

**USING SIMULATION AND ARTIFICIAL INTELLIGENCE TO INNOVATE:
ARE WE GETTING EVEN SMARTER?**

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ABSTRACT

Artificial Intelligence (AI) is spreading into all walks of life and across disciplines. It is being used to explain, predict and optimize, often by creating and experimenting with models derived from data. Arguably, Modeling & Simulation (M&S) has doing this since the late 1950s. Our approaches are different to those used in AI but have some overlap. Both AI and simulation bring significant, different and potentially complementary benefits to end users. However, the majority of work is separate. Is there potential for innovation by bringing together these fields and their associated techniques? This panel explores the potential synergies of these relationships and considers major opportunities and the barriers to realization.

1 INTRODUCTION

The relationship between Artificial Intelligence (AI) and Modeling & Simulation (M&S) is a fascinating one. Although AI has a broader scope than M&S, the two fields do appear to have some common goals. Both seek to analyze systems to find some kind of understanding and ultimately to make informed (and potentially optimized) decisions based on evidence. AI techniques look at system data and derive structure and relationships in that data to analyze past trends and possible future outcomes. M&S techniques place some form of structure on a system and data (e.g., queuing systems, entities, agents, etc.) and then seek to investigate how a system might behave in different scenarios. These techniques have some overlap but are different. The question is whether or not AI and M&S are complementary or separate and what innovations might arise from the combination of the fields.

To investigate this, we bring together four leading experts in M&S and AI. This panel is the second at this conference in the “Using Simulation to Innovate” track. The first considers M&S and Digital Twins and discusses if we are getting “smarter” (in the sense of Smart Cities, Smart Manufacturing, etc.) Following this discussion, will combining AI and M&S lead to us getting “even smarter!”?

2 COMPLEMENTARY USE OF ARTIFICIAL INTELLIGENCE AND SIMULATION (YOUNG-JUN SON)

2.1 Complementary Use of AI and Simulation

Artificial intelligence (AI) and simulation are complementary techniques that can be used in an integrated manner to design, analyze, or control complex systems. This section provides two exemplary cases of such integration (see Figure 1): 1) simulation embedding AI, and 2) simulation embedding AI, which in turn is embedding simulation.

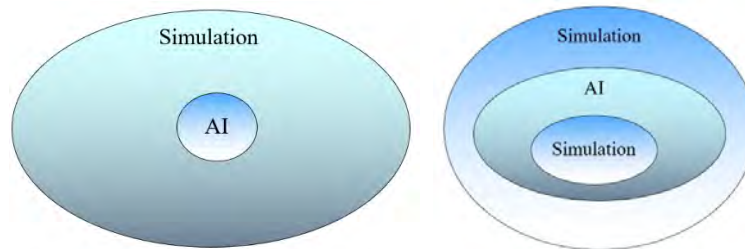


Figure 1: Two cases of Complementary use of AI and Simulation.

2.2 Case I: Simulation Embedding AI

Figure 2 depicts a simulation-based real-time planning and control framework for crowd tracking using unmanned aerial vehicles (UAVs) and unmanned ground vehicles (UGVs) (Lee et al. 2019). In the framework, simulation (three images in the bottom row) is used to devise optimal or near optimal policies via predictive analyses, and the devised policies are used by the control system (three images in the top row) to drive UAVs and UGVs to keep track of a group of targets. In particular, the second and third columns in the top row in Figure 2 depict what the UAV sees and what UGV sees, respectively. The UAV runs an optical-flow-based motion detection algorithm to detect a group of targets (Shi and Tomasi 1994; Lucas and Kanade 1981) while the UGA uses a histograms of oriented gradients (HOG)-based algorithm to detect an individual target (Dalal and Triggs 2005). These two algorithms are contemporary AI algorithms. The simulation systems of UAV and UGV (the second and third columns in the bottom row) in Figure 2 embed each of these AI algorithms, and are used to conduct predictive analyses.

