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HYBRID MODELING INTEGRATING ARTIFICIAL INTELLIGENCE AND MODELING & SIMULATION PARADIGMS

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ABSTRACT

This paper discusses the complementary relationship between Modeling and Simulation (M&S) and Artificial Intelligence (AI) methods like machine learning. While M&S uses algorithms to model system behavior from input parameters, AI learns patterns from correlation in data. The paper argues that hybrid models combining M&S and AI can be more powerful than either alone. It provides a conceptual framework showing how M&S and AI can be integrated in sequential, parallel, complementary or competitive configurations. Several example applications are given where AI enhances M&S and vice versa, such as using AI to optimize simulation parameters, generate synthetic training data for AI from simulations, interpret AI model behavior through simulation, and automate aspects of simulation development with AI assistance. The potential benefits of hybrid AI/M&S modeling span improved accuracy, efficiency, trustworthiness and cross-disciplinary collaboration. The paper calls for further research developing a solid theoretical foundation for merging these complementary paradigms.

1 INTRODUCTION

When I started my career in Modeling and Simulation (M&S) some decades ago, I often heard that only people who were unable or unwilling to come up with a mathematically formulated operations research (OR) solution would use simulation. Textbooks on such OR methods are still used today in new editions (Hillier and Lieberman 2020) and are still very valuable, but the assumption that all problems can be solved by these methods has been proven wrong. A new class of problems emerged under the term *deep uncertainty* (Marchau et al. 2019) that is characterized by the observation that analysts do not know, or the parties to a decision cannot agree on the appropriate conceptual models that describe the relationships among the key driving forces that will shape the long-term future, the probability distributions used to represent uncertainty about key variables and parameters in the mathematical representations of these conceptual models, and/or how to value the desirability of alternative outcomes.

How do we formulate a mathematically accurate solution under these circumstances? If we use big data approaches to collect a set of unbiased training data, we can train neural nets to replicate the observed correlations and interpolate between them. But even overview articles on explainable approaches document that the approaches still fall short, particularly for users with domain expertise, but often with insufficient knowledge about how neural nets work(Samek et al. 2019; Joshi et al. 2021). Gaining deeper understanding still requires algorithmic approaches to transfer observations into predictions codifying the correlations observed as functional interdependence using domain knowledge, which is what simulation do. In summary, if you can formulate and solve a mathematical problem describing the observation, you should do so. If you have a clear understanding of the functional interdependence, you should write a simulation implementing it. If you have data describing the dynamic development of the system, use them to train your neural net.

There are many more Artificial Intelligence (AI) methods than machine learning (ML) based on neural nets (NN), such as expert systems, a variety of heuristics for optimization including genetic algorithms, natural language processing and computer vision, and more. There is no universal definition of AI, and multiple taxonomies do exist. The view on AI methods and paradigms in this paper is shaped by how they can be integrated into hybrid modeling and simulation approaches. An additional reason we focus on ML and NN is that AI solutions that take advantage of neural nets and big data made tremendous advances in recent years (Wang et al. 2020). This includes the rise of large language models (LLM) (Chang et al. 2023). Although the recommended conceptual representation of hybrid AI and M&S solutions is applicable to all methods, the focus of most examples used in this paper will be on the recent AI methods, particularly as they are often seen as competition to simulation solutions.

This paper makes the case that the full potential of these approaches comes to bear when hybrid modeling is applied. As discussed by Mustafee et al. (2017), a hybrid is the result of merging two or more components of different categories to generate something new, that combines the characteristics of these components into something more useful. The paper uses the definitions of hybrid modeling introduced by Mustafee et al. (2018). An example of hybrid modeling using M&S, Artificial Intelligence (AI), and data analytics is published in our documentation of the COVID-19 Healthcare Coalition (Tolk et al. 2021): In the earlier phase, the dynamics of the systems were not known, but slowly more and more data became available, allowing to construct forecasting models based on neural networks. As the COVID-19 Healthcare Coalition's understanding of the system increased, they were able to use more simulation approaches, such as those described by Mucenic et al. (2021), to make theory-based prognoses. In later stages, these complex, computationally intensive simulations were used to provide training data for neural nets, enabling the creation of faster, less resource-intensive substitute or surrogate models.

