ENHANCING DIGITAL TWINS WITH ADVANCES IN SIMULATION AND ARTIFICIAL INTELLIGENCE: OPPORTUNITIES AND CHALLENGES

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ABSTRACT

Simulation is used to investigate physical systems. A digital twin goes beyond this by connecting a simulation with the physical system with the purpose of analyzing and controlling that system in real-time. In the past five years, there has been a substantial increase in research into Simulation and Artificial Intelligence (AI). The combination of Simulation with AI presents many possible innovations. Similarly, combining AI with Simulation presents further possibilities including approaches to developing trustworthy and explainable AI methods, solutions to problems arising from sparce or no data and better methods for time series analysis. Given the progress that has been made in Digital Twins, Simulation, and AI, what opportunities are there from combining these exciting research areas? What challenges need to be overcome to achieve these? This article discusses these from the perspectives of six leading members of the Modeling and Simulation community.

1 INTRODUCTION

Traditionally simulation has been used to investigate physical systems. Connecting a simulation to a physical system with a view to controlling that system has created the concept of the Digital Twin (DT). Separately, there has been a recent and substantial increase in research into Simulation and Artificial Intelligence (AI). There are many advantages to combining the techniques of tools of both areas together. Given this, what are the possibilities of combining these with research into Digital Twins? This article presents views from six leading members of our Modeling and Simulation community on the opportunities and challenges of Simulation, AI, and Digital Twins.

2 POSITION STATEMENT BY CHARLES MACAL

2.1 Simulation, Digital Twins, and AI

We are hearing more and more about developments in AI and DTs in the business press as well as the popular press and the academic press (Science Direct 2023). What do these developments mean for the field of simulation? Do we need to pay attention to these developments? Do we need to *do* something different with respect to our activities in the simulation field?

2.2 Simulation, Digital Twins, and AI: Machine Learning

Barry Nelson made the observation in 2016 that the world had changed in ways that bear on the future of simulation. Paraphrasing Nelson (2016): (1) data storage is cheap and effectively unlimited (we can exploit more of the simulation-generated data than we typically do today), (2) parallel simulation is becoming easy to do (any simulation experiment that requires multiple replications or multiple scenarios can benefit dramatically from parallel simulation), and (3) more users are interested in risk analysis, prediction and control, rather than in [only] system design. All of these developments (and maybe a few more) are coming together to facilitate the development of DT technology.

DT seems to have arisen from the production and manufacturing industry, branching recently into the healthcare industry (Ferdousi et al. 2023). I have not found a formal definition of a DT and there is not widespread agreement on the meaning of the term. My question is: Is DT just another name for: (1) a detailed digital "simulation" model of an object whereby the term simulation is applied to connote he inclusion of dynamic behaviors attached to an otherwise static object, thus facilitating experimentation *in silico*, or (2) a detailed digital representation of a process that can be simulated as it evolved through time?

There is a huge amount of available marketing web sites promoting DT technology and suggesting it will have huge business implications in the future. AWS (Amazon Web Services) offers this description of DT technology:

"A Digital Twin a virtual model of a physical object. It spans the object's lifecycle and uses real-time data sent from sensors on the object to simulate the behavior and monitor operations. A Digital Twin works by digitally replicating a physical asset in the virtual environment, including its functionality, features, and behavior. A real-time digital representation of the asset is created using smart sensors that collect data from the product."

Interestingly, AWS goes on to define different types of DTs: component twins, parts twins, asset twins, system twins, and process twins, and even explicitly draw the distinction between DTs and simulation:

"Digital Twins and simulations are both virtual model-based simulations, but some key differences exist. Simulations are typically used for design and, in certain cases, offline optimization. Designers input changes to simulations to observe what-if scenarios. Digital Twins, on the other hand, are complex, virtual environments that you can interact with and update in real time."

AWS offers a system for creating DTs: AWS IoT TwinMaker "helps you optimize operations and performance by creating DTs of real-world systems". This is of interest because it immediately raises questions regarding the role and relationships of DT development platforms and software and available simulation software platforms.

<u>Bottom Line for DTs</u>: Simulation professionals (researchers, vendors, model developers) need to pay attention to the field of DTs for advances in modeling methods and application development, as well as theory development that moves the DT field forward. DT technology uses machine learning algorithms to process the large quantities of sensor data and identify data patterns. For example, with the inclusion of

real-time data feeds, DTs need to run machine learning algorithms for updating simulation model parameters and adapting the DT representations to reflect those in real life.

