SIMULATION AND MODELING AS THE ESSENCE OF COMPUTATIONAL SCIENCE

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ABSTRACT

Recent developments of computational methods supporting scientific research have led to the rise of a variety of computational science disciplines, such as computational physics, computational biology, computational chemistry, computational social science, and many more. Although simulation is now widely regarded as the third pillar of science, with epistemological status comparable to formal theorizing and experimentation, the insight that computational science is as interwoven with simulation as traditional science is with modeling, has not yet been sufficiently communicated. As a result, important insights from the modeling and simulation discipline are not known or are ignored by traditional scientists entering the computational branch of their discipline. This presentation contributes to closing this gap by giving examples of how modeling and simulated based research contributes to improve computational sciences, including having a look at the supporting philosophy of science perspectives.

Keywords: computational science, epistemology of simulation, philosophy of science.

1 INTRODUCTION

The main thesis of this paper can be summarized as follows: *Computational science of every domain equals applying modeling and simulation methods!* We will see that science is modeling, and computational science is the execution of scientific models on a computer, which is a simulation.

The motivation to point this out is that computational methods supporting scientific research are on the rise. A simple search on Wikipedia pages for articles describing such computational science domains leads to a variety of references to entries on computational archaeology, biology, chemistry, materials science, economics, electromagnetics, engineering, finance, fluid dynamics, forensics, geophysics, history, informatics, intelligence, law, linguistics, mathematics, mechanics, neuroscience, particle physics, physics, sociology, and statistics; and by the time the summer simulation multi-conference is conducted, these list likely grew by some additional fields. Some of these computational science applications are leading to impressive developments that were impossible without using such computational capabilities only a couple of years ago.

An example of the successful application of computational science is the discovery of the Higgs boson particle. Computational physics has been successfully used to guide experiments allowing new observations of this predicted, but so far unobserved elementary particle (Atlas Collaboration 2012). Using the predictions of particle physics, a computer simulation was developed that comprised all aspects of the guiding theory, helping the group of experimenters to look exactly where the theory predicted certain events are expected to occur. The right model representing the right theory was implemented as a computational capability for the experiment, and the experiment was successful: the Higgs boson particle was observed were the computational physics predicted it will happen. These experiments followed the example of Ken Wilson, who's discoveries about phase changes in materials using computational models earned him a Nobel prize in physics (Wilson 1989). The anatomy of successful computational biology software was even the topic of a contribution in the well-known journal *Nature* (Altschul et al. 2013).

Why are such computational success stories of interest to the modeling and simulation (M&S) community? Because they show how intertwined computational science and simulation and modeling are! Currently, there is the danger that important insights from the modeling and simulation discipline are not known or are ignored by traditional scientists entering the computational branch of their discipline To avoid this danger, I make the case that successful computational science applications are grounded in the principles of M&S science and engineering. Equally, lessons learned from M&S research are applicable to domains of computational science as well. I will show that modeling is the essence of science, and also that computer simulations are the essence of computational science.

2 SCIENCE AND MODELS

According to Merriam-Webster, the scientific method is defined by principles and procedures for the systematic pursuit of knowledge involving the recognition and formulation of a problem, the collection of data through observation and experiment, and the formulation and testing of hypotheses. Science is driving the pursuit of knowledge, with the two branches of ontology – dealing with the principles of what we know – and epistemology – dealing with the principles of how we gain knowledge.

But what is the best way to capture knowledge in a way that it can be communicated with others, can be taught to others, and is documented in a way rigorous enough to avoid ambiguities, but at the same time be understandable to a wider audience? As a rule, research results should be documented in a form that is comprehensible, shareable, and reproducible. Scientist use models to do this. According to Rosen (1998), *"modeling is the essence of science and the habitat of all epistemology!"* In his method on the physical sciences, John von Neumann (1955) states that *"sciences do not try to explain, they hardly even try to interpret, they mainly make models."*

The scientific modeling relationship according to Rosen is often used to describe how we generally use formal models to encode natural systems as knowledge. Figure 1 shows these principles and concepts of the modeling relationship.

