The World as a Process: Simulations in the Natural and Social Sciences

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Abstract

Simulation techniques, especially those implemented on a computer, are frequently employed in natural as well as in social sciences with considerable success. There is mounting evidence that the "model-building era" (J. Niehans) that dominated the theoretical activities of the sciences for a long time is about to be succeeded or at least lastingly supplemented by the "simulation era". But what exactly are models? What is a simulation and what is the difference and the relation between a model and a simulation? These are some of the questions addressed in this article. I maintain that the most significant feature of a simulation is that it allows scientists to *imitate one process by another process*. "Process" here refers solely to a temporal sequence of states of a system. Given the observation that processes are dealt with by all sorts of scientists, it is apparent that simulations prove to be a powerful interdisciplinarily acknowledged tool. Accordingly, simulations are best suited to investigate the various research strategies in different sciences more carefully. To this end, I focus on the function of simulations in the research process. Finally, a somewhat detailed case-study from nuclear physics is presented which, in my view, illustrates elements of a typical simulation in physics.

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1 Introduction

Major parts of current research in the natural and social sciences can no longer be imagined without simulations, especially those implemented on a computer, being a most effective methodological tool. Natural scientists simulate the formation and development of stars and whole galaxies [31], the detailed dynamics of violent high-energy nuclear reactions [6] as well as aspects of the intricate process of the evolution of life [15], while their colleagues in the social science departments simulate the outbreak of wars [25], the progression of an economy [2] and decision procedures in an organization [43] – to mention only a few. Recently, computer simulations even proved useful in moral philosophy[1]. In fact, there is almost no academic discipline without at least a little use for simulations.

Although simulations are therefore of considerable importance in science, philosophers of science have almost entirely ignored them. Only recently have whole articles and even conferences been devoted to their metatheoretical analysis[2]. There are, however, some interesting considerations on simulations scattered in the literature pre-dating the works cited above, such as the studies of M. Bunge[3]. Besides, a few scientists working actively with simulations made some more general remarks – mostly in the introductory part of their papers – on the scope and function of simulations[4].

But why should a philosopher of science be interested in simulations at all? I see three main reasons: Firstly, in order to formulate a "theory of science" (R. Giere [18]) one cannot ignore simulations, for they are too important a tool for today's scientists. Secondly, as F. Rohrlich and others [29] have emphasized, computer simulations provide "a qualitatively new and different methodology ... that ... lies somewhere intermediate between traditional theoretical physical science and its empirical methods of experimentation and observation"[5] for the sciences: numerical experimentation.[6] It is the task of the philosopher of science to elaborate this claim. Thirdly, since simulations are used by natural as well as by social scientists, they are best suited to compare critically the different respective methodological strategies.

It is thus worth asking how and why scientists use simulations, what *function* they have in the research process and what their respective advantages and disadvantages are. The purpose of this article is to provide a provisionary account to this task. I shall stress here that it is definitely *not* my aim to urge social scientists simply to copy the blessed methods of their colleagues in the, say, physics departments and everything will be fine.[7] This is – I hold – not appropriate; first of all, every science has its own methods *sui generis*[8]. Instead,

[1] See R. Hegselmann's contribution in this volume and references cited therein.

[2] See the recent work by P. Humphreys [28, 29, 30] and F. Rohrlich [40]. R. Laymon [33] discusses the role of idealizations and approximations in computer simulations.

[3] See [9] and [8], p. 266.

[4] A collection of case-study simulations taken from the social and administrative sciences including some useful methodological analyses can be found in [19].

[5] [40], p. 507

[6] I will come back to this in Sec. 3.

[7] I will leave unanswered the question as to whether scientists really need the advice of a philosopher at all, see [27].

[8] It is a common complaint that current philosophy of science has been developed taking physics [22], or even theoretical physics as the paradigmatic science [13, 16, 17, 20]. Although analyzing physics is surely worth doing, focusing too strongly on it is not without dangers. It is definitely not obvious that, for example,

I suggest we first describe carefully, and thus take seriously, what working scientists actually do. In this context it is worth considering structures of typical problems, exemplary research strategies, the status of empirical tests etc. in the different sciences independently. Later on, ambitious methodologists might reach for "unified" models which fit many sciences. For our purpose, simulations are a good starting point to compare the research strategies of various sciences since the simulation method has become such a generally acknowledged tool.
The term "simulation" has many facets and is used with various meanings [19, 28]. In the following I can only focus on some of them. More specifically, I shall not be concerned with what I call *experimental simulations*. In an experimental simulation a real physical (or biological) process is imitated by another real physical (or biological) process. As an example take the endeavours of M. Eigen and his collaborators to mimick processes which presumably occurred in the early stages of the evolution of life in a specially prepared reactor [15]. Theoretical simulations (that I shall call "simulations" in the remainder of the paper for the sake of brevity), on the other hand, are closely related to theoretical models, as will be pointed out in the next section. These simulations are usually carried out on a computer.
The remaining paper is organized as follows. Sec. 2 deals with the relation between theoretical models and simulations; in this context a definition of the term "simulation" is suggested and confronted with other proposals recently given in the literature. Sec. 3 focuses on the various functions of simulations in the everyday research process. I point out those functions of simulations which are more important for social scientists than for natural scientists and vice versa. In Sec. 4, a typical simulation from physics is presented and analyzed in order to identify some of the characteristic features of simulations in physics.[9] Finally, Sec. 5 summarizes our main results.

2 Models and Simulations

Models and simulations are apparently closely related. But what is the exact relation between both scientific tools? In order to clarify this question, I shall first make some general remarks about theoretical models[10] (Sec. 2.1). Subsequently, I propose a definition of the term "simulation" and confront it with another suggestion given in the literature (Sec. 2.2).

