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LOOK TO THE FUTURE! SIMULATION BY 2050 AND BEYOND

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ABSTRACT

The advancement of Artificial Intelligence (AI) has accelerated the transformation of simulation from a tool for analysis and design into a dynamic partner for decision-making and operation. As AI systems become more capable of learning, reasoning, and adapting, simulation is evolving into an intelligent, autonomous, and predictive framework for exploring complex futures. This paper brings together future-oriented perspectives from simulation scientists and AI experts to discuss the current AI-simulation integration and both near-term and long-term outlooks for innovation, collaboration, and disruption.

1 INTRODUCTION

Advances in disciplines such as computer science, data science, and operations research in recent years have greatly contributed to the field of Modeling and Simulation (M&S). While many people associate simulation with computers and digital technology, its origin can be traced back to the dawn of human civilization (Grieves and Hua 2024). Prehistoric hunters would mentally run through different scenarios when planning their next hunt, such as how best to encircle and drive the mammoth off a cliff without harm. As human knowledge expanded, more mathematical rigor was introduced into M&S. Pierre-Simon Laplace used differential equations to model gravitational forces between celestial bodies, laying the foundation for computational simulations. The invention of computers brought simulation into the modern age, where it has been applied to increasingly complex systems. In fact, modern system complexity has reached a level where mathematical reductionism alone is no longer sufficient to provide meaningful insights.

Artificial Intelligence (AI), on the other hand, is a more recent phenomenon closely linked to the development of computer science. Its goal is to equip computational systems with the capability to perform tasks that traditionally require human intelligence, such as learning, reasoning, and decision-making. AI as a discipline traces its roots to the 1950s, built upon the work of Norbert Wiener, Alan Turing, and Claude Shannon. In the ensuing decades, AI research has undergone cycles of unbridled optimism and periods of tempered skepticism (“AI Winter”), reflecting its competing visions and technical challenges.

Today, both simulation and AI play critical roles in revolutionizing industries and society at large. From a data-centric perspective, simulation can be put into action without requiring large amounts of data *a priori*, whereas AI depends on Big Data. A growing convergence between simulation and AI is also emerging: simulation can harness AI to achieve greater autonomy, while AI development can leverage simulation to study “what-if” scenarios for safe and ethical deployment. Researchers across both fields are collaborating to unlock the full potential of these complementary disciplines in addressing complex problems and developing ground-breaking applications. This synergy is illustrated in Figure 1, which highlights how intelligent simulation arises at the intersection of realistic system representation and intelligent data-driven automation.

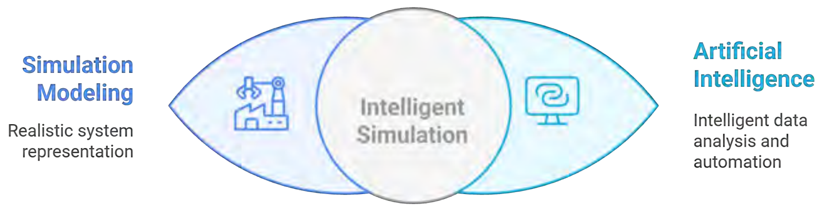

Figure 1: The convergence of simulation modeling and artificial intelligence enables intelligent simulation.

This paper summarizes the current landscape of AI and simulation and outlines a forward-looking vision of their evolving synergy. It explores the roles these disciplines will play in advancing and safeguarding a society increasingly embedded with intelligent, and potentially sentient, machines. The perspectives presented reflect the authors' own views. Throughout this paper, the term *AI* is used broadly to include Artificial Intelligence, Machine Learning, and related data-driven approaches.

1.1 Simulation Principles for AI

Sound principles and theories have formed the foundation for the development of dynamical models (McCarthy 1959; Simon 1962; Von Neumann 1966; Arbib 2012). An underpinning idea has been to conceptualize systems as having *inputs*, *state-based operations*, and *outputs* that involve the passage of time. For example, the underlying principle of event handling at arbitrary times is formalized through different kinds of deductive models to simulate discrete-event dynamical systems (Ho 1989). Such mathematical formalisms are grounded in domain-neutral modeling languages to develop domain-specific models.

The elemental theories and principles, founded on *intuitive* human knowledge and laws of physics, make it possible to formulate and answer questions about specific systems. These models describe the inner workings of systems, for example, as discrete- or continuous-time equations for some acceptable input to predict the evolving (deterministic or stochastic) model's dynamics and output. In contrast, *inductive* models, such as artificial neural networks, are generated based on observed input and output data. Unlike deductive simulation models, generative AI models often require vast amounts of data and computational resources. Incorporating the benefits of the principles and theories embodied in simulation models into the AI capabilities (and vice versa) may lead to more accurate, explainable, and reproducible predictions.

