors have claimed that computer simulations, being a revolutionary new tool of science, call for a new kind of philosophy or require an epistemology of their own that pays due credit to their distinctive character (Humphreys, 2004, 2009; Winsberg, 2001). The acclaimed novelty of computer simulations has been examined in detail by Roman Frigg and Julian Reiss (Frigg and Reiss, 2009), who come to the conclusion that computer simulations do not raise any new or substantially different philosophical question from those that are discussed in the philosophy of science already. Here I am mostly concerned with the issue of validation of models. Frigg’s and Reiss’ most important point regarding the issue of validation comes up in connection with Winsberg’s notion that the specific epistemological features of simulations are that they are constructed “downward” (i.e. starting from a theory), “autonomous” (from empirical data which may not or only sparsely be available for the simulated process) and “motley” (i.e. partially independent from theory, freely mixing ad-hoc assumptions and assumptions from the theoretical backgrounds) (Winsberg, 2001, p. 447/448). With respect to these features, Frigg and Reiss contend:

> . . . it is hard to see, at least without further qualifications, how justification could derive from construction in this way. There does not seem to be a reason to believe that the result of a simulation is credible just because it has been obtained using a downward, autonomous and motley process. In fact, there are

[2] To avoid a possible source of misunderstanding: A theory or model is per se considered to be a theoretical entity notwithstanding its higher or lower degree of empirical accuracy and confirmation. So even a well-tested theory about empirical objects is still something theoretical in this sense. It is only the objects themselves (i.e. the objects a theory describes) as well as the sort of actions that scientists perform in order to study empirical objects (i.e. experiments, observations, measurements) which I count to the “empirical side”.

> models that satisfy these criteria and whose results are nevertheless not trustworthy. (Frigg and Reiss, 2009, p. 600)

An important pragmatic point made by Frigg and Reiss is that putting too much emphasis on the question of novelty of simulations may divert the attention of philosophers of science from more important and relevant questions:

> Blinkered by the emphasis on novelty and the constant urge to show that simulations are unlike anything we have seen before, we cannot see how the problems raised by simulations relate to exiting problems and we so forgo the possibility to have the discussions about simulation make contributions to the advancement of these debates. [. . .]
> For instance, if . . . we recognise that the epistemological problems presented to us by simulations have much in common with the ones that arise in connection with models, we can take the insights we gain in both fields together and try to make progress in constructing the sought-after new epistemology. (Frigg and Reiss, 2009, p. 611)

Frigg's and Reiss' view that computer simulations do not introduce new issues to the philosophy of science has been criticised by Humphreys (2009). Rather than repeating the arguments by Frigg and Reiss, with which I largely emphasize, I am going to discuss the main counter arguments by Humphreys as far as they may have a bearing on the question of validation. What remains to be done is to show that simulations are models and not experiments, for this is an issue with respect to which Frigg and Reiss remain neutral.

Those of Humphreys' arguments for the novelty of computer simulations that are potentially relevant for the validation issue concern 1) the epistemic opacity of simulations, 2) the different semantics of simulations, 3) the temporal dynamics of simulations and 4) the crucial difference between "in principle" and "in practice" that according to Humphreys deserves special attention once simulations enter the scene.

1) According to Humphreys, computer simulations are epistemically opaque because we cannot monitor every single step ("epistemically relevant elements of the process" (Humphreys, 2009, p. 618)) of a simulation that may run through many millions and billions of "epistemically relevant" steps before it produces its result. Does this have any bearing on the validation of simulations? If it does then it can only mean that simulations are a comparatively more dangerous tool than models, because many simulations are opaque in Humphrey's sense. However, since we do know and understand the algorithms programmed into a simulation, and since we can probably at least monitor a few samples of the "epistemically relevant elements" of the simulation process, this kind of opacity may not pose too much of a problem for the justification of the simulation.

2) Humphreys believes that neither the syntactic nor the semantic view of theories are fully adequate to capture just how simulations relate to target systems. According to him this relation differs from how traditional models are applied: "It is in replacing the explicitly deductive relation between the axioms and the prediction by a discrete computational process that is carried out in a real computational device that the difference lies." (Humphreys, 2009, p. 620). The aspect that Humphreys hints at is the "semi-autonomy" of models from theory (see point 2 on page 3). So, this aspect is already taken care of.

I am not sure what exactly falls under the category of "traditional models", but I doubt that it is ultimately just computer simulations that depart from the scheme of an "explicitly deductive relation between the axioms and the prediction". If this is true then it appears to be better to draw the line between simple application of a theory on the one hand side and models and simulations on the other hand side, as I have done before (see page 4), rather than between traditional models and computer simulations.

3) That the temporal dynamics of simulations matter is most obvious for real time simulations as they are used for example in control engineering. Real-time requirements tighten the range of applicable modeling techniques. Often the construction of a real-time simulation involves the development of highly optimized

problem-specific algorithms. While this makes the validation via well-approved modeling techniques more difficult in particular cases, it does not change the situation with respect to validation fundamentally.

4) According to Humphreys, another “novel feature of computational science is that it forces us to make a distinction between what is applicable in practice and what is applicable only in principle” (Humphreys, 2009, p. 623). It is not exactly clear, why this distinction that can become important in many situations should become unavoidable only when computational science is considered. As far as the validation of models is concerned it is, of course, decisive what is “applicable in practice”. But again, there is no difference between models and simulations in this respect.

3.2 Computer simulations are not experiments

Having thus established that the alleged novelty of computer simulations does not distinguish them with respect to validation from models, the question remains how computer simulations are related to experiments. The philosopher’s opinions could not be more diverse on this question. There are those who believe that computer simulations are experiments and can just like experiments be used to test hypotheses. And there are others that believe that simulations are more like miniature theories and therefore – quite the contrary – in need of empirical testing themselves.

3.2.1 The simulations-experiments dispute

As philosophers that take the “simulations are experiments”-side I would just like to quote Margarete Morrison and Uskali Mäkki. Morrsion writes in an article titled “Models, measurement and computer simulation: the changing face of experimentation”:

> . . . hence we have no justifiable reason to assume that, in these types of cases, experiment and simulation are methodologically or epistemically different. As we shall see, the causal connections between measurement and the object/property being measured that are typically invoked to validate experimental knowledge are also present in simulations. Consequently the ability to detect and rule our error is comparable in each case. (Morrison, 2009, p. 43/44) [. . .]
> The conclusion, that simulation can attain an epistemic status comparable to laboratory experimentation, involved showing its connections with particular types of modelling strategies and highlighting the ways in which those strategies are also an essential feature of experimentation. (Morrison, 2009, p. 55/56)

Interestingly, Morrison concedes in a footnote that the account of computer simulations she has argued for may be more appropriate for the natural than the social sciences (Morrison, 2009, p. 56, fn 33).

In a similar vein, Uskali Mäkki compares experiments with models and reaches the conclusion that “Models are Experiments, Experiments are Models” (Mäki, 2005). And the same holds – as we may add without distorting his idea – a fortiori for computer simulations:

> Consider material experimentation as based on causally isolating fragments of the world from the rest of it so as to examine the properties of those fragments free from complications arising from the involvement of the rest of the world. The analogy with theoretical modelling is obvious: while material experimentation employs causally effected controls, theoretical modelling uses assumptions to effect the required controls. (Mäki, 2005, p. 308)

Maeki, however, does not claim that models and experiments can always be equated in this way. And he sees a difference between models and experiments in the fact that in the case of experiments the isolation of causal factors requires material manipulation. A difference that Morrison, in contrast, considers to be rather inessential (Morrison, 2009, p. 54).

That the view that simulations are experiments is not merely an eccentric philosophical point of view is further illustrated by the fact that practitioners often use the term "simulation experiments" as a facon de parler for referring to computer simulations. For example, Hegselmann and Flache use the term "experiment" when referring to results obtained with cellular automata that run on the computer (Hegselmann and Flache, 1998, 3.11). And in a recent simulation of customer experience in retail stores, Siebers, Aickelin, Celia and Clegg use the terminology of hypothesis and experiments when referring to pure simulation studies (Siebers et al., 2010, p. 16ff.). They are aware, however, that these kinds of "experiments" are not empirical – in contrast to what they call the "validation experiments" of their simulation.

