

Towards dialectic models for documenting and conducting simulation studies: a vision

Steffen Zschaler

Department of Informatics,
King's College London
London, United Kingdom
szschaler@acm.org

Thomas Godfrey

Aerogility Ltd
London, United Kingdom
tom.godfrey@aerogility.com

Pia Wilsdorf

Institute for Visual and Analytic Computing,
University of Rostock
Rostock, Germany
pia.wilsdorf@uni-rostock.de

Adeline M. Uhrmacher

Institute for Visual and Analytic Computing,
University of Rostock
Rostock, Germany
adelinde.uhrmacher@uni-rostock.de

Abstract

Validation and documentation of rationale are central to simulation studies. Most current approaches focus only on individual simulation artifacts—most typically simulation models—and their validity rather than their contribution to the overall simulation study. Approaches that aim to validate simulation studies as a whole either impose structured processes with the implicit assumption that this will ensure validity, or they rely on capturing provenance and rationale, most commonly in natural language, following accepted documentation guidelines. Inspired by dialectic approaches for developing mathematical proofs, we propose a vision of capturing validity and rationale information as a study unfolds through agent dialogues that also generate the overall simulation-study argument, as a novel approach to documenting and conducting simulation studies. We illustrate the key ideas in an example simulation study, highlight potential benefits of this novel approach, and identify key next steps towards making the vision a reality.

CCS Concepts

• **Computing methodologies** → **Simulation evaluation; Model verification and validation; Modeling methodologies.**

Keywords

simulation studies, validity, assurance, argumentation, agent dialogue

ACM Reference Format:

Steffen Zschaler, Pia Wilsdorf, Thomas Godfrey, and Adeline M. Uhrmacher. 2025. Towards dialectic models for documenting and conducting simulation studies: a vision. In *39th ACM SIGSIM Conference on Principles of Advanced Discrete Simulation (SIGSIM-PADS '25)*, June 23–26, 2025, Santa Fe, NM, USA. ACM, New York, NY, USA, 5 pages. <https://doi.org/10.1145/3726301.3728411>

1 Introduction

The credibility crisis of simulation (e.g., [24]), has spawned various research activities to improve the documentation of simulation studies and thus their reproducibility [13, 18]. Other approaches go beyond pure documentation, providing guidance and support in conducting credible simulation studies, via workflows [1, 23], and via automatically generating simulation experiments [28].

We aim for an interactive approach towards increasing the credibility and improving the guidance in conducting simulation studies by questioning and probing simulation results. To this end, we propose to adopt an “argumentation-based” dialog, in which participants exchange arguments, using argumentation mechanisms to establish what facts / knowledge can be deemed acceptable [7].

Inspired by argumentation-based approaches for mathematical proofs [3, 4, 10, 20], we explore the feasibility of a dialectic approach to, and discuss their potential for (a) documenting and (b) conducting simulation studies. Therefore, we developed a formal dialectic framework¹ in which a “proponent” can propose artifacts of a simulation study and support them—for example, with theories or experiments—while an “opponent” critically evaluates and challenges the claims made by the proponent. It should be noted that in this framework, both the proponent and the opponent are realized by software. Our working hypotheses are that (a) this approach adds a different yet valuable perspective for *documenting* and communicating simulation studies, processes, and the implied results [26], and (b) when used for *conducting* simulation studies, it directs us towards critically inspecting and probing the results of simulation studies.

We will focus on certain aspects of our approach, and illustrate it based on an example of developing a signaling pathway model first, before discussing our vision, and delineating possible next steps at the end.

2 Arguments for simulations: an illustrated example

We illustrate our overall vision using an example case study on endocytosis [14], which has been used to illustrate and explore other approaches for simulation validation in the past [8, 29], making it

¹An initial version is available at <https://doi.org/10.6084/m9.figshare.28868870>.

