Modeling and Simulation as a Theory Building Paradigm

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Abstract. This chapter makes the case that theory can be captured as a model, which can be implemented as a simulation. This allows composing and recomposing theory components to process new theory out of existing theory. While current modeling and simulation applications focus on simulation as a computational activity that algorithmically produces output data based on valid input data, therefore providing information, the proposed approach utilizes the information and combines the application thereof, which provides knowledge. Relevant work is evaluated, but existing approaches neither us the conceptualization as the central component nor are they applied to ill-defined problems, thus the proposed approach is innovative and closes existing gaps. To show the feasibility and validity, theory is represented as axiomatic structures that can be executed under bounded conditions. As such, the chapter presents a methodological approach for building theory out of existing theory using modeling and simulation.

1 Introduction

Modeling and Simulation (M&S) is an emerging new discipline that is best known for its applications, in particular in the training domain. Most introductory texts focus on these aspects of applications, e.g. Sokolowski and Banks (2009, 2010). Alternatively, the introduction focuses on the computer science fundamentals of simulation development, as well covered in books like Banks et al. (2009) or Wainer (2009). One of the view approaches introducing M&S derived from its own theory, the Discrete Event System Specification (DEVS), has been developed by Zeigler et al. (2000) and represents a systems engineering approach to simulation specification. DEVS builds a significant part of the academic foundations of modeling and simulation. Nonetheless, the emphasis lies on the development and application of simulation systems to be applied as computational activities: a solution for a problem is solved by an algorithm that now can be

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applied to other data describing related problems. The difference between a simulation system and other information systems is that the algorithm implements a model of reality, a purposeful abstraction and simplification introducing assumptions and constraints. Therefore, model-based solutions are harder to compose into a new system than other information services, as the assumptions and constraints of the models need to be aligned in addition to other interoperability aspects. Recent research therefore emphasizes the need for computer interpretable conceptual models, like described in Tolk et al. (2008). But even in this new research, simulations are still perceived as applicable solutions to given problems. In science based disciplines, solutions are applied to solve problems as well, but the emphasis does not lie on the solution itself, but on the method on which the solution is based and the theory from which the method is derived. In general, theories are an important output of the knowledge creation process and finding new good and valid theories is among the most important goals of conducting research. As eloquently put by Popper (1968 p. 59):

> "theories are nets cast to catch what we call 'the world': to rationalize, to explain, and to master it. We endeavor to make the mesh ever finer and finer."

From the M&S standpoint, models and theories have a lot in common, so the question arises if theories can be represented by models. To make theories themselves easier to be accessible to such scientific evaluations, good definitions of theories, methods, and solutions as well as their connections are needed. Bacharach (1989) defines theory as a statement of relations among concepts within a set of boundary assumptions and constraints that are parsimoniously organized and clearly communicated. These concepts are studied in the form of directly observable variables that are related through hypotheses and in the form of constructs that are related through propositions. Hypotheses are concrete and operational statements derived from more abstract propositions; constructs are mental configurations of a given phenomenon that can be measured through variables; variables are observable entities that can take two or more values. Although an empirical perspective, Bacharach's account provide the basic elements one needs to consider when building a theory, namely constructs and propositions and if data is available then variables and hypotheses. It also shows the proximity of theory and model, as Bacharach's definition can be mapped to modeling principles.

However, Bacharach's perspective has different requirements that are not always fulfilled in problem domains: the phenomenon is directly accessible; objectively observable, directly or indirectly measurable, and more importantly the researchers studying the phenomenon have access to all these data. In particular when considering ill-defined problems the researcher copes with phenomena that are not directly accessible and with multiple and sometimes competing accounts on observations. This subjectivity leads to different constructs within different theories, which makes it difficult to determine what data to collect, if data is accessible at all. Recent research has shown that ill-defined problems are commonly found in different disciplines. In particular in new discipline that emerge from overlapping sub-domains of contributing related disciplines, like M&S with its roots in computer science, operations research, systems engineering, artificial intelligence, and more, such ill-defined problems have to be overcome when defining the body of knowledge representing a comprehensive and concise representation of concepts, terms, and activities is needed that make up a professional M&S domain.