2.3 Case II: Simulation Embedding AI Embedding Simulation

Figure 3 depicts an emergency evacuation simulation in response to a terrorist bomb attack (Lee et al. 2010), an extended belief-desire-intention (E-BDI) model to mimic a human behavior (Lee et al. 2010), and an illustration of Decision Field Theory (DFT) (Busemeyer and Townsend 1993), respectively. The behavior of an individual in the emergency evacuation simulation (the first figure) in Figure 3 is based on the E-BDI model, which was originally proposed to represent an optimal AI behavior (e.g., a robot in a robotic soccer team) but later extended by Lee et al. (2010) to represent human behaviors. Four major modules that constitute the E-BDI model are the belief module, emotion module, desire module, and decision module. DFT, which provides a mathematical framework to represent the psychological preferences of humans with

respect to different options during their deliberation process, is a key component of the desire module of the E-BDI. DFT is a micro-level simulator, and results in choice probabilities of each decision option based on the simulation outputs. In summary, the evacuation simulation embeds numerous humanized AIs, where each AI embeds a micro-level simulator as part of its decision-making mechanism.



Figure 2: Simulation-based planning and control framework for crowd tracking (Lee et al. 2019).

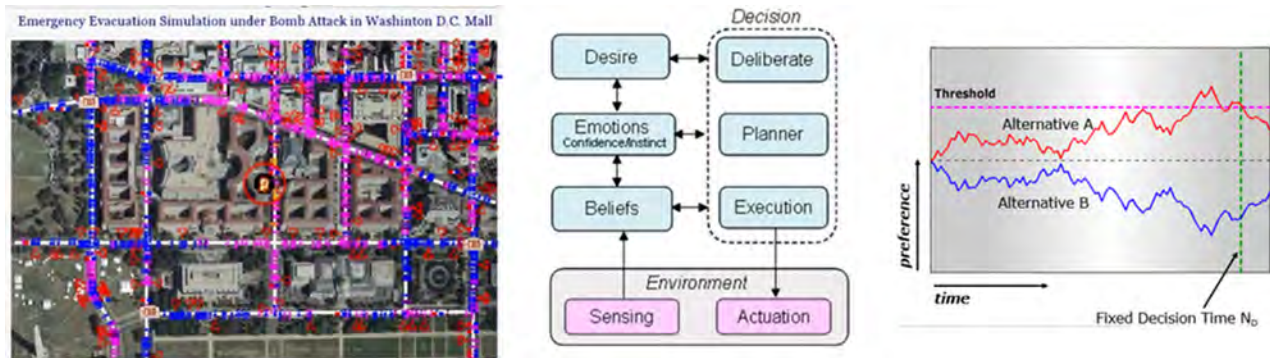


Figure 3: Emergency evacuation simulation (Lee et al. 2010), extended BDI framework (Lee et al. 2010), and Decision Field Theory (Busemeyer and Townsend 1993).

3 SIMULATION AND AI – BETTER TOGETHER! (JUERGEN BRANKE)

There are two primary paradigms of generating knowledge: deduction and induction. In case of deduction, one starts out with a set of generally agreed axioms, and then uses logic to derive (in fact, proof) new theorems which can then be used to derive further theorems. The advantage is that any derived theorems are guaranteed to be true if the underlying axioms are true. Induction, on the other hand, is analyzing data and deriving general patterns. There is no guarantee that the derived patterns are true, but they are often useful in practice and considered reliable until disproved. Research in AI has initially leaned on the first paradigm, using logic and rules to derive conclusions. This has proven difficult, and most of today's AI is following more the paradigm of induction, trying to learn from large datasets. As Axelrod (1997) has already pointed out, simulation provides a third way of generating knowledge. On the one hand, it is related to deduction, as it starts by building a simulation model, which can be seen as agreeing on a set of axioms. Given these axioms, or the inner workings of the model, it is possible to predict what will happen by simply running the simulation model and observing the variable of interest. On the other hand, simulation models are often stochastic, which means every time the model is run, the output is different. To derive general conclusions, one therefore has to run multiple replications, resulting in a possibly large dataset, that can

then be analyzed to derive general insights, just as would be the case for deduction, only that the dataset is not real-world observations but generated by the model. From this perspective, simulation can be regarded as a third approach to prediction and knowledge generation, complementing, even linking the two basic approaches to AI, the logic-based deductive approach and the data-based inductive approach.

Table 1 summarizes the key differences between simulation and the (nowadays predominant) inductive AI approach of deep learning. The key advantages of simulation are that it requires much less data than deep learning approaches, can be used to extrapolate to completely new simulations, and has high explainability. On the other hand, it requires a lot of domain expertise and is computationally time consuming to execute.

Table 1: Comparing simulation and deep learning AI.