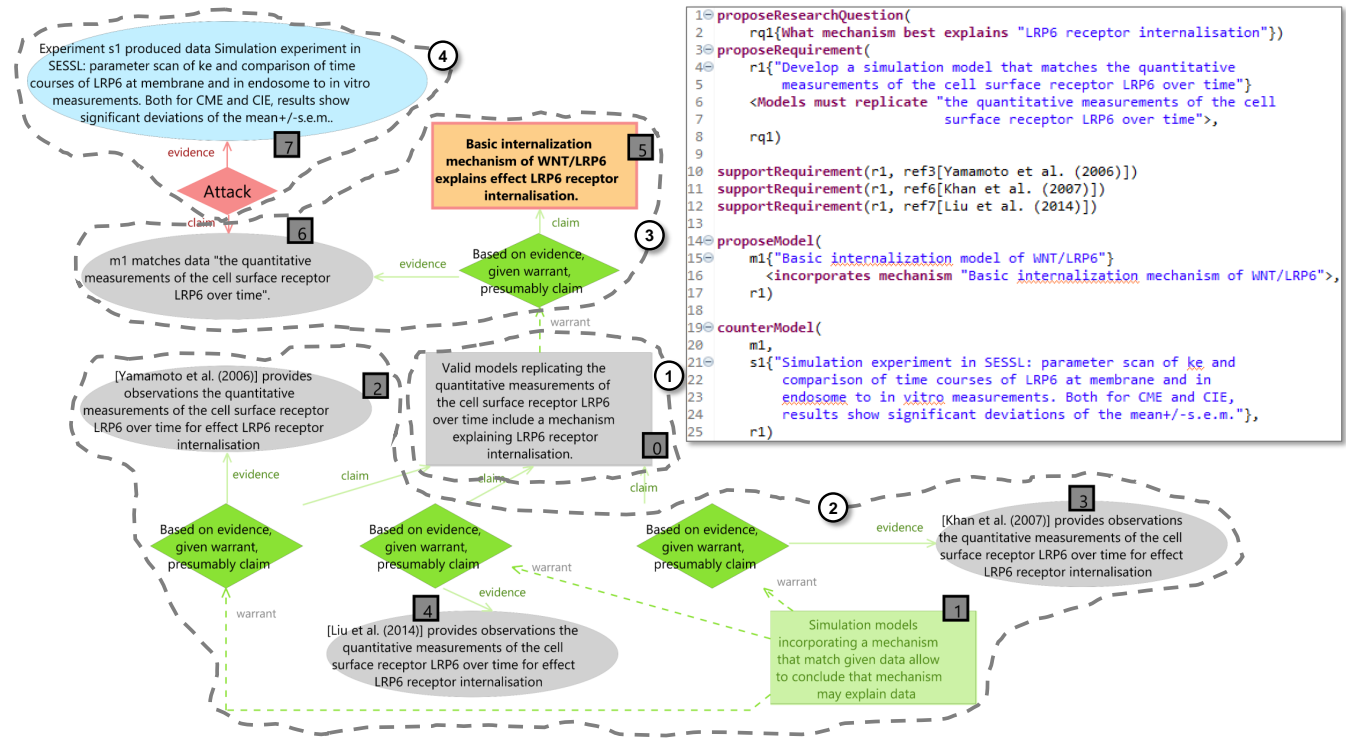


Figure 1: Moves (top right box) and argument graph generated for the beginning of the illustrative case study [14]. Different colors and shapes correspond to different types of arguments.

easier to access relevant information for our purposes. The study required three successive model extensions and various experiments to build a simulation model that represents mechanisms of endocytosis of WNT signaling, fitting to various in-vitro experiments. The model was validated by using it to predict the dynamics of WNT endocytosis induced by a different ligand. Our case study focuses on the start of this simulation study: the first iteration of model building and the failed attempt at output verification. In describing the example, we will refer to Fig. 1 throughout.

Inspired by work in maths [3, 4, 20], we conceive of simulation studies as trying to build an argument to answer a research question. This is achieved through a dialogue between proponent and opponent agents (which may be different people or the same person playing different roles at different times). Agents make ‘moves’ (in the spirit of agent-dialog protocols as proposed in [16]), each of which characterises a step in the development of a simulation study and captures the information of relevance to that step. The box in the top-right corner of Fig. 1 shows some exemplary moves for our illustrative case study: we begin by proposing a research question, followed by proposing requirements for simulation models (which, if satisfied, would allow us to draw conclusions about an answer to the research question), which are supported as relevant by appropriate literature references in line with argument templates discussed in [29]. We then propose a concrete simulation model (m1), which we claim satisfies the requirements. Finally, the opponent provides

a concrete experiment (s1) using our model, demonstrating that it does not satisfy the requirements.

This information is not dissimilar to that captured in provenance graphs, and an example such provenance graph for our example can be found in [14, Fig. 6]. However, moves make explicit the rationale for each step. They also provide additional semantics, in that each move updates the graph of the overall argument maintained about the simulation study.

Specifically, each move adds elements to the argument graph. The argument graph corresponding to the sequence of moves in the top-right box can be seen in the remainder of Figure 1. We are starting at a point where we no longer question the validity of the background knowledge given in various literature references. The proposal of a research question rq1 and refinement to a requirement r1 on the model (Lines 1–8) generates the warrant ①. The requirement is further underpinned by providing various literature references (Lines 10–12) that identify the wet-lab data that needs to be matched, generating the argument structure labeled ②. The simulation experiments try to identify a model with plausible parameter values (according to the literature) that is able to reproduce the data given in references ref3, ref6, and ref7. Unlike the argument graph, the provenance graph in [14] does not include the research question and requirement. Instead, the three data sources (ref3, ref6, and ref7) are directly used as input to the model analysis activity without further clarifying their specific roles.