2.1 Models ...

In his "History of Economic Thought", J. Niehans claims that in 1894 the "era had began in which scientists interpreted their activity as model building."[11] In this very year, H. Hertz published his famous book "Principles of Mechanics". Therein the famous physicist writes:

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metatheoretical insights which were inspired by physics also make sense in other sciences. I would like to remind the reader of the various attempts to make economics fit Lakatos' methodology of scientific research programmes, see [14]; for a critical discussion [22], pp 192.

[9] I have chosen this physics case-study for two reasons. One is expertise (or better non-expertise), the other is that there are already many detailed social science simulations presented in this volume.

[10] In the remainder I will drop the attribute "theoretical" for I am here only interested in this special sub-category of models. For a discussion of other types of models see [18, 34] and references cited therein.

[11] [37], p. 313

> We make for ourselves internal images or symbols of the external objects, and we make them in such a way that the consequences of the images that are necessary in thought are always images of the consequences of the depicted objects that are necessary in nature ... Once we have succeeded in deriving from accumulated previous experience images with the required property, we can quickly develop from them, *as if from models*, the consequences that in the external world will occur only over an extended period or as a result of our own intervention.[12]

In fact, with the end of the late 19th century, model building began to dominate the (theoretical) activity in the field of physics: J.C. Maxwell used hydrodynamic analog models to derive the well known equations of electromagnetism and W. Thompson, later Lord Kelvin, stated that he could not understand a phenomenon until he had succeeded in constructing a (mechanical) model of the system under consideration [46]. Presently, devising and exploring models forms an integral part of theoretical research [18]. Quite often, the term "model" is used – throughout the sciences – synonymously with "theory". By and large, scientists prefer "model", because – as I have spelled out elsewhere – it is safer to label one's thought products "models" instead of "theories" for they are most likely provisionary anyway, and the term "model" seems to acknowledge this right from the beginning [21].
According to J. Niehans, it took some thirty years before the model-method also conquered a social science, viz. economics.[13] Indeed, since the nineteen-thirties model building has been dominating economic theorizing. Other social sciences, such as sociology and psychology, followed somewhat later.
I now wish to explicate the concept of a model in fairly more detail. This is not an easy task, since the term "model" is used with many different meanings in the sciences and in philosophy. Nevertheless, it may be useful to have a precise definition. This is what the Logical Empiricists, such as R. Carnap [11], R. Braithwaite [7] and E. Nagel [36], reached for. These philosophers identified a model in science with a model in mathematical model theory: A model is nothing but an *interpretation of the theory's calculus*[14].
It soon became clear that this definition of "model" is too narrow; it fails, *inter alia*, to illuminate what role models play in the actual research process. Why, then, are models important at all if they are only another interpretation of a given formalism?[15]

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[12] quoted from [37] (translation from the German by J. Niehans), p. 313.

[13] Niehans mentions, however, that the classics, such as A. Smith and D. Ricardo, already used models at several stages of their work.

[14] [7], p. 269. There are, of course, differences between the views of the above mentioned authors, especially between E. Nagel, who is more sensitive concerning the practice of science, and R. Carnap and R. Braithwaite. It is, however, not important for the remainder of this paper to discuss them here in detail, see [38].

[15] This critique is elaborated in [38]. It may, however, be unfair to include R. Carnap in this criticism for he did not intend to provide a reconstruction of the way scientists use the term "model". Carnap attempted to characterize the relation between syntax and semantics of a scientific theory. For this purpose, the model concept proves to be extremely helpful. Among the philosophers who boldly identify models in science with models in the sense of mathematical model theory is P. Suppes. After quoting A. Tarski ("A possible realization in which all valid sentences of a theory T are satisfied is called a model of T"([45], p. 287)) Suppes maintains:

> I claim that the concept of model in the sense of Tarski may be used without distortion and as a fundamental concept in all of the disciplines from which the above quotations are drawn (= physics, economics, psychology etc., *S.H.*). In this sense I would assert that the meaning of

In the course of the general critique of various views of Logical Empiricism starting from the 1960's, philosophers of science such as P. Achinstein [1], M. Bunge [10] and M. Hesse [26] developed conceptions of models which are closer to the scientist's intuition of that concept. All of them stress elements of a typical model that have not been taken into account by the Logical Empiricists.
M. Hesse and P. Achinstein, on the one hand, emphasize the role of *analogies* in the procedure of developing a model, while leaving only insufficient space for general background theories [38], such as Newtonian mechanics or quantum field theory, which often restrict scientist's freedom in the modeling process considerably.
In M. Bunge's approach, on the other hand, general background theories constitute an integral part of a model. According to Bunge, a model (or a special theory) consists of two components:

- A general theory,
- A special description of an object or system (*model object*).

The Billiard Ball Model of a gas illustrates this: In this case the general theory is Newtonian mechanics, the special description contains statements about the nature of a gas, e.g., that the molecules are point-like particles moving in a chaotic way in a given box. With the so characterized Billiard Ball Model it is now possible to derive the equation of state of an *ideal* gas[16]: $PV = RT$
There are many examples of a model à la Bunge in physics. It is harder to find cases in the social sciences, for there often does not exist a general theory[17]. This lack, though, does not prevent scientists from constructing models. I have argued elsewhere [21] that in Bunge's conception, the role models play in these cases is not recognized well-enough. In such cases models prove to be a favorite tool for theorists trying to obtain a (provisionary?) description of an object or system.[18]
For the purpose of this paper it suffices to characterize a model minimally as "a set of assumptions about some system"[19]. Some of these assumptions may be suggested by a general theory (such as symmetry principles), others serve merely as (idealized) descriptions of a special object or system.
It is useful to distinguish between *static* and *dynamic* models. A model is called *static*, if it only covers assumptions about systems at rest. A model is called *dynamic*, if it furthermore includes assumptions about the time-evolution of the system.
Although most systems – be they natural or social – evolve in time, it is nevertheless not generally unreasonable to construct a static model. The main reason for this is that it is

> the concept of model is the same in mathematics and the empirical sciences. ([45], p. 289)

For a forceful criticism of this see [10], p. 111.

