An Extended Research Framework for the Simulation Era

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Abstract
The paper proposes a novel research architecture for social scientists that want to employ simulation methods. The new framework gives an integrated view of a research process that involves simulation modelling. It highlights the importance of the theoretical foundation of a simulation model and shows with the help of the non-statement view and its structuralist theory reconstruction how new theory-driven propositions and hypotheses can be derived from simulations that are empirically testable. It also illustrates the role of theory-based simulation environments. The paper describes the different aspects of the framework in detail and shows how it can help structure the research efforts of scholars interested in using simulation.

1. INTRODUCTION
Business and management researchers are increasingly interested in exploring phenomena that are emergent and/or one of a kind and in studying complex and non-repeatable processes. Simulation modeling is the appropriate methodological approach for this kind of research. Harrison, Lin, Carroll and Carley [2007: 1229] consider simulation modeling to be a “powerful methodology for advancing theory and research on complex behaviors and systems”, while Davis, Eisenhardt and Bingham [2007: 480] point out that “the primary value of simulation occurs in creative and systematic experimentation to produce novel theory”.

As early as in 1997, Axelrod [1997a] called simulation “a third way of doing science”, and even earlier, Ostrom [1988] called “computer simulation: a third symbol system”. Both gave different answers to the question which the other two ways and symbol systems, respectively, were. For Axelrod, simulation was an alternative “way” to both deduction and induction (as he compared it to these two operations); for Ostrom simulation as a symbol system was an alternative both to natural language and mathematics. In this paper we argue that simulation is a way of deduction which is gone by means of an alternative symbol system and that it is not a way of doing science in the sense that it has a starting point of existing knowledge and ends up in new knowledge. Nevertheless, simulation results can be surprising, particularly when they show emerging macrophenomena. However, simulation results are not ‘new’ in a strict sense as they were, so to speak, only hidden in the microspecification from which they were generated [Epstein and Axtell 1996]. Anyway it is questionable whether this holds for deduction without induction or for induction without deduction, to use the two words used by Axelrod. Thus it seems necessary to take a view on simulation which takes the whole research design into account. And we agree with Harrison, Lin, Carroll and Carley [2007: 1229] that simulations is an appropriate means to deal with complex behaviors and system, but we doubt that simulation directly produces novel theory.

In this paper, we propose a novel research architecture, a framework that gives an integrated view of a research process that involves simulation modeling and that draws heavily on recent approach in philosophy of science, called the “non-statement view” [Sneed 1979, Balzer et al. 1987, Troitzsch 1992, 1994, 2012], which helps to formalise the description of research processes and research frameworks. In what follows, we describe the different aspects of the framework and show how it can help structure the research efforts of scholars interested in using simulations.

2. AN ‘EXTENDED’ LOGIC OF SIMULATION AS A METHOD
Carley [2002: 254] gives a detailed explanation for “why so many social and organizational scientists and practitioners are turning to computational modeling and analysis as a way of developing theory and addressing policy issues”. Among the many reasons she advances is that “social and organizational systems are complex non-linear dynamic systems; hence, computational analysis is an appropriate technology as models can have these same features.” [2002: 254] Harrison, Lin, Carroll and Carley note that “the academic field of management has been slow to take advantage of simulation methods” [2007: 1229]. But looking at the increased number of recent articles based on simulation research in management journals and of simulation-specific workshops and papers at management conferences, it seems that management theorists are finally discovering the benefits of simulation methods. Davis, Eisenhardt and Bingham [2007] and Harrison, Lin, Carroll and Carley [2007] give guidelines for simulation research in the field of management. Gilbert and Troitzsch [2005] put forward the following framework (see Figure 1 which is a version modified by Drogoul, Vanbergue
and Meurisse [2003: 5] from Gilbert and Troitzsch [2005: 17]) to explain the logic of simulation as a method in their authoritative book on simulation for the social scientist.

Starting at the bottom left, the real world ‘target’ under study is modeled by abstracting characteristics from it, and then a computer model is used to run simulations in order to produce simulated data. This data can then be compared with data collected in the ‘real’ social world.