2.3 Simulation and AI: ChatBots

Barry Nelson also once said in a Winter Simulation Conference (WSC) keynote address "Why can't I talk to my simulation?" (Nelson 2017). We can also now ask: "Why can't my simulation talk to me?" Answering these questions is now in the realm of AI ChatBots and large language models. The very recent rise of ChatGPT has caused a sensation and started a rethinking of its impact in many fields of knowledge, and human endeavors. A ChatBot is a program based on a "large-language model." To take some of the mystique away, ChatBot are not sentient, they simply use massive amounts of text (thus the term large language model) to predict one word after another, are generally trained over a period of many months via deep learning neural networks, on a very large and powerful GPU-enabled computer. ChatBots may return results that mix truth with falsehoods, or even be non-sensical. The breakthrough of ChatGPT was that it actually works, and it works well a very large part of the time. ChatGPT began producing reasonable and plausible answers in response to questions of a very general nature posed by users. According to the developers at the OpenAI (2023) web site:

"We've trained a model called ChatGPT which interacts in a conversational way. The dialogue format makes it possible for ChatGPT to answer follow-up questions, admit its mistakes, challenge incorrect premises, and reject inappropriate requests."

So, I put the question to ChatGPT: "Why can't I talk to my simulation?" ChatGPT provided a threeparagraph, cogent, and sensible answer, showing quite an understanding of simulation I have to admit, reply excerpted here:

"As an AI language model, I can understand and respond to your queries because I have been specifically designed and trained to do so. However, simulations, which are virtual replicas of physical objects or systems, are typically designed to simulate the behavior of the real-world object or system, and do not possess the ability to communicate independently.

... While simulations can provide valuable insights and predictions, they are limited to the inputs and parameters that are programmed into them, and cannot exceed those limits. Furthermore, simulations are typically designed for specific purposes and are not capable of independent thought or action. *Therefore, it is not possible to have a conversation with a simulation, as it is not capable of understanding or responding to natural language queries in the way that an AI language model like myself can.*"

Bottom Line for AI: ChatBots: As we have seen with ChatGPT successes, we cannot predict the ultimate value or even limitations, if any, of this technology. Many surprises lie ahead. ChatGPT can also do coding and programming in a number of computer languages. The prospects for having a conversation with a ChatBot about a simulation model you would like it to build for you are not far-fetched; having a ChatBot automatically summarize, analyze and interpret the results from a large corpus of simulation model results or from a large numbers of simulation experiments seem to be within reach, or at least a worthy goal of continuing research in the simulation field. ChatBots that are trained on a large corpus of simulation-related content, discourse, grammars, text, and even non-textual materials such as images, schematics, and flowcharts have enormous potential for achieving the goal of being able to talk to your simulation and have your simulation talk back to you.

3 POSITION STATEMENT BY ANDREA MATTA

3.1 BACKGROUND

The recent years have seen a significant acceleration of information and communication technologies (ICTs) together with a diffusion of artificial intelligence (AI). Access cost to ICTs has dramatically decreased as well as their required implementation time, thus allowing small and medium companies to easy install sensors in their processes and automate data collection & management. This facilitates data flow and model sharing in network of enterprises linked by B2B (business to business) relationships, but also large companies will benefit, being often the major players of these networks of commercial interests and material and information exchanges. At the same time, AI approaches have been suddenly and rapidly adopted in several fields, and implemented in software applications easily customized by practitioners who do not necessarily need to have a deep knowledge of AI theory. Another barrier is fallen, automated knowledge extraction and decision making is now enabled and can be accessible for small and medium companies too. And, very likely, this is only the beginning of a much more extensive use of AI in business processes.

DTs are a recent emerging technology that replicates the behavior of physical entities, processes, systems, and organizations. Originally conceived by Grieves in 2003 for descriptive purposes of a physical counterpart (Grieves 2014), the DT concept has been enriched of other advanced features such as prediction of system performance, prescription for control and optimization, ability to adapt to changes, lightness of models thanks to its different fidelity levels (Matta and Lugaresi 2023). Not all the advanced features need to be present in a DT. On the contrary, other fundamental features that characterize DTs, in addition to description, are the synchronous alignment with the physical system (synchronization) and its digital nature (i.e., a DT is a computer code). DTs leverage the models of their physical counterparts to fast process real time acquired data and obtain accurate problem diagnosis, predictions, and recommend prescriptive actions. Considering the complexity to manage DTs together with their high investment cost, the actual trend is to couple DTs with important assets such as productions systems, power plants, airplanes, and cars. The expected benefits are many, among these the most significant are increased availability of the asset, higher efficiency, and lower cost.