	Simulation	Deep Learning
Domain knowledge	Requires a lot of expert domain knowledge to formulate the causal logic	Little domain knowledge required
Data	Little data required	Large amounts of data required
Computational speed	Slow to execute	Slow to train, but quick to predict
Explainability	Good explainability, model can be understood and traced by humans	Mostly black box and difficult to explain
Extrapolation and Interpolation	Can extrapolate to completely new situations	Very good at interpolation, struggles to generalize to previously unseen situations

However, often it is not a question which of the two techniques is preferable, but simulation and AI have to work together to achieve the best results. Below are some examples for typical combinations.

- **AI within a simulation.** If the system to be simulated includes intelligent machines then obviously an AI component has to be part of the simulation model. Similarly, if the system includes humans, and their adaptive behavior and learning ability are to be modelled, an AI component is needed within the simulation model, although in this case the purpose is more to replicate human behavior than to learn as quickly as possible, so the AI models human intelligence rather than machine intelligence.
- **Simulation within AI.** As explained above, standard deep learning techniques are not so good at extrapolating to completely new situations. Thus, if planning for new situations is required, a simulation model can be included in an AI for this purpose.
- **Simulation before AI.** To speed up exploitation, one can use a simulation model to generate data for many (also previously unseen) situations, then train an AI to derive general patterns.
- **AI before simulation.** To calibrate simulation models efficiently, AI techniques such as evolutionary algorithms or Bayesian optimization can be used.
- **Reinforcement learning.** In reinforcement learning, simulation and AI are tightly integrated, with simulation being used to simulate paths through the state space and the AI deciding on the actions to take and learning about the reward structure.

Let us look at two concrete examples for a successful interplay between simulation and optimization. Bongard, Zykov and Lipson (2006) describe a four-legged robot that can recover from mechanical failures. It has a simulation model of itself. If after a failure the actuator-sensor data doesn't match the expected data given the simulation model, the robot can adapt its simulation model, actively experimenting with its actuators to understand the new situation. Once the simulation model has been adjusted, the robot can use

it to quickly come up with a new gait that still works despite the failure. Prothmann et al. (2009) describe an observer-controller architecture for an adaptive traffic light system. On the lowest layer, a reactive traffic light controller is employed. The traffic is continuously monitored at the layer above, and this layer uses an AI to learn which of a set of reactive traffic light controllers is best suited depending on the traffic situation. So, if for example the traffic pattern has changed from morning traffic to evening traffic, the AI would simply replace the controller in use at the lowest layer by one more suitable for the new traffic situation. In order to handle completely new traffic situations such as after an accident or the end of a football game, a simulator in combination with an evolutionary algorithm is used to generate a new controller optimized for this new situation. This new controller would then enter the pool of controllers available to the AI on the middle layer, thereby broadening the range of situations it can react to.

4 SIMULATION AND AI – OUR ROAD TO SIMULATION-BASED DECISION MAKING (OLIVER ROSE)

Instead of starting a philosophical essay about getting smarter by means of technical artifacts, we will discuss some ideas about the principal strengths and weaknesses of simulation and AI to solve real world engineering problems, where AI means machine learning approaches in this section. If you are confronted with a problem the rough goal of your work is already given. In our (simulation) community, there is some kind of consensus that computer models are helpful in finding solutions to almost all sorts of engineering problems because they provide a rather well-defined way to describe the system where our problem lives in with respect to its structure and its behavior. This model is a reasonable way to discuss about its characteristics, in particular, about its performance. Because an abstract model is much simpler than the real world system, chances are high that we find a solution to our problem by means of experimenting with our computer model. If the model is valid, i.e., it is appropriate for our purpose, it should be possible to transfer the model-based solution back to the real world. The amount of abstraction or the level of detail, respectively, lies completely in the hands of the modeler and can be easily explained to an interested audience. The validation will be mainly based on measurement data from the real world system. When data is not available convincing assumptions will have to be made which require critical assessment. As a consequence, simulation models are white-box models where the modeling concepts, input data and assumptions are accessible even to practitioners who claim to have issues with abstract mathematical approaches. Apart from all those benefits, the main drawback of simulation models are their long run times. That is no problem for most of our performance analysis work but inhibits their application for online decision making.

