BIAS EX SILICO – OBSERVATIONS ON SIMULATIONIST'S REGRESS

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ABSTRACT

The scientific community is aware of the experimenter's regress: a research bias that occurs when the researcher unconsciously affects results, data, or participants in an experiment. Bias in simulation based experiments is no exception, but maybe even be the rule. The paper evaluates to what degree bias plays a role for the selection of simulation systems, or if bias played a role when the simulation system was developed. The paper provides a discussion on whether simulation based experiments increase or decrease the chance for bias. Epistemological and computational constraints and their implications are presented. It is concluded that in particular the epistemological constraints result in unique challenges for simulation based experiments.

Keywords: epistemology of simulation, philosophy of science, research results.

1 INTRODUCTION

In philosophy, regress is a series of statements in which a logical procedure is continually reapplied to its own result without approaching a useful conclusion. A typical example is a definition of a term by the means of the term itself. In other words, assuming that one is correct it is proven that one is correct!

Within the scientific community, conscious as well as unconscious bias can occur at any phase of the research process, from the underlying literature research over formulating the hypothesis and setting up experiments to the publication of the results. To reduce the likelihood of bias influencing research, double blind studies, independent data collectors, peer reviews, and other means to support scientific rigor have been introduced.

Within this paper we will evaluate if simulation based experiments increase or decrease the chance of bias. The main objective is to increase the awareness of the danger to uncritically use simulation systems as a surrogate for real world experiments, because they may implement a biased conceptual world view (Shermer 2017), are applied outside the capability of epistemological or computational constraints (Tolk 2015), or expose systemic errors in the simulation implementation (Oberkampf et al. 2002).

To increase awareness, we first describe the classic experimenter's regress. In the next section, the use of simulations to conduct experiments is evaluated, followed by a look at the epistemology of simulation to discuss the core question of this paper: How significant is the problem of simulationist's regress?

2 EXPERIMENTER'S REGRESS

The term experimenter's regress was coined and communicated to the wider scientific audience by Collins (1975). In the book "Changing order: Replication and induction in scientific practice" (Collins 1985), his

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ideas were introduced to a broader audience, including in particular the engineering community. Collins' argument was that whenever we use instrumentation in our experiments, we need good tools to observe the desired facts, but we can only define a tool to be good if it produces the desired effects, hence we are in a circle well known from the philosophy of skeptics. Collins (1985, p.84) describe this problem as follows: *"We won't know if we have built a good detector until we have tried it and obtained the correct outcome. But we don't know what the correct outcome is until [we observe it with the detector]. . . and so on ad infinitum."* For Collins, the experiment and its result are not independent, but logically, mutually dependent, hence the term of experimenter's regress, borrowed from philosophy. The underlying problem was the lack of any formal criteria independent of the experiments outcome. He saw no way to decide if the tool was working properly or not, as the facts observed couldn't be observed without the tools, hence could not be used to demonstrate the usefulness of the tool. In the face of any phenomenon that could only be observed by this one tool, scientists cannot be sure that they actually can label this phenomenon as a fact, and the tool as the appropriate tool. Collins (1975) example is Joseph Weber's experiment to prove the existence of gravitational waves, and how other scientists couldn't replicate or corroborate the original findings:

> According to Cervantes-Cota, Galindo-Uribarri, and Smoot (2016), Albert Einstein predicted in 1915 the observability of gravitational waves, which are tiny ripples in the time-space continuum caused by cosmic cataclysmic events, such as the collision of highly condensed stars or black holes. Weber constructed a device to detect such waves made up of large cylinders of ultrapure aluminum. Gravitational waves were supposed to make these bars hum, on a similar intensity like thermal waves would do, but if the gravitational wave would be the reason, the pattern could be observed by several bars humming in concert. He claimed success in 1970, but no other sciences could replicate or otherwise confirm the results. An experimental proof was not observed until 2015, 100 years after their prediction by theory, in the Laser Interferometer Gravitational-Wave Observatory, using a way more complex experimental setting.

Collins (1985) generalized these observations as described above. He claimed that bias was the main reason that Weber observed something he believed in, but which had no unbiased empirical evidence otherwise. Observations and facts were not based on the scientific principal, but they were mutually dependent.

The scientific community recognized the danger of such biases, in particular in social science settings. This bears the question: are we in similar danger when we conduct simulation based experiments? Are we eventually even in more danger due to the nature of simulation based experimentation and the epistemology of simulation? Can we determine if simulation is the right tool to conduct an experiment? These questions will be addressed in the following sections.