In this paper, these approaches using M&S and AI methods and paradigms to support common research are generalized, extending the framework for a conceptual representation of hybrid methods introduced by Mustafee et al. (2020).

2 HYBRID MODELING AND THE DIKW PYRAMID

The introduction to the Data, Information, Knowledge, and Wisdom (DIKW) Pyramid is attributed to Ackoff (1989), as shown in Figure 1.

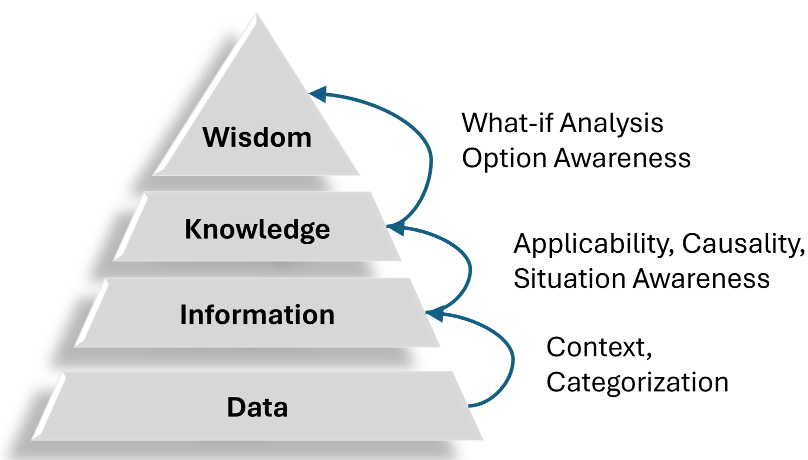

Figure 1: The Data, Information, Knowledge, and Wisdom Pyramid.

Ackoff proposes that data themselves are merely a collection of facts that need contexts to be interpreted. Only in their context, data make sense and become information. This is the realm of data analytics: creating information from data. Without data analytics, we do not have a real understanding about what the data we are working on mean, where it comes from, how reliable the sources are, how old the data is, etc. Neither AI nor M&S can provide credible results without reliable data.

To gain knowledge, information must not only comprise factual data, but also causality, relations, and more system specific data that can not always be captured exclusively by pure data analytics. There are sub-fields of data analytics, often referred to as diagnostic data analytics, that are interested in identifying causalities behind observed correlations, but this always requires a creative element of generating hypotheses that can be tested on the given data set. In any case, moving from data modeling to system modeling is a necessary step to gain knowledge from information. This knowledge then allows the conceptualization and implementation needed to develop simulation systems, which are needed for the next increase.

Wisdom, which is at the top of the DIKW pyramid, requires not only knowing what is and how we got there, but also being aware of options and their consequences (Pfaff et al. 2013), possible developments in the system that do not require active participation, and uncertainty quantification. Awareness about possible emergent behavior also falls into this category.

Methods from various disciplines contribute to this process. Hybrid modeling already has been identified as an enabler for cross-disciplinary work (Tolk et al. 2021). In the next sections, several examples will show how hybrid modeling can support the successful collaboration between M&S and AI.

3 FORMS OF HYBRID SOLUTIONS

Examples for hybrid M&S applications are often describing complementary contributions using different paradigms that are executed in parallel to provide hybrid solution for the given challenge. That is not the only option, as this section shows, which extends the ideas presented Byrne et al. (2023).

3.1 Complementary and Competitive Hybrid Solutions

Beside scope, structure, and resolution, different simulation solutions can not only differ in the simulation paradigm, but also in underlying assumptions and constraints underlying the solutions. As demonstrated in Tolk et al. (2013), it is possible to capture the characteristics of simulation solutions using ontological means. Such an ontological reference model allows for the identification of inconsistencies in the underlying assumptions and constraints. If such solutions are composed into a new hybrid solution, these inconsistencies in the assumptions can potentially lead to unjustified decisions based on contradicting theories.