Continuing with the agent argumentation dialogue, a first model m_1 is proposed, claiming that it satisfies the requirement (Lines 14–17). This generates the orange claim of an initial overall answer to the research question, supported by the argument labeled ③. Note that this argument uses the warrant previously established by accepting the requirement r_1 . At this point, no experiments have been performed yet; the argument graph only represents the claims currently accepted by the team undertaking the simulation study.

A simulation experiment s_1 is then executed and turns out to show that the model does *not* satisfy the requirement; the experiment thus counters the model (move shown in Lines 19–25). This adds the argument ④, which attacks the claim that m_1 matches the wet-lab data. In the provenance graph in [14], the attack is denoted less explicitly by a model analysis activity that produced an experiment specification and a “findings” entity, which contains simulation data from the experiment execution as well as a remark whether the output verification was successful. Overall, the provenance graph delineates sequences of steps with their inputs and outputs, whereas the argument graph in Fig. 1 comprises detailed claims, evidence, and warrants about the artifacts, which enables an analysis of what statements the simulation developers currently accept about the system being simulated.

This analysis can be undertaken by automatically translating the argument graph into an abstract argumentation framework [11] and using standard argument solvers (we specifically use `plato` [22]) to obtain the set of all ‘acceptable’ arguments; that is, those statements that can be considered valid and are not contradicted by other statements. Doing this analysis for our example, reveals that the orange argument is not currently part of the set of acceptable arguments and, thus, cannot be considered valid. Thus, in the current state of the simulation study, we do not have an acceptable answer to our research question.

We can do this analysis at any point during the simulation study. For example, one move earlier (that is, when the counterModel move on Lines 19–25 hasn’t been made yet), argument ④ would not be part of the argument graph yet. Using `plato` to obtain the acceptable arguments produces a set that includes the orange argument ‘Basic internalization mechanism of WNT/LRP6 explains effect LRP6 receptor internalisation.’ This correctly reflects the fact that at this point, the simulation-study team still believes (albeit without explicit evidence) that they may have found a mechanism explaining the wet-lab data.

Note that more work is needed to correctly capture the semantics of Support relations in simulation studies. For example, assume we were to attack one of the literature references, which supports warrant ①. Because we have translated each of the Support relations separately, even attacking one of them would be sufficient to make the warrant become invalid. As a result, the overall conclusion would also be deemed unacceptable by the formal analysis. This does not necessarily reflect real-world practice, where multiple references may add strength, but attacking one will not necessarily make the overall conclusion invalid, either. Other forms of argumentation frameworks are available [17], which provide more subtle differentiations of possible relationships between arguments.

3 Vision: new possibilities for documenting and conducting simulation studies

Simulation studies are inherently complex and iterative, involving the interplay of diverse artifacts, activities, and decisions. To avoid pitfalls [19] and to support the documentation of simulation studies as well as their execution, we envision a dialectic model based on a structured exchange of arguments and counter-arguments.

3.1 Documenting

A record of the conducted moves and the corresponding argument graph can serve as a highly detailed documentation of the simulation study: by scrutinizing each step and product, the dialectic approach prompts modelers to disclose critical context information that would otherwise remain implicit. This is what distinguishes it from other methods of documentation, where the exact content and level of detail in the documentation depend on the modeler’s preference (reporting guidelines) or are ingrained in the capturing software (provenance). Thus, our dialectic approach may complement existing forms of documentation with additional detail and—foremost—explicit pro and contra reasoning. Using the approach in the WNT/LRP6 simulation study, for instance, allows clearly articulating the rationale for omitting certain intermediate reactions and entities, and linking evidence from the literature.

In the design of our approach, we deliberately leave the dialogues (and thus the simulation studies) open-ended, i.e., we do not define any explicit termination rules for our dialogues. This is because, similar to the ideas of ‘proof-events’ and ‘fluents’ (sequences of proof-events) from [3], we think of a simulation study as a socio-temporal phenomenon, where new moves may be introduced by different agents at different points in time. This is where argument graphs and their automated analysis can be particularly useful. For example, assume we have produced a complete sequence of moves for our study and have generated the corresponding argument graph. At this point, we publish the paper [14], where we make a claim about the mechanism underpinning LRP6 receptor internalization. This corresponds approximately to Almpani’s notion of a ‘proof-event’²: a public announcement of a specific claim with an underpinning argument [3]. Assume that a year later, someone finds a problem with the experiments described in reference 5 (see Fig. 1). How would this affect the validity of the claims in [14]? Adding a corresponding move explicitly to the documentation of our study and incrementally updating the argument graph would allow us to analyze which arguments remain acceptable and, in particular, whether the acceptability of our overall claim has been affected.

With the described reasoning support, also changes within the validity of specific arguments would be propagated throughout the network of arguments and counter-arguments, thus providing a living documentation of a simulation study and its validity.