Indeed, there is a growing interest in inductive AI models that can incorporate various kinds of knowledge (e.g., algebraic equations and predicate calculus) to reach or exceed the capabilities of deductive simulation models (Von Rueden et al. 2021; Wu et al. 2022). A basic expectation for generative models is to achieve or surpass the accuracy of simulation models, particularly for safety-critical real-time systems such as automated transportation (Yan et al. 2025). By mid-century, combinations of simulation and AI models may reach the capability to match the complexity and scale of their real-world counterparts. Self-generating models could conceptualize and predict the structures and behaviors of futuristic systems (e.g., socially aware robotic nurses) and existing systems (e.g., human biology). This highlights the need for the development of executable models capable of (self-)reasoning for diagnostic and prognostic purposes.

Outlook 1: A promising direction is the development of simulation-informed foundation models that embed system constraints and governing equations into learning architectures. These hybrid models could offer stronger generalization, particularly for physical systems where data are scarce or costly to collect.

Achieving near scale-free computation with today's simulation engines and host platforms remains impractical. As a result, combining simulation and AI can enable *hybrid models* where each part has its own data, operation, temporal, and spatial resolutions (Davis et al. 2000). However, hybrid modeling introduces challenges because the composed models often differ in their structural representations, behavioral logic, and interpretation of time and events (Alur 2015; Zeigler et al. 2018). These challenges become even more critical when such models are developed for safety-critical, real-time socio-technical systems.

Outlook 2: To ensure trust in hybrid AI-simulation systems, future research must focus on standardizing model integration frameworks. This includes defining interoperability protocols, data fusion standards, and verification and validation methods suited for multi-resolution, multi-temporal environments.

1.2 Key Enablers for AI-Driven Simulation

When discussing simulation enablers, the focus is typically on the tools and methodologies necessary for building scenarios and explicitly understanding system limitations. For experienced practitioners, it is important to follow a systematic process and carefully address data details, parameter definitions, and abstraction of the system under study. This applies mainly to Discrete Event Simulation (DES), but also broadly to Agent-Based Simulation (ABS) and System Dynamics (SD), where systems are modeled as sequences of events that change system states at specific times. Key steps include (with potential future enablers noted in parentheses):

1. **Define Objectives and Scope**, including limitations.
2. **Map the Process and Identify Components** (future: ontologies and tailored digital twins).
3. **Collect, Provide, and Analyze Data** (future: Qualified Synthetic Data (QSD) and digital twins).
4. **Build the Simulation Model**. Simulation software like AnyLogic or Simio is highly useful.
5. **Verify the Model**. Assess whether the model delivers expected results, often using simplified or estimated data initially.
6. **Validate the Model**. Compare simulation outputs with real-system data to ensure accuracy.
7. **Run Experiments and Analyze Results** to verify or falsify experimental hypotheses.
8. **Implement Findings**.

A comprehensive overview of the evolution of simulation practice is given by McGinnis (McGinnis et al. 2011; Ehm et al. 2009; McGinnis and Rose 2017). The main challenge remains how simulations relate to real-world systems and how stakeholders interact with simulation experts to solve practical problems.

A growing implication of this evolution is the increasing convergence of AI and digital twin models. Digital twins—digital representations of physical entities that mirror behavior and status in real or near-real time—are becoming central to simulation, particularly in domains like manufacturing and logistics. These models not only enable real-time monitoring but also create opportunities for AI-driven decision-making and adaptive control.

The study by (Lugaresi and Matta 2021) explores this evolution, showing how traditional simulations are transforming into digital twins in the manufacturing sector. Building on this, Leon highlights the need for new modeling approaches and integrated cross-domain analyses to support digital twins, particularly for discrete-event logistics systems. He introduces the concept of "analysis-agnostic system models" (McGinnis 2020), which are standardized system representations not tied to any specific analysis type.

Although the general approach to simulation may not change dramatically in the coming years, fundamental shifts in how models are designed, interpreted, and integrated—especially with AI—will significantly improve simulation practices.

Outlook 3: In the future, overarching ontologies may become as essential as today's definitions and entity-relationship models. An early example is the Digital Reference (DR) from the European Productive 4.0 project, which acts as a *lingua franca* for digitizing semiconductor supply chains, enabling human- and machine-readable knowledge sharing.