Hofmann et al. (2011) already introduced the idea of referential and methodological ontologies earlier. While a referential ontology describes *WHAT* is modelled, capturing what parts of the real-world referent are modelled and at what resolution, a methodological ontology describes *HOW* the referent is modelled, capturing the paradigm and abstraction level. As the resulting ontologies are machine readable, they provide the mathematical basis to decide if two solutions are dealing with the system of interest on the appropriate abstraction levels, using paradigms that do not lead to inconsistencies.

This provides the necessary tools to decide if two – or more – hybrid solutions are complementary, as they contribute to different facets to the understanding of the system of interest, or competitive, as they provide answers based on different assumptions and constraints. The former justifies building compositions of the hybrid solutions that are also referred to as federations. They provide based on consistent theory, from which the assumptions and constraints are derived, that allow to understand the system of interest from different facets and even on different abstraction levels, leading to multi-scale simulation that allow to evaluate systems across various scale in scope, space and time (Qu et al. 2011). However, while multiple approaches assume consistency of theory, assumptions, and constraints, the ontological structures allow to prove them.

The consistent representation of truth was used to define composability by Taylor et al. (2015). When two contributing components both define a truth value regarding the state a system is in, these values must be identical. One component cannot contradict another, nor can the truth value depend on which component is used. To ensure this, the underlying models need to be conceptually aligned (Tolk 2024). This holds true for all model-based methods, i.e., for M&S as well as for AI methods.

However, while conceptual alignment is a requirement for the development of compositions or federations, competitive solutions can still provide insight when applied in the form of ensembles, which extends the idea of differently parameterized simulation solutions (Matković et al. 2018). Instead of showing the spread of results based on different initialization of the initial parameters, these ensembles show the result based on different assumptions and constraints, possibly representing different theories behind them. This is of particular interest for applications in cross-disciplinary teams and in support of social sciences, as described in (Wildman et al. 2017; Tolk et al. 2021), among others.

3.2 Sequential and Parallel Hybrid Solutions

The next distinction involves the use of hybrid solutions either sequentially or in parallel. While simulation interoperability standards traditionally focus on parallel execution of hybrid solutions, where two or more solutions are synchronized or orchestrated via the standard – as described by Zhang et al. (2006) –, such complex solutions aren't always necessary.

For many purposes, which will be detailed in the following section, a sequential application of the solution is possible. Even though synchronization or orchestration of events and time advances isn't required for such common use, the application of common theoretical foundations, along with their assumptions and constraints, is still necessary. It's essential to map the data provided by the first solution to the initial parameters needed for the second solution, at least for the overlapping scope. This is necessary but not sufficient, a fact often overlooked because the use of a common theory is assumed, which isn't always the case.

3.3 AI within M&S, and M&S within AI

In practice, AI algorithms and heuristics are often applied within M&S solutions and vice versa. For instance, agent-based simulations frequently use AI methods to enable their synthetic software agents to act more intelligently, as described by An et al. (2023). The use of expert system like rule sets and neural nets to create situation adequate behavior has long standing traditions. In defense applications, the term *semi-automated forces* is often used to express that the simulated forces do not follow a script but some form of decision rules.

This principle also applies to AI methods. For example, AI solutions can generate a set of potential courses of action and then use M&S to simulate each one to determine which is most likely to succeed, which is most stable, etc. In complex adaptive decision spaces, estimating the effects and side effects of decisions is not straightforward, making simulation a viable option.

The concept of integrating of AI within M&S, and M&S within AI, can be fractal: A simulation can use internally an AI solution that itself uses an M&S solution, which uses internally an AI solution, and so on. Figure 2 shows a conceptual view of the combinations of AI and M&S discussed in the subsections.