This framework nicely illustrates the core logic of simulation as a method that underlies all the different kinds of simulation approaches that Gilbert and Troitzsch [2005] review in their book. However, they acknowledge that the figure is only a shortcut. For example, researchers usually start with “presumed social processes” which are already mental models (informal theories) of real social processes [Drogoul et al. 2003]. The framework does not capture the entire simulation research process that scholars encounter, especially for complex agent-based modeling approaches. In particular, it does not highlight the role of existing theory — insights and frameworks from the literature — when it comes to modeling, nor does it talk about theory development. It also does not show where simulation environments — software toolkits that help researchers create, run, and analyze simulation models — come into play.

In this paper, we divide simulation toolkits into two different classes: multi-purpose toolkits (Class-1 environments) such as Repast, NetLogo or AnyLogic which can be used for nearly all simulation approaches developed for the social sciences at large (including management science and economics as well as psychology, anthropogeography and archeology), and theory-related toolkits (Class-2 environments) such as EMIL-S [Lotzmann et al. 2012] or SimISpace [Ihrig and Abrahams 2007]. While theory-related toolkits do not have so many members, we shall argue that they have distinct advantages. A simulation environment that is based on a theory can be used to create various application-specific simulation models. This stands in contrast to the many little simulation programs that can only be used for one particular research question, and new models have to be always created from scratch. SimISpace is a simulation environment that lets researchers model knowledge flows and knowledge-based agent interactions based on Boisot’s [1998] conceptual framework that describes the properties of knowledge assets. With this simulation toolkit, one can create many different models for all kinds of research questions that concern the knowledge economy — from intellectual property (IP) policies to research and development (R&D) processes to innovation strategies. EMIL-S, on the other hand, is an implementation of EMIL-A, a theoretical architecture of a normative agent which describes how agents learn about the norms of the group or society they live in and how norms evolve in such a group or society [Andrighetto et al. 2007; Andrighetto et al. 2013]. Both EMIL-A and EMIL-S have also been applied to various contexts and scenarios.

To account for those issues and provide a more detailed picture of the simulation research life-cycle, we constructed an expanded framework (Figure 2) to extend the logic of Gilbert and Troitzsch’s [2005: 17] basic model of the modeling and simulation process. This framework is meant to not only provide future simulation researchers with a research architecture that can assist them in their modeling efforts, but also help the wider research community put simulation methods into perspective. The following sections explain the different building blocks of the research architecture and its relationships.

3. FROM THEORY TO SIMULATION MODEL

In contrast to Gilbert and Troitzsch [2005: 17], we propose to start the simulation research ‘adventure’ with a real-world issue backed by prior theory in the two right-hand columns of Figure 2. We assume that some new, unexplained feature of the real world (Gilbert’s and Doran’s ‘target system’ [1994: 4]) in the middle of the third column awakens a researcher’s interest. The researcher then becomes aware of the existing approaches to explaining this or similar features in the existing literature (fourth column of Figure 2). From both, a mental model is formed in the researcher’s mind. After this first occurrence of the word model in its dedicated meaning we try to give a more formal definition of this word.

The creators of the ‘non-statement view’ defined theory — to be more precise: a theory-element (T) — as a mathematical structure consisting of a theory-core (K) and a domain of intended applications (I): K = (K, I) [Balzer et al. 1987: 39]. K in turn is another mathematical structure containing three sets of models, a set of constraints and a set of links: K(T) = (Mpp,(T), Mpp(T), Mppp,(T), GC(T), GL(T)) [Balzer et al. 1987: 78–79]. The fact that the ‘non-statement view’ defines three classes of models to describe the contents of a theory goes back to the observation that

- some terms used in the theory are measurable or observable no matter whether the theory has ever been formulated or tested — the list of these terms defines a set of partial potential models Mppp(T);
- other terms used in the theory become meaningful only after the theory was formulated — the list of these terms extends the elements of Mppp to elements of the set of potential model Mpp(T); and
- the relations between both kinds of terms need to be defined as axioms — full models which conform to such axioms form the set M(T).