Simulation is widely considered among the most utilized approaches to study the behavior of products and systems. Since the 1960s (Tocher 1963), simulation is widely used to numerically estimate the product or system performance and make diagnostics, predictions, and ranking of alternatives in control and optimization problems. Thanks to these capabilities, simulation can be considered the core technology of DTs (Monostori et al. 2016). The rapid and continuous increasing of processors will consolidate the relevance of simulation and help to spread real-time simulation approaches embedded in DTs (Lugaresi and Matta 2018).

These mentioned technologies have their origins in different areas. More precisely, ICT and AI in computer science, DTs in product design, and simulation in operations research. This has led to almost independent developments with minor connections among areas, redundancies and overlapping of developed models and methods, and no common vocabulary. Therefore, positioning these technologies in a same framework in order to unify models, methodologies, tools, and terminology should have high priority in the research agenda of academic communities and standard institutions.

3.2 SYNERGIES OF SIMULATION, AI, AND DIGITAL TWINS

In the described technology trend, it is undoubtedly that these technologies are constantly evolving and spreading, and will give place to new products and alternative ways of managing business processes. Therefore, it is right and proper to investigate simulation and its future scenarios considering also the coevolution of the other technologies. A possible and reasonable evolution is that each technology will be used for its strengths but modified to remove its weaknesses. In the following, it is discussed how AI and DTs can be used to mitigate simulation's weaknesses and vice versa toward an evolution of better technologies.

3.2.1 AI and DTs To Improve Simulation

Focusing on simulation, AI, and DTs will help to mitigate its weaknesses as explained in the following.

Data requirements. Simulation normally requires data inputs that are not easy to gather. With the spreading of ICTs, data is now available at affordable cost and simulation experiments will be less expensive and more accurate thanks to the sample size increase of gathered data. Further, real-time simulation applications will be enabled by automated data feeding. Indeed, simulation models in DTs can be easily instantiated and initialized thanks to the synchronization service provided by DTs. This is also a great chance for including simulation-optimization approaches in DTs that provide prescriptions in real-time. The faster simulation-optimization approaches are, the smaller the time scale applications; for instance, the real-time machine assignment in semi-conductor manufacturing systems can be supported by simulation-optimization experiments aligned with the physical system state.

Simulation model development. Creating conceptual models and implementing them in computer codes require high skills and may take considerably long times. AI can help to develop approaches that learn the physical system from the gathered data, make abstractions, and generate conceptual models that can be successively transformed into simulation software codes. Process mining approach, originally conceived to discover processes from data logs (van der Aalst 2016), can be extended to automatically mine the physical system from data logs and describe the new acquired knowledge into formal models such as Automata, Petri Nets, Entity Relationship Graphs, or Knowledge Graphs (Lugaresi and Matta 2021). This automated discovery of the system is also known as system identification in control theory. This learning may be needed only for some portions of the systems, in this case AI contributes to develop the code locally in the existing simulation model. Generative AI approaches can also create more general models without having observed all the patterns of the physical system. In conclusion, it is not difficult to image that, in a near future, simulation models will be generated from data collected from existing systems and a few existing knowledge from experts. Even the update of simulation models, needed to keep consistency with a changed physical system, can be supported by AI approaches, thus decreasing skill level, cost and time of simulation model maintenance.

Simulation model validation. Validation of simulation models is a costly activity. The continuous data flow from physical system to simulation model, provided by the DT synchronization service, will facilitate model validation activity. Invalid models will be fast detected and improved using AI approaches that can reconstruct the logic or the input data distributions.

Cost and time of simulation execution. Simulation experiments can be very computationally intensive and often lead to long experimental times. This time can be reduced if surrogate models are generated from simulation and used instead of it. Machine learning is widely used among regression techniques to fit functions from data, it can replace simulation models when fast responses are required, or used jointly with simulation in multi-fidelity settings. Other regression techniques can be used for model lighting, an investigation on which technique fits better with simulation experiments would be necessary. In this way, simulation models are reduced and its light surrogates can be used in optimization approaches or easily transportable to other actors and executed on another server. When simulation is coupled with an optimization algorithm, times can drastically become unaffordable. Reinforcement learning is a quite a general framework in which observed data and simulation experiments can be used to find optimal policies for the physical system.

3.2.2 Simulation To Improve AI

Focusing on AI, simulation will help to mitigate its weaknesses as explained in the following.

Data bias. Most of AI approaches are model free, built from data, light, and easily transportable. However, the lack of model is also a limitation that can be easily compensated by simulation. In other words, simulation will help to mitigate the data bias by using its structural information, particularly in those unexplored areas without observed behavior. Of course, AI model-based approaches already exist, but simulation can reinforce them thanks to its capacity to take into account of randomness, adaptability to the requested detail level, and facility to model complicated systems.