Outlook 4: There is a growing need for Qualified Synthetic Data (QSD)—artificially generated datasets that replace real data, reducing privacy risks and preventing irrelevant events from dominating simulation. QSD enables faster verification and more efficient validation of simulation models.

2 SKILL DEVELOPMENT AND WORKFORCE EVOLUTION

AI is expected to play a transformative role in the evolution of simulation. As simulation and AI practices continue to converge, this section discusses the changing demands on simulation professionals and the emerging roles needed to bridge the gap between traditional modeling and data-driven techniques.

2.1 New Roles and Competencies for the Future Workforce

The rise of AI-integrated simulation calls for new technical competencies, particularly in relation to data, systems modeling, and decision evaluation. The following areas highlight some of the most critical shifts in simulation-related skill sets:

- **Data Availability and Quality:** Large volumes of high-quality data are essential for AI models. There is growing emphasis on labeled data for supervised learning tasks.
- **Computational Power:** Rapid progress in hardware is essential to support the increasing complexity and size of AI-enhanced simulation systems.
- **Talent and Expertise:** Beyond traditional simulation skills, the workforce must now include specialists in data labeling, model interpretation, and scenario management. New roles such as labelers, decision reviewers, and exception handlers are becoming more prominent.
- **Governance and Ethics:** As AI plays a bigger role in decision-making, ethical and legal considerations must guide its deployment. Understanding regulatory frameworks, explainability, and risk boundaries is now a critical requirement.

Outlook 5: Future simulation professionals must combine domain knowledge with AI literacy. Understanding how labeled data serves as the foundation for learning systems will be vital in ensuring trustworthy, high-performance models.

Outlook 6: Explainability remains a core concern. Despite their impressive predictive power, advanced models such as CNNs can produce misleading outputs. Professionals must learn to evaluate AI suggestions critically and intervene when necessary.

Alongside these technical shifts, we anticipate the emergence of several new job profiles to address the needs of hybrid simulation–AI environments:

- **Ontology Specialists:** These professionals transform expert knowledge and conceptual representations into machine-readable semantic models. The process, sometimes called “DrOWLing” (from “Drawing” and “OWL”), is key to formalizing knowledge across domains.
- **Ontology Integration Experts:** Responsible for aligning and connecting diverse domain ontologies to overarching semantic frameworks such as the Digital Reference used in manufacturing.
- **Synthetic Data Designers (QSD Generators):** Tasked with generating realistic, privacy-preserving datasets that maintain statistical integrity. These datasets enable safe model verification and validation where real data is unavailable or restricted.
- **Labeling Professionals:** Provide consistent and meaningful annotations to training data. These annotations form the “ground truth” for AI models and directly impact simulation reliability.
- **AI-Aided Decision Analysts:** Evaluate the relevance and reliability of AI outputs, especially in partially explainable systems. They act as interpreters of AI-generated recommendations.
- **Exception Handlers:** Operate in VUCA (Volatile, Uncertain, Complex, Ambiguous) environments. These professionals step in when AI predictions fail or when unprecedented cases arise that require human reasoning beyond the model’s scope.

Outlook 7: To prepare for these emerging roles, simulation professionals must gain familiarity with semantic technologies, data synthesis techniques, and human-in-the-loop AI workflows.

2.2 The Role of Simulation Experts for the Implementation of Models

A professional field closely related to M&S and highly impacted by the advancements in generative AI is software engineering. Generative AI, particularly LLMs, is transforming software development workflows, roles, and skills. The same transformation applies to simulation professionals involved in implementing models.

We assume the model is already conceptualized, with defined entities, properties, relationships, and processes, and is ready for implementation (i.e., coding, debugging, documenting, maintaining). Though natural language can describe such a model, machine-readable specifications are preferable.

- **Code Generation:** LLMs assist in writing code by leveraging vast software development resources. They support auto-completion, pattern abstraction, and retrieval of relevant code snippets. Advanced use cases include transforming natural language into executable code for specific domains (Frydenlund et al. 2024; Jackson and Saenz 2022). While promising, further research is needed for reliability.
- **Testing and Debugging:** LLMs identify bugs (Li et al. 2024), suggest fixes with rationale, optimize performance (Gao et al. 2024), and trace code logic. They also support creating unit and interface tests, mapping data structures, and harmonizing program data (Santos et al. 2025).
- **Documentation:** Documenting code, often viewed as burdensome, is eased with LLMs. They detect inconsistencies (Zhang 2024), generate documentation (Luo et al. 2024), and adapt tutorial content to learner maturity (Bhat et al. 2024; Jackson and Rolf 2023).
- **Code Maintenance:** LLMs simplify code, suggest structural improvements, and assist future maintainers. Their use is critical when original developers are unavailable or models use heuristics/numerical approximations (Oberkampf et al. 2002; Winsberg 2019). Digital twin-inspired methods show promise (Peng et al. 2025), and custodial work may be reduced as LLMs act as digital collaborators (Barry et al. 2022).

