Simulation on Digital Twin: Role of Artificial Intelligence and Emergence of Industrial Metaverse

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***Abstract*—Digital Twins (DTs) are cutting-edge technological design principles of Industry 4.0. They elevate the representation level of physical systems backed up by accurate real-time data in virtual environments and empower the simulation capabilities of these systems through Artificial Intelligence (AI) for their analysis, monitoring, and optimization. This work comprehensively explores the intrinsic interaction between simulation and AI in DTs, meticulously covering the current literature status and categorizing these symbiotic interactions into three different groups that cover AI to support DT-based simulation, AI for optimization of simulation within DT, and simulation to support AI approaches in DT. In addition, a deeper look is taken at the role of simulation and AI in the emerging concept of the Industrial Metaverse, which promises to extend DTs beyond discrete virtual representation of physical systems to encompass the industrial ecosystem from end-to-end. Finally, the main research challenges for achieving the full integration of simulation and AI in DTs and at the Industrial Metaverse are discussed.**

Keywords: Digital Twin, Simulation, Artificial Intelligence, Machine Learning, Industrial Metaverse

I. Introduction

The digitalization process in Industry 4.0 (I4.0) represents the strategic adoption of innovative technologies, such as the Industrial Internet of Things (IIoT), advanced simulation, Artificial Intelligence (AI) and Digital Twin (DT), for transforming manufacturing companies into smart manufacturers [1]. The linkage of all assets comprising the manufacturing process – devices, machines, systems, and operators – via IIoT technologies facilitates the creation of virtual environments composed of DTs, offering AI-based data analytics to enhance production processes and predictive maintenance, leveraging by historical and real-time data collected from the physical assets and by performing realistic simulations [2].

A further aspect guaranteed by the connection between the physical asset and its virtual copy is the bi-directionality of data, which allows the simulation model in the DT to be a high-fidelity replica constantly updated based on the real-time changes in the physical asset. The simulation results guarantee the DT can act and provide feedback for the physical asset performing corrections and optimization of its operation [3]. Simulation procedures integrated with AI approaches in DTs enable the generation and execution of accurate models and what-if scenarios, providing decision-makers with deeper insights under a wide range of configurations and potential hypothetical situations associated with the manufacturing systems' behaviour [4].

AI models can further be applied to optimise what-if simulations by eliminating irrelevant scenarios and providing decision-making support. This is particularly useful since the manual decision-making process in each possible scenario can be time-consuming and require intensive computational resources [5]. The proper and deeper integration between AI and the simulation process under DTs is still an advancing field that is beginning to define how to formalise its iterations with the modelling of complex manufacturing systems [6]. These advances, combined with the expansion of the representation of the digital environments of the manufacturing process to the entire production chain through more complex modelling in a network of connected DTs, are leading the I4.0 to embody a new paradigm known as the Industrial Metaverse [7].

Industrial Metaverse proposes a broader and more dynamic perspective of DTs in industry, not limited to discrete physical systems that represent separate Cyber-Physical Systems (CPS), but the whole industrial system across elements outside the factory, departments, processes, assets and players. Moreover, it opens up a premise for extensive what-if simulation functionalities that can cope with the dynamism and complexity of these evolutionary virtual models and the interconnections required between simulation and AI for encompassing these end-to-end manufacturing ecosystems [8].

The effective integration of simulation and AI in DTs and Industrial Metaverses still depends on developing more robust integration methods to deal with highly complex industrial systems, effectively guaranteeing the real-time exchange of feedback between the simulation and the physical assets and ensuring interoperability between these systems. For this reason, this article aims to comprehensively understand the association between AI and simulation capabilities in DTs and how these interconnections can result in mutual relationships between them regarding an improvement of efficiency, optimization and accuracy. For this purpose, the related literature will be reviewed and duly organized into different categories that cover their main aspects and advantages. Moreover, it is intended to contribute towards establishing a clear understanding of the role of simulation-based AI within the Industrial Metaverse, highlighting the existing gaps at the current stage of development of Metaverse and DT technologies, and defining which research lines can be pursued to exploit the potential of these concepts in the next stage of I4.0.

The rest of the paper is organized as follows: Section II provides a detailed specification and classification of the existing interactions between the simulation and AI principles within DT. A contextualization of the Industrial Metaverse and its vital role in fostering the simulation through its fusion with AI for end-to-end DT of complex industrial systems is made in Section III. Section IV identifies some open issues and future research lines for AI-assisted simulation in DTs and Industrial Metaverse. Finally, Section V rounds up the paper with the main insights and conclusions.