Explainability. Many AI approaches suffer of interpretability issues, users can have difficulties to understand results generated by AI. These problems can be mitigated by use of simulation models that can increase the confidence of AI results with their graphical representation of the modeled physical systems.

Data quality. AI approaches suffer of poor data quality. Simulation models of the physical system can be used for data validation purposes.

3.2.3 Simulation and DTs

Focusing on DTs, simulation models represent their kernel that, together with the continuous data flow gathered from synchronization, are able to describe the physical system. Without simulation models, a DT can only provide analysis using data and simple models, often analytical, of the physical system. Such systems fit with the definition of DTs (Grieves 2014), but they are not known or considered as DTs. Famous examples are Programmable Language Controllers (PLCs) to control devices using very simplified models, or Computer Numerically Controls (CNCs) to control the axis drives of machine tools using kinematic models. In conclusion, we can say that simulation provides to DTs depth for analysis of the physical system behavior.

3.3 CONCLUSION

These coming years represent a great opportunity for a new cycle of simulation. After the significant developments in the last decades, simulation is a well consolidated approach with several technologies offered in the market, and robust enough to be used in real time applications where DTs operate to analyze, optimize, and control a (or a set of) physical system(s). This means to shift simulation from the design phase, where simulation is mostly used nowadays, to the operational phase of the product or system. This shift is not for free, extensions to modeling and analysis methodologies for simulation need to be extended and revised. However, the revisitation of simulation-based methodologies represents also a great opportunity for the simulation community that will face with the new research challenges toward a pushed usage of simulation in real time operation of complex systems.

4 POSITION STATEMENT BY MARKUS RABE

In the context of applications in production and logistics, covering the scope from supply chains down to intralogistics, simulation has become a standard for planning purposes (Fleischmann et al. 2015). However, simulation just provides an experimental what-if technology. For an effective integration into the enterprise's continuous improvement, (i) promising scenarios have to be identified, (ii) good solutions applied for simulation forecasts based on current enterprise data, and (iii) the resulting changes transferred back to the real system. Such integration requires suitable simulation-optimization approaches as well as a maturity growth from digital factory models up to fully interactive digital twins. This section discusses the single elements and some of their current application barriers.

For the underlying *simulation*, applied technologies are in the first line discrete event simulation (DES), but also time-slicing approaches often combined with agent-based modelling and even Monte Carlo simulation (MCS), e.g., for many types of vehicle routing problems (cf. Balci et al. 2017). The planning horizon is usually on a tactical level, because for strategic questions the data granularity is not sufficiently detailed for simulation, while planning engineers typically will plan the future to come in a few months or even years. These digital models are characterized by enabling experiments, but require engineers to define

which experiments to conduct and to finally approach a solution that appears sufficiently good. An optimum can never be guaranteed by an experimental technique; worse, the engineers have no measure how far they might be from a theoretical optimum.

In order to support these human decisions, optimization techniques have been combined with simulation. From the four possible classes of such simulation (cf. VDI 2016), this is Case D where optimization is driving the overall process, while simulation is in a slave mode providing the results of the objective function to the master optimization algorithms. A major issue of this approach is performance, because simulation models require comparatively long computation times to calculate the objective function, and simulation runs must also be replicated to achieve statistically reliable outputs. Therefore, an intelligent procedure is mandatory to reduce the amount of required experiments, e.g., by a suitable design of experiments. One possible approach to improve the performance in stochastic simulation-optimization systems is simheuristics. A broad overview on simheuristics has been given by Juan et al. (2015). The approach is based on the expectation that good deterministic solutions might also be candidates for the stochastic case. Thus, a typical simheuristic procedure will include three phases: (i) reduce the model to a deterministic case (fixed value approach) and search for a set of reasonably good solutions without any replications; (ii) further optimize with the stochastic model starting from the previously built solution set with only a few replications (accepting quite broad confidence intervals); and (iii) finally conducting simulation runs with the full number of replications to reliably detect the most-promising solutions. Simheuristic approaches are especially promising in systems that can be analyzed statically, because MCS is by dimensions faster than DES and allows for much more experiments. Frequent applications are found for vehicle routing tasks (e.g., Juan and Rabe 2013).

In terms of the optimization technologies, *evolutionary algorithms*, especially genetic ones, have seen specific attention (e.g., Jackson et al. 2018; Gutenschwager et al. 2018). However, there is also first research on *machine learning* approaches like reinforcement learning (cf. Rabe et al. 2017). For large trading networks, Rabe et al. (2021) compared a genetic algorithm adapted to the huge number of parameters with a deep reinforcement learning solution. However, such huge systems require an adapted approach. For very simple systems with a few parameters, classic approaches of genetic algorithms that identify each parameter with a gene can provide acceptable results. For huge systems like supply chains, the parameter space is, however, far too large for such approaches. Here, the selection of the parameters to be changed must become part of the decision algorithm. This leads to an integrated 2-level structure, with one level defining the set of parameters and the second one defining good values for them. However, the simulation run time of supply chains also tends to be very long, in the range of minutes or even hours. A very interesting approach for large materials trading networks has recently been published by Ammouriova (2021), who formalized domain-specific additional information to speed up her genetic algorithms.