The approach proposed and described in this chapter uses the idea to represent theory components as models. This allows implementing the components as simulation components that can be recombined under validity constraints. The main objective of the approach is to generate a theory, from existing theory, that can explain a phenomenon of interests by making explicit what the phenomenon is and how it works. The applicable phenomena, as mentioned, are those that have no forms a being measured, non-physical, no direct access to data, and due to these characteristics, multiple and often competing theories that attempt to provide an explanation. As a form to formalize the process and gain insight into these phenomena, M&S is presented as the conduit to develop the theory.

As a knowledge generation activity, Ören (2009, p.18) states that "from an epistemological point of view, simulation is a knowledge generation activity with dynamic models within dynamic environments." This suggests that M&S provides a way of exploration in areas of study that may not be accessible through empirical means while providing a formalism that rationalist means may not be able to achieve. The correspondence vs. coherence perspective provided by empiricism and rationalism is, therefore, also valid for simulation models. As Schmid (2005) states, a simulation model is accepted as true if these is correspondence to reality; the perspective of coherence also applies to simulation, in which a simulation model can be true only if it consists of a coherent system of believes.

When dealing with complex phenomena simulation becomes extremely useful given that allows the researcher to explore possibilities and test the boundaries of theories in development. Gilbert and Terna (2000) have stated that the reason why social sciences have not benefitted from computer simulation as a methodological approach enough may be that the main value of simulation in the social sciences is for theory development rather than for prediction. The proposed approach is a way of formalizing the use of modeling and simulation for the purpose of theory development. The flow of the chapter is as follows: In Section 2, three example approaches that are found in literature are discussed and critiqued. The proposed approach is described and explained in detail in Section 3. The validity of this proposed approach is discussed in Section 4, followed by the conclusions section.

2 State of the Art in Theory Building Using M&S

Within the body of knowledge of theory development, various approaches exist that propose methodologies and/or methods that use M&S. Davis, Eisenhardt, and Bingham (2007) propose a roadmap for developing theory using simulation methods. Simulation's primary value is in creative experimentation to produce novel theory. They suggest the following method:

- Research Question
- Identify simple theory (conceptual modeling)
- Chose simulation approach
- Create computational representation
- Verify computational representation
- Experiment to build novel theory
- Validate with empirical data (if available)

Davis et al. roadmap departs from an existing simple theory that can be simulated. The main purpose of the simulation is to generate data that can later be analyzed and if possible compared with empirical data. However, this approach's assumption of an existing simple theory may be more appropriate for theory testing than for theory building. If a theory already exists is usually suggested to proceed with its testing for which M&S can provide basis. In this sense, the testing of the simulation is equivalent to the testing of the theory. This approach does not elaborate on what a simple theory is or how to assess its level of simplicity to be able to be explored using the suggested roadmap. The simple theory for a researcher may be a complex theory for someone else. Lastly, this approach seems to focus its attention more on the simulation aspect than on the modeling aspect. Although simulation is key to establish a computer experimental environment and to generate the needed data to study, the modeling component may bear much of the biases of the researcher if this is not made transparent.

Bertrand and Fransoo (2002) present a methodology that builds objective models that partly explain the behavior of real-life operational processes or that can partly capture decision-making problems. They propose a methodology that follows axiomatic research using simulation:

- Conceptual Modeling
- Justification of research method
- Scientific model
- Justification of the heuristic or hypothesis
- Experimental design
- Analysis of results
- Interpretation of results

This approach focuses on the use of existing models or variant of models that have been studied before. This brings two assumptions: that there exist models that can be used and that they are correct for the problem at hand. This assumption is correct within the Operations Management community where new models are built on existing models that can be proven to be correct. However, this is not necessarily the case in areas where theories and models about those theories are scarce.

Sousa-Poza, Padilla, and Bozkurt (2008) present a methodology and a method. The rationalist/inductive methodology consists on generalizing from patterns found in the body of knowledge towards theory building, instead of generalizing from observations as it is the case of induction in empiricism. The method consists in building premises from these generalizations and put them together in a coherent system of premises where assumptions are made explicit and no contradictions are created. Coherence is then established via modeling and simulation and from the results of the simulation an interpretation is conducted. This approach is based on the traceability of the resulting theory to the set of premises and the set of premises to the body of knowledge as a form of validation of the theory. The Rationalist Inductive Methodology and Method is similar to the proposed approach in this study in terms of its focus on developing theory out of theory. However, it lacks the sufficient amount of detail needed for proper application. Figure 1 highlights the methodology and method.