> *"Another way to characterize what we are trying to do here is the following: we seek to encode natural systems into formal ones in a way which is consistent, in the above sense. Via such an encoding, if we are successful, the inferences or theorems we can elicit within the formal systems become predictions about the natural systems we have encoded into them; consistency then means that these predictions will be verified in the natural world when appropriately decoded into linkage relations in that world. And as we shall see, once such a relation between natural and formal systems has been established, a host of other important relations will follow of themselves; relations which will allow us to speak precisely about analogy, similarity, metaphor, complexity, and a spectrum of similar concepts."* Rosen (1985, pp. 73-74)

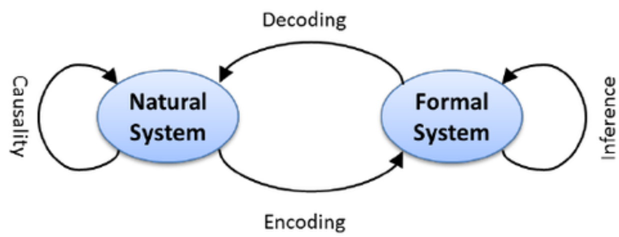

Figure 1: Modeling Relationship according to Rosen (1985).

Scientific work is therefore working with formal models of the world capturing our current knowledge. During evolutionary progress, we modify the models, making them better, adding attributes or relations, providing better transition functions, and improving accuracy and fidelity. From time to time, revolutionary changes lead to new models replacing old ones, namely when new theories evolve that capture our empirical observations better than the old theories, and new theories come with new models. Goldman (2006) describes science therefore as a series of models.

The usefulness of models is measured by their ability to make reliable predictions. If a model can make a prediction that can be evaluated within a scientific experiment, we call this process the validation – if the prediction becomes true – or falsification – if it doesn't come true – of a hypothesis. If a sufficient amount of hypotheses have been successfully validated, we perceive the underlying model to be valid, and it is no longer a collection of hypotheses, but it becomes a theory. However, Popper (1935) already observed that *"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 state that all predictions made *so far* were validated, but as we never know if this will be true for of future predictions as well, the search for a general validated theory in general is futile. Nonetheless, many of our theories have been proven to be stable enough for practical applications.

Another aspect of using models in science has been described in detail by the philosopher of science Gelfert (2016), who observes in his philosophical primer on models in the summery the following:

> *"Whereas the heterogeneity of models in science and the diversity of their uses and functions are nowadays widely acknowledged, what has perhaps been overlooked is that not only do models come in various forms and shapes and may be used for all sorts of purposes, but they also give unity to this diversity by mediating not just between theory and data, but also between the different kinds of relations into which we enter with the world. Models, then, are not simply neutral tools that we use at will to represent aspects of the world; they both constrain and enable our knowledge and experience of the world around us: models are mediators, contributors, and enablers of scientific knowledge, all at the same time."* (Gelfert 2016, p. 127)

Models are used in the scientific community as mediators, contributors, and enablers of scientific knowledge, contributing to the comprehensive and concise representation of concepts, terms, and activities that make up the scientific domain, also known as the body of knowledge. They allow to comprehend, share, and reproduce research results, presenting theories in a more generally comprehensible and testable form. Modeling is intrinsically tied to scientific work.

But what are models in the context of M&S? First, like any other model, they are a representation of the "real thing," a conceptualization focusing on the important concepts, properties, and relations of entities and processes of interest. But other than general models, M&S models are developed with the purpose to create a simulation that should support a task, such as an experiment, training, education, etc. As such, as captured in Tolk (2015), the model is a result of the *task-driven purposeful simplification and abstraction of a perception of reality*. The perception of reality reflects our understanding and is shaped by physical, cognitive, and sometimes legal or moral constraints on what data we can collect, and how we interpret the data in the context of our views and background. The purposeful, creative activities are driven by the task we have to support, or the simulation-based experiment we have to conduct. This task defines the desired abstraction level, hiding unnecessary details from other abstraction levels that could be of interest – think about the macro, meso, and micro-levels of systems –, as well as what concepts, properties, and relations are important, and which can be excluded to simplify the model. While this definition focuses on models intended to be the foundation for computational implementations, and other domains, such as engineering for design and control purposes likely will use different definitions, the essence remains the same: our models are subsets and abstractions that focus on the important concepts driven by the problem at hand. While in engineering studies the importance is usually driven by requirements, it is possible that the perceive importance is shaped by cognitive constraints, maybe even bias, as will be discussed later.