The opposite position with regards to the simulation-experiments question is, among many others, taken by Kleindorfer and Ganeshan, who place simulations firmly on the theoretical side of science by declaring them with reference to Naylor and Finger (Naylor and Finger, 1967) as "miniature scientific theories":

> To simulate means to build a likeness and the question as to the accuracy of the likeness, one version of the validation problem (some might argue the only version), is never far behind. The validation problem is an explicit recognition that simulation models are like miniature scientific theories. (Kleindorfer and Ganeshan, 1993, p. 50)

If simulations are understood in analogy to theories rather than experiments it appears only natural to also consider the validation requirements of simulations in analogy to that of theories. This is what Troitzsch does when he maintains that "Validation of simulation models is thus the same (or at least analogous) to validation of theories." (Troitzsch, 2004)[3] And Naomi Oreskes, Kristin Shrader-Frechette and Kenneth Belitz even warn that "Any scientist who is asked to use a model to verify or validate a predetermined result should be suspicious." (Naomi Oreskes, 1994, p. 644) Given that one denies that simulations are experiments this warning is important, because then, rather than being able to "verify or validate" given assumptions, models and simulations are in the need of verification and validation themselves.

3.2.2 Resolving the simulations-experiments dispute

Which of the two positions on the relation between models and experiments is the right one? Or how can these views be reconciled? In my opinion the dispute can be decided very clearly in favor of those who deny that simulations are experiments. The reason is straight forward: Simulations cannot generate any results that are not already implied in the theories and assumptions that enter into the simulation setup. Typically, these implications are not known to us and the simulation results may therefore be surprising just like the results of an experiment. Still, computer simulations cannot deliver anything that was not built into them. There is no causal influence from nature or, more precisely, from the investigated target system itself on the results of the simulation. And therefore there is consequently also no transfer of information from nature to the simulation results.

That there is a fundamental and irreconcilable categorial difference between simulations and experiments becomes most apparent when we think of the special kind of experiment which is called "experimentum crucis", i.e. the kind of experiment which we use to test our most fundamental theories. For example, there is obviously no way how Young's double-slit experiment (wikipedia, 2010), which was conducted in order

[3] See also Küppers and Lenhard (2005), where I took these references from, in this context.

to decide between the corpuscular and the wave theory of light, could be replaced by a computer simulation. Other than in the experiment, the outcome of a computer simulation would simply depend on which of the alternative theories is preferred by the programmer of the simulation.

But if there is such a fundamental and obvious difference between simulations and experiments, why do so many people then believe that simulations are experiments? A possible reason is that many experiments are indeed just simulations. If, for example, scale models are used to study the properties of some physical system, then one can reasonably maintain that the scale model is a simulation of the "real" system. This is nicely illustrated by a Quotation from John von Neumann, who explained the purpose that experiments in wind tunnels had at his time:

> The purpose of the experiment is not to verify a proposed theory but to replace a computation from an unquestioned theory by direct measurement. . . . Thus wind tunnels are used . . . as computing devices to integrate the nonlinear partial differential equations of fluid dynamics." (quote taken from (Winsberg, 2003, p. 114))

One could say that in such cases the experimental setup is in effect an analog computer to perform certain calculations. It is no surprise that experimental setups that function as analog computers can safely be replaced by digital computer simulations. The quotation of von Neumann also nicely highlights an important prerequisite for simulations to replace experiments: There must already be an "unquestioned theory" the laws of which can safely be assumed to govern the phenomena that are simulated. As we will see later, this is one of the main problems of "simulation experiments" in the social sciences.

Admittedly, as there exist similarities as well as dissimilarities between simulations and models, the answer to the question whether simulations are experiments or not becomes somewhat relative because it depends on whether greater importance is attributed to the similarities or to the dissimilarities between the two. A very important reason for emphasizing the dissimilarities, however, is that if the differences between simulations and experiments become blurred, scientists (or the broader public for that matter) might much easier be inclined to overestimate the cognitive value of simulations and prefer to stick to pure simulation studies instead of carrying out the often much harder work of empirical or experimental testing of their hypotheses. A remark by Peter Hammerstein about the uselessness of the sort of simulation studies of the "evolution of cooperation" that became fashionable in the aftermath of Robert Axelrod's pioneering work (Axelrod, 1984) vividly illustrates this problem:

> Why is there such a discrepancy between theory and facts? A look at the best known examples of reciprocity shows that simple models of repeated games do not properly reflect the natural circumstances under which evolution takes place. Most repeated animal interactions do not even correspond to repeated games. (Hammerstein, 2003, p. 83) [. . .]
> Most certainly, if we invested the same amount of energy in the resolution of all problems raised in this discourse, as we do in publishing of toy models with limited applicability, we would be further along in our understanding of cooperation. (Hammerstein, 2003, p. 92)

It is indeed well-nigh impossible to apply any of the results of the simulations of this particular simulation-tradition empirically, if by empirical application more than just drawing vague and superficial analogies is meant (Arnold, 2008, p. 145ff.). What is even more worrisome is that in some instances simulation scientists even appear to be rather insensitive to the importance of empirical validation, as another example illustrates, where a journalist summarizes his discussion with a scientist who has simulated opinion dynamics:

> None of the models has so far been confirmed in psychological experiments. Should one really be completely indifferent about that? Rainer Hegselmann becomes almost a bit embarrassed by the ques-

tion. "You know: In the back of my head is the idea that a certain sort of laboratory experiments does not help us along at all." (Grötker, 2005, p. 2) [4]

This attitude is even more surprising because the way the simulation model is constructed it does not appear principally impossible to submitt it to some form of empirical testing (Hegselmann and Krause, 2002).[5] Normally one would expect a scientist to have a natural interest in the question whether his or her model is true or not. It stands to reason that the anti-empirical attitude of some simulation researchers is fostered by confounding the categories of simulation and experiment.

The pragmatic aspect of directing research in the wrong or right direction has not been paid much attention to in the philosophical discussion about the relation between simulations and experiments. If this aspect is taken into account then another important reason for distinguishing these two categories is the danger of drawing premature conclusions about the world from empirically unconfirmed simulation studies.

Summing it up: While certain types of experiments can indeed be replaced by simulations, there remains a fundamental difference between simulations and experiments in so far as in experiments we can put nature to the test, which we cannot do with simulations. Therefore, instead of thinking of simulations as experiments or experiment-like it would be more adequate to think of simulations as tools for analysing the consequences of theories.

But before we examine what consequences these results about the simulations have for the employment of simulations in the social sciences, I am going to illustrate what has been said about the epistemology of simulations so far with an example from the natural sciences.

4 The epistemology of simulations at work: How simulations are used to study chemical reactions in the ribosome

The example from simulations in the natural sciences that I am going to discuss comes from the field of biochemistry. It concerns ongoing research about how peptid bonds between amino acids are formed in the ribosome molecule.[6] The *ribosome* is a macro molecule in the cells of living organisms which assembles amino acids to proteins according to the information on the *messenger RNA* (mRNA), which in turn is a copy of the genetic information stored in the cell's DNA. The process proceeds roughly as follows: The ribosome receives a new *transfer RNA* (tRNA) molecule with an attached amino acid at a specific location called the ribosome's *amino site*. At the amino site the tRNA molecule is bound to the chunk of mRNA that is currently "read" by the ribosome. (Which kind of tRNA molecule and therefore which amino acid can enter the amino site depends on the chunk of mRNA that occupies the amino site during this step of the whole process of protein formation.) The amino site is spatially close to the *peptide site* of the ribosome, where another tRNA molecule is located, the amino acid of which is already attached to the evolving protein. In a process called peptide bond formation the amino acid of the "new" tRNA at the amino site is connected to the amino acid of the "old" tRNA at the peptide site. Finally, the tRNA at the peptide site is released (having given away

[4] The German original of this passage reads: Keines der Modelle wurde bisher in psychologischen Experimenten bestätigt. Sollte einem das wirklich völlig egal sein? Rainer Hegselmann macht diese Frage fast ein wenig verlegen. "Wissen Sie: In meinem Hinterkopf ist die Idee, dass eine bestimmte Sorte von Laborexperimenten uns gar nicht weiterhilft."