It is noted that in all three cases modeling takes a supporting role to the simulation effort. In other words, modeling is important as long as the simulation is the one providing the insight. However, the approach proposed in this chapter

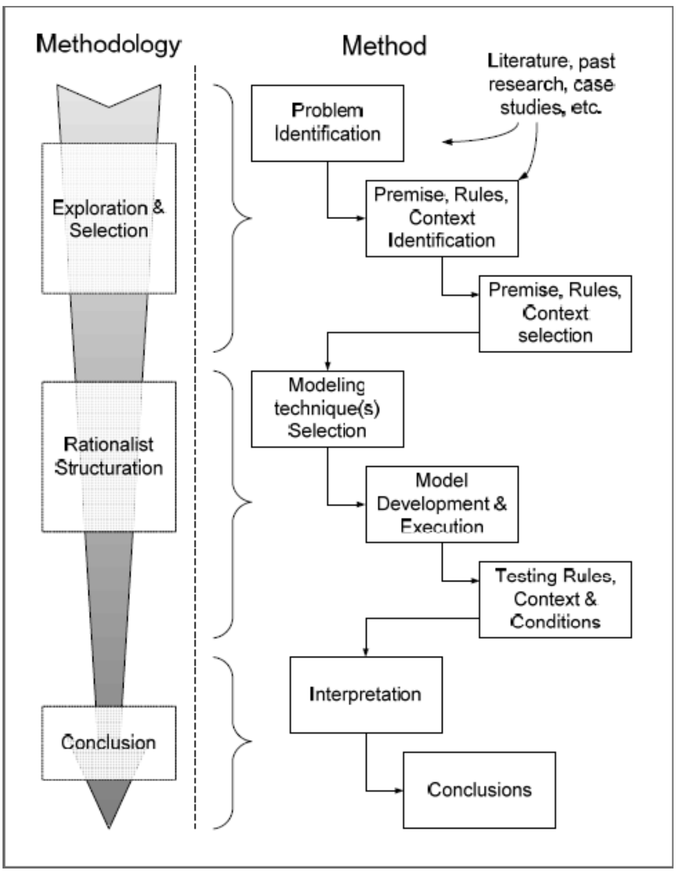

Fig. 1 Rationalist/Inductive Methodology and Method (Sousa-Poza et al., 2008)

in the following sections utilizes the modeling process to create theory that can be enriched with results from the simulation process. In addition, these approaches described in this section do not explicit provide mechanism for studying ill-defined problems. The proposed approach covers the development of theories for this kind of problems. As such, the explicit use of conceptualizations as dominant parts of theories and the application to ill-defined problems are innovative components of the proposed approach that have not been observed in related research.

3 M&S for Theory Building

The proposed approach has the advantage that does not assume an existing simple theory and does not depart from variants of existing models. In addition, it provides an additional level of detail making directly applicable where the following conditions are present:

1. Multiple and sometimes competing theories about the phenomenon of interest. Competing theories are due to the lack of consensus on the phenomenon
2. No direct access to data.
3. No measurable constructs and/or variables due to the lack of agreement of what the phenomenon is and how it works.
4. No existing models.
5. Non-physics-based phenomenon.

If one of these conditions is not met, there are still other options to follow. For instance, if all conditions, but condition two (2), a researcher could use grounded theory, for instance, given that there is access to data. The researcher could also depart from direct observations and speed up the process through M&S. If it is a physical phenomenon, more likely there are data to collect then empirical experimentation is the best candidate. However, if the physical phenomenon is expensive or dangerous to conduct, the option of M&S is also available. It is important to mention that although M&S is an option in many of these cases, they may be different flavors of M&S, namely, live, virtual, or constructive. A live M&S example is that of a wind tunnel where a prototype can be tested for real life conditions; a virtual M&S is that of a flight simulator where a user is immersed in a virtual world; a constructive M&S is where user and world are a creation of the modeler. The option suggested in this chapter is constructive M&S where a world is created given that there is no direct access to reality. The address the issues above, the proposed approach builds, with those competing theories, a world that allows the researcher to explain those theories and create new insight. Figure 2 shows the major processes and the inputs and outputs of the proposed approach.