Overall, models in the context of M&S are usually not as broad as general theory models, but as they become the conceptual foundation of the simulation in the M&S context, they are usually more rigorous and precise regarding the intended task to be supported by the resulting simulation. Ören (2011) compiled a critique of definitions that is particularly useful in this context.

In summary, models are a way to capture our knowledge. This can be tailored to support a task that may require a simulation, resulting in a more focused and detailed conceptualization that becomes the foundation of our simulation. Models are representing the ontological branch of knowledge, as discussed in the introduction to this paper.

3 SIMULATION AND EXPERIMENTS

After this look at the role of models in science, let's have a closer look at experiments and the role that simulation play. The US Department of Defense defines a simulation as "a method for implementing a model over time," and a computer simulation as "a simulation that is executed on a computer, with some combination of executing code, control/display interface hardware, and, in some cases, interfaces to real-world equipment." This tight coupling of model and simulation is even more obvious in the definitions used by NASA. They address the simulation as the "functional model," while the model as we talked about it in the last section is referenced as the conceptual model. In any case, our interest in this paper lies with computer simulations, in which the concepts, properties, and relations of entities and processes are implemented as data and algorithms.

For a long time, theory and experimentation were the two pillars of gaining scientific knowledge. Lynch (2013) describes scientific research as *"the process of (1) developing an empirically answerable question, (2) deriving a falsifiable hypothesis derived from a theory that purports to answer the question, (3) collecting (or finding) and analyzing empirical data to test the hypothesis, (4) rejecting or failing to reject the hypothesis, and (5) relating the results of the analyses back to the theory from which the question was drawn."* The objective of this process is epistemological: we have to create new knowledge! Aligning two theories is not research, or the pure collection of data – including conducting a literature research – is not research, as no new knowledge emerges. However, if we use empirical data to discover new propositions that require an update or extension of the existing theory, we created new knowledge. Likewise, if we extend the theory and collect data to verify or falsify our claim, we create new knowledge.

Today, simulation is considered to be the third pillar of gaining scientific knowledge. Ihrig (2016) shows not only the connections, but also the mutual complementation between theoretic, experimental, and simulation settings, extending the model proposed by Gilbert and Troitzsch (2005), as shown in the following figure.

In the theoretic setting, propositions are derived from an existing theory, which also drives the design of experiments. In the experimental setting, the real world issue provides access to the empirical data and also is the source for the desired insights. Finally, in the simulation setting the model provides the simulated data within the context of the simulation environment. As such, there are epistemological similarities between the existing theory, the real world issue, and the model, the propositions, the empirical and the simulated data. The design specifications are comparable to the desired insights driving the design of the experiments, and the simulation environments that does the same for the simulation-based experiments and insights. Ihrig (2016) concludes that simulation-based experiments and epistemology is not only consistent with theoretic and experimental methods, they also add value and richness to the traditional approaches.