In the last years, the term *Digital Twin* has appeared in newspapers and also some research reports, not always with a clear and unique understanding what the term means (van der Valk et al. 2002). From the many aspects that can be found in recent works (cf. Cimino 2019), some can be identified that help to find sound classifications and, thus, common understanding. Van der Valk et al. (2020) have provided a taxonomy to achieve more transparency. The perhaps most important classification is based on the type of connections. Basically, all *digital models* are, finally, a mirror of a real system or a system that is currently only planned on paper or an IT-based design system. With simulation, dynamic models represent the (planned) systems behavior.

If a real system is already available, the digital model can be further exploited to monitor the running system, predict its expected further progressing, and potentially derive alerts when critical situations are likely. For this purpose it is mandatory that the model does not only mirror the system's structure and attributes, but also its *status*. This requires communication from the real system to the digital model, e.g., by suitable sensors and a – unidirectional – interface to the model, which can analyze these data and update its own state accordingly. The digital part of the couple follows the real development like a shadow follows the animal that throws it, and this enriched model is called a *digital shadow*. The shadow can "speed up" and analyze what will happen in the system in the near future. Always aware of the current system state, a

digital shadow can at any point of time give real-time advice for the system's operation. Early applications have been reported for space vehicles (Rosen 2015), and current implementations are today available, e.g., in the sector of supply chain management (cf. Enders 2019).

While currently there are not too many digital shadows outside theoretical research, implementations of a DT are even sparser. As the major criterion, a shadow follows; never will something follow its shadow. In contrast, twins are equal individuals. While a shadow follows the original, twins will follow each other. Therefore, the DT requires a bidirectional connection between its components (Grieves and Vickers 2017): Changes in reality influence the model – like in the case of the shadow – and *changes in the model operate reality*. For example, stopping a machining center in the model will mean that the real process is interrupted, and changing the sequence of orders in front of a machine in the model will change the real processing sequence. Still, a simulation component would allow for exploring the potential consequences before such changes are transmitted and, thus, made effective. This feature has been identified as a major research trend (Rosen et al. 2015, Enders and Hoßbach 2019). New research investigates Labeled Property Graph models to simulate logistics networks in a DT framework (Wuttke et al. 2023a) and the integration of data farming into a DT for the purpose of condition-based maintenance (Wuttke et al. 2023b). However, such a digital twin, which actually builds up an advanced control system for the real production, will raise massive challenges that have not been sufficiently explored yet. Actually, the implementation of digital twins in production and logistics would lead to completely new architectures of manufacturing execution systems, warehouse management systems, or supply chain execution systems.

The conclusion is that considering the real application in current enterprises, the goals to integrate improvement processes in a digital twin are not at all mature. With simulation finding quite broad application and simulation-optimization being in operation for a significant number of real cases, digital models can be declared a kind of standard. Digital shadows that really connect to the factory (and not through time-delayed data warehouses) are rarely reported. Digital twins, notwithstanding the current fashion discussion in the newspapers, are still a challenge for the future. Actually, a digital twin will require a more or less complete redesign of tactical and operational planning as well as control of enterprise systems into fully integrated IT systems. This is an important goal for the future. However, if we remember the goals and approaches of CIM in the eighties – which have not been too far from those of the DT – we should be aware that this maturing process has to be estimated in decades.

5 POSITION STATEMENT BY SUSAN SANCHEZ

My first recollection of hearing the term 'digital twin' was from a speaker at a Science of Test Workshop in 2016, and I remember thinking at the time that the excitement they portrayed boded well for the further augmentation of field experiments with simulation experiments. I was unaware that term had been coined in 2010 (IBM 2023; Glaessgen and Stargel 2012); indeed, the term "digital twin" was synonymous with "simulation" in my mind. Fast forward another seven years, and this term has taken off like wildfire. A Google search for "digital twin" yields 13 million hits – an order of magnitude more than the 1.22 million hits for "discrete event simulation" or the 846 thousand hits for "agent based simulation."