[16]Here, p, V and T represent the pressure, volume, and temperature of the gas respectively, R is the gas constant.

[17]An exception is – as H. Lind [35] has pointed out – economics. Microeconomic theory / general equilibrium theory is, Lind maintains, *the* fundamental theory in economics. To study concrete systems in detail, special model assumptions have to be made. See also [2] for a critical assessment of this approach.

[18]Some of these aspects are, however, evaluated somewhere else in Bunge's Œvre, see [8].

[19][39], p. 146.

commonly much easier to acquire a thorough understanding[20] of a system at rest. Unfortunately, it often does not make much sense to study static aspects for the considered system is inherently dynamic. This holds especially true in the social sciences.

2.2 ... and Simulations

Simulations are closely related to dynamic models. More concretely, a simulation results when the equations of the underlying dynamic model are solved. This model is designed to imitate the time-evolution of a real system. To put it another way, *a simulation imitates one process by another process*. In this definition, the term "process" refers solely to some object or system whose state changes in time.[21] If the simulation is run on a computer, it is called a *computer simulation*.

I maintain that the definition given above is in agreement with the scientists' usage of that term. It emphasizes the function of a simulation to investigate real dynamic system. In a recent article, P. Humphreys concentrates on another decisive feature of a computer simulation, viz. the possibility to explore otherwise untractable models. After critically examining several alternative definitions of a computer simulation, Humphreys suggests the following *working-definition*:

> A computer simulation is any computer-implemented method for exploring the properties of mathematical models where analytic methods are unavailable.[22]

Hence, having simulations as a tool it is not necessary any longer to make dubious approximations in order to obtain analytically solvable equations. In fact, most interesting, i.e. "most non-linear ODE's (= ordinary differential equations, *S.H.*) and almost all PDE's (= partial differential equations, *S.H.*) have no known analytic solution"[23].

I shall mention two objections to Humphrey's working-definition: Firstly, Humphrey's working-definition does not stress the dynamic character of the model in question. As far as I see, scientists reserve the term "simulation" exclusively for the exploration of *dynamic* models. Secondly, a computer simulation may also be helpful even if analytic methods are available. Visualizing the result of a simulation on a computer screen is just one advantage.

[20] It is notoriously hard to explicate the notion "understanding". I certainly mean more than R. Carnap did when writing:

> An "intuitive understanding" ... is neither necessary nor possible. ... He (i.e. the modern physicist, *S.H.*) knows how to use the symbol 'ψ' in the calculus in order to derive predictions which we can test by observation. ... Thus the physicist, although he cannot give us a translation into everyday language, understands the symbol 'ψ' and the laws of quantum mechanics. He possesses that kind of understanding which alone is essential in the field of knowledge and science. ([11], p. 69)

A adequate explication of "understanding" is certainly a *desideratum* of contemporary philosophy of science for this concept is of utmost importance in actual scientific practice.

[21] I should say that in using the notion "process" here, as well as in the title of this contribution, I do not intend to allude to the metaphysics of A.N. Whitehead [48]. I restrict myself to a methodological analysis of simulations in the various sciences.

[22] [28], p. 501

[23] [28], p. 499

This may increase our understanding of the system more than complicated formulas written down on a paper would ever do.
It is convenient to distinguish between *continuous* and *discrete* simulations. In a continuous simulation the underlying space-time structure as well as the set of possible states of the system is assumed to be continuous. The corresponding dynamic model is conveniently formulated in the language of differential equations [40]. Discrete simulations are based on a discrete space-time structure right from the beginning [50]. Moreover, the set of possible states of the system is assumed to be discrete. The appropriate language for discrete simulations are cellular automata (CA) [40]. Here, the state of a cell of the system at time t_{i+1} follows from the state of the neighboring cells at time t_i according to certain rules.[24]
It should be mentioned here that the numerical integration of a differential equation also uses a discrete space-time resolution. The aim is, however, to extrapolate to zero resolutions.
In recent years, the availability of computer simulations has supplemented the methodology of the natural sciences. Furthermore, the delay to the social sciences was much shorter than in the case of models. This volume documents the impressive work that has been done so far. There is no doubt that we are at the beginning of the "simulation era".

3 The Functions of Simulations

In this section I shall discuss the various functions of simulations in science. The following are – as far as I see – the main motives to run simulations:

1. Simulations as a technique: Investigate the detailed dynamics of a system
2. Simulations as a heuristic tool: Develop hypotheses, models and theories
3. Simulations as a substitute for an experiment: Perform numerical experiments
4. Simulations as a tool for experimentalists: Support experiments
5. Simulations as a pedagogical tool: Gain understanding of a process

While discussing these functions in detail I shall pay special attention to the different weights of them in the natural and social sciences. Besides, I will point out some inherent drawbacks of computer simulations. It is interesting to note that both, the advantages as well as the disadvantages, result from the fact that simulations are run on powerful computers.