\(^{1}\)We will not discuss the latter two in detail here.
Elements of the domain of intended applications (I) are partial potential models, as applications in the real world can only be described in terms which are meaningful before the theory is defined (describing, observing and measuring these terms necessitates, of course, other theories, connected to the theory in question by links $\in \text{GL}(C)$).

To give an admittedly simplistic example of how one can describe the research process in the terminology of the ‘non-statement view’ we remember that some unexplained feature of the real world awakens a researcher’s interest. Quite recently a British newspaper reported that currently 18 pubs have closed per week between March and September 2012, that 52 pubs closed per week in 2009 and that only some 58,000 pubs still existed in the UK, due to the rising cost of beer since the previous Labour administration introduced an automatic increase of the beer tax by 2 per cent above inflation every year.\footnote{\textit{The Telegraph}, 01 November 2012, \url{http://www.telegraph.co.uk/foodanddrink/foodanddrinknews/9646395/Pub-closures-rise-due-to-beer-tax-campaigners-warn.html}, last access on 30 January 2013 10:00.}

This casual observation (middle of the third column of Figure 2) is an intended application of the ‘pub closure’ theory $\text{PC}$ (still to be created). In our researcher’s mind a mental model forms, partly from the casual observation (in column 3), partly from background knowledge and desk research (in column 4) by abduction as the most economic explanation of the fact of pub closure under respective background knowledge is the increased beer price: the higher the beer price the less the propensity of potential pub visitors to go there for a drink, and the less the pubs’ sales volumes and the landlords’ profits, with the result that more and more pubs become needy and will be closed. While the casual observation only spoke about the beer price and an increasing rate of pub closures, both observable without knowing any economic or management theory, the mental model already contains at least one variable which is not directly measurable, namely the propensity to visit a pub (not even thirsty people can give a numerical value to this variable).

Formalising this mental model leads to the definition of a potential model $M_{\text{PC}}(\text{PC})$ of a pub closure theory, listing terms such as beer price, pub closure rate, number of remaining pubs, pub sales volume, landlords’ profits — and propensity to visit a pub. The mental model already contained the idea that these terms should be related in some way, but there are of course several different ways to formulate these relations. The most simplistic way could be a regression analysis over time between the annual pub closure rate $c(t) = \dot{n}(t)$ and the beer price $p(t)$, for instance, assuming that the pub death rate is proportional to the current beer price: $c_t = \dot{n}_t = \lambda p(t)$.

\footnote{Perhaps the latter is measurable with some statistics from questionnaire surveys asking how often the interviewee visited a pub during the past six months, from which a probability can be calculated that an average British person of a certain gender and age went to a pub during the following ten days, and this probability could be interpreted as an average propensity. This would be a link to another theory with applications which do not intend to explain the pub closure rate.}
\( \alpha p_t + e_t \) and \( p_{t+1} = \beta p_t, \ t = 2008..2012 \), introducing \( \alpha \) as a new PC-theoretic term — which only has a meaning with respect to this version of the pub closure theory — and \( \beta \) as a term which is non-theoretical with respect to PC, as it is annually published by the government. This regression equation with a fixed \( \alpha \) would be an axiom of a specific element of \( \mathbf{M}(\mathbf{PC}) \).