Outlook 8: By 2050, simulation engineers will shift from traditional coding to AI-assisted model implementation. AI tools will enable executable simulations as part of pragmatically linked solution networks.

2.3 Challenges of AI in M&S education

Teaching, learning, and practicing modeling and simulation invariably depend on creating useful abstractions. LLMs, as teaching machines, should be introspective and retrospective in addition to being pedagogical. They should be skilled in core modeling, simulation, and computing subjects, but also disciplinary (e.g., cancer biology) and multidisciplinary subjects (e.g., built-natural-social systems of systems). Rigorous and repeatable studies of teaching machines should demonstrate that their questions and answers to them are explainable and understandable in educational settings, including university classrooms. Incomplete and contradictory knowledge can mislead instructors and students alike to believe the needed skills are taught and gained to develop correct and useful M&S artifacts.

Inclusion of AI in educational settings is complicated – it involves students, curriculum, accreditation, assessment, teachers, and a myriad of policies and rapidly changing infrastructures and technologies for content delivery (National Science and Technology Council 2023). Studies in computer science (Meyer, Bertrand 2023) and M&S (Yan et al. 2024; Tolk et al. 2023; Lesage et al. 2024) show varying understandings and expectations of AI, such as its use in personalized and team learning. Either way, the practical use of AI in educational settings should be grounded and demonstrated with useful and measurable studies with outcomes such as assignments, exams, and projects that require critical thinking as part of the Bloom taxonomy. AI can bring useful change to education when its knowledge and the means to deliver it can be shown to complement what has been the foundation of education. AI models should be subject to external audit and evaluations as is currently possible through bodies such as the Certified Modeling & Simulation Professional (CMSP) certification program.

AI as teachers (or teaching assistants) should have soft skills and common-sense reasoning in addition to technical skills. Teaching machines are likely to be highly specialized. However, they may prove to be revolutionary in teaching the knowledge and practice for inter-/trans-disciplinary M&S research and development.

Anecdotal teaching experiences in a graduate-level modeling & simulation and research suggest that student learning using AI tools is confined to simple and well-understood knowledge (e.g., facts, examples, and procedures). Currently, the models, code, and examples lack evidence of correctness, explainability, and repeatability, making them unsuitable for use in educational settings. Looking into the future, on the one hand, AI may reach a stage to serve teachers, students, and researchers to gain sound M&S knowledge. Teachers, on the other hand, may be unaware that students are learning materials that lack scientific rigor and are impractical to measure.

Outlook 9: AI will transform M&S education through intelligent tutors and assistants, but only if their outputs are auditable, explainable, and grounded in sound pedagogical practices. Otherwise, they may hinder rather than enhance deep learning.

3 FUTURE PERSPECTIVES ON AI-SIMULATION INTEGRATION

As AI capabilities expand and simulation systems evolve, their convergence will influence not only technological tools but also the roles of practitioners, workflows, and organizational strategies. This section explores emerging perspectives on how AI-driven simulation may transform modeling practices and ecosystem dynamics in the years ahead.

3.1 Impact of AI and Simulation Merging on Users in the Next 5 to 25 Years

There are three primary applications with the merging of AI and simulation as follows:

1. *Generative AI* (GenAI) to augment/perform model and experiment generation.
2. Reinforcement Learning (RL) to find optimal input parameters for a simulation model.
3. Neural Networks (NN) embedded in a simulation model to optimize decision-making.

In the following sections we will discuss the challenges and promises of these primary use cases.

3.1.1 Generative AI for Building Models and Running Experiments

The idea of asking AI to build models and run experiments to answer questions seems a bit far-fetched, but just a few years ago so did the idea of asking AI to drive a car, write papers, create art/videos, write poems, or write computer programs. A lot has changed in a short time, and the pace of change remains high. Over the past few years there has been dramatic progress in the development of AI/ML, particularly in the advancement of *Generative AI* and Large Language Models (LLMs) that are trained on massive amounts of data, with an underlying Transformer comprised of a set of Neural Networks that provide an encoder and decoder with self-attention capabilities. GenAI can understand a wide variety of inputs including text, voice, pictures, and videos, and can summarize and generate new content in a variety of formats. A key to the rapid progress has been the ability to train ML algorithms with extremely large data sets using massively parallel data training centers. Given the broad and rapid success of GenAI, the natural question is: Can it create simulation models, and design and run simulation experiments to answer specific questions?