²Albeit not specifically in mathematics

3.2 Conducting

Inspired by Osman Balci’s approach to simulation credibility—where each product and sub-product is subject to verification, validation, and accreditation [6]—counter-arguments carefully scrutinize every artifact and step in a simulation study regarding its meaning and role as well as the methodology and context information used. Rather than taking artifacts and processes at face value, our approach encourages their critical examination, reinterpretation, and refinement, thereby fostering creativity and deeper understanding [3]. For example, in the endocytosis study, the exchange of arguments has been a driving force for model development: a counter-argument evidenced by a simulation experiment prompted the modelers to think about new hypotheses to explain the discrepancy between simulation results and experimental in-vitro measurements [14], which led to the creation of an improved simulation model.

The dialectic model can be easily extended to support interactive thinking and communication as it makes the reasons in support of claims explicit, possibly with specific stakeholders in mind. This makes it a powerful tool for collaborative model development and stakeholder engagement. The importance of interaction has already been acknowledged in fields such as visualization [25] and human-computer interfaces [2]. In simulation studies, the interactive exchange of arguments allows different types of users—including modelers, reviewers, and external stakeholders—to challenge specific parts of a study, explore alternatives, and to construct a common understanding and overall answer(s) to the research question(s).

Besides communication, another key objective in simulation methodology is automation [26]. Given the current argument graph, the involved models, requirements, assumptions, and literature references, new arguments and counter-arguments may be automatically generated and applied, allowing for a (semi-)automatic progression of simulation studies. Additional input to the generation may come from the documentation of related simulation studies and web-based sources.

4 Next steps

We introduced a vision for a dialectic model of simulation study validation based on an exchange of arguments and counter-arguments. Compared to checklists for documenting and conducting simulation studies [13, 18], this offers a complementary and more detailed view of the reasoning behind conducting simulation studies.

To make this vision a reality, the first step will be to refine and extend the formal dialectic framework. This will lead to an agent dialogue protocol defining a catalog of *moves* that proponents and opponents may make as part of a simulation study; *rules* describing how each move extends an *argument graph* encoding the current state of the simulation study; and analysis of argument graphs based on *abstract argumentation theory* to identify the set of arguments that are currently agreed to be valid by both proponent and opponent.

Another key next step would be to provide tools that make the approach accessible to developers of simulation studies. Following Schneiderman’s mantra of visualization—“overview first, zoom and filter, details on demand”—will help manage the complexity of documenting and conducting simulation studies: More coarse-grained

approaches, such as the checklists provided by TRACE [13], provide a good high-level overview, which could then be underpinned by more detailed arguments and dialectic documentation as and where required. An integration with TRACE—for example, realized in Jupyter notebooks [5]—would allow users to zoom in and filter on critical aspects and, subsequently, based on the presented approach, to hone in on arguments and counter-arguments to ensure validity.

Equally, tool support can allow a dialectic model of a simulation study to drive the development of the study and improve its documentation. For example, we can envision a tool that automatically generates suitable simulation experiments (building on existing work like [27, 28]) and executes them to generate moves that counter or support a proposed simulation model. Alternatively, tools could identify aspects of a simulation study that need to be reinvestigated when new information becomes available.

All such tool support needs to be developed in ways that cause minimal interference with the efficient development of simulation studies. To this end, co-creation with simulation developers and qualitative (possibly ethnographic) studies of simulation developers will be essential future steps. In addition, based on the prototypes, it needs to be evaluated, what benefits an argumentation-based approach (+ automation) brings to simulation studies. Key questions include: Do the different stakeholders, given this documentation, trust the results more? Has reproducibility been improved? When conducting a study with this approach, does a modeler reach the answer to their research question earlier? Have they gained additional insights? And how does this compare to other approaches for supporting and documenting simulation studies, such as using a workflow with provenance capturing?

An approach that allows scrutinizing simulation studies is particularly valuable in domains of high societal relevance and political dispute—for example, climate change [21], epidemics [12], or studies leading to the development of medical devices, where certification is essential [9]. This requires mechanisms and tools for making dialectic models of simulation studies accessible to non-technical stakeholders, including certification bodies, political decision makers, and the general public. Here, it will be valuable to explore what role generative AI and large language models can play both in extracting easily understandable, natural-language arguments from structured models, and in creating such structured models from natural-language narratives [15]. This has great potential for interactively and more effectively communicating and conducting simulation studies taking context and different users into account [26].

Acknowledgments

This work was partly supported by a seed-corn fund awarded through the EPSRC-funded MDENet network (grant reference EP/T030747/1) and the DFG (grant 320435134). We thank Peter McBurney, Odinaldo Rodrigues, and Sanjay Modgil for helpful discussions and feedback about agent dialogue and argumentation.

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