On the left side, M&S is central and can use AI to pre-process and post-process data sequentially, or can form a federation in parallel. As mentioned, AI and M&S methods can also be used internally. The right side displays the version with the AI solution at the center. It's important to note that this conceptual view assumes that conceptual alignment has been confirmed for the combinations. If this is not the case, the solutions must be conducted individually and their results projected into a common solution map for comparison.

Depending on which paradigm the driving force is, the Gartner Report (2023) on innovation insight on AI simulation addresses these combination as simulation-assisted AI and as AI-assisted simulation.

3.4 Examples for the mutual support of AI and M&S

AI and simulation can mutually support and enhance each other in several ways. The following are non-exclusive examples of such support, as well as the different forms of hybrid solutions discussed earlier.

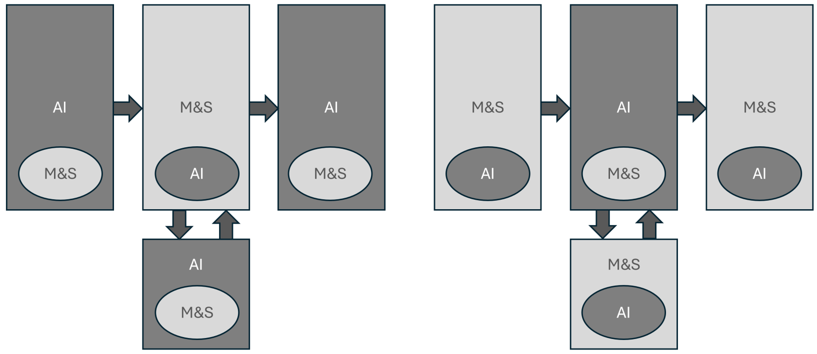

Figure 2: Conceptual view of combinations of AI and M&S.

- Machine Learning for Simulation:
  - Machine learning algorithms can be used to build accurate simulation models by learning patterns and relationships from real-world data (Osoba et al. 2020). These surrogate models can then be used to simulate complex systems, processes, or scenarios more realistically (Rackauckas et al. 2022) and usually significantly faster. It also allows to transfer surrogates of simulations requiring high-performance computing environments to personal computers or laptops, so that users can benefit from the simulation results without requiring the expensive environment.
  - The surrogate model reproduces not only the training sets but interpolates solutions in between the observed training data. The requires less computational resources than the original simulation system (Koziel et al. 2011).
  - To avoid becoming a victim of hallucinations, i.e., the LLM provides a reasonable but nonetheless incorrect solution, the simulation can be used to validate such results and – in case the LLM solution deviates too much from the simulation result – used to generate additional training data.
- Simulation for Training AI/Machine Learning Models:
  - Simulations can be used to generate large amounts of synthetic data for training machine learning models. This is particularly useful when real-world data is scarce, expensive, or difficult to obtain. In particular in medical applications, the provision of realistic while not being real data is pivotal due to privacy concerns and legal constraints (Walonoski et al. 2018; Al-Ars et al. 2023).
  - Simulations can also be used to create diverse and controlled environments for training AI agents, such as in reinforcement learning for robotics or game AI. This is particularly important for safety-critical applications, such as autonomous vehicles or robotics, where real-world testing may be risky or impractical. As such, they can become realistic testing grounds (Nhan et al. 2015).
  - Simulations can also be used to stress-test AI systems under various scenarios and edge cases, including scalability of solutions.
- AI for Simulation Optimization:
  - AI techniques, such as optimization algorithms and heuristic search methods, can be used to optimize and improve simulation models. The use of genetic algorithms or heuristics like simulated annealing is described in a myriad of publications.
  - AI can help find optimal parameter settings, identify key factors influencing the system, and explore different scenarios more efficiently (Page et al. 2012).