GenAI is being applied today in simulation studies to perform specific project tasks that were done manually in the past. Here are some example prompts that might be used in a simulation study:

- *"Write me a Python program to pull the first 500 records from an Excel spreadsheet with columns named Material and Quantity and write them off in a CSV file for input to my model."*

- *"Write me a program in C# that I can call from my model to send a message to an MQQT broker to specify an AMR name of type string to move to a destination location of type string."*
- *"I have exported output data for multiple responses from my model into a CSV file. Write me a Python program to display a histogram of each response along with the 10, 25, 50, and 75, and 90 percentile values."*

Although there are valuable and time-saving benefits from working with existing GenAI tools, these tools are not currently capable of building a simulation model or designing and running experiments to answer specific questions. Consider, for example, the following prompts to a GenAI system.

- *"I have as input a 3D CAD drawing of my factory along with Enterprise Resource Planning (ERP) data and Manufacturing Execution System (MES) historical production data. Create a model of my factory that allows me to evaluate changes in demand and the impact of system changes or the introduction of new products."*
- *"I have a model of a new factory, and I am selecting between Autonomous Mobile Robots (AMRs) with differing prices and performance characteristics. Run an experiment to determine which AMR model I should choose and how many units I need to purchase to deliver 99% of orders on time with 99% confidence."*

The question is, how close are we to having GenAI tools that can accept prompts like these that build our models and run our simulation experiments, and what challenges do we face in getting there? Will we see this capability in the next 5 or 25 years?

Outlook 10: Within the next two decades, Generative AI will evolve from task-specific assistants to full simulation collaborators, capable of interpreting complex system inputs and autonomously generating valid simulation models and experiments. While current tools fall short, the trajectory of GenAI suggests a future where simulation modeling becomes prompt-driven, interactive, and significantly more accessible to non-experts.

3.1.2 Reinforcement Learning for Simulation Optimization

Reinforcement Learning (RL) is a type of ML where an agent learns to make decisions by interacting with its environment, taking actions, receiving rewards/penalties, and then adjusting its behavior to improve performance.

RL has shown compelling results in board and computer games, receiving considerable attention for potential simulation applications (Belsare et al. 2022). A key advantages is that it does not require massive amounts of labeled training data since it learns from its environment, real or simulated. Due to the challenges with creating a reward/penalty for embedded decision making, RL has primarily served as an alternative to classic search methods for simulation optimization (Wang and Liao 2023; Lim and Jeong 2023; Castrignanò et al. 2024), finding optimal decision variables to maximize/minimize objective functions such as throughput or cost. Here, the RL reward function is straightforward: the improvement in the Key Performance Indicator (KPI) of the system being modeled.

In this application, RL competes with existing simulation optimization search tools such as OptQuest. Optimization search tools and RL simulation optimization applications share many similarities: both explore an unknown search space and adjust their decisions based on that exploration. RL and tools like OptQuest also compete with running large simulation experiments of the full solution space, which becomes increasingly practical with advanced statistical methods reducing required replications and expanded access to massively parallel cloud-based data centers. Despite its successful applications with simulation optimization, RL faces challenges achieving broad success. For example, PathMind, a well-funded startup specialized in RL for simulation optimization with interfaces to several commercial simulation tools, shutdown after years of effort and tens of millions in funding due to lack of progress.

Outlook 11: RL will continue to evolve as a complementary approach to traditional simulation optimization methods, particularly in domains where labeled data is scarce but well-defined reward structures exist. While challenges remain, future advancements in reward shaping and hybrid integration with classical search methods may unlock broader adoption of RL in simulation contexts.

3.1.3 Neural Networks for Optimal Decision Making

Neural Networks for decision logic and simulation are ideally suited for each other. On the one hand, Neural Networks excel at making predictions and optimizing decisions, but are handicapped by requiring massive amounts of high-quality labeled data for training, since a Neural Network model is only as good as the training data on which it is based. On the other hand, simulation models require high-quality decision logic to optimize the system performance, but can generate endless synthetic training data. Hence, the appeal of embedding Neural Network models for decision optimization within a simulation model and using the simulation model to self-train the Neural Network. This area has already had some success, and is one of the most promising short-term opportunities.

Decision logic is often a major component of a simulation model, created with significant modeling effort. For example, some typical decision logic that must be built into a manufacturing simulation model includes logic for:

1. Selection of the next job to work on at a workstation.
2. The selection of a production line for a new job.
3. Deciding if a job can be released now and be completed within a maximum makespan (otherwise it expires).