3 SIMULATION BASED EXPERIMENTATION

How to set up and conduct a simulation based experiment is among the topics of well-established and often referenced textbooks, such as Kleijnen (2008), Law (2014), and Zeigler, Praehofer, and Kim (2000). They agree on the basic principle that in a simulation based experiment the system of interest is replaced by a valid simulation thereof, which means that by variation of the free input parameters and observation of the same bound input parameters the same output parameters with – where appropriate – the same temporal behavior should be observed. An experimental frame binds the overall system, sufficient parametric variations allow for a good understanding of solutions and their sensitivity, and uncertainty can be captured by choosing and calibrating the appropriate probability functions.

Simulation has matured to a point where it is widely accepted as an analysis and design tool complementary to theoretical considerations and experimental investigations, becoming the third pillar of gaining scientific knowledge. In his work, Ihrig (2016) proposed a framework bringing theory building, simulation, and experimentation into the common context of epistemological insight, as captured in figure 1.

- In the theoretic setting, shown on the left side of the figure, propositions are derived from an existing theory, which also drives the design.

- In the experimental setting, shown on the right side of the figure, the real world issue provides access to the empirical data and also is the source for the desired insights.
- In the simulation setting, the model provides the simulated data within the context of the simulation environment.

It is worth mentioning that the traditional connection between theoretic and experimental setting is omitted in the figure, but was explicitly mentioned in the discussion of related ideas in Tolk et al. (2013).

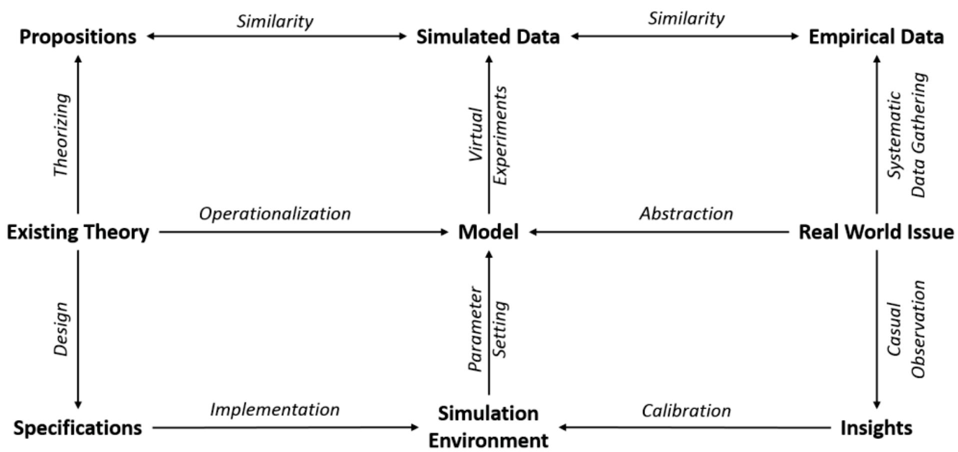

Figure 1: Research Architecture proposed by Ihrig (2016).

Ihirig (2016) shows that these settings provide a consistent reference frame to understand simulation experiments in the context of the conventional research approach, pointing also to the duality of simulation experiments: Looking at simulation from the theoretic settings, it is perceived as a way to conduct experiments. From the experimentation side, a simulation can be perceived as a theory capturing tool.

As such, Ihrig's framework is a logical extension of the modeling ideas of Rosen (1998). Rosen postulates that in order to understand a natural system we are interested in, we model it using a formal system. We use that formal system to understand the natural system better. Observed correlations are assumed to result from a causality embedded in the natural system. By encoding our understanding of the natural system using symbols and rules of a chosen formalism, we can make inferences in the formal system that by decoding help us to understand the natural system better.

However, there is an important difference between conventional experiments and simulation experiments: while conventional experiments are using experimental settings to exclude unwanted influences from the natural setting, they can never exclude not-assumed – but nonetheless existent – natural influences within the experiment. In a simulation experiment, we can only simulate what has been modelled and implemented for this experiment. If we did not include an important concept or if we assume the wrong causality, we cannot detect these errors by conducting a simulation based experiment. In other words: a simulation experiment can only provide insights that have been modeled and implemented – explicitly or implicitly – within the simulation. The reason lies in the epistemological constraints of simulations, which are captured in the next section.