II. AI-Integrated Simulation within DT

To obtain more profound insights into the current positioning, trends, and applications related to the fusion of simulation and AI under DTs and define which trends and forthcoming challenges must be addressed to meet this topic concerning the emergence of the Industrial Metaverse, a meticulous literature analysis was carried out, considering some of the leading scientific datasets in the field of technology, namely Scopus, WoS, and IEEE Xplore. The search query covered publications between 2016 and November 2023 (the start date of the work), selecting papers with the following keyword variations: “Digital Twin*” AND (“Simulation*” OR “What-if”) AND (“Artificial Intelligence” OR “Machine Learning” OR “Reinforcement Learning” OR “Neural Network”). After removing duplicate entries, 801 articles were identified. From these, 220 peer-reviewed articles were selected for initial analysis based on their abstracts. Afterwards, 19 articles were chosen for complete analysis as they were deemed highly relevant.

Based on the literature review, the symbiotic interactions between simulation and AI in the DT context were categorized into three distinct clusters, as illustrated by the Venn diagram in Figure 1. The first cluster deals with AI to support DT-based simulation, which centres on the generation of what-if scenarios and simulation models in an accurate and realistic way, besides the adoption of AI for real-time analysis of simulation to predict and prevent anomalies and to support decision-making and feedback for physical assets. Moreover, this cluster addresses AI to improve simulation scenarios by merging real and simulated data and the joint use of AI and simulation to generate datasets that describe future scenarios and conditions that could occur and affect the physical asset.

The second cluster addresses the use of AI for simulation optimization within DT, where AI can act in the autonomous setup or dynamic reconfiguration of simulation parameters to reduce the computational consumption and setup time, besides increasing the simulation efficiency. In addition, AI can continuously improve the simulation model performance or even assist in decision-making or the autonomous choice

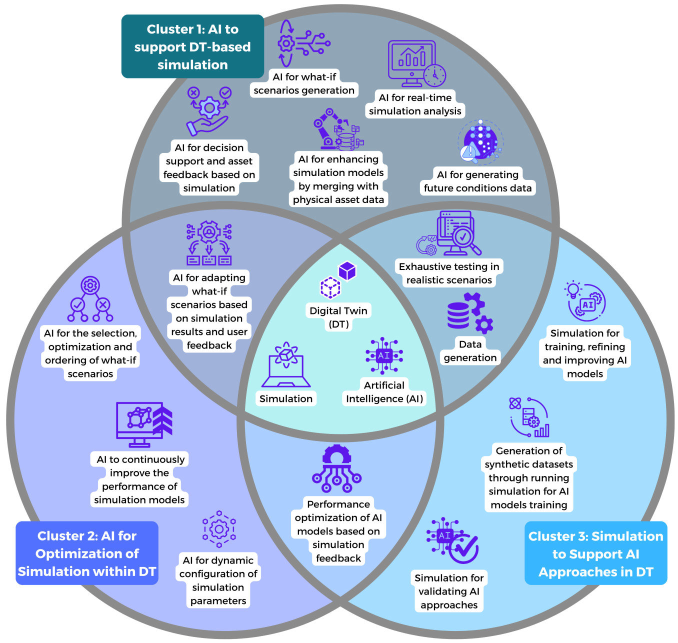

Figure 1. Venn diagram representing the clustering of co-relations between AI and Simulation within DT.

of what-if scenarios to eliminate irrelevant scenarios or define priority orders. Finally, the third cluster addresses simulation to support AI approaches in DT, where simulation can be used to train, refine and improve AI models. The training of AI models can take place by generating datasets through the use of simulation, which can also be applied to validate AI approaches through exhaustive testing.

Some noteworthy characteristics stand out in the intersections areas of the Venn diagram. For instance, AI can be applied to adjust and adapt what-if scenarios and simulation models based on the user feedback or through the learning resulting from the simulation process (intersection of clusters 1 and 2). Furthermore, data can be generated or AI models can be tested in realistic scenarios by running simulations (intersection of clusters 1 and 3). Additionally, AI models can be optimized based on the simulation feedback (intersection of clusters 2 and 3). In the following subsections, each cluster will be further discussed in detail, along with a perspective of the existing applications in the literature.