[5] It should be considered less embarrasing for a scientist to test a model and fail the test than not to test one's own models at all. One notices a difference of attitude and research design between Hegselmann's and Krause's simulation study (Hegselmann and Krause, 2002) and the earlier quoted study by Siebers, Aickelin, Celia and Clegg (Siebers et al., 2010). To be sure, Hegselmann and Krause did not have the same man-power at hand as the other team, but Hegselmann should at least be aware that empirical testing is essential in science.

[6] I am greatly indepted to Professor Johannes Kästner from the Institute of Theoretical Chemistry at the University of Stuttgart for explaining this fascinating area of research to me. Needless to say that what I write here is my own summary of this research for which I take the full responsibility.

its amino acid) and the ribosome moves forward along the mRNA chain so that the tRNA that was received at the amino site now occupies the peptide site. This whole process is catalysed by the ribosome. Just how the peptide-bond formation is mediated is a question that researchers currently investigate. With the means available today it is extremely difficult if not impossible to investigate this question experimentally. Experimental data is only available on certain features of the reaction, most notably on the reaction barriers (i.e. the difference in energy levels that must be surpassed so that the reaction takes place). Therefore, molecular dynamics simulations are used to study how the peptide bond formation is catalysed by the ribosome.

In the following I am going to look at one such simulation study (Kästner and Sherwood, 2010). The questions that concern me here is under what kind of "epistemic situation" these simulation studies take place and whether the previously established epistemological categories can roughly capture this situation. In order to answer these questions, we shall work our way backwards from the results that were optained in this study to how these results were optained.

The results that were found in the study are:

1. The ribosome performs its catalytic function of reducing the energy barrier of the peptidyl bounding reaction "by the electrostatic influence of the environment rather than just a favorable positioning of the reactants. The high concentration of mobile ions …in the ribosome …was found to be the key to the catalytic activity of the ribosome" (Kästner and Sherwood, 2010, p. 304). The conclusion was reached by comparing the simulations of the reaction in the ribosome with simulations of the reaction in the gas-phase.[7] The average reaction barrier that was found in the simulations was "in good agreement with experimental data" (Kästner and Sherwood, 2010, p. 304).
2. Both of the two different reaction mechanisms ("direct proton transfer" and "proton shuttle") that were studied may indeed account for the proton transfer. "Both were found to have similar activation energies. They may compete in the real system." (Kästner and Sherwood, 2010, p. 304) At least the simulation results do not allow to exclude one of these results definately for the time being.
3. The possible occurrence of a certain "tetrahedral intermediate" in the course of the reaction is "irrelevant for the reaction mechanism". This conclusion could be drawn from the simulations, because "no minimum corresponding to a tetrahedral intermediate was found on the free-energy surface" as it should have been the case if it played a vital role in the reaction. The diagnosis of irrelevancy is furthermore strengthened by results in the literature. (Kästner and Sherwood, 2010, p. 300)
4. For one scenario a discrepancy between simulation results and experimental data occurred: " The free-energy simulations for the direct proton-transfer mechanism resulted in a significantly higher free energy of activation than the potential energy barrier." (Kästner and Sherwood, 2010, p. 304)

How were these results arrived at and how do the above mentioned "sources of credibility" come into play here? In order investigate the process of peptid bond formation the researchers conducted series of computer simulations of the ribosome of the *Thermus Thermophilus* bacteria. The fundamental scientific theory upon which these simulations rest is *quantum mechanics*. Needless to say that quantum mechanics is a both quantitatively and qualitatively extremely well confirmed scientific theory with no competitors in the applicable areas of physics and chemistry. Researchers believe this theory to realistically describe on the most basic level just how things happen in physics. Unfortunately, quantum mechanics is computationally

[7] Drawing a rough analogy one could say that the reaction in the gas-phase amounts to what in the social sciences what be termed the "null hypothesis". Regarding in how far the comparison is warranted, the authors state: "Of course, here the comparison was done with respect to the gas phase. A fairer comparison may be with the reaction in water. However, we doubt the validity of common continuum solvation models for this system, as many of the interactions are hydrogen bonds and interaction with ions (see below) that cannot be covered by continuum solvation models. Taking solvation in water or salt solutions into account explicitly is computationally rather demanding and, therefore, outside the scope of this work." (Kästner and Sherwood, 2010, p. 8)

much too expensive to simulate a whole ribosome molecule. (The ribosome of Thermus contains roughly 2.6 millions of atoms.) A feasible approach to keep computational costs in check is, therefore, to use combined quantum mechanics and molecular mechanics simulations (*QM/MM-simulations*) where only the crucial parts of the reaction are rendered with quantum mechanics. This was also done here. Molecular mechanics is not a fundamental theory but can be considered as something of a simplified theoretical approximation that works good enough for some purposes. Just as quantum mechanics it has demonstrated its suitability in many application cases. Thus, as far as the credibility of the background theories goes, we have here the ideal case of extremely powerful and at the same time very well-confirmed background theories that cover the phenomenon under study. This situation seems to be typical for some areas of the natural sciences though not for all of them (e.g. climate simulations).

Apart from the background *theories*, there is quite a bit of factual background *knowledge* that enters into the simulations. The basic function of the ribosome has been understood since the midst of the 20th century and its structure is known since the 1970s. Thus, if scientists simulate the ribosome today they can draw on a wealth of more or less reliable background knowledge that has already been collected. Just how reliable some parts of this knowledge are, is almost impossible to judge for a non-expert. A non-expert can at best rely on the general trustability standards of the science concerned. In order to do so, some general knowledge of the science concerned is still necessary. The only other alternative for assessing the reliability of scientific knowledge as a complete non-expert would be to wait for technical applications of this knowledge, the success or failure of which is obvious even for the most ignorant and uneducated person. It suffices, however, if at least experts – if in doubt – are able to trace back the assumed background knowledge to its sources.[8] The simulation study discussed here, could not have been done if a model of the ribosome did not already exist. Also, the background knowledge was important for deciding which alternative mechanisms of peptide bond formation ("direct transfer", "proton shuttle") to examine in the first place. And it was used as a source of credibility by notifying agreement with results in the literature.

The application of a theory to a particular problem is by no means a trivial task and often requires no less inventiveness than the development of a new theory. In the example case discussed here, numerous different problems had to be solved and quite a range of different technologies had to be applied. This is where what Eric Winsberg calls the "tricks of trade" (Winsberg, 2001, p. 444) come into play and where the simulation relies on what I have termed the credibility of simulation techniques before (see point 2 on page 4). I am going to point out just a few of these:

1. In order to build a "hybrid" QM/MM-simulation it must be decided which parts of the reaction are to be included in the quantum mechanics part and which are calculated with molecular dynamics and how these parts are to be linked (Kästner and Sherwood, 2010, p. 295). This choice is still considered by the scientists as rather straight forward, though.
2. While the ribosome model used already existed, the simulation system needed to undergo a complicated procedure of preparation and equilibration (Kästner and Sherwood, 2010, p. 295).
3. The simulations made use of the so-called density functional theory (DFT), an approximation to quantum mechanics. For some parts of the simulation the respective calculations would have required far too much time. For these parts, the simplified "semi-empirical" SCC-DFTB method had to be used. Although it has been compared to DFT and found to deliver similar results, the use of this less exact method is considered as one possible explanation for the discrepancy with empirical data which was detected at one point (Kästner and Sherwood, 2010, p. 304).

[8] Still, the problem of assessing reliability should not be taken lightly. In the social sciences there exist whole simulation-traditions which at no point seem to have a secure foundation in reality (see Arnold (2008)).

4. Finally, the simulation is realized within the "Chemshell" simulation framework (P. Sherwood, 2003), which of course also falls under the heading of "simulation techniques". Summing it up, the simulation makes use of well reputed techniques, and where in doubt (as in the case of SCC-DFTB), further testing is done.