Decisions such as example 1 can be done with standard rules such as Critical Ratio (i.e., remaining processing time divided by the remaining slack time). However, rules are not easily created for examples 2 and 3, as the correct choice depends on many factors such as the number and mix of work orders, the required product changeovers at all the downstream stations in product routing, and operator and material availability. Building good custom rules to handle these cases is difficult and time consuming to do, but, as we will discuss in Section 4.1.3, it is easily done using a Neural Network by transforming the selection problem into a prediction problem.

Outlook 12: Neural Networks will become integral to simulation-based decision-making by leveraging self-generated synthetic data from simulations. This synergy allows complex, data-hungry models to be trained without external datasets and enables simulations to evolve beyond rule-based logic into prediction-driven optimization engines.

3.2 The Convergence of Simulation, AI, and Engineering Disciplines

Several publications already investigate the benefit of close collaborations among various disciplines, such as (Onggo et al. 2018; Taylor et al. 2021; Mustafee et al. 2023; Tolk 2024). As discussed in (Mustafee et al. 2017), a hybrid is the result of merging two or more components of different categories, combining their characteristics into something more useful.

In addition to the potential of AI methods discussed in the previous sections, Large Language Models (LLMs) promise to converge a variety of engineering disciplines, becoming a "melting pot of cross-disciplinary ideas." Following the argument discussed in (Tolk et al. 2021), this requires the conceptual alignment of the models being used and the interoperability of their implementation. It is worth pointing out that different engineering disciplines all follow this principle of conceptualization and implementation, where conceptualization is the creative process of creating a model of the object of interest within its context, while the implementation focuses on creating an executable artifact representing this object in a computer. For example:

- In M&S, the modeling part results in the conceptualization while the simulation part implements this model.
- In AI, the various algorithms and heuristics work on models of the objects of interest, not on the real-world object.
- Digital twins use digital models and their implementation to implement their functions.
- Big data works on data models that are implemented in data products. In more recent approaches, such as the data mesh, it is a common semantic understanding, a conceptualization, that allows to find, share, and mediate the different implementations to each other (Dehghani 2022).

As discussed in (Giabbanelli et al. 2025), LLMs have the potential to become universal translators between implementations if they have access to the underlying conceptualizations. This capability can support the convergence of several engineering principles, but aligning the different conceptualizations remains an open challenge for the human expert.

Nonetheless, the use of standardized ontological methods combined with the ever-increasing power of GenAI will augment human experts' capabilities in this creative process as well. For simulation, some ideas already are discussed in (Benjamin and Akella 2009), and there are promising recent developments in the integration of ontology methods. Ontologies allow us to communicate conceptualizations in a standardizable and unambiguous form, which is needed by generative AI to access them.

Furthermore, a white paper by the Google DeepMind group (Novikov et al. 2025) describes how their AlphaEvolve approach combines the creativity of an LLM with algorithms that can scrutinize the model's suggestions to filter and improve solutions, supporting many disciplines.

These observations motivate the notion that we will continue to witness the convergence of many engineering disciplines, in which simulation expertise needs will likely shift to the conceptualization tasks. By 2050, the role of a simulation engineer may have changed into a conceptualist for computational sciences, as envisioned in the Keynote for the 2018 Summer Simulation Multi-Conference (Tolk 2018).

Outlook 13: Engineering disciplines will converge through AI-mediated conceptual alignment, with simulation experts evolving into computational science conceptualists who focus on model abstraction and cross-disciplinary integration rather than implementation details.

4 TECHNICAL CHALLENGES AND SOLUTIONS

This section highlights the key obstacles and bottlenecks in implementing AI within simulation frameworks, along with emerging techniques to overcome them.

4.1 Near-Term Impediments and Solutions for AI in Simulation Models

This analysis considers impediments for advancing these three areas for merging AI and simulation.

4.1.1 Challenges with Generative AI and Simulation

In most AI applications, the biggest implementation challenge is the quality labeled training data, and the same is true with merging GenAI and simulation. If the goal is to create a GenAI tool for building simulation models and running simulation experiments to answer specific questions, training the GenAI model will require a labeled training set with a massive number of models and experiments, with detailed textual descriptions of each. This approach would also require separate large datasets for each modeling tool that needs support. The current set of LLMs could be trained using billions of documents available on the web, but it is not clear where massive datasets of models/experiments can be found, since most industries consider their models to be proprietary. As a result, progress towards a generic GenAI solution is expected to be slow and will require the creation of large datasets of sample models with detailed descriptions.