1. Simulations as a Technique

One major advantage of simulations is that they allow scientists to explore the detailed dynamics of a real process. In many cases it is not possible for pragmatic reasons to extract this information experimentally: the relevant time scale turns out to be either too large (e.g. for the evolution of galaxies) or too small (e.g. for nuclear reactions). For this purpose,

[24]F. Rohrlich maintains that CA's "are necessarily of a phenomenological nature rather than of a fundamental one" ([40], p. 516). I could not find any argument for this statement in Rohrlich's paper. Maybe Rohrlich considers a discrete space-time to be an approximation. However, it has been suggested that Nature itself is in fact discrete. Then, a special CA would indeed be fundamental, see also [23], chap. 7.3.

simulations are often the only appropriate tool to learn something about a system's time-evolution. This applies particularly for very complex systems, systems that are composed of many interacting sub-systems. These sub-systems may, for example, be atoms (as in the case of solid state physics) or human beings (as in sociology). In these cases it is practically impossible to derive analytical solutions of the corresponding equations that have been formulated to describe real systems.
Furthermore, certain approximation schemes may wipe out effects that would otherwise occur in a full treatment of the model. Well known instances from chaos-theory illustrate this point. For example, the famous Russian physicist L.D. Landau failed to explain the phenomenon of turbulence because he cut off curls with very high frequencies in his harmonic-oscillator-treatment. We now know that a thorough description of turbulence can only be achieved when curls at all scales are taken into account. In many cases this can only be done by solving the corresponding equations "exactly" with the help of high-powered computers. I used quotation marks here to indicate that a numerical solution is not exact in the same sense as an analytical solution is. Indeed, in a computer-aided solution of, say, a differential equations space and time are always discretized. However, the corresponding lattice spacings can – in principle – be made arbitrarily small. At least, extrapolations to vanishing lattice spacings are possible.
The possibility to obtain very accurate solutions of equation in a simulation procedure has an interesting consequence: It allows a test of the underlying model or theory. I will explain this by distinguishing two cases:
1. Discrete simulations: In this case any difference between the simulation and empirical data directly blames the model assumptions, i.e. the transition rules of the CA. This enables a critical assessment of these rules. Besides, there is no way to make approximations in a CA simulation that may be called into question for the deviation [50].
2. Continuous simulation: This case is more complicated. Let us therefore distinguish two other cases:
(a) There is no background theory: Then, any disagreement between data and theory can blame – in principle – any of the model assumptions. However, by "playing around" with the different assumptions etc. one may be in the position to detect the wrong one.[25]
(b) There is a background theory: Then, we have to distinguish between that background theory and the model assumptions (or the model object – to use Bunge's term). Now, any disagreement between theory and data can be either due to the theory or due to the model or due to both. Is it then possible to test the underlying theory? R. Laymon answers this question in the affirmative. In a recent article, Laymon suggests the following criterion for the confirmation (or disconfirmation) of a theory.

> A scientific theory is confirmed (or receives confirmation) if it can be shown that using more realistic idealizations will lead to more accurate predictions.
>
> A scientific theory is disconfirmed if it can be shown that using more realistic idealizations will not lead to more accurate predictions.[26]

[25]This sounds perhaps a bit naive for *aficionados* of the Duhem-Quine Thesis. However, as A. Franklin demonstrated convincingly, scientists usually have strategies (within a specified context) to detect wrong assumptions [16].

[26][32], p. 155

I take Laymon here to identify his “idealizations” with my “model assumptions”. A theory is then, according to Laymon, confirmed when a better model object leads “to more accurate predictions”. This sounds plausible. Take, e.g., the Billiard Ball Model of a gas mentioned in the last section. Idealizing the gas particles as point particles leads to the well-known equation of the ideal gas. Now, it is well known that molecules are *not* point-like particles. They have a finite volume V_0 and this volume affects the system's equation of state, too. A modification of the model object along this line leads to the van der Waals equation:

$$(p + \frac{a}{V^2})(V - b) = RT$$

with adjustable parameters a and b depending on the special system under investigation. This equation accounts for much more phenomena and leads “to more accurate predictions”. Therefore, Newtonian Mechanics is confirmed.

But what exactly does it mean to make the model assumptions “more realistic”? It certainly does not mean to add more and more terms to the equations of the model which exhibit additional free parameters that can be adjusted suitably to experimental data.

There is, however, a strong temptation in science to complicate the underlying dynamic model in order to increase the simulation's empirical adequacy. I wish to confront this practice with N. Cartwright's fine discussion of models. In her book “How the Laws of Physics Lie” Cartwright claims that

> [t]he beauty and strength of contemporary physics lies in its ability to give simple treatments with simple models, where at least the behavior of the model can be understood and the equations can not only be written down but can even be solved in approximation.[27]

This romantic picture may change soon since high-powered computers facilitate the treatment of very complex models. That is the dilemma of using computers in science: People no longer spend that much time thinking about “simple treatments” but just complicate the model in order to increase its empirical adequacy. At this point it is worth noting that we need *independent* evidence for the terms involved: “A simulation is no better than the assumptions build into it.”[28] Every term in the model has to be interpreted thoroughly. There is no understanding of a process without a detailed understanding of the individual contributions to the dynamic model. Curve fitting and adding more and more ad hoc terms simply doesn't do the job.[29]

There is still another (psychological) problem with many “realistic” simulations which fit all data well. They make us forget that – as always in science – idealizations and approximations were involved in deriving the model. A serious appraisal of computer simulation has to pay attention to this fact.

In closing this sub-section I shall mention that the term “simulation” is sometimes also used in the context of mathematical-statistical algorithms. A special example is the technique of so called Monte-Carlo-Simulations[30]. It has often been emphasized [19] that a Monte-Carlo-

[27] [12], p. 145

[28] [42], p. 18

[29] I hasten to add that in some cases curve fitting is also valuable, mainly if there is no better alternative in sight. It does not, however, facilitate real understanding.

[30] A description of this technique or method is given in [5]. A special example, the treatment of the Ising model, is analyzed from a philosophy of science point of view in [29].

Simulation is in fact *not* a simulation at all. It is an effective numerical technique to tackle, say, complicated integrals. After all, this technique is often used in simulation procedures. In a way one can try to "save" the label "simulation" here: The problem of evaluating an integral with the Monte-Carlo method is *dynamized* in so far as one has to select successive random numbers, then calculate the value of the respective function, sum all the values up, do the same again for a new set of random numbers, ... and finally average over all those preliminary results.