At first glance, AI/machine learning models are completely different. Most of them are typical black box models. There is some input and you will receive the related output quickly but you don't see what is happening inside. They are abstract models of the structure and behavior of real systems, too, but there is not much to see at first glance what can be compared to the structure and behavior of a real system. In this perspective, machine learning models are typical forms of rather abstract mathematical models. They work well, often outperform more accessible problem solutions like simulation-based approaches with respect to accuracy and run time, but are less appealing to most human spectators. There is another difference: the whole model development cycle is completely data driven: the model selection, the model parameterization and the model evaluation are completely based on well-known statistical procedures. This is a big advantage because the modeler is not forced to work with assumptions about the system under consideration. The disadvantage, however, is that in the case of a lack of data it is not possible to overcome this problem by useful assumptions as in the case of simulation models. Thus, we need to find a way how to generate missing data for machine learning approaches. Here, simulation models come into play again. As soon as we have a validated simulation model, we are able to create huge amounts of basically any data about the real system at almost no cost, at least, compared to collecting data directly from the real system.

This generation process is called data farming because it is like harvesting data from a computer simulation field after growing the data crops under controlled experimental conditions. Data farming can

support all kinds of machine learning approaches. In this context, it might be useful to outline that briefly for dispatching jobs in a job shop as a sample problem.

- Unsupervised learning: create data for the clustering of state vectors which are needed to judge the current situation in the job shop. This is a reasonable approach to simplify the problem via dimensionality reduction of the input data.
- Reinforcement learning: create as many (clustered) state – action pairs as possible and assess their future reward, where actions are dispatching decisions. This will become the data basis for an approximate solution of the related Markov decision process optimization.
- Supervised learning: create data for learning the functional relationship between a dispatching decision and its resulting performance. This will facilitate future online decision making.

On one hand, the application of simulation-based data farming can solve one of the biggest issues of machine learning: the lack of appropriate data. On the other hand, it introduces the dependence on potentially questionable assumptions through the backdoor because we no longer have to deal with real data but simulated data, where the generating model might depend on assumptions. Therefore, both the simulation model and the machine learning model have to be validated very carefully. Depending on the type of computer simulation models, the ability to do data farming at a large scale with hundreds or even thousands of simulation replications running in parallel may also require a considerable investment in computer hardware and simulation licenses.

Nevertheless, this combination of simulation models, (offline) data farming, and (offline) machine learning is a big step forward in simulation-based decision making support. So far, online decision making by means of running a number of simulation experiments was practically impossible due to the prohibitive run times. Performing data farming independently from the decision making process and saving the data which will be required for future decisions in a data base or, even better, teaching a machine learning approach from it, can become a viable solution for simulation-based online decision making.

5 INTEGRATE TO INNOVATE (SUSAN M. SANCHEZ)

A panoply of prepositions can be used to describe how AI and simulation might be integrated. AI can be used *before*, *within*, or *after* simulation for different purposes. Simulation can be used *for* or *over* AI. Finally, the external perceptions of simulation and AI may influence the ways that tools and methods from these fields are (or are not) used synergistically in the future.

AI can be used *before* running a simulation model as a way to improve the way we represent complex, interdependent simulation input data. It may find patterns in the real-world data that merit modeling. Additionally, it may generate questions that could guide the use of a simulation model by pointing out experiments that might need to be run. Consider a simulation of an urgent care clinic where patients may need a variety of screening tests before receiving medical treatment. If data are available only at the aggregate level, input modeling may focus on marginal distributions, such as the numbers of patients sent for x-rays, blood draws, or other types of labs; or the service times for these procedures. Requirements for simulated patients obtained via independent draws from marginal distributions may not pass a Turing test for face validity. A great deal of interaction with subject matter experts (health care workers) may be required to understand key dependencies in the data. In contrast, applying AI to detailed patient-level data may be a better and faster input modeling approach. For example, clustering algorithms could create patient subgroups with different sets of needs for separate input models, or neural networks could predict service times based on patient demographics or the current state of the clinic. One guiding question this raises relates to the appropriate level of detail. How many patient subgroups are appropriate? What subset of the clinic state information is sufficient? Issues such as these may arise during conceptual model development, but sometimes running the simulation can answer these “what if?” questions directly.

AI can also be used *within* a simulation in several ways, as other panelists describe. In the future, we need more learning agents and living simulation models. Many of the agents in current agent-based

modeling platforms use rule-based decision making, but most often these rule sets are static. There are opportunities for leveraging AI to have agents evolve during a simulation run, and have the models themselves evolve over time. But there is larger question that needs to be addressed by an integrated AI and simulation approach—namely, what will happen as greater numbers of *learning* systems and devices with embedded AI are released into the world? Over time, these may behave very differently based on their individual uses and local environmental conditions. Imagine multiple self-driving cars with identical embedded learning AI algorithms. Some are used primarily for short trips in urban environments, others primarily for longer highway travel. Traffic simulations must incorporate this learning behavior if we hope to understand the safety these AI algorithms will provide in the future.