Progress may occur first in specific application domains or with specific modeling tools. A simulation tool that is designed for a narrowly defined application area may see earlier progress. Although a generic

LLM is challenging because it requires massive amounts of quality labeled data, much can be done with Small Language Models (SLMs) that are more narrowly focused. In the near term, simulation-specific SLMs will likely emerge that are trained using simulation textbooks, simulation software user manuals, example models, etc., to enhance the learning and building of simulation models. Users can then ask SLM questions such as: *How do I model reneging from a queue?*

4.1.2 Challenges with Reinforcement Learning

RL applications in simulation optimization face challenges from the well-developed competitive alternatives in search algorithms such as OptQuest, as well as the evolving competitive alternative of running the full experiment with statistical pruning on a parallel bank of processors.

Although most RL applications in simulation have been for simulation optimization, it is also possible to implement RL for embedded decision logic (Kuhnle et al. 2021; Liu et al. 2022). For RL applications in decision logic within a model, RL eliminates the need for having a large dataset of labeled training data, but replaces it with the challenge of devising a reward structure and associated decision rule that will lead to an optimal strategy. For example, in selecting the next job to work on at a workstation, it is difficult to measure the reward for each candidate action, since the decision impacts not only on the selected job, but on all the other jobs in the system, and is only known once all jobs have been completed. A reward that only looks at the short term impact on the selected job may lead to sub-optimal performance.

4.1.3 Challenges with Neural Networks for Decision Logic

A Neural Network takes a set of numeric inputs and generates a set of one or more outputs. In many cases, the outputs are probabilities that each candidate is the correct choice, and the highest probability is selected. This structure aligns well with decision logic in simulation models, where a system state is used to choose the best option—such as the next job or production line.

However, generating labeled training data is a challenge. To know the “correct” decision, one would need to simulate every possible choice, which becomes impractical for large models with numerous embedded decision rules. A more scalable strategy is to recast selection problems as prediction problems—using the Neural Network to predict a value (e.g., makespan), and choosing the option with the optimal predicted value.

To support this approach effectively in simulation, the following are key:

- **Self-training from synthetic data:** Use simulation to generate inputs (e.g., current workstation states) and true outcomes (e.g., actual makespan), enabling Neural Network training.
- **One-hot encoding and feature capture:** Handle categorical variables (like job type or material) using one-hot encoding and track all input states required for accurate prediction.
- **Prediction-first mindset:** Focus Neural Networks on predicting values, not direct selection, to simplify training and integration.
- **Model generalizability:** Allow use of ONNX format to import externally built ML models.
- **Operational logic separation:** Use broader data during training and apply decision logic constraints (e.g., shift end checks) only during live simulation.

Compared to other AI-simulation integrations, Neural Networks for embedded decision logic offer the most natural fit and can be incrementally adopted using self-generated data within the simulation.

Outlook 14: Overcoming AI-simulation integration challenges will require domain-focused approaches. Small, targeted models and simulation-generated synthetic data can help address the lack of large training sets, while hybrid strategies may simplify reward design and decision logic.

4.2 Architectural Principles for Simulation-AI Hybrid Systems

The principles of architectural complexity, including hierarchy, choice of components, and intra-/inter-component linkages, are omnipresent in natural and artificial systems (Simon 1962). Simulation models, built on these principles, are created as a collection of interacting components. These principles help tame model complexity and enable scalability, at the cost of longer simulation time and increased computational and communication demands. They should also serve as the foundation for composing simulation and AI models.

There exists an extensive body of theories on the composability of continuous-discrete time models (Alur and Henzinger 1997; Lynch et al. 2003; Zeigler et al. 2018). Simulations of such hybrid models are supported using High Level Architecture (HLA) and Functional Mock-up Interface (FMI) interoperability standards. The composability and interoperability are distinct—the former for creating composable models, the latter for managing separate simulation protocols. Standards should provide services like data, time, and ownership management. Domain-specific hybrid models can be developed by mapping domain knowledge onto continuous and discrete models simulated with interoperability implementations. Higher layers for domain-specific and neutral models, combined with lower layers for interoperability and computing hosts, provide a foundation for conceptualizing, constructing, and verifying models through simulations, validation, and evaluations in an autocatalytic process.

The heterogeneity between inductive AI models and deductive simulation models presents unique challenges. While component-based simulation models have formal structures for inputs, outputs, and interactions, time-series ML models remain black boxes. New principles are needed to bridge these paradigms, particularly since hybrid simulation models combine continuous and discrete time bases, suggesting AI models should support continuous time as well.