2. Simulations as a Heuristic Tool

Simulations play an important role in the process of developing hypotheses, models or even new theories. Analyzing the results of very many runs of a simulation model with different parameters *may* suggest new and simple regularities that would not have been extracted from the model assumptions otherwise. Some of these hypotheses can, in turn, serve as basic assumptions of, say, an easier model. This happens quite often in the natural sciences. Simulating the dynamics inside hadrons at finite temperature starting from the fundamental model[31], quantum chromodynamics (QCD), reveals, for example, that there are certain phase transitions. Starting from this result, physicists intend to explore the consequences of these phenomena by modeling them in a simpler way.
The following quote illustrates the corresponding role computer simulations play in the social sciences:

> Even if the processes under study are not complex, simulation can give a better picture of them because of its greater likeness to them than other models, and this is useful not only for instructional purposes but also for research. Where the causal relationships are not well understood (that is, where theory is not well developed), sometimes the best one can do is attempt to imitate the change process itself in the hope of learning more about such relationships. Thus, the model becomes an aid of theory development. Guetzkow ... has given this as a chief reason for using simulations in the study of international relations. With such a model one can also try out a theory through manipulation of the model processes to see if results conform to real-world observations.[32]

In this context "theory development" refers to the task of guessing suitable assumptions that may "imitate the change process itself". Confronting the outcome of a certain simulation with the "real-world" helps to critically assess the "theory" in question. The idea here is – as far as I see it – to establish theories by using the well known trial-and-error strategy (educated guesses). This sounds a bit blue-eyed; let's just try out as many assumptions as

[31] I here use the somewhat queer notion "fundamental model" for two reasons: Firstly, QCD is a model in the sense of Bunge since it is a special realisation (interpretation) of a general quantum field theory [49]. To make QCD a model it is necessary to specify the special fields (quarks and gluons), their respective symmetry groups (e.g. flavor $SU(3)$ and color $SU(3)$) and their interaction (gauged color $SU(3)$) [21]. Secondly, I added the specifier "fundamental" since it is often claimed that there is nothing more to be said about strong interactions than QCD does. However, this is not true in general, because – for example – Grand Unified Theories (GUTs) presumably modify the physics at high energies.

[32] [41], p. 10

possible (remember: we have huge computers!) and as a result of this process we will finally get the aspired theory.
There are at least two problems with this approach: Firstly, as I mentioned already, one might not learn much from a simple reproduction of data with assumptions that are not satisfactorily understood.[33] Secondly, the social world is so complex that it is probably even with high-powered computers not possible to get close to "real-world observations". This raises again the problem of how to assess the model assumptions independently.
There is still another heuristic function of simulations that I shall mention here. S. Wolfram [50] maintained that the analysis of simulations may suggest an *ansatz* for an analytical solution of a given problem. Of course, there is no guarantee that this will lead somewhere; nevertheless, it may work. This aspect reflects the strong interaction between analytical and numerical endeavors - at least in the natural sciences.

3. Simulations as a Substitute for an Experiment

Simulations may help scientists to explore situations that cannot (yet?) be investigated by experimental means. The performance of an experiment might be impossible for pragmatic, theoretical or ethical reasons. An example of a *pragmatically* impossible experiment is the study of the formation of galaxies; we simply cannot do much to manipulate galaxies. An example of a *theoretically* impossible experiment is the investigation of counterfactual situations. Theorists ask what happened, when some fundamental constants (such as the charge of the electron) had other values. These questions are also relevant for philosophers who study the so-called anthropic principle [4]. An example of an *ethically* impossible experiment is to ask for the long-term consequences of a raising of, say, the income tax by a factor of 1.5 or so. This question may well be of some interest for economists. However, it is hard to imagine that those experiments have a realistic chance of being performed in the future. In all these cases, an appropriate simulation is the best scientists can do.
In his article "Numerical Experimentation" P. Humphreys claims that "the computational methods of numerical experimentation constitutes a new kind of scientific method, intermediate in kind between empirical experimentation and analytic theory."[34] In fact, simulations help us to theoretically approach regions in a parameter space that are inaccessible by normal experiments. This novel possibility supports the thesis that a methodology is nothing fixed but something that evolves in a similar way as our scientific knowledge evolves.
Although social scientists have experience in performing laboratory experiments for several years[35], it is apparent that numerical experiments on a computer prove to be an appreciated complementary way to approach social systems. Now scientists can easily vary different kinds of parameters, visualize the effects and eliminate disturbing influences that unavoidably show up in real systems. It is precisely the lack of conclusive experiments that motivates social scientists to run computer simulations.
What is the difference between numerical experiments in the natural and social sciences? Methodologically there is no big difference. However, it is probably not too unfair to note

[33] Compare, however, H.A. Simon's elabortation of the role of simulations of poorly understood systems in [42], pp. 19.
[34] [29], p. 103
[35] For a survey of (laboratory) experiments in economics see [44].

that numerical experimentation is much more founded in the natural than in the social sciences. What reasons do we have to believe in numerical extrapolations? In the natural sciences models are (often) well confirmed in a certain parameter space and, furthermore, embedded in strong theories. Starting thus from such "solid ground" makes extrapolations in realms beyond experimental reach more trustworthy. In the social sciences, on the other hand, there often is no such "solid ground" to start with; this makes it much harder to trust numerical experiments.

I should stress again that it is important when running a simulation to have reason to believe in the details of the underlying model or theory which are independent of the results of complete simulations.