The simulation study discussed here does not exclusively rely on background theory, background knowledge and simulation techniques. Where possible and in so far as it is possible its results are compared to experimental data. (Experimental data does introduce questions of reliability of its own, which would lead too far to go into here. But even if it is not totally reliable, the comparison with empirical data is meaningful, because the experimental results are generated independently and if they match the simulation results then this does at least add some mutual "holistic" credibility to both of them.) The fact that the experimentally determined reaction barrier matches the barrier found in the simulations (within the error bar), strengthens the credibility of the first two above mentioned results concerning the role of mobile ions and the relative importance of the two alternative mechanisms of proton transfer in the peptid bond formation. The third result, concerning a "thetrahydral intermediate", seems to be more or less a purely theoretical result. The fourth result in turn is obviously due to empirical testing. Just as if done by the book (and as it would please philosophers of science such as Karl Popper or Imre Lakatos), the contradictory empirical evidence is taken as a discrepancy (though for good reasons not already a total disconfirmation) that demands explanation and gives rise to new research questions.

Where does this all leave us? First of all, the exmple (hopefully) shows that the above stated categories ("sources of credibility") allow by and large for an analysis of the epistemic situation of a typical computer simulation. All three sources of credibility come into play here, and at the same time nothing important seems to have been left out. The example, furthermore, seems to support the contention that even when empirical data is too sprase to conclude what mechanisms are at work in the target system from empirical data alone, it may still be good enough for the validation of computer simulations that serve as a tool to identify these mechanisms. If this can be granted then the example provides evidence for the "synergy of sources of credibility" as stated above (point 2 on page 4).

This is not to say that merely on the basis of such an analysis an evaluation of the credibility of the simulation would be possible. (This would require expert knowledge of the field under study and of the technologies employed in order to evaluate each of the sources of credibility in this particular case.) It is merely meant that these categories help us to understand the general research logic underlying simulation studies such as this one. Although the simulation study itself is quite complicated, its research logic seems to be very straight forward: The simulation is meant to simulate more or less "realistically" how the process of peptid bond formation takes place. It is built upon powerful and empirically confirmed background theories as well as on background knowledge. It employs well-reputed or otherwise tested simulation techniques. Where possible and so far as possible, the results are compared to empirical data. Discrepancies to the empirical data are properly taken care of. In fact, the basic research logic is so clear that there does not even need to be much debate about it. In the following we will see that quite the opposite is true for the research logic of many models and simulations in the social sciences.

5 How do models explain in the social sciences?

It is much harder to see how models or simulations contribute to the understanding of phenomena in the social sciences than in the natural sciences, because in many cases social science models are highly stylized. Often the degree of idealization is so strong that the models are obviously unrealistic and it becomes hard to see how they represent their target system at all (see Hammerstein (2003) for an example of this problem). The textbook literature on economics, which is the social science in which the use of models is the most pervasive, defends the use of strongly simplified models with the standard argument that because reality is much too complex to be described directly, we would not be able to gain any understanding at all without strongly simplified models (Mankiw, 2004, p. 22ff.). As it is at the same time obvious that not any arbitrary simplifications are permissible, the question inevitably arises what kind of simplifications are permissible and what kind of simplifications are not. Unfortunately, the economic textbook literature offers no satisfactory answer to this question. To rely on the predictive success of otherwise unrealistic simulations offers no solution, because the predicitive success of economic models is notoriously weak (Betz, 2006). And if this is true for economics then the situation for models in other social sciences like sociology or political sciences must be expected to be even worse.

Not surprisingly, therefore, the ongoing debate about the proper use and the epistemic value of models in the social sciences is characterized by a wide diversity of different and often contradictory viewpoints. To an outsider it could almost appear as if mathematical models and computer simulations are used in the social sciences without a common understanding of what they are good for. Among the views taken in this debate are the following:

1. *Models as predictive devices*: As just mentioned, Friedman defends models as tools for generating empirical predictions (Friedman, 1953). Unfortunately, due to the usually poor predictive success only very few social science models can seriously be defended on this ground. This is especially the case if the predictive success of elaborated models is no better than that of simple naive prediction methods (Betz, 2006, ch. 2/3).
   The basic rationale of this concept of models can be described as this: *Models help us to understand the world by generating successful predictions. Other than that they do not need to be particularly realistic.*
2. *Models as experiments*: Some authors strongly emphasize the analogies between models and experiments (Morrison, 2009; Mäki, 2005). In their view most models and most experiments share more or less the same features (e.g. more or less close resemblance to a target system, controlled environment, potentially unpredictable and surprising results) and it is therefore often more a matter of convenience and feasibility which of the two is to be preferred under which circumstances. But, as has been argued earlier, the analogy quickly breaks down if we consider experiments that test the empirical truth or falsehood of fundamental theories (*experimentum crucis*). Most of the authors advocating this view are, of course, aware that it does not work for all types of models and experiments. But even if this is taken into account, there is the constant danger of forgetting about the epistemic primacy of the empirical side of science. (After all it is the empirical world that our theories must be adjusted to and not the other other way round.)
   The bottom-line of the "models as experiments" conception is: *Models and Simulations help us to understand the world much like experiments do, e.g. by representing a real-world target system in a controlled environment that allows us to test assumptions.*
3. *Models as isolating devices*: The view that models are "isolating tools" has some likeness to the "models are experiments" view, because when conducting experiments one often tries to isolate the causal relation under study as good as possible from all disturbing influences. To the adherents of this view it does not matter, how the isolated system is arrived at; if by shielding from other influences (experiments) or by including just as much as is needed to model the causal relation in the first place (models) (Mäki, 2009). The value of this analogy is disputed by others, however (Kourikoski and Lethinen, 2009, p. 127). And with regards to the epistemic situation the same caveats as for the analogy between models and experiments hold.

If models are understood as isolating tools then the important question is, if and how we can learn something from isolating models about the real world. As Nancy Cartwright argues, this depends on the scientific field. According to her, in comparison with physics very little can be learned from isolating models in economics. And one can probably safely generalize this finding to all social sciences. The possible explanation for this limitation that compared to the natural laws in physics economics has only few general principles (Cartwright, 2009) links well with our previous contention that strong background theories provide a good ground for successful modeling.

Models help us to understand the world, because they allow us to study the functioning of causal mechanisms in isolation which in the real world are usually mixed up with other mechanisms.

4. *Models as credible counterfactual worlds*: Robert Sugden's "credible world" account of models (Sugden, 2000, 2009) is motivated by the observation that models in the social sciences often do not represent any particular target systems. Rather surprisingly, "authors typically say very little about how their models relate to the real world" (Sugden, 2009, p. 25). Determined to find a rationale behind this modeling practice nonetheless, Sugden develops his "credible worlds" account. According to Sugden models are neither isolations or abstractions nor do they merely serve the purpose of "conceptual exploration". But they constitute "counterfactual credible worlds". Because the models (in economics) are by their very nature "counterfactual" it would be misplaced to demand that they be realistic. Yet, they need to be "credible" in order to allow us to draw inductive conclusions from them.

   This account of models raises more questions than it answers: In what sense can a world that is "counterfactual" still be credible? And what are the criteria by which the credibility of a "counterfactual" model must be judged?

   Regardless of how these questions might be answered, the role of models according to this view can be characterized as follows: *Models do not represent particular target systems but they constitute paralell counterfactual worlds. By being "credible" they allow us to draw inductive conclusions about the real world.*

5. *Models as incredible counterfactual worlds*: In contrast to Sugden, Kourikoski and Lethinen (2009) do not assume that the counterfactual worlds of models need to be "credible" to be of good service to our understanding of the real world. Quite the contrary, a model may very well contain counterfactual or even incredible assumptions. Varying counterfactual assumptions plays a crucial role in what Kourikoski and Lethinen call "derivational robustness analysis". This is a procedure by which the robustness of a model's "substantive" assumptions can be tested by varying its "auxiliary" assumptions. If the the substantive assumptions still produce the same result no matter what varying counterfactual auxiliary assumptions are made in the model, they can be considered robust and we are entitled to draw the inductive conclusion that even if the counterfactual auxiliary assumptions would be replaced by realistic assumptions, the same results can be expected.[9]

   Though it does raise questions, this is an interesting robustness concept that certainly deserves further exploration. If it proves to be sound than it offers a strategy how a model can be hardened – up to a certain limit, if the substantive assumptions are not to be tautologies – by a pure model to model comparison.