The potential model can be given a dynamic mathematical form — \( c(t) = \dot{n}(t) = \alpha p(t), \dot{p}(t) = C e^{\beta t} \); \( n(2013) = 58,000 \) or \( n(2008) = 63,8000 \) and \( p(2007/6/30) = £2.57 \) and \( p(2012) = £3.09 \) with a solution for this differential equation which turns out to be \( n(t) = \alpha e^{\beta t} + C \)
where \( \alpha, \beta \) and \( C \) can easily be calculated from the data given in the source mentioned in the footnote. Otherwise the mental model can already be converted to an again simplistic theory-based simulation environment — in the current case this could be a System Dynamics model with beer price and number of remaining pubs as level variables, the tax increase and the pub closure rate as rate variables where the right-hand sides of the level and rate variables are not yet filled, just as in the GUIs of commercial products for System Dynamics simulation when only the diagram has been drawn on the screen (see Figure 3). The regression equation forming part of the full model \( \mathbf{M}(\mathbf{PC}) \) instantiates the environment (here mainly by parameterisation of \( \alpha \) and \( \beta \), but perhaps also by replacing the linear function by another type of function, thus switching between different elements of \( \mathbf{M}(\mathbf{PC}) \)) and results in an executable System Dynamics simulation model of the pub closure theory. Both the differential equation and the System Dynamics simulation yield testable propositions for the number of remaining pubs in, say, 2015, which can be compared to empirical data measured at the end of that year.

An extended version of PC would also give operationalization hints at what kind of data should be collected to gain new research insights leading to a new mental model in which, for instance, the individual behaviour of potential pub visitors...
and of landlords (and, perhaps additionally, of the current British government which might change the automatic increase of the beer tax to save pubs from closure are modeled). This version would then result in an agent-based simulation environment of an extended pub closure theory.

The example should have shown that a research framework like the one postulated here defines the role of simulation in a different and more precise way than in Axelrod’s seminal presentation during one of the first international conferences on social simulation [Axelrod 2007, Axelrod 1997a, Axelrod 1997b]. Our approach extends Balzer’s [2009: 327–328] definition of the role of simulation in scientific research from the ‘non-statement’ point of view where (for the sake of brevity) he does not make a difference between the runs of an executable simulation program and the data generated by these runs. Balzer also discusses theory-based simulation environments (which he calls “abstract simulations”, contrasted to “Einzelsimulationen, die für ein ganz bestimmtes, reales System konstruiert werden” (single simulation programs constructed for a specific real system, Balzer 2009: 326)), which are more or less the same as our executable simulation models.

4. SIMULATION RESEARCH IN ACTION

The basic component of simulation research concerns running the executable simulation model and conducting many virtual experiments by varying the parameter space. The resulting simulated data can then be compared to both theoretical and empirical assessments, which is the first step in generating new research insights that will help improve existing theories and eventually create new ones. With agent-based models for example, the researcher specifies well-defined micro-behaviors of agents (based on the theoretical assumptions). The macro-level results that emerge from those individual-level activities cannot be predicted (especially when exploring different boundary conditions), and the researcher may gain valuable new insights from analyzing the outcome. Another example are agent-based models that do not rest on formal theories. In these — quite numerous — cases the agent-based simulation program is the first attempt ever at formalising a mental model using Ostrom’s [1988] third symbol system. For those, unambiguous conclusions cannot be derived and simulation results may reveal unexpected outcomes. More often than not, simulated data cannot be compared to purely theoretical assessments as a classical mathematical formulation of the axioms of the theory has no analytical solution (and a numerical solution of, for instance, a system of non-linear differential equations is also the result of a computer simulation for a specific combination of parameters), such that simulation sometimes is the only possibility to generate deductions from theoretical assumptions.

This simulation exercise will result in theory-driven hypotheses that are empirically testable. Although an executable simulation model is a full model of the theory and makes all T-theoretical terms (as in “theory-element” of the non-statement view) and their values visible, it also generates hypotheses from which the T-theoretical terms were eliminated. Subsequently, the T-non-theoretical simulated data can be compared to empirical data. In an empirical follow-up study, the real world issue that is being investigated can be further examined by obtaining empirical data through systematic data gathering on a basis that is informed by the previous simulation research, and perhaps ways can be found with the help of a link to another theory to measure terms which are theoretical with respect to this theory T, but not to the other (linked) theory T’ (as the propensity to go to a pub in our simplistic example above, perhaps measured with some psychological theory T’ about the relation between price and propensity to buy).

The research architecture described above is more comprehensive than conventional approaches that do not employ simulation tools, and so is better suited for studying complex phenomena and obtaining new theoretical insights.