5.1 Digital Twins are not Identical Twins

One reason for the rapid rise in the popularity of digital twins may be the perception of different terms. Consider these excerpts from the New Oxford American Dictionary (Oxford University Press, 2015):

- A twin is a "person or thing exactly like another,"
- A simulation is "an imitation of a situation or process" or "the production of a computer model of something, especially for the purpose of study,"
- A model is "a simplified description, especially a mathematical one, of a system or process to assist calculations or predictions."

Consequently, a layperson might think that a digital twin is an exact replica, while a simulation or model is a simplification or abstraction. George Box's well-known mantra "all models are wrong, some are useful" (Box 1987) concisely indicates that modeling is not perfect and can be a difficult process requiring expertise. However, the presumption often appears to be that if you have a digital twin, it is good – if it is not good, then it is either not being fed the necessary data or it is not sufficiently detailed to truly be a twin.

Is the fact that digital twins are not identical to their physical counterparts a showstopper? Certainly not – like other computer models, they have proven beneficial for a variety of application areas, including manufacturing, robotics, aerospace, health care, and urban planning. They were beneficial in practice even before the term digital twin was coined; the application to biopharmaceutical manufacturing of Johnston et al. (2008) is just one example.

5.2 Identical Twins are not Identical

Identical twin siblings share the same DNA, and studies have found strong similarities even among identical twins separated at birth. However, they are distinct individuals with distinct life experiences. Similarly, no digital twin can possibly be identical to its real-world counterpart. This is important because some people have the misconception that digital twins will make it possible to predict exactly what will happen to their physical counterparts. For example, consider the reliability-based maintenance field. A digital twin of a physical drone will not be able to perfectly predict where crack propagation will start, or when crack propagation will abruptly result in catastrophic failure. A good (albeit non-identical) digital twin would enable us to identify better preventive maintenance protocols than either a regular schedule (e.g., at time-based or flight-time-based intervals) or breakdown-based approach. However, even if our digital twin could predict with certainty that the next gust of wind of over 50 miles per hour would cause a breakdown, we would not be able to predict exactly when that would occur.

5.3 Twins can be Good, "Evil," or Both

I view a digital twin as a model with connections – one that can be characterized as good if these connections provide insights or cause actions that are useful and timely. This applies to digital twins of the environment, as well as digital twins of the entities, systems, or processes operating within it.

One potential role for a twin is to put pressure on the others. For example, a hospital might subject its digital twin of an intensive care unit to an "evil" virtual environment by greatly increasing the arrival rate of patients, a retailer with a digital twin of its supply chain could explore the impact of supply-chain disruptions on its sales and inventory, or a drone manufacturer could investigate the effects of different weather patterns and operating protocols on the digital twin in a virtual environment rather than limit itself to field testing a physical prototype. This type of "what if?" analysis, similar to accelerated testing, can best be done using designed experiments in a data farming approach rather than by trial and error (Sanchez, Sanchez, and Wan 2021). The idea of purposefully varying uncertainties (a.k.a., "noise factors") in the environment underpins the concept of robust design (Sanchez and Sanchez 2020).

In summary, a suitable digital representation can be more useful if it is sometimes exercised in adversarial ways. Consequently, a digital twin can be both good and "evil" – and that is a good thing!

5.4 **Opportunities**

The rapid growth in digital twin applications is a chance for the simulation community to vastly broaden its reach by disseminating our current knowledge, while challenges that arise from digital twin implementations will raise interesting new lines of research. Nine years ago, in a WSC panel on the future of computerized decision-making, I predicted "a growth in automating linkages between real-world data and simulation modeling environments" would increase "the potential for using simulation as a real-time decision support and control system," and posited that as common interfaces and data exchange protocols made it easier to link simulation models to external data in real time, they could also facilitate the use of analysis apps including data farming, simulation optimization, and big data visualization (Elmegreen,

Sanchez, and Szaley 2014). Those opportunities remain today. We need thoughtful dialogue and collaboration with those developing and using digital twins outside of the simulation community. Understanding subconscious reactions to the language used may ease this communication.

6 POSITION STATEMENT BY GUODONG SHAO

6.1 Various Applications of Digital Twins

In recent years, DTs have become more prevalent in a wide variety of industries including manufacturing, construction, smart cities, healthcare, and business for a wide range of purposes such as monitoring, anomaly detection, prediction, optimization, and control. Various DT applications are shown in Figure 1. These include descriptive, diagnostic, predictive, prescriptive, and intelligent DT. From left to right, Figure 1 represents digital twins, from monitoring to intelligent control, to support more valuable decision making and automation. With the advancements in simulation, optimization, and AI, DTs can become more and more powerful. In the context of manufacturing, each category is described as follows (Shao et al. 2014).