   The bottom line is: *If a model is counterfactual or even incredible it can still help us to understand the world.*

[9] This procedure is somewhat similar to the "de-idealization" procedure proposed by Ernan McMullin 25 years earlier (Alexandrova, 2008; McMullin, 1985). Only that when "de-idealizing", the auxiliary assumptions must gradually be replaced by more realistic assumptions. One can conjecture that when both alternatives are available "de-idealization" is the safer method. Derivational robustness analysis could then be understood as a kind of second-best alternative to "de-idealization" when the latter is not available.

6. *Models as partial explanations*: Drawing on the conceptual framework of C.G.Hempel, Aydinonat describes models as partial explanations (Aydinonat, 2007). This means that models capture one possible cause of a phenomenon that can have several causes which may differ from instance to instance. Aydinonant gives this account in the course of a case study on Schelling's neighborhood segregation model, a model that explains the macroeffect of segregated neighborhoods with the micromotive of individuals having a weak preference against living in a neighborhood that is dominated by an ethnic group other than their own. Saying that this model provides a partial explanation means that particular instances of neighborhood segregation may have been caused by the factor that the model describes but could also have been caused by other factors. For, neighborhood segregation can also result from housing prices in connection with a difference in average income levels of different ethnic groups. An empirical assessment is needed to decide which causes were effective in a particular instance of the phenomenon.
   Although it is probably not appropriate for all types of models, Aydinonat's account is a very convincing one: It provides a clear and convincing idea of how and why models may contribute to explanations in the social sciences. And it can almost immediately be transformed into a research design.
   Summarized, this account of models says: *Models are partial explanations that describe possible causes of phenomena of a specific type. For providing a full explanation of a particular phenomenon, the model must be sufficiently robust and it must be chacked empirically against other possible causes of the phenomenon.*
7. *Models as "open formulae"* An even more defensive reading of the role of models in social sciences that has been suggested by Alexandrova (2008) who treats them as open formulae. By this it is meant that models are merely templates or schema to generate causal hypotheses about the world. If models are only templates for causal claims then they do not carry any direct burden of epistemological justification any more, but the burden lies on the hypotheses that are produced from the template-models.
   Just as the previous one this account has the merit of suggesting a research design where the use of models interacts with that of experiments. The kind of iterative research that results is described by Alexandrova with respect to the example of auction design (Alexandrova, 2008, p. 384ff.).
   Summary: *Models serve as templates for the generation of hypotheses.*
8. *Models as tools for conceptual exploration*: Finally, and at the other end of the spectrum models and simulations can be regarded as a purely theoretical device that serves the purpose of conceptual exploration. There is no doubt that models and simulations can be used to explore the implications of our theories and concepts. The question is whether they are good for anything else. What is assumed here is that, unless they are empirically applied to particular target systems, models and simulations do not serve any other purpose than that of conceptual exploration.
   Bottom line: *Models serve primarily theoretical functions like that of exploring the implications of concepts and theories.*

The diversitiy of views on simulations, exemplified by the above list, is not simply a consequence of the fact that models and simulations are used for different purposes in the social sciences. For, some of the contradictory views like the "credible worlds" (Sugden, 2009), "incredible worlds" (Kourikoski and Lethinen, 2009), "isolation" (Cartwright, 2009; Mäki, 2009) and "partial explanation" account (Aydinonat, 2007) have been proposed by their authors in the same discussion and under consideration of exactly the same examples.

The situation is somewhat embarrassing because as Sugden has observed "authors typically say very little about how their models relate to the real world" (Sugden, 2009, p. 25). And it is not because the answer is so obvious that they remain silent. Otherwise, why would there be such a debate? One obvious approach to resolving the debate would be to go through the accounts that have been advanced one by one and either find an account that is the most adequate or to arrive at some kind of synthesis. But, apart from the fact that this procedure would be rather tedious, it is also not guaranteed that it leads to the desired result. For, it is unclear which criteria a good account of models ought to fulfill. Therefore, before entering into any discussion about epistemological accounts of models it might be advisable to ask for the reasons why the research logic of models and simulations in the social sciences is not at all obvious.

So, how is it possible that scientists use models, yet nobody seems really able to tell “how their models relate to the real world” (Sugden, 2009, p. 25)?

6 Common obstacles for modeling in the social sciences

A possible explanation why it is so difficult to grasp the research logic behind social simulations is that the models and simulations do themselves face much stronger obstacles in the social sciences than in most of the natural sciences. If it proves hard to justify models and simulations in the social sciences then the simple reason may be that very often there is no justification for using these models. In the following a number of common obstacles for modeling in the social sciences will be examined and the possible epistemological consequences for modeling will be discussed.

It is not claimed that these obstacles are exclusive for the social sciences. Some of them may to a lesser or greater degree also plague some simulations in the natural sciences as well. In this case presumably also the epistemological consequences will be the same. If one is aware of these obstacles it becomes easier to understand the specific epistemological conditions of models and simulations in the social sciences.

6.1 Lack of universal background theories

In the social sciences there exist hardly any empirically well confirmed background theories that fully cover the phenomena in their domain. There simply is nothing in the social sciences that compares to Newtonion mechanics or quantum theory in physics. If a physicist wants to explain some mechanical phenomenon it is no question that she must apply the theory of mechanics. In the case of the simulation of the ribosome discussed earlier, there was no question that quantum mechanics is the right theory for the problem. The challenge consisted in how to apply this theory to the problem at hand.

In contrast to that, the first challenge in the social science is to pick the right theory or the right set of theories. One usually has a whole range of theories to chose from. In their book on the Cuban misile crisis, Allison and Zelikow (1971/1999) present three different paradigms, each of which encompasses a host of different theories and scientific approaches, partly overlapping, partly contradicting and partly complementing each other. The way, how social scientists deal with this situation is to pragmatically select from the theoretical supply whatever deems them appropriate, then to look at the question at hand from different angles suggested by different theories and, finally, to assemble this patchwork to a reasonably comprehensive picture.

The best candidate for a universal theory in the social sciences would probably be utility theory in economics. But even if we take this prime example of an axiomatized and highly universal theory, we will not have a theory that could rival the importance and success of Newtonian mechanics in physics. The difference is obvious: Newtonian mechanics can be confirmed empirically in many different constellations and it has at least for a certain well defined range of phenomena (i.e. macroscopic phenomena where the velocities involved are much smaller than the speed of light) never been disconfirmed. Therefore, we can safely draw the inductive conclusion that Newtonian mechanics remains true even in those constellations that have not or cannot be tested directly. Utility theory on the other hand can at best roughly be confirmed in some select scenarios and its general truth or at least its empirical applicability in other cases remains doubtful. One important reason for this state of affairs is that reliable measurement procedures for (cardinal) utility do not exist. It is hard to confirm a theory without being able to measure its central magnitudes. A further reason is the scarcity of principles (i.e. the analogues of natural laws in economics) that come with utility theory, which means that a great part of the explanatory work of models based upon this theory is in effect be done by auxiliary assumptions and situation-specific rules. (See also Cartwright (2009, p. 48/49) and Cartwright (1999).)

What are the epistemological consequences then? The most important consequence is that reliance on theoretical validation (i.e. proven or tested compliance with a well-confirmed background theory) remains insufficient, because there are no sufficiently credible background theories to rely on. The more important, therefore, becomes the direct empirical validation of models and simulations in the social sciences.