If software “hooks” are built into simulation models in order to pull in either raw data or AI products, that opens up possibilities for deeper (and potentially more insightful) analysis. Automated links between data capture devices and simulation modeling environments will certainly permit allow real-time or near-real-time reflections of the status (traffic congestion on a city-wide road network, work-in-process in a manufacturing facility, etc.). They also facilitate other types of exploration and analysis. Software hooks would also make it easier for federations of models to share information. In many defense and homeland security applications, for example, we have observed that detailed results from engineering-level models may be summarized into a single statistic (such as mean performance) before passing things up to an operational-level model. This can result in greatly underestimating the operational risks. Making it easy to switch back and forth between trace-driven inputs, empirical input distributions, and parametric input distributions may improve the insights gained from the simulation study. It may also increase the buy-in from decision makers if we can answer “what if we had done this in the past?” and “what if we do this in the future?” using a single simulation model.

There are huge potential benefits for employing AI to the simulation output data *after* running a simulation, particularly if you have conducted a data farming experiment. Smart analysis agents could search through mountains of multidimensional output data for interesting patterns, and alert the analyst of their findings. This could greatly accelerate the process of verification and validation during model development, and streamline the process of extracting actionable information from a mature simulation model. Similarly, AI findings from a massive metamodel sensitivity analysis might suggest the next round of questions an analyst or decision maker might ask, or identify interventions for direct experimentation, or identify situations where a metamodel should be updated or its region of applicability expanded or contracted. There are many research opportunities for developing AI methods that leverage the special structure of output data generated from well-designed simulation experiments.

Simulation *for* AI refers to the use of data farming experiments to transform some of the art of current machine learning methods to more of a science. For example, data farming can be used to support algorithm development and testing via either synthetic data generation or via systematically investigating the choices of the many algorithm parameters and their joint effects on its performance (Sanchez 2020). These might be considered way of “optimizing” an AI algorithm for a particular application, or “robustifying” the default parameter choices for that algorithm. Simulation for AI also includes sharing the best practices our community has developed over the years, as we have wrestled with ways to deal with complex problems. These include the concepts of repeatability, traceability, uses of randomness, model verification and validation, common random numbers, and more.

It is important to recognize that not all studies need to involve AI—there are times when simulation should be preferred *over* AI. Simulation and data farming provide “better big data” for decision making, by identifying the most important cause-and-effect relationships between the inputs and outputs. This inferential big data differs from the observational big data and digital dust that surround us, where relationships are correlative and not causal. The understanding that simulation can be used to make investigate systems and situations that do not yet exist, or that are too dangerous or costly for real-world experiments to be viable, is a foundational simulation concept—but may not be obvious to those with an observational big data worldview (Sanchez and Sanchez 2017, Sanchez 2018).

Perceptions of AI and simulation are important. On one hand, the general public may be becoming more comfortable with computerized and computer-based decisions, and the rapid increase in the number of data science and analytics professionals may mean that decision makers are more likely to rely on AI or simulation (Elmegreen et al. 2014). On the other hand, some will remain skeptical of model-based approaches. The simulation community must continue its outreach efforts so the benefits of causal model-based decision making do not get overlooked.

Combining simulation, data farming, and AI creates a very powerful approach for problem solving. As the saying goes, “with great power comes great responsibility.” Let us take this responsibility seriously as we seek to address some of the big problems the world faces. As researchers and analysts begin to explore the joint use of AI and simulation, this may lead to other and even more innovative ways of melding tools and methods from these fields. In other words, we may need a longer list of prepositions to capture the types of integration that will occur in the future.

6 CONCLUSIONS

This panel has discussed the relationships between AI and M&S. Son discussed using these in an integrated manner to design, analyze, or control complex systems and gave examples of AI embedded within simulation and vice versa. Branke considered the theoretical bases of both fields and discussed how these complement each other. His views extend Son’s examples with a wider range of AI/M&S relationships. Rose continued these examples and highlighted the issues of black-box AI versus white-box M&S methods and their roles with respect to situations where data are rich or sparse. Finally, Sanchez provides a wide range of views to consider the relationship between AI and M&S from other perspectives. Overall, the conclusion to this panel is that there are major advantages to creating combined AI and M&S approaches and that by developing these we could indeed become “even smarter!”

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