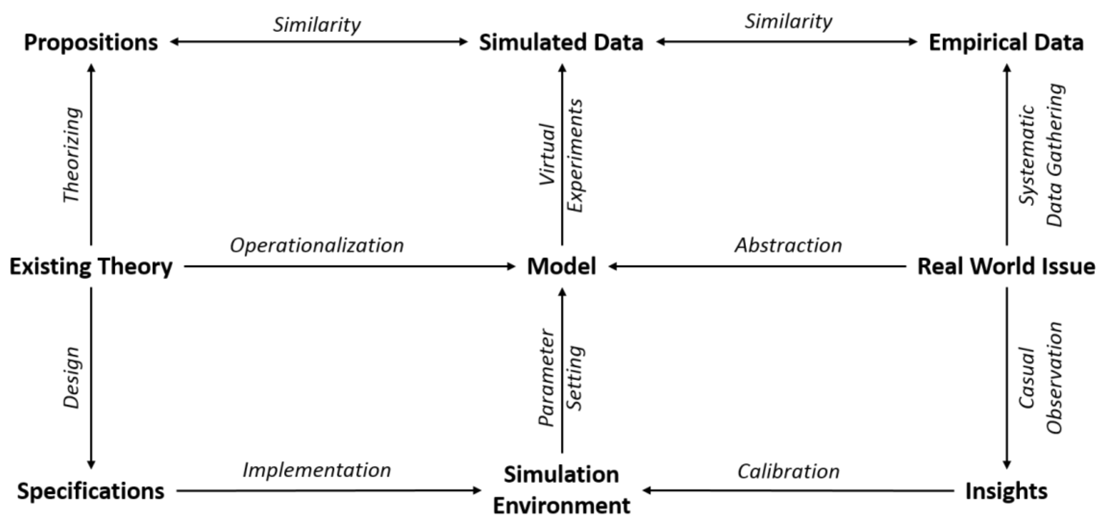

Figure 2: Simulation Research Architecture (Ihrig 2016).

These insights are not new. Carley (2002) already observes that a research architecture that employs simulation tools is more comprehensive than conventional approaches and the classic deductive and inductive reasoning that go with them. As such, this simulation-based architecture is better suited for studying complex phenomena and obtaining and documenting new theoretical insights, as the objects of interest themselves are complex, non-linear, dynamic systems, and simulation systems can reproduce exactly this behavior. It may be of interest that for the same reason, the International Council on Systems Engineering (INCOSE) recommends currently the use of simulation methods – complemented by artificial intelligence methods – in support of complex systems engineering (Sheard et al. 2015).

Even before, Axelrod (1997) posited simulation as an often superior way of doing science: "*Like deduction, it starts with a set of explicit assumptions. But unlike deduction, it does not prove theorems. Instead, an agent based model generates simulated data that can be analyzed inductively. Unlike typical induction, however, the simulated data come from a rigorously specified set of rules rather than direct measurement of the real world.*" These are just some of many examples of recent – and some not so recent – publications showing the use of simulation based experiments. More examples were recently compiled by Mittal et al. (2017). Glotzer (2009) summarizes the current views on simulation in her executive summary to the international assessment of simulation-based engineering and science as follows:

> *"Today we are at a 'tipping point' in computer simulation for engineering and science. Computer simulation is more pervasive today – and having more impact – than at any other time in human history. No field of science or engineering exists that has not been advanced by, and in some cases transformed by, computer simulation. Simulation has*

> *today reached a level of predictive capability that it now firmly complements the traditional pillars of theory and experimentation/observation. Many critical technologies are on the horizon that cannot be understood, developed, or utilized without simulation."* (Glotzer 2011, p. 1)

In summary, 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, representing the epistemological branch of knowledge, as discussed in the introduction to this paper. Additionally, it has been recognized as a mature method to cope with complex systems as the object of study, as such showing tremendous potential for current scientific challenges.

4 COMPUTATIONAL SCIENCE CHALLENGES

In section 2, we showed how tightly *science* and *modeling* are interrelated. In section 3, I gave evidence that *computational science is simulation*, i.e., the execution of models representing theory. Simulation and modeling are therefore essential to computational science. This implies that all the encouraging research results of our modeling and simulation discipline will benefit the computational science community as well, but also that the same assumptions and constraints apply. This section will therefore out some of the pitfalls and dangers for this approach point.

4.1 Computer Programs, Creativity, and Research

One of the underlying philosophical questions is if computers even can conduct research? As discussed in section 2: The objective of the research process is epistemological, which means that we have to create new knowledge! Can this be accomplished by a computer program?