4. Simulations as a Tool for Experimentalists

I now discuss a function of simulations that is of significant importance for the natural sciences. Computer simulations nowadays constitute an essential tool to support real experiments. These are the dominant tasks:

- Inspire experiments
- Preselect possible systems and setups
- Analyze experiments

A simulation *inspires* experiments when, say, a new regularity or hypothesis has been found by analyzing the results of simulations for many different parameter sets. It is then worth confronting this hypothesis with a real experiment.

A simulation helps to *preselect* possible systems and setups for pragmatic reasons. It is simply too difficult to find the parameters that demonstrate the effect experimenters are after most clearly in a real experiment, especially in cost (and time)-expensive high-energy physics [3]. Then detailed simulations of possible experimental setups and arrangements are performed before the actual experiment is executed.

A simulation helps to *analyze* experiments when trivial or well-understood effects have to be subtracted in order make the actual effect visible. Simulations often prove to be useful for identifying these contributions. My example is again from high-energy physics. Physicists use standard methods to simulate so called "background"-processes. Subtracting their contribution from the experimental data (cross sections etc.) helps them to identify "non-trivial" contributions. In a way this is also done in the social sciences. Effects that are of entirely statistical origin can be identified (and then subtracted) by performing appropriate computer simulations.

5. Simulations as a Pedagogical Tool

Simulations prove to be extremely useful in instucting students. By "playing" with a simulation model and visualizing the results on a screen, students increase their understanding of the underlying processes and develop an intuition for what might happen in similar circumstances. Learnig things this way is both much cheaper and faster than performing real experiments (if this is possible at all!). Once again, all this only makes sense when we have good reasons to trust the underlying model.

With respect to this function there is no difference between the natural and social sciences.

4 Case-Study: The Simulation of Heavy-Ion Reactions

I now wish to present a somewhat detailed case-study from nuclear physics that shall illustrate some typical features of a simulation in physics.[36]
Nuclear physics has, so far, not attracted philosophers of science much. Particle physics, which separated from nuclear physics in the 1940's, seems to be much more attractive to the philosophical mind. The reason for this preference is, I suppose, that particle physics is directly concerned with the fundamental problems of the constitution of matter, questions which have been worrying philosophers for a long time. Nuclear physics, on the other hand, is more applied and less fundamental and hence – one might infer – not worth looking at from a philosophical perspective.
Nevertheless, since physics is surely more than particle physics, a complete picture of science also has to include the efforts, say, in solid state physics and in nuclear physics. Besides, those branches of physics that deal with complex systems raise fascinating new philosophical questions.
In his recent book "Explaining Science", R. Giere also argues that nuclear physics is worth looking into:

> [N]uclear physics is itself a paradigm of twentieth century science. In its use of mathematical techniques, of computers and other advanced technology, as well as in its organization into research groups, nuclear physics resembles many other contemporary sciences.[37]

Giere carefully analyzes the development of relativistic models of nuclear structure (Dirac phenomenology) and confronts the upshot with his meta-scientific model, thus presenting an interesting example for a "naturalized" philosophy of science at work.
There are even more reasons why nuclear physics is challenging for philosophers of science:

- The models of nuclear physics are a colourful mix of fundamental theoretical principles, phenomenological assumptions and bold analogies. In this respect nuclear physics is, in my view, more representative for physics as a whole than, for example, particle physics.

- Nuclear physics is closely affiliated with other sub-disciplines of physics, such as particle physics (for high energy reactions), astrophysics (nucleosynthesis), solid state physics (nuclear solid state physics), statistical physics (as an underlying theory for the description of nuclear reactions) and quantum field theory (which is the "fundamental" background theory). It is thus a good starting point to examine the relations between the different branches of physics.

[36] Presenting this case-study I will be a bit more technical. It is often claimed, in philosophical analyses of scientific theories and in popular science books, that it is possible to *understand* the essentials by just over-reading the formulas. I think this is plainly wrong! Without at least a little grasp of the mathematical structure behind it is hopeless to gain an adequate understanding. Nevertheless, it is important to present the respective technicalities as simple as possible.

[37] [18], p. 180

- Nuclear systems are special insofar as they are neither fundamental nor highly complex. The number of particles involved in a typical nuclear reaction is of the order of ten or hundred.

The following case-study is about heavy-ion reactions. After some introductory historical remarks (Sec. 4.1) I present the model (Sec. 4.2), discuss the detailed simulation process (Sec. 4.3) and point out what one can learn from this case-study concerning the function of simulations in physics (Sec. 4.4).

1. Some Historical Remarks

After E. Rutherford's crucial discovery in 1906 showing that there is a tiny but very heavy nucleus in the center of each atom, experimental physicists started systematically collecting a tremendous amount of data about masses, charges and other observables of numerous nuclei. These data sets could be structured in a variety of models such as the liquid drop model, the optical model, and the shell model, to mention only a few. All these models were designed – inspired by quantum mechanics – to help understanding static properties of nuclei, such as their masses and binding energies.

After some time physicists realized that the analysis of dynamic phenomena (nuclear collisions, scattering of electrons and photons on nuclei etc.) reveals even more about the nuclei in question. Consequently, experimentalists studied transition probabilities by exciting one nucleus in the field of another in peripheral reactions and later – once higher energies were available in the laboratory – direct nucleus-nucleus reactions. The corresponding observables turned out to be much more sensitive to the details of certain models. Thereby physicists learned more about the properties of nuclear matter, about matter under extreme conditions, and many other interesting topics.

The most modern of these experiments use heavy ions (up to uranium), systems that consist of several hundred protons and neutrons. Complementary to the "real" experiments in the laboratories (such as GSI near Darmstadt/Germany), theorists run extensive numerical simulations of the very processes.

2. The Model

There are some models which describe the dynamical behaviour for low energies fairly well. One of them is the so called Boltzmann-Uehling-Uhlenbeck (BUU) model that I will sketch now.[38] For the sake of simplicity I will be concerned only with the non-relativistic version of this model.