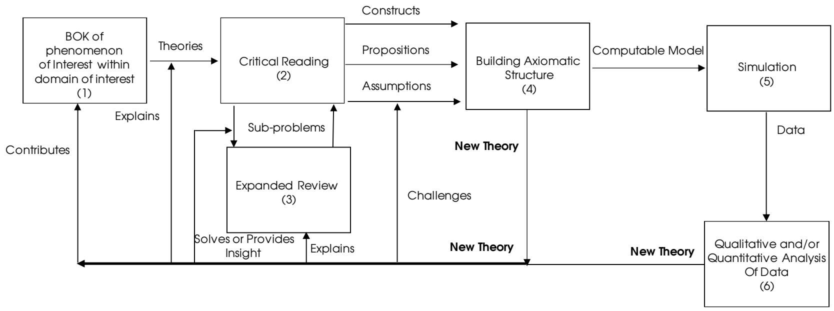

Fig. 2 Approach for Theory Building

Process one (1) refers to scouting the body of knowledge of the phenomenon of interest within a domain of interest. This means that the researcher first needs to identify the context within which the research is conducted and establish the boundaries of the domain of interest. This step allows the establishment of where the theory is intended to be applicable. This step is guided by the research problem for which a theory is needed and a research question that helps bound the scope of the research. The research problem establishes the need for a theory providing the significance of a possible solution. The problem is posed as a statement or series of related statements that must be supported by the BOK. The research question serves as a guide to address the problem within the domain of interest. For instance, a research problem related to interoperability would state: there is no theory of interoperability as it applies to M&S that explains what interoperability in an unambiguous and formal matter. This sentence is made up of concatenated statements that posit the problem at hand and for which a theory of interoperability is needed. As a follow up, a research question would read: what is interoperability and how it can be identified? Although it appears as two questions, the second one cannot be answered without the first and both need to be answered to explain interoperability. As the BOK is scouted, it has been identified that there is no accepted theory that provide a formal explanation of interoperability, but there have been attempts to an explanation. These attempts are mostly theories that need to be evaluated. These theories are the output of the study of the BOK that serves as the input of the process of Critical Reading (2).

Critical Reading is a key process within the approach. It is the process that evaluates explanations of how the phenomenon is defined and how it works within the BOK. From theses definitions and descriptions of the phenomenon, the researcher needs to evaluate their inadequacies and contributions by identifying within the selected theories:

- Lack of Precision: most theories instead of defining what something is they describe what something does. Further, they lack precision when presenting definitions. This is reflected by the use of undefined and ambiguous terms that may lead to subjective interpretations and/or circularities. Additionally, some attempts tend to classify or establish categories of the phenomenon when it is still undefined. This categorization adds to the lack of precision of the phenomenon.

- Perspective: identifying, if possible, the worldview of the proposer of the theory is important because it tells details about the mindset under which the theory was developed and its untold limitations. In the BOK of understanding, for instance, a group of researchers is focused on studying understanding as a process, whereas other group is focused on studying it as an output. In the BOK of interoperability, some definitions are presented as the ability to exchange information while others are presented as the state when information has been exchange.
- Assumptions: researchers postulate their theories and usually leave out the assumptions they use to build them. Most assumptions, although untold, are valid within the context of the theory. However, they are also weak points that may need to be challenged. Assumptions have different origins. One is the research method used to conduct the research. When the research is conducted via experiments, for instance, the main assumption is that the phenomenon can be directly observed and measured. This is regardless of the possible non-physical nature of it. Using the example of understanding. One of the observable processes used as a proxy for studying understanding is problem solving. However, the assumption that the identification of a solution is a reflection that a person understood is flawed given that a person can arrive to a solution by luck or by trial and error. Further, perhaps understanding is simply the identification that no solution is the solution to the problem in question.
- Preconceptions: during theory development, researchers are tempted to posit characteristics of the phenomenon that are neither the reflection of generalization from data, nor a logical deduction, nor a generalization from literature. These are ideas of how the phenomenon "should" work. In this case, this is no longer a theory building effort, but a theory testing effort where the how the phenomenon "should" work need to be tested first.
- Unique characteristics of the phenomenon: these are the components and processes that are part of the phenomenon. Common characteristics' selection is extremely important given that these are the main candidates for the constructs and propositions to be used to explain the phenomenon. For instance, when referring to understanding, one important construct that is commonly found in the literature is the concept of knowledge. Knowledge then becomes a construct used to explain understanding. The process of mapping is also commonly found in the literature when referring to understanding and its descriptions may become a proposition of how the process works. The combination of characteristics must identify the phenomenon in question uniquely and also isolate and bound the phenomenon from similar or concurrent phenomena. For instance, the phenomenon of understanding is usually defined as part of learning or as part of problem solving. However, its combination of characteristics must be different than the combination of characteristics of those processes; especially when components are shared, such as knowledge.