Dowek (2011) observes that building a proof and applying an algorithm are two well-known mathematical techniques that can be mutual supportive or even be equivalent. With the recent developments of computational methods, we are now able to apply algorithms on a scale unimaginable only a couple of year ago. Dowek uses proof theory, computability theory, model theory, and set theory to show the power of formal approaches that can be applied to show the validity of possible approaches. But he also shows the limitations of computer programs regarding decidability of problems by computers.

Mathematically, computer programs are compositions of computable functions, in which each of these functions maps a discrete set of finite input data to a discrete set of finite output data. Since the formulation of the Church-Turing thesis (Church 1936) we know that every computer program can be solved using the lambda calculus, which is equivalent to the use of general recursive functions, which is equivalent to using a Turing machine. In other words: computer programs map input data to output data. Whatever they do must either be part of the *algorithm*, or it must be part of the *data*. Computers cannot be creative; they simply transform data. This is true for all computer programs, no matter which simulation paradigm is supported: discrete event simulation systems, system dynamics programs, and agent based simulation are all data transformers. Therefore, by definition a simulation – as every other computer program – cannot create new knowledge!

But does this mean that computer simulation are not useful for research? Absolutely not, as the famous examples by Wilson (1989) and the Atlas Collaboration (2012) demonstrate. In the general research setting, computer simulations enable us to study more complex processes by simulating propertied concepts, relations, and behaviors that individually are well-known and act straightforward, but their composed behavior results in unpredictable outcomes. Providing such quasi-empirical data to gain insight into the dynamic behavior of complex systems is invaluable to researchers of many domains dealing with the challenge of complexity. Often, the transformation and visualization provided by simulation systems may mathematically just result in an alternative view on knowledge that is captured in the sum of data and algorithms, but cognitively this alternative view may result in new insights to the user: based on the experiment we now know what we know, while before the experiment we did not know what we know, as what we know was still hidden in the data and algorithms. We did not create knowledge, but we brought knowledge into the awareness of the user, maybe even in a “blinding flash of the obvious.” While we do not create new knowledge, we create additional information, and it is the interpretation of this alternative view of information that may trigger new insights leading to knowledge.

An example is given by Padilla (2010). He applied agent-based simulation to evaluate the question of building a theory of understanding. The current literature identifies *knowledge* needed to solve a given problem, the *worldview* allowing perceiving the problem, and the *problem understanding* and definition as such as the driving components for such a theory. Defining an axiomatic structure for knowledge, world view, and problem definition, the current interpretations of understanding were evaluated and used to represent the axiomatic structures for knowledge as agents. This allowed to derive theories for understanding by recomposing the axiomatic structures of matching agents: agents representing knowledge, world view, and problem definition in agreement with the axiomatic structure clustered, representing a valid knowledge representation as currently known. The computational intensive experiments did not only reproduce known theories – such as understanding based on the knowledge needed to solve a problem, or understanding based on recognizing a problem to be similar to another problem for which a solution is known that can be applied to the current problem as well –, but new clusters emerged that are not captured in detail in literature, such as the dominance of having the ‘correct’ worldview in order to solve new problems (a problem known as ‘cultural awareness’ to many current defense related operations). In other words: the simulation did not only reproduce known patterns, it showed additional patterns not yet discovered in the supporting literature. Subject matter experts supporting the PhD thesis evaluation agreed that all new clusters are indeed consistent with the axiomatic structure and valid – and new – interpretations that help to understand knowledge better. In Padilla’s example, all patterns were derived by the algorithms from the data, no new knowledge was created, but it did lead to new insights that actually supported theory development.

In summary, computational constraints limit simulation and computational sciences as they do with any other computer program. Beside decidability, in my recent tribute to Dr. Ören (Tolk 2015) I also mention the challenges of computational complexity and chaotic functions as possible pitfalls. Despite these constraints, applying simulation is the best method to address complexity, which is at the heart of many computational science challenges, as shown in the examples used in this section.