The conventional research approach can be depicted by leaving out the second column of our framework (Figure 2). Predictions and analyses are made based on existing theories in Ostrom’s [1988] first and second symbol systems of natural language and mathematics, and the empirical data gathered on real world issues is compared to these theoretical accounts or propositions. What is lacking is the power of computer tools that enable us to study more complex processes by modeling micro behaviors that individually might be straightforward, but may result in unpredictable outcomes when considered together.
5. VERIFICATION AND VALIDATION

Our framework can also be used to illustrate the important processes of verification and validation, both of which have been explained in detail in the literature [Carley 2002, Davis et al. 2007, Gilbert 2008, Gilbert and Troitzsch 2005, Harrison et al. 2007]. Gilbert and Troitzsch [2005] give a concise definition:

While verification concerns whether the program is working as the researcher expects it to, validation concerns whether the simulation is a good model of the target.

Our framework allows us to identify multiple instances where verification and validation come into play. There are three layers of interest: verification, validation, and ascertaining the two.

Verification. Starting at the bottom left, the obvious area where the model needs verifying is in the building of the software, where the researcher has to ensure that the program’s technical specifications have been properly implemented. The simulation environment has to perform exactly as described in the technical document derived from $M_p(T)$, without errors or ‘bugs’. The simulation processes, in their abstracted form, also have to work like and be consistent with the real world social processes they represent. Thus verification is mainly the comparison between columns 1 and 2 of Figure 2.

Validation. The middle layer of the framework depicts the areas of interest in validation terms. Most researchers will look to the right, and ensure that the application-specific model fully represents the real world issue or target under study. But there is another important area: since the simulation environment is underpinned by a theory, they also have to make sure the model is a fair representation of the theoretical constructs. Thus from the point of view of the researcher using simulation, validation is mainly the comparison between columns 2 and 3 of Figure 2.

Ascertaining Verification and Validation. The factors noted above will be difficult to ascertain without comparing the simulated data to theoretical predictions (verification) and empirical data (validation), respectively. Therefore, simulation researchers have to pay attention to the top layer of the framework. They have to infer and draw conclusions from the actual results of the simulation runs to assess whether the program is working as intended, and represents the actual phenomenon studied. Great care must be taken here because — as Gilbert and Troitzsch [2005] point out — mistakes can occur at any step in the research process.

6. SIMULATION CAPABILITIES BEYOND A SINGLE RESEARCH PROJECT

Considering our research framework further, the top half of Figure 2 (starting at executable simulation model) maps the area usually covered by research employing simulation methods. The core research activities classically conducted in scholarly work based on simulation modeling as described by Gilbert and Troitzsch [2005] are those depicted in columns 2 and 3. Many recent simulation studies also base their modeling on theoretical modeling, columns 1 and 2. (a fine example of this would be Caszar and Siggelkow [2010]). Generally however, simple simulation models are programmed that can only be used for and applied to the particular research topic of the study. An increasing number of researchers turn to pre-existing modeling and simulation tools (multi-purpose toolboxes, Class-1 environments) that support the construction of simulations (e.g., RePast for agent-based systems [North et al. 2006]), which enable researchers to take a short-cut from mental model to executable simulation model. Very few simulation research projects cover the purposes of a theory-based simulation environment (bottom of column 2). Most researchers do not build an entire simulation environment that can be used for many different research topics and purposes (theory-based toolboxes, Class-2 environments), far beyond the subject of the immediate research needs, but supporting research in theoretically related areas. This is a pity because future research projects studying different scenarios, different intended applications of the same theory, could also employ the simulation environment created to derive new theory-driven hypotheses that are empirically testable and which range across numerous applications such as the different scenarios on norm-related behavior simulated with the EMIL-S toolbox Lotzmann et al. 2012, Mohring and Lotzmann 2009, Markisic et al. 2012.