A. AI to Support DT-based Simulation

AI-powered approaches have outstanding potential for supporting simulation in multiple manners, including generating accurate hypothetical simulation scenarios [4]. The study described in [9] employed Generative Adversarial Networks and diffusion models to create realistic road traffic scenarios under different environmental conditions; these scenarios are applied to validate autonomous driven systems, avoiding the need for conducting dangerous tests on the actual environments, besides cover situations of complex replication. Additionally, AI models can precisely define situations and changes that may occur in the system under study as part of what-if simulations, thus generating scenarios and data that reflect these abnormalities, making it possible to make predictions during the simulation process or its identification through real-time data analysis. For example, a trajectory prediction learning model is used to minimize the risk of accidents in a human-machine cooperative driving system in dynamic traffic scenarios [10], considering historical trajectory data to determine risk situations that could affect the vehicle.

Deploying advanced AI capabilities in real-time analysis of simulations, both for feedback to physical assets and to support decision-making, for the prognosis and prevention of malfunctions and anomalies in the production process [2], is the foundation behind the Zero-Defect Manufacturing (ZDM) concept. An allusion to this aspect is presented in [11], where a Markov model is applied to answer what-if scenarios in real-time, delivering the probability of abnormal states occurring in different stages of a femtolaser ablation manufacturing procedure and demonstrating the DT's adaptability in monitoring and prevent failures in the running process.

Moreover, AI can enhance the simulation models' accuracy by integrating real-time data from physical assets. As a result, the DT can effectively provide feedback and operate over the physical component or even assist decision-makers through AI-enabled visualization technologies [12]. These aspects are covered in [1], where a DT of a collaborative robot is created to provide iteration and decision support to the user through an immersive mixed-reality application. The DT gathered data in real-time from the robot through IIoT-based sensors, which are used to simulate, plan and validate the robot's movement according to the user feedback before its deployment.

B. AI for Optimization of Simulation within DT

The predominant advantage of performing what-if simulation is the ability to test and explore numerous alternative scenarios, including production line arrangements and worst-case situations [13]; however, running each scenario can be time-consuming and require significant computing resources. These simulation procedures can be optimised by employing AI solutions that allow scenarios to be prioritized or even eliminated, depending of their relevance. What-if simulation optimization in industrial logistics scenarios can use trust-based recommendation systems, particularly reinforcement learning approaches, such as the Q-Learning algorithm, along with similarity measures, to support the user's decision-making process [5]. The system provides target scenarios based on the user's trust in the system, which reduces the decision-making time and increases the system efficiency by eliminating irrelevant hypothetical scenarios.

Besides prioritizing scenarios, AI can be used to autonomously and dynamically configure simulation inputs and parameters, reducing the setup time and computational consumption. A discussion on machine learning models to speed up the what-if analysis for optimising production chains is presented in [14]. The models are adjusted according to the evaluation of input parameters from the generated synthetic data, improving the system's responsiveness to execute the what-if processing. This perspective also outlines how AI can be leveraged to continuously improve the simulation performance, as demonstrated in [15]. The authors propose an approach based on Active Learning, where metamodels are progressively trained with selected data sets, reducing the computational resources required for the simulation execution.

C. Simulation to Support AI Approaches in DT

Simulations have a significant role in generating synthetic datasets used to train, refine and improve AI-based models in DTs. For instance, in [16], a fast fashion company's operational planning is modelled through discrete event simulation (DES) in FlexSim; the generated data is used to train an artificial neural network, which is validated through the simulation process, allowing the improvement and reorganization of the company's operational system. Another example is discussed in [17], which evaluates the intelligent navigation of drones to reduce the time and energy required to visit moving targets. A 3D simulation model based on the physical scenario is developed to train a Deep Reinforcement Learning (DRL) approach in the OpenAI Gym structure so that the drone can learn the mobility pattern of the moving target and create a more efficient approach strategy for battery consumption. DRL algorithms are validated by running exhaustive DES considering the variation of different parameters of the physics-based DT, such as the drone operating area, the number of moving targets and the randomness of the movement.

Performing exhaustive testing of AI models through simulation is paramount to validate their robustness and performance under different parameters and situations, ensuring that the models fulfil their roles as accurately and realistically as possible. This principle is illustrated in a multi-purpose robotic manufacturing cell [18], where AI models undergo a series of comprehensive simulated tests to ensure their suitability for the robotic cell. These models are responsible for dynamically optimizing and reconfiguring the parameters, layout, and operating time to meet the process requirements.