4.2 Epistemological and Hermeneutical Challenges

Shermer (2017) observes that 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 worldview. Our perception is at least unconsciously shaped by our biases, such as identified by Ross (2014). These biases in domains that we are personally of emotionally affected by shape not only the way we see the world, they only can shape our research. As discussed in (Tolk 2017), for computational sciences using simulation this is of particular concern, as it can lead to simulationists’ regress. 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. In computational sciences, regress can happen if 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. By doing so, 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: simulation regress. In practice, we build a simulation to test an idea that is emotionally and morally affecting us. As a result, the simulation may reflect our world view more than an unbiased, scientific view of the research domain would require. This starts with the selection of data, continues with the interpretation of correlation with causality, and ends with the interpretation and presentation the observations and results, leading to epistemological and hermeneutical challenges.

Epistemological challenges deal with including all important information into the simulation-based experiment. The simulation is based on a model, which is according to (Tolk 2015) a *purposeful, task-driven simplification and abstraction of a perception of reality*, which is constrained by physical, legal, ethical, and cognitive aspects. This model, designed with the intended purpose in mind, becomes the reality of the simulation. If something is in the model, it can be evaluated and drive the experiment, but if something is not in the model, it cannot be discovered. If we overlook an important functional connection, we make an epistemological mistake, as an important aspect needed is not included in our model. The same is true if we implement a function based on a potentially coincidental correlation: we include something in our model that is not part of reality. Irvine et al. (1998) state that such biases can be introduced into the model in the characterization of model requirements phase, the data collection phase, the preliminary design phase, and the final design validation phase. They believe that such bias can dilute the effectiveness of the resulting simulation beyond being useful. In summary, there may be many undiscovered elements or correlation that are important in reality, but as we don't know them, we cannot include them into our computational science models, hence the simulation can provide no insights regarding this undiscovered things. Simulation can still help by providing projections that can be compared to real world observations, and if the predicted state differs from the observed state, we know that something in the model is missing. Also, if the predicted state is based on a valid model, an expected observation should occur, just like it was successfully used in the search for the Higgs boson particle.

Hermeneutical challenges extend these ideas to the interpretation of the simulation results. Hermeneutics copes with methods of interpretation, originally of sacred texts. Today, the hermeneutics as the theory and method of interpretation to discover truth is more generally applied, including the interpretation of simulation results, often in the light of validity evaluation, see, e.g., (Aarseth 2001; Kleindorfer et al. 1998). Following the same arguments as above, it is human to perceive support for one's – possibly biased – worldview in observations, inclusive simulation results. If we interpret something into a simulation result that is not part of the underlying model, we are making a hermeneutical mistake: we see something in the result that cannot be in there, as the necessary concepts are not part of the producing system! In practice, using intuitive reasoning familiar to the user or sponsor of a study help to make results persuasive, but this reasoning must part of the model structure and the data.

Epistemological and hermeneutical challenges are more human than technical issues. Computational science based solutions do need peer review as much – if not more – than traditional science results to ensure that all relevant concepts are included in the model, biases are reduced to the maximal extend in the model, and the result interpretation is aligned with the model. Ören (2010) describes these challenges from the perspective of how simulation can – or cannot – reflect reality, which goes to the essence of the heart of the epistemological and hermeneutical challenges.

4.3 The Limits of Computational Thinking

Denning (2017) observes that the *Computer Science for All* education movement began around 2006, mainly spawned by the influential article of Wing (2006), and was motivated by two premises:

- First, that computational thinking will better prepare every student for a better living in an increasingly digitalized world, and
- Second, that computational thinkers will be superior problem solvers in all fields.

This movement led to many accomplishments getting computer science into all schools and promote algorithmic thinking and problem solving. Going through rigorous analysis of the problem and coming up with well-specified solutions that could be implemented in steps with clearly defined metrics was interpreted by many as the vital ingredient of science, technology, engineering, and mathematics (STEM) learning. It also contributed to a better documentation of solutions and being able to communicate them across the borders of application domains, as computational thinking was perceived to be the common foundation.

However, Denning's critique is about the vague definitions resulting from trying to be too general and too inclusive, and the unsubstantiated claims promoted by enthusiasts. Computational thinking wanted to solve everything for everyone. This critique can be made for simulation and computational sciences as well: by trying to serve all possible scientific domains and application domains, general definitions often lose any connection to an application field, leaving them abstract, academic, and often not valuable for the practitioner in the field. Furthermore, promises made by simulation enthusiasts did oversell the current capabilities, resulting in disappointments with the user.