6.2 Pluralism of Paradigms

Social sciences are typically characterized by a pluralism of paradigms and a multitude of competing theories about the same domain. This is a fact that it is often lamented about, but it can also be seen as a chance, because the limits of one paradigm often become apparent only in the light of other paradigms. This can also nicely be illustrated by the previously quoted study on the Cuban missile crises (Allison and Zelikow, 1971/1999), because each of the three therein discussed paradigms (rational actor, organizational behaviour, governmental politics) lends itself to a comprehensive story about the Cuban missile crisis. And it is only by considering the other paradigms that one really becomes aware that there is more to it.

What consequences does the pluralism of paradigms in the social sciences have for modeling and simulating? First of all, there is a danger of exclusively paying attention to only those paradigms that allow for mathematical modeling. Now, as there is no reason a priori why these paradigms should be any better than other paradigms, choosing a paradigm merely on the basis of the relatively irrelevant criterion of technical implementability bears the danger of getting a seriously distorted image of reality. Many of the associated problems have become apparent in the heated debate about rational choice explanations in political science that started in the midst nineties. They are most clearly pointed out in Shapiro's "The Flight from Reality in the Human Sciences" (2005).

Thus, before a model is accepted as the proper description or explanation, other alternatives, and this includes also non-mathematical depictions of the object under study, should be considered, too. In this respect, theoretical models (i.e. models that mostly rely on some background theory or paradigm or, worst of all, on "plausible assumptions") are probably much more dangerous than models of phenomena or data. For, if one is directly working with the empirical subject matter, one becomes easier aware of the insufficiencies of theoretical assumptions.

6.3 Multiple and varying causes for the same effect

Many important phenomena in the social sciences are characterized by the fact that they may be caused in many different ways. While this can happen in physics, too, it seems to be a standard case in the social sciences. Take for example, the outbreak of war. There are many different reasons why a war can break out. In each single instance of an outbreak of war there is usually a bundle of different causes involved. And in different instances of an outbreak of war probably different bundles of causes lead to the same effect, namely, the outbreak of war. Finally, it is in most instances difficult to determine which of a number of possible causes were decisive. How can historians deal with these problems?

The best way to deal with this situation is to consider all reasonable assumptions about what the causes in a particular instance of the outbreak of war are. And where the evidence remains insufficient as to whether a particular possible cause was indeed relevant, it is better to at least mention this cause as a possibility than to leave it out completely.

Because multicausality in the just described sense as well as the evidential underdeterminacy of particular possible causes are typical features of historical explanations, the discipline of history has developed a scientific culture that in some respects runs contrary the scientific culture of the natural and technical sciences. Most importantly, historians do not consider an explanation as better just because it is simpler. Quite the contrary, an explanation in history is the better the more "differentiated" it is. The reason for this attitude is that it is always easy to cook up a simple story. (The most simple explanations are those that rely on ideologies, e.g. "history is the history of class struggles.") But it is usually much more challenging to get all the details right. It is therefore no surprise that among social scientists the charge of "monocausality" is almost a kind of an insult. In history as well as many other social sciences, explanatory *parsimony is a vice and not a virtue*.

This conclusions can be generalized to all cases where multicausality is involved and where it is practically impossible check the relevance of all potential causes. In this situation, it does not make any sense to demand that explanations should be as simple as possible. For, there is no way of determining when an explanation has become too simple.

What consequences does this have for the employment of models and simulations in generating explanations. One consequence is that simple models that demonstrate merely logical or – as the practitioners sometimes prefer to say – "theoretical" possibilities are at best a small piece in the puzzle. They are "partial explanations" in the sense of Aydinonat (2007). And before they can be considered a part of a full explanation it must be checked whether the so demonstrated theoretical possibility is a real possibility in the given situation and how it compares to other possible explanations.

Often, unfortunately, the surplus in explanatory power to be gained by simulation models that merely demonstrate logical possibilities is almost negligible. This can be seen, for example, when comparing Robert Axelrod's account of the informal truces between soldiers of opposing forces on large parts of the western front in World War I in terms of his simulations of the repeated prisoner's dilemma with the original historical study by Tony Ashworth on which Axelrod based his account (Arnold, 2008, p. 180-189).

Linking to the discussion whether in the social sciences KISS ("keep it simple stupid") models are better than KIDS ("Keep it descriptive stupid") models, one might now conclude that this is a problem of KISS models in particular (see Pyka and Werker (2009) with further references). Without entering into the full discussion here: From their approach and their own aspiration KIDS models do indeed avoid to be overly parsimonious. Yet, they are plagued by many problems of their own like being more difficult to understand, often lacking robustness or, despite being more complex, still not coming close enough to empirical reality to be of explanatory value.

6.4 "Wholistic" nature of many phenomena in the social sciences

There is good reason to assume that many phenomena in the realm of social sciences are of a wholistic nature. By "wholistic nature" it is meant that the effect which a particular "entity" or "force" produces changes from one occasion to another and depends on the particular circumstances of each occasion. It is an empirical question whether this is true of many or most phenomena in the social sciences. But if it is true then it explains why explaining phenomena by breaking down their cause into single causes and then determining their joint effect by some law of combination does hardly ever work in the social sciences (see Alexandrova (2008, p. 390/391) and Cartwright (2009, p. 48ff.)).

In physics one can break down the forces acting upon a body into different components and then combine them with the rules of vector calculus. This works quite well in practice. The same thing does not work in the social sciences. The question can be left open whether it does not work because the “wholistic nature” of social phenomena poses an epistemic barrier, which merely makes it extremely difficult for us to find the right “capacities” (Cartwright) and rules of combination, or whether there is more to it and the “wholistic nature” of social phenomena raises an ontological barrier to the very existence of processes that could reasonably be broken down into single components. The epistemological consequence remains the same: One has to be very careful with drawing general conclusions from models about “capacities” or regularities.

As a sidenote it can be mentioned that this feature, too, is reflected in the scientific culture of some social sciences. Historians typically have a strong sensitivity for the individuality of events and historical processes. The idea was taken to its extreme by the school of historism which denied that there are “laws” in history.

6.5 Difficulties of measurement

The empirical data in the social sciences does often not have the form of measurable quantities and where it does, it is often difficult to measure it precisely.

An example for non-quantitative data would be historical sources like international treaties. Examples for quantitative data that are well defined and can be measured precisely are money or the number of inhabitants of a country at a given time. Quantitative magnitudes that are less well defined and hard to measure would be the power a state has in relation to other states or the utility a consumer derives from the consummation of a certain good. To make this point a little clearer the latter examples shall be discussed in slightly more detail.

While power seems to be a magnitude that has an order of greater or smaller, any comparison remains almost inevitably vague. This is especially true when different forms of power like economic power and military power are to be compared. Thus, despite of what Bertrand Russell had hoped some time ago (Russell, 1938/2001, p. 10), it is impossible to form a concept of power that works similar to that of energy in physics, where different forms of energy, say potential energy and heat energy, can be measured and compared precisely.

As regards utility: In order to apply utility theory in the same way as, say, the concept of force in physics, one would have to determine peoples’ preferences and measure the cardinal utility values they attach to them with a reasonable degree of accuracy. Even in purely economic contexts this is often well-neigh impossible. Money, to be sure, can be measured, but then what prompts peoples’ actions is not money but the utility they derive from money or other means.

Now all this is of course well known, but what is easily overlooked are the restrictive consequences these facts have for the range of reasonable modeling in the social sciences. Assume, for example, a scientist wants to explain why the victorious powers of the Second World War were willing to agree to the unification of Germany in 1990 and she wants to do so by using a game theoretical model of the negotiation process. Now, the raw data available consists of protocols (if available) of the two plus four negotiations, communiques and news releases of the involved parties, treaty drafts, the final treaty and the like. Before any game theoretical model can be fed with these data they would need to be transformed into quantitative parameters through a careful process of interpretation. Given that there is always a certain range of reasonable interpretation the interpreted data must be considered quite noisy. The need of interpretation also occurs on the way back when interpreting the results of a formal model so that they make sense in terms of the phenomena that the model is about.