From critical reading there are four major outputs: generalized common components, generalized common processes, generalized assumptions, and generalized common sub-problems that were not addressed in the BOK. Common components are elements that can be turned into constructs of the phenomenon. As previously explained, constructs are not-directly measurable components of a phenomenon. Common processes are turned into propositions that bind constructs together. Propositions are statements that are believed to be true about the phenomenon. Assumptions allow theories to be formed, but they also limit their generalization. From the BOK, they are the main candidates subject to challenge given that some of the limitations need to be lifted for the new theory to take place. Sub-problems are issues about constructs and propositions that are not resolved within the BOK. They can be explained either on an expanded review of a broader BOK (3), through the construction of the axiomatic structure (4), or possibly through the simulation (5). A review of a broader BOK, and its corresponding critical review, means that the researcher needs to go beyond the boundaries of its disciplines and domain of interest to find an explanation for these sub-problems. In the understanding example, for a psychology researcher to investigate the concept of knowledge, it may need to seek supporting information in areas where knowledge has been studied such as epistemology and knowledge management among others. Sub-problems, if possible, must be addressed with the expanded review in order for constructs and propositions to be clearly defined and assumptions to be properly challenged within steps (4) and (5).

Building the axiomatic structure is a full modeling process and a major step in theory creation. Here, constructs and propositions brought over previous steps are formally defined in order to eliminate any ambiguity found within the BOK. This means that a construct and a proposition must be identified uniquely and mean only one thing. The axiomatic structure either solves some of the sub-problems that were carried over from (4) or it is the basis to become a computable model that later can be simulated. If a sub-problem is solved by means of the axiomatic structure, then a new theory has already been created. This is of extreme importance and of difference with traditional approaches that use M&S to build new theory. This means that theory is created "during" the modeling process. Traditional approaches generate theory based on the analysis of data from the simulation only (Davis et al., 2007; Bertrand & Fransoo, 2002; Sousa-Poza et al., 2008).

It is important to note that the axiomatic structure should explain existing theories from where constructs and propositions where derived. This means that the phenomenon is being explained within a general theory and not another instantiation of the theory. An explanation of existing theories with the axiomatic structure then becomes a test of the new theory. Theory and axiomatic structure are not the same. The explanation of the phenomenon through the axiomatic structure becomes the theory. The structure is just the conduit for that explanation.

It is suggested that this axiomatic structure be built in a manner that reflects a formal modeling process. Set theory or predicate logic are considered good candidates. Another candidate is modeling towards a computable implementation. In this case, the axiomatic structure is formal enough to be processed by a computer. This implies that the modeling can be done oriented towards a simulation using systems dynamics, discrete event, or using agents. Figure 3 roughly shows an algorithm for selection of the modeling paradigm.