  - In the context of systems engineering, AI can be used to optimize the design of simulated systems, such as aircraft or vehicle designs, by exploring a vast design space of respective digital twins (Tolk et al. 2022).
- Interpretability and Explainability:
  - Simulations can be used to understand and interpret the behavior of complex AI and machine learning models. By simulating the input-output relationships and internal dynamics of these models, researchers can gain insights into their decision-making processes and identify potential biases or limitations. This can aid in the development of more transparent and trustworthy AI systems.
  - Moving from data-driven forecasting using AI solutions towards knowledge-driven prognosis of M&S solutions increases the understanding of complex socio-technical systems (Tolk et al. 2021).
- AI Supporting Simulation Development
  - Generative AI has been shown to increase productivity when utilized in the simulation development process (Giabbanelli 2023).
  - Fully automated simulation development is a topic of ongoing research, but generally still in its infancy (Frydenlund et al. 2024). Nonetheless, for some specialized application domains that are well documented and understood, some promising results have been published (Jackson et al. 2024).
  - An interesting application is also to translate existing simulation code back into English (Jackson and Rolf 2023).

Overall, the synergistic combination of AI, machine learning, and simulation can lead to more accurate and efficient modeling, improved training and evaluation of AI systems, and deeper understanding and interpretability of complex models and processes. The topic of mutual support is not new and discussion in the OR field go back several years, as presented by O'Keefe and Roach (1987). Accordingly, the enumeration provided here only scratches the surface and invites further research.

4 UNIFYING CONCEPTUAL REPRESENTATION OF HYBRID AI/M&S SOLUTIONS

Mustafee, Harper, and Onggo (2020) provide an inclusive definition for the various types of hybrid M&S solutions and give classification examples. In their work, they follow the example of the OR community, as introduced by Shanthikumar and Sargent (1983), by integrating hard OR methods, working with quantitative methods, and soft OR methods, applying qualitative methods. The various types of hybrid M&S solutions all fall into the quantitative method sections, as simulations provide numerical insight into the dynamic behavior of the simulated system of interest.

There is no generally accepted taxonomy for AI methods, and the borders between them are fluid. One of the pioneers in AI, John McCarthy, is attributed with the phrase *"As soon as it works, no one calls it AI anymore."* Several optimization algorithm that originated in the realm of AI are today accepted OR methods. Rule sets developed in expert systems become standard solutions for control algorithms. This overlap between hard OR methods is prevalent for heuristics and symbolic – or algorithmic – AI. Logic-based AI solutions include such methods as well, but are already extending towards qualitative applications. Neural nets, machine learning, and LLMs are applied in both quantitative and qualitative application fields. Figure 3 extends the conceptual representation of Mustafee et al. (2020) with these three broad taxonomic groups.

Adding AI methods to the recommended unifying conceptual representation is challenging, as their categorization can easily become ambiguous. Like simulation, AI is a computational tool that predominantly uses quantitative methods, but using methods that support reasoning with uncertainty clearly touches the realm of qualitative support. Furthermore, AI methods do not only support decisions, but often bear the promise to become real decision tools, including their use in high-consequence areas, such as defense

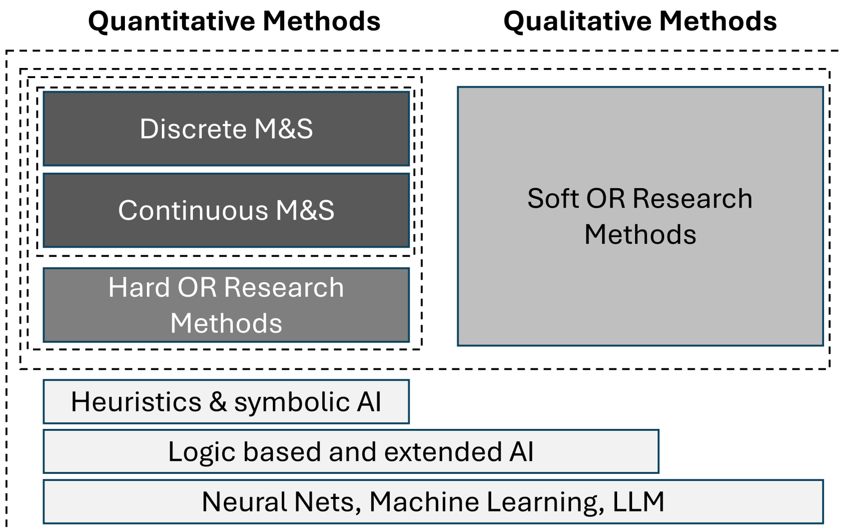

Figure 3: Conceptual representation of hybrid AI and M&S solutions.