Designing and implementing a full simulation environment or platform (including a simulation execution and reporting suite) that can be used for a variety of research projects in the same subdiscipline is a difficult and laborious process (Figure 4, Gilbert 1996). This probably explains why many people shy away from developing them. Problems can occur at various places, especially if researchers are not able to write the actual software code themselves, but have to rely on software engineers who may not necessarily understand the theory fully. In fact, completely debugging a simulation environment can take several years. However, once developed, it benefits the many researchers who are interested in simulation methods but lack the computer science skills that are necessary to build the software. They can use the graphical user interface to easily set up, run, and analyze simulations that model their particular research questions.

To help build such a theory-based Class-2 simulation environment, some of the lessons learned from difficulties the
authors encountered during this effort are listed below (items 1 through 3 certainly apply to all kinds of software projects, but in the case in question, where researchers in the social sciences at large are not typically familiar with software development, they are particularly crucial). Attending to these four points will help simulation researchers to get closer to the proper computational representation of the theory they want to model and avoid losing too much time on software development.

1. If the software development project is inherited, or there are multiple authors, the researcher will have to revisit the specifications thoroughly and check whether they are all correct and appropriate, a process which involves uncovering and repairing inconsistencies, errors and omission in the spec.

2. If the researcher has to work with successive generations of programmers, and proper documentation is not in place, coherent knowledge about what has been implemented and how it has been implemented may be lacking. The software development process must be either very closely monitored over its entire development cycle, or rigorously and consistently documented.

3. Software bugs are an inevitable part of the development process, but having the program properly designed by a good software architect can at least avoid faulty code and inappropriate architecture.

4. Misrepresenting theory is dangerous: a researcher who is not their own software architect must attend to the specifications and technical document closely to ensure the computer algorithms really implement the theory the researcher wants to model.

Figure 4. The long road to a simulation environment

7. CONCLUSION

This paper describes our unique research architecture and discusses the applicability of its framework, and looks ahead to many future research projects that could be structured using this approach. Being able to navigate the research space presented by this framework is a first step in using simulation methods to produce novel theory. We hope that the framework will help other researchers conceptualize the different tasks required to realize good simulation studies.

REFERENCES


**Biographies**

**Martin Ihrig** is an Adjunct Assistant Professor at the Wharton School and a Senior Fellow at the Graduate School of Education of the University of Pennsylvania (USA), a Visiting Professor at Lappeenranta University of Technology (Finland), and President of I-Space Institute, LLC (USA). He holds a Master of Business Studies from UCD Michael Smurfit School of Business (Ireland) and a Doctor of Business Administration (PhD) from Technische Universitã­t Berlin (Germany).

The research initiative he manages at Wharton’s Snider Entrepreneurial Research Center focuses on the strategic and entrepreneurial management of knowledge. In his simulation research, he is studying entrepreneurial opportunity recognition strategies with the help of agent-based models.

**Klaus G. Troitzsch** has been a full professor of computer applications in the social sciences at the University of Koblenz-Landau since 1986. He studied sociology and political science in Cologne and Hamburg. After taking his first degree as a political scientist, he was a member of Parliament of Hamburg from 1974 to 1978. In 1979, after having taken his PhD in political science from the University of Hamburg, he returned to academia, first as a senior researcher in an election research project and from 1986 as full professor of computer applications in the social sciences. In March 2012 he retired but continues his academic activities.

His main interests in teaching and research are social science methodology and, especially, modelling and simulation in the social sciences. Among his main research projects there are MIMOSE which developed a declarative functional simulation language and tool for micro and multilevel simulation (1986–1992), FIRMA, an EU Fifth Framework funded international research project named Freshwater Integrated Resources Management with Agents (2000–2003) where his team was, among others, responsible for the simulation aspects, EMIL, an EU Sixth Framework project on the emergence and innovation of norms in social systems (2006–2009), This project, too, used agent-based simulation, OCOPOMO, an EU Seventh Framework project on open collaboration in policy modelling (2010–2013) and GLODERS, another EU Seventh Framework project on the global dynamics of extortion racket systems (2012–2015) where his team is responsible both for text and data mining and for agent-based simulation.

He is author, co-author, and co-editor of a number of books on simulation, author of a number of articles in social simulation, and he organised or co-organised a number of national and international conferences in social simulation.