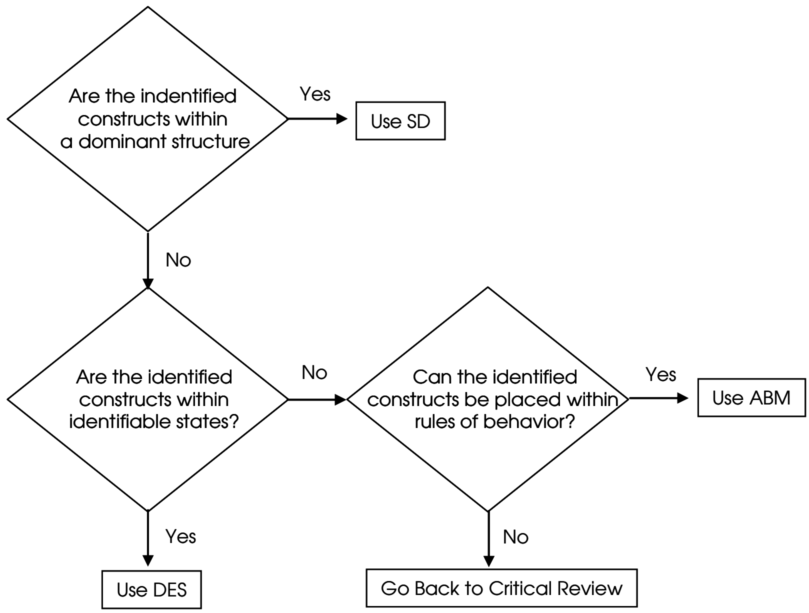

Fig. 3 Selection of the M&S Paradigm

The axiomatic structure then can be simulated. Simulation provides a glimpse into how the phenomenon works under bounded conditions contributing to the theoretical development. This is where this approach is the same as traditional approaches that use M&S. Simulation is mainly used to generate data that can be either assessed qualitatively and analyzed quantitatively used statistical analysis. Through this analysis, further theoretical insight about how the phenomenon works is derived.

Through generalizations from data, theory is created. This theory jointly with the theory created during the modeling process make the new theory. The new theory should address any existing sub-problem, be able to explain existing theory, and provide insight not foreseen before. This is particularly the case when emergence takes place during the simulation. Emergence, in this case is just a pattern that was not considered previous to the simulation, but that can be explained within the axiomatic structure.

Finally, either through the axiomatic structure or through the simulation means of how to measure the constructs of the phenomenon should be presented. However, given that these are still constructs, the accessibility to techniques and tools to measure them may not yet be available. Nonetheless, they provide the basis for future research and further empirical studies.

Padilla (2010) applied this approach systematically to evaluate the question of building a theory of understanding. The current literature identifies knowledge needed to solve a given problem, the world view 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. Using a simple agent based approach, in which agents were used to represent the axiomatic structures for knowledge; theories for understanding were derived by re-composing the axiomatic structures of matching agents. Computational intensive experiments did not only produce know 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 theories emerged that are not captured in detail in literature, such as the dominance of having the 'correct' world view in order to solve new problems (a problem known as 'cultural awareness' to many current defense related operations). Although the example used in Padilla (2010) is limited in its applicability and cannot be easily generalized to other domains, it presents a first application example proofing the feasibility of the approach.

4 Validity of the Proposed Approach

As most researchers in M&S would attest, validity is a contentious issue mainly because it mostly refers to its empirical roots. According to Moss (2008):

> Although model validation has been an ongoing issue in the social simulation literature, there has so far been no systematic consideration of whether different approaches to validation are appropriate to different approaches to modeling and whether some validation approaches, and their associated modeling approaches, are preferable to others.

Empirical validation of models is that in which "validation involves comparison of simulation results with empirical data. If the results of the simulation match the empirical evidence, then the simulation is validated for that empirical context" (Davis et al. 2007). Because of the reasons presented before, empirical validation by comparison with real world data is not possible. This is because until the constructs where postulated there were no objectively agreed constructs to measure. Further, given that the problem is ill-defined in the BOK, establishing an experimental case where it can be tested may not be possible. It is noted however, that the resulting theory is a generalization that considers the different instantiations of the theory. A testing of the theory will irrevocably result in falling into one of those instantiations. Empirical research departs from instantiations to establish generalizations. The theory in this case is already a generalization, an abstraction of the concept that reverts to one of the particular cases when tested. If this is the case, the researcher must identify which of the particular cases is being tested.