One might of course deny that this is a suitable problem for the application of a game theoretical model. But if this is denied then already one important lessen is learned: Due to the nature of the data occurring in the social sciences, formal modeling is sometimes not a reasonable option. And if it is not denied then it does at least highlight some of the specific challenges that the application of mathematical models faces in the social sciences due to difficulties of measuring data quantitatively.

The epistemological consequences can be summarized as follows:

1. Establishing a link between a model and empirical reality can be difficult as it may require careful interpretation of empirical facts. Other than in the natural sciences the last step in the chain of models leading from theory to empirical reality may not simply be a model of data or phenomena but a hermeneutical interpretation of data. (By "hemerneutical" I mean "involving the interpretation and understanding of a product of human cognition by a human agent".)
2. Because of the difficulties of quantitative measurement, great strain is placed on the robustness of models. In order to draw valid conclusions, a model must be robust with respect to variations of the values of its input parameters within the range of measurement inaccuracies. The larger the measurement inaccuracies or – in cases where hermeneutical interpretation takes the place of measurement – the range of acceptable interpretations, the more robust, therefore, the model must be.

6.6 Pluralism of scientific styles

Social sciences in general are characterized by a multitude of different styles of presentation like rich narratives or "thick descriptions", stylized verbal descriptions, mathematical descriptions. Often explanations in the social sciences work completely without formal models. If an example is seriously needed[10] then Orlando Figes "The Whisperers" could be cited (Figes, 2008). In this book Figes describes how the persecution in Stalinist Russia formed the habits of its citizens in everyday's and family life and he explains why it did so. The book is a fine example of "oral history" that rests mainly on interviews with contemporary witnesses. Even though he explains things in his book, Figes does, of course, not have any use for mathematical models or computer simulations whatsoever.

But even in cases where mathematical models might help us to understand social phenomena, they typically operate in a field that is also covered by theories and descriptions of a very different scientific style. To put the content and the results of mathematical models or simulations into relation to theories and descriptions that are rendered in a completely different scientific style requires a considerable interpretative effort. Getting around these difficulties by confining oneself to a modeling approach and ignoring descriptions and theories that do not fit a mathematical style of research is not recommendable, because it can lead to omitting relevant information. In non-economical contexts, where the description of the empirical subject matter to which the models are related usually has a narrative form it is not an option at all, anyway.

A good example for this situation is the interpretation of mathematical results in social choice theory. The most famous of these results is Arrow's theorem which shows that a mapping from individual preferences to a collective preference relation is impossible if mild and seemingly self-evident restrictions are placed on the mapping function (such as that it should be "non-dictatorial", guarantee "pairwise independence" and allow any kind of well-formed individual preference relations in its domain) (Mueller, 2003, p. 583ff.). But what does this abstract mathematical result mean in terms of voting and decision making in a democracy? Does

[10] It seems that it is, because Epstein (2008) denies that social science without modeling is possible. Epstein's argument that one has only the choice between either implicit or explicit models, wherefore it is better to make explicit models, fails for several resons: 1) An implicit model can be better than an explicit model, if one fails to render one's implicit model in explicit terms properly. Just as the formalization of a verbal theory is a highly non trivial task so is the rendering of implicit assumptions in explicit terms. 2) Implicit assumptions about human behaviour and human nature often work quite well. We use them every day in our life with considerable success. 3) The question that is at stake when discussing social simulations is not whether a model is implicit or explicit but whether it must be mathematical or not. My claim is that for many connections that we can perfectly well describe verbally we do not (yet) have acceptable mathematical equivalents. No formalization is better than poor adhoc-formalizations. Epstein, however, is right in so far as explicetness is desirable.

it mean that democratic decision making procedures are unavoidably precarious, as some authors believe (Riker, 1982/1988)? In order to answer these questions the mathematical results need to be related to empirical descriptions of democratic elections and democratic decision making as well es philosophical concepts of democracy, liberalism, political participation and the like. Many things can go wrong if the task of interpreting the mathematical results in terms of empirical and philosophical concepts is not done carefully (see Mackie (2003) for a comprehensive portrayel and an acute criticism of misinterpretions of Arrow's theorem). Again, this interpretative task is not the same as the respective task in physics of interpreting the results of a calculation with respect to the physical situation, if only because the hermeneutical gap between the language of the models and the language of the empirical descriptions is much larger in the social sciences than in physics.

The epistemological consequences that the plurality of scientific styles in the social sciences has for modeling can be summarized as follows: 1. Specific attention must be paid to the task of integrating mathematical models with the results obtained by other methods. 2. In some cases mathematical models might not be a reasonable option at all. This should best be evaluated before embarking on the task of constructing models.

7 Conclusions

There are two kinds of conclusions that can be drawn from the previous considerations: Conclusions that directly concern modelers in the social sciences and conclusions that concern philosophers of science that seek to understand and reconstruct the modeling practice of the social scientists.

7.1 Consequences for modellers in the social sciences

As far as the consequences for the practitioners are concerned, one can find two quite different research strategies in the social sciences: Research that is method centered and research that is problem orientated.[11] The consequences to be drawn for these types of research strategies are somewhat different, but follow the same general principle as a guideline, which I call the "principle of appropriate method":

> *Principle of appropriate method:* The use of a certain method for investigating a specific research question is justified if no superior method for investigating the same question exists and if the results that it yields are more reliable than mere guessing.

The rationale behind this principle is that ultimately the goal of science is to find something out about reality, i.e. to describe, to understand and to explain pieces of reality. In order to do so all kinds of methods are employed. Now, as a result of the division of labour in science, some scientists specialize on the development of theories, of models or of methods while other scientists specialize on the empirical research. There is good reason for specializing in this way, especially if the mastering of particular methods, like computer simulations or mathematical models requires specific skills that it takes years to learn. But the study of models and the development of methods is not an end in itself. Because the ultimate goal of science is to generate knowledge about reality, all of its activities must either directly or indirectly be related to this goal. And a certain scientific activity is justified to the degree in which it is appropriate to serve this goal. The "principle of appropriate method" substantiates this idea with respect to the employment of specific methods. Even under the conditions

[11] This distinction is motivated by Green's and Shapiro's criticism of method centered research (Green and Shapiro, 1994; Shapiro, 2005). Rather than dismissing method centered research in general, as Green and Shapiro do, I consider method centered research as a different kind of research strategy and try to catch the defects of the method centered strategy by placing specific requirements on the research design of method centered research.

of scientific division of labour a scientist has a certain responsibility for making sure that the scientific activity she is engaged in serves the ultimate goal of science.

7.1.1 Consequences for problem orientated research

Under "problem orientated research" I understand the kind of research where scientists try to answer a particular empirical research question. If a scientist follows a problem orientated research strategy then the problem is fixed and the methods should be chosen or disposed of as appropriate. From what has been said before about the specific conditions for modeling in the social sciences, two obvious conclusions follow:

1. *Keep your options open*: Other options than the use of models or simulations should be evaluated as well. It might even be a good idea to use several different methods to get the most comprehensive view on the problem.
   A possible exception to this rule is the science of economics, where there seem to be few methodological alternatives to modeling. It almost seems as if in economics, any answer of an economical question needs to be rendered in the form of a model in order to be acceptable to the community. (I am not in a position to judge whether what appears to be the common understanding of economists about their science is misguided or not. Therefore, I am just mentioning this fact.)
2. *Choose wisely*: If models or simulations do not work for a particular problem, then models or simulations need not and, in fact, should not be used. For some types of research questions (as in the aforementioned example of Orlando Figes' oral history of Stalinist Russia (see page 21)), formal models are simply inappropriate.
   But even in those cases where the kind of research question does not preclude a mathematical approach prima facie, modeling is not always worth the effort. If a model can neither be validated empirically nor vindicated theoretically then there is no point in modeling.