Denning (2017) also observes that many professions, although they will use computers, do not really have the need for understanding all details to use computer systems effectively, such as physicians, surgeons, psychologists, architects, artists, lawyers, ethicists, realtors, and more. While Wing's (2006) vision included the idea that every student should be able to think like a computer scientist, Denning (2017) recommend that computer scientist should be more aware of the needs of other groups than computer scientist, and how to construct computer systems to make them easier and effectively accessible. Accordingly, computational thinking is today more understood as a conceptual framework enabling students to think of algorithms as recipes on how to conduct tasks, not necessarily limited to programming or being aware of any computer models. Denning closes his observations with the following recommendation, applicable to computational science and modeling and simulation as well: *"It would do all of us good to tone down the rhetoric about the universal value of computational thinking. … Adopting computational thinking will happen, not from political mandates, but from making educational offers that help people learn to be more effective in their own domains through computation."* (Denning 2017, p. 39).

There is a deeper challenge that should be addressed in this context: how can computational scientist as well as simulationists connect better with the users of their products and insights? How can we better elicit knowledge to become the scientific foundation of our simulation systems that provide the computational components of our computational science approaches? While computer generated images are used in movies to support the story, and immersive visualization makes training more realistic for soldiers and surgeons, we still seem to fall back on flow charts and causal loop diagrams when it comes to conceptual modeling. We should be able to do better than this.

Padilla et al. (2017) give an example on how to use the ideas of storytelling to communicate science to nonexpert audience in the context of simulation, as already suggested by Dahlstrom (2014). While such non-traditional approaches are in their infancies, they have a huge potential to reach new audiences. Gibson et al. (2018) make similar recommendations using narration and dramaturgy to provide better training using simulation. Although their application domain is defense, the principles *"composing, storing, sharing, and debating renditions of the past as well as producing rapidly-updating, profusely-disseminated and widely-debated accounts of the present"* are applicable in other domains as well. In the United States, the Institute for Creative Technologies (IST) at the University of Southern California is working on the use of high-tech solutions to use this kind of ideas, such as described by Cavazza et al. (2002) and Rickel et al. (2002). The IST also evaluates "Hollywood" methods to immerse users more into simulation. And why stop here? Brain-machine interface-based solutions are still waiting to be applied, why not aim at those to create a natural interface to every user? As Long et al. (2012) demonstrated, the technology is rapidly moving to make such a vision a reality.

5 CONCLUSION

Computational science is modeling and simulation. The scientific domain must be the foundation for the modeling efforts, and the modeling must capture the theories derived from the science. For a model to be valid, it must be valid in the scientific domain. In order to become computational, the models must be executed on a computer, which means to apply the means of computer simulation. This implies that all computational, but also the philosophical constraints of the epistemology of simulation are valid for computational science as well, from the limits of computational decidability and computational complexity to the challenges introduced by numerical approximations and computational implications of chaotic functions (Oberkampf et al. 2002; Winsberg 2010).

But despite these shortcomings, computational science and modeling and simulation are the best tools we currently have in support of reaching beyond current frontiers. Humphreys (2004) provides an excellent motivation for the full integration of computational means into the toolbox of scientist: like the microscope and telescope helped us to observe thinks not accessible to the naked eye, computers are providing us with the power to solve mathematical challenges describing our scientific problems in a way not doable without them. They are extending our abilities.

It is my personal conviction that despite the success stories we already witnessed the computational science and simulation era has just begun. The tidal wave is still to come as soon as people understand how computational science can help them to solve their problems that are unsolvable with traditional means. It is the responsibility of the simulationists to contribute to this discussion by clearly stating what our constraints are, but also what we can help to accomplish, preferably in the language of the user, using vicarious and empathetic representations like immersive visualization and storytelling, continuously adding to the list of simulation-based disciplines and supported scientific domains.

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