4 EPISTEMOLOGICAL AND COMPUTATIONAL CONSTRAINTS OF SIMULATION

Winsberg (1999) and Humphreys (2009) are among those who started the discussion about epistemology of simulations, looking at the special challenges when we rely on simulation based experiments, but also the resulting advantages. Interestingly enough, this discussion was mainly driven by philosophers, and not so often by simulationists. An exception is captured by a panel that tried to bring both worlds together (Tolk et al. 2013). The resulting epistemological constraint are captured in the following subsection. As we are in the context of this paper primarily interested in computer simulation, the computational constraints are another important factor. Computer simulations are executions of computer programs. As such, they are bound by the same laws and insights as other computer programs. This will be captured in the second subsection.

4.1 Epistemology of Simulation

Simulations are based on models. A model is a purposeful, task-driven simplification and abstraction of a perception of reality, which is constraints by physical, legal, ethical, and cognitive aspects (Tolk 2015). The underlying terms are defined as follows:

- *Task-driven:* a model is generated for a task, such as to answer a question within the domain of analysis or providing a certain functionality, such as supporting training. Like the question that initiates the scientific method, the task drives the modeling process.
- *Purposeful:* modeling is a creative act. The various activities are driven by the task and are done knowingly and purposefully to reach the goal to the greatest extent possible.
- *Simplification and abstraction:* just like in an experimental setting, elements that are not important and only distract from the main event are eliminated from the model. Furthermore, components that may have an effect but are considered secondary or less important can be combined as a form of data reduction techniques. The task also defines the level of detail needed for the important elements, which also shapes the level of abstraction needed.
- *Reality:* our work shall be rooted in empirical observations. If a real world referent exists, this shall be the yardstick. If no such reference exists – or cannot be accessed to gain empirical data –, at least all assumptions and constraints need to be consistent with the underlying theory.
- *Perception:* our perception is shaped by physical, legal, ethical, and cognitive aspects and constraints. The physical aspects define what attributes of an object are observable with the sensory system of the observer. Legal aspects are regulating which and how data can be collected. Ethical aspects may furthermore limit the amount of data that can be obtained. Cognitive aspects are shaped by the education and the knowledge of the observing team, their paradigms and even knowledge of related tools associated with the tasks.

The result of the modeling phase is a conceptualization shaped by the task, as well as by the physical-cognitive abilities of the modeler and legal-ethical constraints when gaining empirical data. *This model becomes the reality of the simulation.* It seems to be simple, but if something is not represented in the model – or not implemented in the simulation – it cannot be observed.

Another important aspect is the *creative process of deriving causality from correlation*. As discussed earlier, our general insights about how a system works is not based on the natural system its, but on the formal system we use to explain it (Rosen 1998). Causality is a feature of the formal system, correlation a feature of the natural system. If our assumed causalities are able to produce all observed correlations, and also are only producing correlations that are observed in the natural system, we have a consistent theory.

If applied with these constraints in mind, simulation can be a powerful tool. In some recent cases, simulation was successfully used to guide experiments to allow for new observations, such as it happened in search of the Higgs-Boson elementary particle (Atlas Collaboration 2012). Simulation comprised all aspects of the guiding theory, and therefore could help to look exactly where the theory predicted certain events to occur, and they did: the right model representing the right theory was used. However, it is worth mentioning that the history of modern science is also the history of many such models that replaced each other due to new observations, which required better models, or new theories that even predicted new observations (Tolk 2015). Having to update or replace a model is scientific progress. In general, simulation shall represent the currently best theory to explain the real world. It helps to generate all possible observations that should happen under this theory and, as such, can guide our experimentation. However, it will never generate anything outside of this theory, and if something is observed that cannot be generated by the theory, the theory is falsified and needs to be replaced with a better one, which also requires a new model. As Popper (1935) points out: *"Theories cannot be proven to be generally correct, but we can state that they have not been falsified so far by new observations or insights!"* We can always observe something new in the real world that we cannot simulate, as it is outside of the scope of the theory that builds the foundation of the model and the implementing simulation.

4.2 Computational Constraints for Simulations

Another aspect often underestimated by those interested in conducting simulation-based experiments is that computer simulations obey the same limits and rules as all computer programs regarding decidability, computability, and computational complexity. In addition, numerical issues have huge effects on chaotic functions, which are generally observed when non-linear functions are folded back onto a limited domain.