Heterogeneous composition of simulation and AI models requires coordinated mechanisms to preserve model integrity and interactions. Key considerations include (Sarjoughian 2006):

- **Data Transformation:** Align diverse data formats between simulation and AI models.
- **Communication Protocols:** Define clear interaction rules via Knowledge Interchange Brokers.
- **Execution Regimes:** Allow models to run with independent prediction horizons rather than lock-step execution.

As an example from semiconductor supply chains (Huang et al. 2009):

- Discrete-event modeling manages manufacturing operations step by step.
- Model-Predictive Control handles tactical decisions over short timeframes.
- Linear programming guides strategic planning across long horizons.

LLM time-series models, such as Temporal Fusion Transformers (TFT) and Temporal Convolutional Networks (TCN) (Pendyala et al. 2024), can achieve high accuracy with rich datasets and extensive training. These models are orders of magnitude faster than simulations but lack fine-grained event handling, operating on discrete time bases. This suggests small LLMs may assist with individual parts, while computation-intensive components can be replaced with ML counterparts (Sarjoughian et al. 2023). However, inaccuracies in ML proxies can ripple across hybrid systems, affecting fidelity.

LLMs are also proposed for generating simulation models from text (Jackson and Saenz 2022). Frameworks like agentic LLM-assisted DEVS show potential (Carreira-Munich et al. 2024), but require expert oversight for model creation and verification. While careful selection of sample models may improve correctness, assembling them remains challenging for complex, multi-scale domains. Ensuring logical reasoning and explainability is critical for domains such as cyber-physical systems, where precision and validation are essential.

Real-time execution adds another layer of complexity. Models supporting near real-time operation are vital for live digital twins. AI/ML models must address worst-case execution time to align with diverse simulation and environmental constraints.

Outlook 15: Composing simulation and AI models requires frameworks that balance temporal accuracy, interoperability, and real-time responsiveness. Domain-aware solutions, integrating component-based simulations with AI/ML proxies, will be key to enabling robust hybrid systems for applications like digital twins.

5 LONG-TERM OUTLOOK AND STRATEGIC INSIGHTS

As this paper concludes, this final section presents the strategic opportunities emerging from AI-simulation integration and examines the critical challenges that will define the future of trustworthy AI adoption in simulation contexts.

5.1 Current Insights and Strategic Outlook

The integration of simulation and AI in recent years has led to a flourishing of applications, opening new horizons in model development and decision-making. Although we are still at the infancy of GenAI, its rapid rise has introduced many application-specific tools that are beginning to reshape simulation modeling practices. LLMs show promise as "universal translators," enhancing cross-domain integration and collaboration. As these technologies mature, they are expected to play an increasingly critical role in supporting decision-making and improving the efficiency of simulation modeling across industries.

In the next five years, AI will provide new automated techniques and methods—along with frameworks and tools—to develop and evaluate simulation models more efficiently. The expanded use of simulation-embedded neural networks will optimize decision-making within models, such as selecting the best job to process next or determining the appropriate production line for a given job. Additionally, specialized SLMs, trained on specific modeling tools, will assist simulation practitioners in learning concepts and building models more effectively. AI will also significantly increase the automation of running and evaluating simulation experiments in collaboration with stakeholders, streamlining both analysis and decision support processes.

Looking ahead to the next 25 years, GenAI is expected to evolve to the point where it can autonomously build complete simulation models directly from system sketches, problem descriptions, and enterprise data. It will be capable of designing and executing simulation experiments needed to answer complex analytical questions without human intervention. However, this advancement may come at the cost of diminishing the trust traditionally placed in simulation models, as the growing complexity of AI-driven solutions challenges transparency and explainability. Despite this, the use of AI in simulation will likely continue to grow, requiring new standards for validation and responsible adoption.

5.2 Speculative Challenges and Quality Standards

This section speculates on what standards, expectations, and technologies might emerge to ensure the trustworthy use of AI in simulation contexts by 2050.

When considering the quality requirements for AI or AI-based simulations, the fundamental question arises: *What level of quality is acceptable?* Humans tend to accept malfunctions more easily when a responsible person can be held accountable. However, the closer we approach scenarios involving potential casualties, the higher the required quality standard becomes.

In cases involving legal prosecution or mourning, the quality standard should be up to ten times higher. Significantly more research and resources are needed in this area. This will benefit both those advocating for the implementation of AI—who often face resistance despite AI frequently outperforming classical methods on average—and those who hesitate to accept AI solutions.

Defining a clear threshold for how much better AI needs to perform compared to classical approaches under specific circumstances would greatly facilitate transparent communication and informed decision-making.

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