and healthcare. As mentioned in the introduction, in current discussions AI methods are often reduced to LLM and ML approaches, as these are the methods that are providing very promising results, but expert systems, heuristics, and other related methods rooted in symbolic AI still have their place, and logic remains a common building block of many AI methods. But there are extended AI methods that are touching quantitative methods, and NN, ML, and LLM already bridging the gaps between qualitative and quantitative approaches. As the application of hybrid solutions is well known in the AI community and often referred to as multi-modal AI (Acosta, Falcone, Rajpurkar, and Topol 2022). This should facilitate integration into the conceptual representation, as more detailed taxonomies for multi-modality are being developed. Such a taxonomy needs to be more detailed and address the many AI methods and paradigms we did not even touch in this paper, such as natural language processing, computer vision, knowledge representation, and additional methods extended probabilistic and logic-based reasoning.

In the context of this paper, the emphasis lies on the quantitative AI methods, but as argued by Mustafee et al. (2020), extending our possible support beyond the traditional boundaries is worth to exploit further. If we can use LLMs and other generative AI methods to not only elicit knowledge from groups that we want to model but create valid simulation solutions, such as envisioned in recent publications (Jackson et al. 2024; Frydenlund et al. 2024), the objective of better participatory integration of all relevant stakeholder groups becomes possible (Tolk et al. 2022).

5 DISCUSSION AND CONCLUSION

M&S contributes significantly to challenges addressed by OR and related disciplines (Mustafee et al. 2020). The breadth of our discipline has recently been captured in a first compilation of the Body of Knowledge for M&S (Ören et al. 2023). Within this book, the section on "Synergies of Artificial Intelligence and M&S," which is part of the chapter "Synergies of Soft Computing and M&S," provides additional insights, but many open research questions remain.

As demonstrated by the references of this paper, there are already multiple examples of the successful hybrid combination of M&S and AI methods and paradigm. What is missing is a systematic literature review to provide a solid foundation for future steps. In addition to identifying these papers, a significant portion was published several years ago and could not foresee the recent developments in the field of generative AI and machine learning. Although this paper could only provide a limited survey, it hopefully can serve as a starting point to conduct such a review.

A topic that deserves more attention in both communities is the question of trust. The traditional view that humans trust and technology is trustworthy is currently reviewed by the human-machine collaboration community. Interestingly, the M&S community increasingly has to address this challenge as well, as the results of simulations -– particularly of complex adaptive social-technical systems -– become as hard to explain as the results provided by neural networks or LLMs. The ideas covered by Harper et al. (2021) may help to address the issue of trust in AI as well, such as described among others by Rossi (Rossi 2018). Such synergies are not in the traditional scope of hybrid solutions, but may prove to be very important due to their practical implications.

Another topic of shared concern for M&S and AI is obtaining and curating data, as recently discussed by Mustafee et al. (2023). The challenge of data carrying a bias is well known, as discussed among other by Roselli et al. (2019). As published by Tolk et al. (2021), such observations are documented for M&S as well. As already observed by Roman (2005), data are as important for simulation as the algorithms, and in the age of supporting cyber-physical systems and digital twins, the importance of obtaining and curating data has not diminished.

In summary, the current conceptual representation of hybrid M&S solutions must extend beyond the OR methods and embrace AI methods as well. These ideas have a long standing at the Winter Simulation Conference (Lavery 1986; Rothenberg 1989). In practice, the synergy of M&S and AI is already utilized, but we as a coalition of both disciplines must now provide a solid foundation. The domain of hybrid modeling and simulation is the forum to make this happen. This paper is a call to action, providing arguments and an extended conceptual representation of hybrid solutions to shape such efforts.

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