Schmid (2005) defines rational validation of a model if the model is true due to its membership of a coherent system of believes, in this sense a simulation must be consistent and non-contradictory in that system of beliefs. Schmid says that a model may be wrong in what regards to its correspondence with reality, but truth using coherence if it satisfies its subjective purpose. He presented two concepts in validation, *specific purpose* and *sufficient accuracy*; a model can be valid from one perspective (serves its purpose), but inaccurate on the other (lack of empirical data). In this case, the model is accurate and true (ergo valid) from the viewpoint of coherence while invalid from the viewpoint of correspondence. This position is consistent with Sousa-Poza et al., (2008). They suggest that the validity of this type of approach is based on the capability of the new theory to explain the theories from which it was derived and on the coherence of the new theory. Coherence, they suggest, is assessed by how well constructs and propositions fit together. From figure 2, the arrows that depart from New Theory that explain existing theories and explain the expanded review are forms of rationalist validation. In addition, the axiomatic structure and its formal structure is a form of rationalist validation as well.

One pragmatic form of validity built into this approach is the solution of the identified sub-problems. If the sub-problems are completely or partially solved, then the theory is found to be useful. Being useful is the base of pragmatism which is a common form of validation found in disciplines such as engineering; as long as it works it is valid. In figure 2, the arrow that solves or provides insight about sub-problems is a form of pragmatic validation.

5 Conclusions and Future Work

In summary, this chapter presents a methodological approach for building theory out of theory using modeling and simulation. The approach serves for conducting research in ill-defined domains of non-physical phenomena where: there are multiple and sometimes competing theories about the phenomenon of interest, no direct access to data, no measurable constructs and/or variables, and no existing models. The approach starts with scouting the Body of Knowledge, goes through a critical review thereof, formulates constructs, propositions, assumptions and sub-problems, incorporates them into a model, and conducts a simulation which result in a New Theory. This New Theory is a generalization of previous existing theories. This means that the theory developed using the proposed approach not only explains and encompasses all existing theories, but also provides explanations to sub-problems and bring new insight to the non-physical phenomenon at hand. The advantage of using M&S for theory building is highlighted. M&S provides formality and traceability making it a robust approach.

The proposed approach is more than a new application of M&S, it is a paradigm shift from applying M&S as a computational activity that applies algorithmic knowledge to solve problems by generating output data based on provided valid inputs towards real knowledge processing. In his well know chapter, Ackoff (1989) distinguishes between data, information, and knowledge: data are simply a set of symbols, facts or figures, while information is data that are processed in context to be useful and provides answers to questions such as “who,” “what,” “where,” and “when;” and applying information useful results in knowledge. Computational simulation can only derive output data from input data, those providing information. By using the approach described in this chapter, the next quality leap from information to knowledge is supported, as the recombination of models representing theory is based on the application of useful information. Hence, M&S moves into the category of intelligent decision technologies with the potential not only to reproduce and conserve knowledge, but actually to produce new knowledge. Although predicted by visionaries like Yilmaz and Oren (2004), the chapter describes a real application of such ideas and proves the possibility thereof.

In order to take full advantage of this new application paradigm of M&S as an intelligent knowledge processing method, the conceptualizations of simulations need to be made explicit to allow their computer supported re-composition to derive new knowledge in a systematic way. First ideas are captured in Tolk et al. (2010) and the recent dissertations of Diallo (2010) and Padilla (2010), but more research in this direction is needed. However, the interpretation of models as representations of theory and knowledge allows perceiving model bases to extract knowledge as today we use data bases to extract information. As the structured query language (SQL) today allows to define what information is needed, based on metadata describing the formal specification of the conceptualization of simulations in the future the knowledge needed can be defined using something like a "model query language" (MQL). Such efforts will significantly impact domains of knowledge management, risk management, and many other fields. This will truly introduce a new intelligent decision technology envisioned in Tolk et al. (2009), namely decision support simulation systems. While the traditional view on decision support systems is still dominated by collecting and presenting data, simulation added a new feature by adding the model-based development of these data over time, focusing on the processes. Therefore, Tolk and colleagues define "*Decision Support Simulation Systems* as simulation systems supporting operational (business and organizational) decision-making activities of a human decision maker with means of modeling and simulation. They use decision support system means to obtain, display and evaluate operationally relevant data in agile contexts by executing models using operational data exploiting the full potential of modeling and simulation and producing numerical insight into the behavior of complex systems." (Tolk et al. 2009 p. 405). In particular in combination with the agent metaphor the approach described in this chapter will enable a new category of intelligent decision technologies.

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