7.1.2 Conseqeunces for method centered research

The method centered approach can be understood as a research strategy where a certain methodology is developed and investigated with regards to its ability to answer different research questions. If a scientist follows a method centered research approach then the method is fixed and the problems are chosen or disposed of according to their suitability for applying the method. The conclusions that can be drawn for method centered research are symmetric to those for problem orientated research:

1. *Chose the right problems for your method, make sure that relevant scientific problems for the method exist*: The "right problems" are problems where the success of the models can be tested. A common danger of method-centered research is the irrelevancy of its results (Shapiro, 2005). This happens, if problems are chosen only because they fit the method and not because they are relevant problems in any other sense.
2. *Keep in mind that the model needs to be validated*: Models and simulations should be designed so that they can be validated. This implies that free parameters should be avoided and measurement inaccuracies should be taken into account. The burden of attuning models to measurement restrictions clearly rests on the shoulders of the modelers and not of the empirical researchers that develop measurement techniques, because the possibilities for developing measurement are limited by the empirical world.
3. *Validate your model, take failures seriously*: Models need validation. It is insufficient to base a model – as is often done (see Hegselmann and Krause (2002) for an example) – merely on "plausible assumptions" without either systematically testing the validity of these assumptions nor empirically validating the results. A model that has not been validated does at best have the epistemological strength of a metaphor or a just-so story. Admittedly, this may be sufficient in certain contexts.

Failures of validation ought to be taken serious: A model that fails validation is a false model. A model that cannot even be validated should be considered as not yet a scientific model in the same sense as an unfalsiafiable theory is considered as unscientific.

7.2 Consequences for philosophers of science

The object of the philosophy of models and simulations is to reconstruct how models and simulations contribute to the generation of scientific knowledge. In order to do so the philosophy of models asks what models are and, more importantly, how models prove. The latter question is more important, because it helps us to draw the line between proper use and improper use of models. In this respect the philosophy of models takes up a similar task as the philosophy of science in general does with the demarcation problem. To draw a line between proper use and improper use of models is a particularly important task for the philosophy of simulations in the social sciences, because, as a matter of fact, the scientific value of many social simulations appears to be rather doubtful (Arnold, 2008; Hammerstein, 2003).

>From what has been said previously, it should be clear that the epistemic situation for models and simulations in the social sciences is somewhat different from that in the natural sciences and engineering, although the transition is of course smooth and interlocking. Paying proper attention to this difference leads, as I believe, to the following conclusions for the the philosophy of models and simulations:

1. *Models "mediate" differently in the social sciences.* While in the natural sciences "models as mediators" are linked to exact and well-confirmed background theories on the theory-side and to precisely measurable data on the empirical side, the standard case in the social science appears to be quite different.
   On the theory-side there are no precise, well-confirmed and content-rich background theories. Often modelers help themselves with plausible assumptions to feed their models (Hegselmann and Krause, 2002), which unfortunately adds quite a bit of arbitrariness to the models right at the beginning. In other cases the assumptions are result of a careful empirical assessment of the target system (Siebers et al., 2010).
   On the empirical side, the data that the models are related to are only sometimes precisely measurable quantities. Often the "data" consists of or is embedded in narrative descriptions of situations which need to be strongly stylized before they can be fed into models.
   Summing it up: The "mediation" concept of models is of comparatively more limited applicability in the social sciences, because i) there are no theories on the one end of the "mediators" and ii) there is more involved in the process of mediation than merely models or a cascade of models.
2. *The analogy between simulations and experiments is harder to justify.* In an experiment we learn something about nature from nature. A simulation in contrast "generates new knowledge on the basis of existing knowledge"[12]. This is not to say that we cannot learn something about nature from simulations. We can do so if the existing knowledge already is fairly comprehensive and well-assessed. In the natural sciences, part of the existing knowledge consists of powerful and empirically well-confirmed theories. Under this condition we can learn something about nature from "computer experiments" that apply these theories to particular research questions (as in the ribosome example) or that put more specialized theories to the test. Because of the lack of well confirmed and powerful (i.e. structure-rich) background theories, simulations in the social sciences usually do not have this quasi-experimental status. The may attain such a status if the assumptions that are built into the simulation are – even without a background theory – at least empirically well-assessed for the simulated scenario. But frequently this is not the case and if it is not the

[12] This is the very clear expression used by Jen Schellinck and Richard Webster in their talk at the Models and Simulations 4 Conference in Toronto, May 2010. To avoid any kind of misunderstanding one might add that "simulations generate knowledge *exclusively* on the basis of existing knowledge".

case then the “experimentation”-terminology used in connection with mere computer simulations (as in (Hegselmann and Flache, 1998, 3.11) for example) can be misleading. For, what these simulations show are only the consequences of more or less arbitrary assumptions, but not the behaviour of the simulated entities in nature.

Philosophers of science should be aware that there is a categorial distinction between experiments and simulations. The analogy between experiments and simulations works only under certain favorable conditions such as the existence of comprehensive and reliable background knowledge. These conditions are usually not met in the social sciences.

3. *Validation and research designs for models and simulations differ in the social sciences.* As far as validation ist concerned, the lack of empirically well confirmed background theories means that the assumptions entering into the model need to be assessed individually for the scenarios to which the model is to be applied. (The not uncommon practice to rely on merely “plausible assumptions” is rather unsatisfactory and should not be sanctioned by a critical philosophy of science.) Also, because the model input (e.g. assumptions, measured parameter values, tried and trusted modeling practices) is typically less reliable in the natural sciences, direct empirical validation of the simulation results becomes more important.

   It stands to reason that as a consequence of these differences the kinds of research design that are most successful in the social sciences are different form those in the natural sciences. If we follow Alexandrova’s examination of the use of auction models (Alexandrova, 2008) then a successful research design is one where models function as “open formulae” for generating causal hypotheses in a trial and error approach that includes models as well experiments as complementary elements of the research process. At the same time other accounts of modeling which are somewhat more in line with the research logic in the natural sciences fail to adequately capture the showcase of the auction design (Alexandrova, 2008, p. 387-393).

   While similar trial and error research can also occur in the natural sciences, it might turn out that it is the standard case of a successful simulation-research design in the social sciences. This suffices to give the activity of modeling or simulating a distinct flavor in the social sciences.

4. *Philosophers of science should refrain from rationalising bad practices.* Philosophy of science is not so much a descriptive but a critical enterprise. Its aim is to reconstruct how science generates reliable knowledge about the world. But the philosophy of science should also criticise scientific practise when it is flawed. In this respect the aim of the philosophy is not only to understand how science generates knowledge but also to critically examine whether it actually does.

   If, as in the case of Robert Sugden, one has reason to wonder that “authors typically say very little about how their models relate to the real world” (Sugden, 2009, p. 25) then the most salient explanation is that these models are simply not fit to teach us anything about the world (Cartwright, 2009, p. 48ff.). Philosophers should allow for this possibility and refrain from rationalising bad methodological practice. This is the more important, because some of the common research designs for simulations in the social sciences appear to be heavily flawed. For example, the (implicit) research design that lies at the basis of many simulations of “the evolution of cooperation” in the tradition initiated by Robert Axelrod (Axelrod, 1984) which works by constructing purely theoretical simulations and then drawing generalizing conclusions from the results is flawed, because the generalizing conclusions are not sufficiently warranted (Binmore, 1998, p. 313-319). And a more modest variant of this research design, which consists in constructing purely theoretical simulations and then never drawing any empirical conclusions at all, is also not convincing, because it raises the question why we should be interested in models from which we cannot learn anything about the world.

> As in science and philosophy rational argument ought to decide about the truth and falsehood of opinions and not the number of supporters, philosophers of science need not to be impressed by how widespread certain faulty research designs are.

But why is it important to be aware of these epistemological differences of simulations in the social sciences and simulations in the natural sciences? The answer is that our explicit or implicit epistemological ideas have a regulatory function when designing research programs. Wrong epistemological ideas can entail the long-term failure of research program. If we believe that the epistemological conditions in the social sciences are just the same as in the natural sciences then we will expect simulation studies that are designed on the role model of the natural sciences to sooner or later yield good results. Any failure to do so will in the first place be considered as a failure of the particular simulation study and not of the research program. If we are aware of the differences between social sciences and natural sciences, then we might still consider it worth while to learn and apply techniques for social simulations that have been sucessful in the natural sciences. But in cases where these fail we will much sooner consider the possibility that the research design was inappropriate and that the research program needs to be readjusted.

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