The BUU model provides an equation for the phase space density $f(\vec{x}, \vec{p})$ of the nucleons, the constituents of the colliding nuclei. With the phase-space density in hand one can subsequently work out all interesting observables that can later be compared to experimental data.

Let us consider first the (highly idealized) case where no collisions between the nucleons occur. Now, a basic theorem of (classical) statistical mechanics ("Liouville's Theorem")

[38] I follow the presentation given in the review [6] where further details can be found. In this article, alternative models are shortly discussed as well.

demands that $f(\vec{x},\vec{p})$ has to be a constant in time:

$$\frac{df}{dt} = \sum_{\mathrm{i}=1}^{3}\left[\frac{\partial f}{\partial p_{\mathrm{i}}}\frac{dp_{\mathrm{i}}}{dt} + \frac{\partial f}{\partial q_{\mathrm{i}}}\frac{dq_{\mathrm{i}}}{dt}\right] + \frac{\partial f}{\partial t} = 0$$

Including the general Hamilton equations of classical (!) mechanics (with a position and momentum dependent mean field potential $U(\vec{x},\vec{p})$), one obtains the Vlasov equation:

$$\left[\partial_t + (\vec{\nabla}_p U)\vec{\nabla}_x - (\vec{\nabla}_x U)\vec{\nabla}_p\right] f(\vec{x},\vec{p}) = 0$$

The Vlasov equation describes the time evolution of the phase space density in the presence of the mean field $U(\vec{x},\vec{p})$. This mean field results from a self consistent treatment of the motion of the particles.
Thus far there are no collisions in the model. Besides, this treatment is completely classical. However, it is sometimes argued that quantum mechanical interactions alone are responsible for the generation of the mean field potential $U(\vec{x},\vec{p})$. The rest can be understood using classical physics.
Now it is clear that in a real heavy-ion reaction there are also collisions between the individual nucleons. Formally, the right hand side of the last equation does not vanish once collisions are taken into account. Particles can be scattered into another phase-space cell or scattered out of one respectively. Considering only two-body collisions one gets the BUU equation:

$$\begin{aligned}
&\left[\partial_t + (\vec{\nabla}_p U)\vec{\nabla}_x - (\vec{\nabla}_x U)\vec{\nabla}_p\right] f(\vec{x},\vec{p}) = \\
&\frac{4}{(2\pi)^3}\int d^3p_1 d^3p' d\Omega\ v\ \frac{d\sigma}{d\Omega}\ \delta(\vec{p}+\vec{p}_1-\vec{p}\,'-\vec{p}_1\!')\\
&[\ f(\vec{x},\vec{p}\,')f(\vec{x},\vec{p}_1\!')(1-f(\vec{x},\vec{p}))(1-f(\vec{x},\vec{p}_1))\\
&-(f(\vec{x},\vec{p})f(\vec{x},\vec{p}_1)(1-f(\vec{x},\vec{p}\,'))(1-f(\vec{x},\vec{p}_1\!'))\ ]
\end{aligned}$$

This equation governs the time evolution of the phase space density $f(\vec{x},\vec{p})$ in the presence of the mean field potential $U(\vec{x},\vec{p})$ and two-particle collisions. The term on the right hand side is the so called *collision term.* $d\sigma/d\Omega$ is the corresponding two-particle collision cross section. We will come back to it below. The factors of the form $(1-f(\vec{x},\vec{p}))$ in the collision term take the Pauli principle into account, guaranteeing that no two particles occupy the same phase-space cell. This is in fact the only place where quantum mechanics explicitly enters the scene.
It is important to point out the different ingredients of the BUU-equation:

1. The gross structure of the BUU equation is a general demand of statistical physics that acts as a background theory.

2. The collision term is modeled in order to respect features of quantum mechanics.

3. Two components of the BUU model are fed in by other models:

(a) The mean-field potential

$$U(\vec{x},\vec{p}) = A\left(\frac{\rho(\vec{x})}{\rho_0}\right) + B\left(\frac{\rho(\vec{x})}{\rho_0}\right)^{\sigma}$$
$$+2\frac{C}{\rho_0}\int d^3p' \frac{f(\vec{x},\vec{p}')}{1+\left(\frac{\vec{p}-\vec{p}'}{\Lambda}\right)^2} \quad ,$$

where A, B, C, Λ and σ are constants, is suggested by nuclear structure calculations. These parameters reflect *static* properties of the nuclei. It is therefore essential for the later simulation of heavy-ion reactions to have a solid description of the relevant nuclei at rest.

(b) The "elementary" cross section $d\sigma/d\Omega$ is either taken from "fundamental" calculations in the framework of quantum field theory or it is just extracted from experimental data (data fits).

Thus, our (dynamic) model is a complicated combination of an inhomogenious set of theories and model assumptions: Simulations are an interplay between "real" experiments and theoretical considerations.

3. The Simulation-Procedure

The BUU equation describes the full dynamics of the model system. The equations are, of course, not analytically solvable. In order to solve them, theoretical physicists use what I call a *meta-simulation*. Applying the *test-particle method* one approximates the continuous phase space density $f(\vec{x},\vec{p})$ by a phase space density of a large number of imaginary test-particles with phase-space coordinates $(\vec{x}_i(t),\, \vec{p}_i(t))$, i.e.

$$f(\vec{x},\vec{p}) = \frac{1}{N}\sum_{\mathrm{i}=1}^{NA} \delta(\vec{x}-\vec{x}_{\mathrm{i}}(t))\delta(\vec{p}-\vec{p}_{\mathrm{i}}(t)) \quad .$$

N is the number of test particles per nucleon and A is the total number of nucleons described by $f(\vec{x},\vec{p})$.
With this *ansatz*, the BUU equation can be solved numerically. One finally obtains a sequence of phase-space density profiles that imitate the real process in the laboratory.
The philosopher S. Toulmin stated that it is a typical feature of a model that it "suggests" how to extend it.