- *Incompleteness:* Kurt Gödel proved in 1931 that a not trivial system supporting mathematical reasoning will necessarily contain true statements that cannot be proven within the system. Introducing rules producing these truths will generate inconsistencies: the systems can either be complete or consistent.
- *Decidability*: Alan Turing showed in 1936 that some problems never can be solved with a computer, as no algorithm can exist to answer the related question.
- *Computability*: Lambda calculus, the Turing machine, and recursive function theory define computable functions that have a limited and discrete range and domain. Only computable problems can be addressed by computer programs.
- *Computational Complexity*: Computational complexity studies the use of resources, in particular computer memory needs and computing time, leading to the insight that not everything that can be computed in theory can also be computed in practice.
- *Chaos*: Chaos theory describes the behavior of chaotic dynamical systems that are bounded and show some degree of order, but are not predictable over time. Two points can be arbitrarily close to each other in the beginning, they will follow different trajectories (Devaney 1989). We cannot reliably predict the long term behavior of any truly chaotic dynamical system.

4.3 Implications of these Constraints

In this section, we want to discuss some of the implications of epistemological and computational constraints for simulation-based experimentation. Let us first consider the epistemological implications:

- *The model is the reality of the simulation.* When observing microscopic particles, like tiny smoke or dirt particles, in a fluid through a microscope, we witness the erratic random movement of this particles in the conventional setting. The reason for this Brownian motion is that the microscopic particles are continuously bombarded by the molecules of the surrounding fluid. The experiment originally helped to gain insight into the makeup of fluids, namely that they indeed are made up of rapidly moving molecules. Only if we model the fluid in our simulation as a collection of randomly fast moving molecules that bombard the microscopic particle, pushing it into the respective direction, will our simulation experiment show the erratic movement of the particles we know from the conventional experiment. The difference is: we do not have to know about the real nature of a fluid to observe Brownian motion in reality, but we have to know and explicitly model it to observe it in the simulation.
- *Deriving causality from correlation.* As captured before, we cannot observe causality in nature, only correlation. We use a formal model that contains our causality to explain the observations (Rosen 1998), and as long as our experiments and observations do not contradict our predictions,

we can assume it to be correct. But while in nature such new observations are possible, in a simulation the causality implemented as a computable function mapping input to output parameters can never lead to the observation of a contradiction to the implemented theory.

- *Computational Constraints.* Not all true statements of a sufficiently complex system can be derived with a computer system that is based on consistent logic. Furthermore, some questions are not decidable by an algorithm, and therefore not by computer simulation as well. As pointed out by Oberkampf et al. (2002), numerical approximations lead to systemic uncertainty and errors in simulation programs. Deterministic chaos furthermore implies the impossibility to predict the long term behavior using simulation.

The following figures demonstrate the implications of computational constraints. The left graphic shows the approximation of a differential equation using two different heuristics. The right graphic shows the computed trajectory for the logistic map using exactly the same algorithm, but executed on two processors with different precision (32 vs. 64 bit).

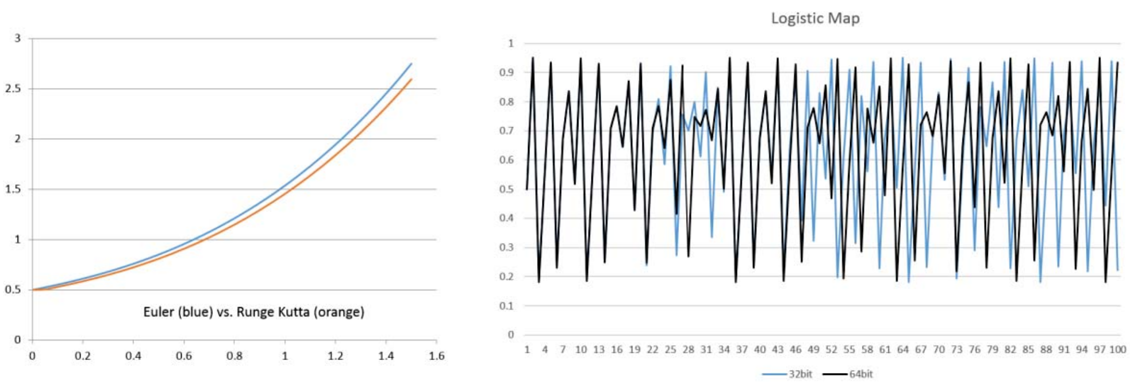

Figure 2: Implications of Computational Constraints.

5 SIMULATIONIST'S REGRESS – A DISCUSSION

After having highlighted some of the dominant constraints for modeling – bounded by epistemological constraints – and simulation – bounded by computational constraints – in this final section, we come back to questions whether there is something like simulationist's regress: which would dispute the validity of simulation based experimentation. Similar to the challenges of experiment's regress as defined by Collins (2012), do we have to ask ourselves if no conclusive criteria other than the simulation outcome itself exists for deciding if the simulation was the correct method and tool to conduct the experiment?