Observe	Analyze	Predict	Influence	Automate
Descriptive Digital Twin	Diagnostic Digital Twin	Predictive Digital Twin	Prescriptive Digital Twin	Intelligent Digital Twin
What happened or happening?	What's wrong and why is it happening?	What is likely to happen?	How can we make it happen?	How can we make it adjust itself?
 Data stream Database queries Reporting & dashboards 	 Simulation Data mining & forensics Real-time analytics & mining 	 Simulation Statistics & linear regression Predictive data mining Forecasting & trend reporting 	 Simulation Machine learning Optimization 	 Simulation Optimization Artificial Intelligence (AI) Automation Control

More decision support, greater value

Figure 1. Various applications of digital twins

- *Descriptive* DTs help identify what happened or is happening. These kinds of DTs can provide various views of the data collected using device sensors to identify patterns and trends in such data. These views may be data visualization in forms of text, tables, and charts, e.g., average throughput and cycle time by product types in manufacturing.
- *Diagnostic* DTs help identify why it happened or is happening. This includes understanding the impact of the input factors and operational strategies on the performance measures. For example, the increase in cycle time of a product may be tracked down to factors such as machine breakdowns, worker absenteeism, or rework of defected parts.
- *Predictive* DTs help identify what is going to happen and when. For example, these kinds of DTs can be used to estimate the cycle time and throughputs for various products based on current strategies for order release and dispatching, scheduled material arrivals, and machine and worker availabilities.
- *Prescriptive* DTs help decide how we can make it happen and what the consequences could be. These kinds of DTs can help identify the strategies and inputs that will lead to the desired performance. For example, prescriptive analytics may include identifying changes in input

parameters and strategies that will enable cycle-time reduction and throughput increase to the desired levels.

• *Intelligent* DTs will automatically control the physical counterparts based on the strategies and parameters identified by the prescriptive DTs. These kinds of DTs may also be able to dynamically adjust themselves to keep themselves valid and trustworthy. AI is the main modeling technique for this kind of DTs. Of course, stringent verification and testing must be performed before the DTs can be applied to the production environment to ensure operational safety. In the human-in-the-loop cases, human operators may be required to validate the actions before applying them.

Which kind of DT should be implemented and used will depend on the use cases and be driven by the objective and scope of the DT. In addition, use cases of DTs can be at any stage of the lifecycle of the real-world entity. For example, in the design stage, a DT can digitally represent the real-world product or system for simulation and analysis to support design decisions. In the operation stage, a DT can digitally represent the real-world system and process for monitoring, managing, and controlling the equipment or system to support operational decisions. Data can also flow between lifecycle stages, a DT in the operation stage can provide feedback to a DT in the design stage.

6.2 Standardization for Digital Twins – From Requirement to Credibility

Because DTs are still in their relatively early stage, the ecosystem of DTs has not been well established. Manufacturers, especially SMEs (Small and Medium-sized Enterprises), face challenges to implement their DT applications efficiently and effectively. Current implementations are mostly using ad-hoc approaches. Standards are required in order to go beyond expensive, custom DTs to an affordable marketplace of products and tools for DTs. Standards for DTs will facilitate the composition and integration of DTs by providing guidelines, methodologies, frameworks, common terminologies, architectures, and interface specifications. They help make the creating, integrating, updating, and validating of DTs more accurate and consistent, ultimately to achieve "plug and play," i.e., enabling interoperability between DTs and supporting software and hardware from different vendors. This can, in turn, significantly reduce the development time and effort required to create and use DTs. Standards can help formalize requirements for DT projects; enable the use of building blocks for DT implementations; analyze DT performance; communicate between suppliers, partners, and customers; and secure DT information and protect privacy.

For example, a recently published DT framework standard series, ISO 23247: Digital Twin Manufacturing Framework, is to facilitate the implementation of digital twins in manufacturing (ISO 2021). The standards have four parts: (1) Overview and general principles, (2) reference architecture, (3) Digital representation of physical manufacturing elements, and (4) information exchange. The standards provide guidelines, methods, and approaches for analyzing modeling requirements, defining scope and objectives, and promoting the use of common terminology and a generic reference architecture when implementing digital twins in manufacturing. The standards also help facilitate the composability of digital twins and interoperability among various domains and entities by applying existing relevant standards. It provides examples of data collection, modeling and simulation, communication, integration, visualization, and control.

Future work of the standards may include new additions that can support the development and validation of DTs. The new topics include: (1) digital thread for DT, (2) composition of multiple DTs, (3) ontologies of the DT framework to clarify the entities and relationships, (4) building DTs from reusable components to increase the consistency and reduce the development time, (5) credibility assessment of DTs to increase the trustworthiness and value for decision-making, (6) providing guidelines that enable the integration between DTs and the industrial metaverse, (7) a DT core that enables plug and play software/hardware integration by standardizing interfaces with customers' environment and application platforms, and (8) extending the framework to specific sectors, e.g., semiconductor manufacturing, biomanufacturing, and additive manufacturing to address domain specific needs (Shao et al. 2023).