> It is in fact a great virtue of a good model that it does suggest further questions, taking us beyond the phenomena from which we began, and tempts us to formulate hypotheses which turn out to be experimentally fertile.[39]

Like any good model, the BUU-model has also been extended in several directions:

[39] [47], p. 38

1. Relativistic Formulation

   In order to study heavy-ion collisions with collision energies above, say, 1 GeV it is necessary to make the model consistent with relativity. The result is the RBUU (=relativistic BUU) model [6]. These investigations were initiated once experimentalists were able to produce heavy-ion beams with such high energies. Before this energy regime was experimentally accessible nobody thought seriously about developing a relativistic extension of the model.[40] This again stresses the main motivation for those studies: phenomenological success. Deeper theoretical understanding can only be gained by carefully analyzing and simulating thorough experimental studies.

2. Many Particle Scattering

   There is no reason why only two-particle collisions should show up. It is natural to also include three and more particle scattering effects [6]. This, however, makes the model much more complicated and – in a way – less intuitive.

3. Inclusion of Particle Production Mechanisms

   At very high energies new particles, such as strange mesons and other exotic particles, are produced in heavy-ion reactions. The different production rates strongly depend on the explicit structure of the interaction. Since electromagnetic interactions are well known it is especially interesting to study the production of electron-positron pairs and photons. So theorists hope to determine properties of the still (almost) unknown structure of the strong nuclear interactions.

4. Discussion

Having introduced the BUU model and the procedure how to simulate heavy-ion reactions with its help, I shall now identify the motives to run simulations in the process of investigating the physics of heavy ions.
First of all, simulations of this kind are, so far, the best one can do as a theorist. It is impossible to derive cross section and related observables from first principles. The systems are too complex and we do not yet know exactly how the strong force works. Because of the complexity of the problem it may be seriously doubted that one can ultimately learn something about the nature of the strong force. However, experiments are surely not compatible with every assumed force.
What one can learn from these studies is the relevance of certain physical processes. Is it possible to generate the spectra etc. by neglecting three-particle scatterings?
The following more general claims about simulations can be extracted from our discussion of the BUU model. Performing simulations is an intermediate step between theoretical and experimental work. They are inspired by experimental findings as well as by theoretical principles. On the other hand, simulations help both theoretical and experimental physicists. Computer simulations (e.g. of the BUU type) help *theorists* to

1. develop an understanding of the relevant processes by calculating "macroscopic" properties (cross-sections etc.) from some assumed microscopic dynamics.

   In our example scientists study details of nuclear dynamics.

[40] See also R. Giere's insightful remarks in [18], p. 185.

2. develop new models.

   In our example theorists try to discover regularities by varying the model parameters. These regularities may serve as an input ("model assumptions") in a modified model.

3. perform numerical experiments.

   In our example scientists do, for example, interpolate between known data regimes or extrapolate into regions that are experimentally inaccessible (such as the physics inside a supernova).

Computer simulations help *experimentalists* to

1. design new experiments.

   Experiments in nuclear and particle physics are so cost-intensive that it is common to perform detailed simulations in advance in order to determine the "best" experimental setup. Simulations help, e.g., to find the optimal detector location and to single out the best suited nuclear system for real experiments.

2. interpret real experiments.

   For given experimental data in high-energy physics (cross-sections etc.) researchers wish to know what part of the spectrum is simply "background". The contributions of those processes can be readily determined in computer simulations and then subtracted. What remains is the result of nontrivial dynamic interactions.

Summing up, this example demonstrates the involved interplay between fundamental theoretical concepts, model-inspired assumptions about the detailed dynamics and experimental inputs in a typical computer simulation in physics. An essential prerequisite for the phenomenological success of these simulations is definitely that the static aspects of nuclei are (theoretically) well under control.

5 Conclusions

In this paper, I proposed and explicated the following definition of a simulation: *A simulation imitates one process by another process.* The basis of a simulation is a dynamic model that specifies – besides some static properties – assumptions about the time evolution of the considered object or system. There are simulations that assume a continuous dynamics, and others that assume a discrete one. The first are formulated in the language of differential equations, the latter in the language of cellular automata (CA). Both types of simulations are applied in the natural as well as in the social sciences. So far, natural scientists (especially physicists) still prefer models based on differential equations, while social scientists frequently employ CA's that reflect the essential decision aspect right from the beginning.
Besides this difference there are many parallels between the various sciences concerning the question why simulations are an important tool at all. This is why the focus of this paper is on the *function* of simulations in the research process. Besides their pragmatic function to supply a description of the time evolution of a real system, simulations serve to perform numerical experiments that allow the extrapolation of data into experimentally inaccessible

realms, they support experiments and provide useful heuristics to develop new models and – maybe – theories.

The final case-study from nuclear physics demonstrates that simulations in physics are often deeply grounded in models of the static aspects of the system whose time evolution is now in question. These static models are often well-established in physics, providing a solid basis for the dynamic part. The dynamic parts of the model assumptions is often severely constrained by the demands of statistical physics (such as Liouville's Theorem). However, there are still many free parameters that have to be (or can be) adjusted to experimental data.

Obviously, life is much harder for the social scientist. There are neither good descriptions of static aspects (if they make sense at all), nor are there generally accepted hypotheses for the details of the dynamics.

There is substantial evidence that computer simulations will become even more powerful in the foreseeable future. Progress in this field, at least progress in the descriptive power of computer simulations, is closely linked to progress in the development of new generations of high-powered computer systems. However, simultaneous progress in *understanding* natural and social phenomena can only be achieved when we use this mighty tool properly.

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