Gelfert (2012) observes that simulation success can often be assessed in the light of their external validity against experiments and observations against the real world referent of the target system; an argument shared in particular by Ihrig (2016), Law (2014), and Zeigler, Praehofer, and Kim (2000). If the access to the reference target system is not possible, simulation systems can still serve as providing analytically derived results which can serve as mathematical reference points (Humphrey 2009), which assume that computationally challenges have been overcome and the numerical approximations or applied heuristics results in sufficiently similar simulated data to the analytically derived data. In his conclusion, Gelfert (2012) observes that worries regarding a systemic simulationist's regress appear exaggerated, overstating the 'detachedness' of computer simulation from conditions of real inquiry.

While Gelfert (2012) makes valid observations on robustness of solutions, emphasizing the need for rigor in coping with the data and their pedigree, and arguing that simulation introduces a qualitatively new step in the multi-step process of investigating nature, the epistemological argument that simulation experiments are only including conceptually captured knowledge that is correctly implemented seems not to be addressed with the necessary rigor: If the implemented theory regarding contributing concepts, their properties, and their relations – including causality that produces observable correlation – is correct, simulation can be an increasingly valuable tool, as the Hibbs bosom example convincingly demonstrates, but we have no general means to prove this validity. For a simulation, a hypothesis is not different from a theory. As a result, in cases where no common theory has been established, there is a significant danger that a simulation system can be used to proof its own underlying assumptions. The scientific method accepts ideas based on supporting evidence, or rejects ideas based on refuting evidence. If new evidence or perspectives require it, those conclusions may be revised. Reproducible experiments are still the cornerstone new scientific insights. In particular, a theory should make empirically observable predictions.

The danger of the simulationist's regress is that such predictions are made by the theory, and then the implementation of the theory in form of the simulation system that is used to conduct a simulation experiment is used as supporting evidence. This, however, is exactly the regress we wanted to avoid: *we test a hypothesis by implementing it as a simulation, and then use the simulated data in lieu of empirical data as supporting evidence justifying the propositions: we create a series of statements – the theory, the simulation, and the resulting simulated data – in which a logical procedure is continually reapplied to its own result.* Mathematically, we gain no new insight at all, as the statements that are true/false under the theory must be true/false in the simulation, resulting in true/false enumerations in the produced data. If this is the case, we can assure transformation accuracy between these viewpoint, also known as verification. But this has nothing to do with representational accuracy, also known as validation.

In particular in cases where moral and epistemological considerations are deeply intertwined, it is human nature to cherry-pick the results and data that support the current world view (Shermer 2017). Simulationists are not immune to this, and as they can implement their believe into a complex simulation system that now can be used by others to gain quasi-empirical numerical insight into the behavior of the described complex system, their implemented world view can easily be confused with a surrogate for real world experiments.

In physics-based simulation experiments, we have well established data for real word referents as well as theories that are documented, agreed, and supported by empirical evidence. In other application domains, such as social sciences, humanities, etc., there are still many gaps. Simulation experiments have their place in these domains to evaluate what-if scenarios, as discussed among others in Epstein (1999). They also help to fully understand all implications of a hypothesis when it is implemented as a simulation system, but it cannot serve to represent reality. The epistemological constraints of generative simulation require additional research to avoid the danger of interpreting possible model artificialities as real world phenomena. Some related efforts on the import aspect of verification and validation in this context has been summarized among others by David (2009).

As simulationists, we have the responsibility to be aware of these dangers, and also to educate users of our simulation systems accordingly. Simulation experiments are powerful tools, but they are not surrogates for reality. They are implementations of a theory, that identifies which concepts are important, which properties are needed to describe the concepts, how the concepts are related, and what functions operate on these concepts. They transform input parameters into output parameters, using computable functions. They can create quasi-empirical data, but these data are generated by the underlying, implemented theory and cannot serve to justify this theory. Like the theory, simulations are interpretations of nature, based on the purposeful abstraction and simplification of the perception thereof. They can be used to better understand the implications of the theory, but not to gain insight about nature outside of the boundaries of this theory.

The resulting challenge shows the necessity for simulationists to have a solid understanding of philosophy of science and the epistemological foundations of their discipline. Simulationist's regress is not a computer science or computer engineering problem, it goes straight to the in-depth understanding what the role of simulation is – or should be – within the multi-step process of investigating nature and, as such, it is a general challenge for every form of computational science.

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