7 POSITION STATEMENT BY SIMON J. E. TAYLOR

As noted by others in this article, there have been many advances in Simulation and AI (see for example the many papers in the new Simulation and AI Track introduced in the 2022 Winter Simulation Conference in Singapore). Arguably research in this area dates back to the 1990s (e.g., Doukidis and Paul 1985). More recently, advances in virtualization and Cyber-physical systems/the Internet of Things have made possible DTs (again see many examples in the Digital Twin track of the Winter Simulation Conference over the last few years). If the combination of Simulation and AI is leading to novel methodologies and applications then one might assume that similar contributions could be made to DT research, at least to the simulation component of the DT. Branke (in Taylor et al. 2021) presented a comparison between simulation and one of the main areas of AI, machine learning. Borrowing from this, Table 1 shows some thoughts comparing DTs (specifically the simulation component) and Machine Learning.

	Digital Twins	Machine Learning (ML)	
Domain Knowledge	A lot of domain knowledge needed	Little as models are derived by	
	(e.g., to formulate causal logic, routing,	applying ML approaches (assuming	
	machine breakdowns, etc.)	data is available).	
Data	Can be little if domain knowledge used	Large amounts needed (for	
	but will increase can be more if	training/developing the model). A	
	distributions derived from historical	problem if there is little data.	
	data (e.g., efficiency, breakdowns, etc.)		
	Can be used if there is little data		
	(leveraging domain knowledge).		
Computation Speed	Can be slow due to model size – a	Slow to train due to processing of	
	particular issue if replications/	training sets, quick to use.	
	experiments used		
Speed up needs	Can use parallel simulation methods	Can use GPUs but expensive.	
	and grids of generally available CPUs		
	(e.g., clusters, desktop PCs)		
Explainability/	Good, model can be understood by	Black box, difficult to explain. Issue	
Trust	humans. Confidence/error/etc.	about clearly stating robustness/error.	
	techniques well understood. Can be	Difficult to trust on this basis.	
	trusted on this basis.		
Extrapolation/	Can extrapolate to completely new	Very good at interpolation, struggles	
Interpolation	situations (what-if experimentation).	to generalise to unseen situations.	

Table 1: A Comparison of Digital Twins and AI (Machine Learning)

It can be argued that the two areas are complementary. For example, AI/ML can develop quick-to-use metamodels that could be incorporated into a simulation by leveraging available data. This could reduce the run time needed for a simulation by reducing parts of a large model to mathematical models. Complementing this with specific domain knowledge in a simulation might in turn lead to better trusted and understood AI/ML models that are capable of what-if analysis. There are many opportunities. However, what is not generally reported are two issues that need urgent investigation and understanding.

Model development. The simulation component of a DT is developed using techniques that date back to the 1950s (e.g., iterative model development, verification, and validation, etc.) Sometimes this "hand-crafted" approach has been criticised for being time consuming and expensive. However, it does create well understood and trusted models. There seems to be a general assumption that this is the same for AI techniques. This may not be the case. Many articles proposing new AI/ML algorithms or AI/optimization approaches tend to compare several techniques and suggest one that produces the best metamodel for the dataset presented in the work. It is difficult to generalize on this basis. This strongly suggests that AI

approaches are "hand-crafted" as well and are in turn time consuming and expensive. This aspect of AI does not seem to be widely reported.

Confidence. How certain are we that a simulation or DT gives results that we can be confident in? There are established techniques to reporting confidence in simulation, especially verification and validation. This does not seem to be widely discussed in DT research. However, in AI it appears that common approaches to capturing the confidence that one might have in a metamodel or optimization seem to be in their early stages. Common approaches to robustness seem to be a long way away (Hamon, Junklewitz and Sanchez 2020).

In summary, there is a strong argument that combining DTs and AI research can lead to interesting complementary innovations. However, in this context one needs to be aware that AI model development methodologies and robustness techniques are in their early stages, despite widespread claims to the contrary.

8 SUMMARY

This article has presented views from six experts on the potential innovations and challenges of combining research into Simulation, AI, and Digital Twins.

DISCLAIMER

No approval or endorsement of any commercial product by NIST is intended or implied. Certain commercial software systems are identified in this paper to facilitate understanding. Such identification does not imply that these software systems are necessarily the best available for the purpose. The opinions, recommendations, findings, and conclusions in this publication do not necessarily reflect the views or policies of NIST or the United States Government.

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