III. Simulation Boost in the Industrial Metaverse

The Industrial Metaverse is an emerging field that represents a new step in intelligent manufacturing systems and the integration between physical factories and the virtual world [7]. Through the digitalization of manufacturing operations, the Industrial Metaverse can potentialize the adaptability and agility of the supply chain, enhancing collaboration and promoting the development of more sustainable businesses [19].

Despite being closely related to the DT concept and other I4.0 enabling technologies, the Industrial Metaverse can be defined as a connected whole system of DTs that can represent real industrial systems throughout the entire value chain – from inbounding logistics to the manufacturing process and across the whole product life cycle. The Industrial Metaverse enables the convergence and evolution of DTs, especially considering aspects such as connectivity, complex systems simulation, scaled-up AI, and process visualization, enhancing the decision-making strategic level in the design, development, operation and optimization of the industrial process [8].

Companies at the forefront of the Industrial Metaverse, such as BMW and Bosch, have already employed advanced DT replicas of their factories for a tight convergence of the digital and physical systems, covering the simulation process at a macro factory level [19]. NVIDIA and Siemens have launched the NVIDIA Omniverse platform, which integrated with the Siemens Xcelerator, aims to connect and develop OpenUSD applications – an extensible ecosystem for describing, composing and simulating high-realistic 3D models – to provide photorealistic visualization of simulation models for the design and operation of industrial systems comprising a wide range of software tools for the description and realistic visualization of processes, besides the AI-enabled simulation acceleration. The platform enables the DT design and simulation of production systems in various scenarios, including numerous models of autonomous robotic systems, as well as the real-time connection with data from IIoT devices [20].

Despite the tremendous opportunities for AI-enabled simulation in the Industrial Metaverse, the literature still lacks research studies dealing with developments in this field. In [2], it addressed the deployment of DT as part of the Metaverse for Additive Manufacturing, where the 3D printing process can be monitored and simulated to optimize the process and for fault detection by using Convolutional Neural Networks. The work presented at [21] discusses the significance of Deep Neural Networks and Generative Adversarial Networks concerning their use in creating hypothetical scenarios within the Industrial Metaverse context. The models are explicitly explored for configuring industrial automation layouts and verifying compliance with the established Service Level Agreement. For its part, [22] refers to the Industrial Metaverse to parallel manufacturing, where DT is responsible for understanding the interactions between operators and robots in customized production systems, which require a high level of reconfiguration of the production line. The paper uses a customized shoe production line as a case study, where simulation and neural networks optimize processes and the robot's performance in real-time, thus reducing waste in production.

Some works have focused on performing AI-enabled simulation in the Metaverse but in a non-industrial setting. For example, [23] describes the components needed to build a DT network on the NVIDIA Omniverse platform for 6G wireless networks, including what-if analysis for the dynamic modification of network parameters, the generation of synthetic data through simulation and AI that reflects diverse operating conditions such as climatic and environmental factors, and network operating parameters, as well as the application of synthetic data and real data to train AI algorithms responsible for predicting and analyzing the operation of 6G networks. Meanwhile, [9] addresses the Vehicular Metaverse in an architecture where the DT is responsible for assisting and training autonomous driving systems, generating multiple driving and traffic scenarios through empowered simulation by generative AI and the combination of data from autonomous car sensing.

The Industrial Metaverse symbolises a radical shift in the scalability of simulations in DT, extending it far beyond the portrayal of discrete physical industrial assets towards multiple connected assets and internal processes at the end-to-end of the industry [8]. In fact, the increase of simulation scalability and the complexity of modelling closed-loop industrial systems raises exponentially the difficulty of handling and processing the volumes of generated data, as well as the formulation and execution of what-if scenarios. This context makes AI an even more valuable and powerful enabling technology, not only for data analysis but also for optimising the simulation process. The computing power needed to carry out large-scale, complex and realistic simulations is highly substantial, so it is crucial to have AI mechanisms to optimize the simulation process or reduce the number of alternative scenarios, especially when considering the need for real-time iteration between the real and virtual worlds.

An Industrial Metaverse's technological ecosystem representation is portrayed in Figure 2. The bottom layer, referred to as the "Physical Industrial System," showcases the various elements that compose the production chain in the physical spectrum, encompassing CPS, manufacturing procedures, collaborative robotics, logistics, the product life cycle, the value chain, virtual commissioning, and the operators and decision-makers involved in the manufacturing process.

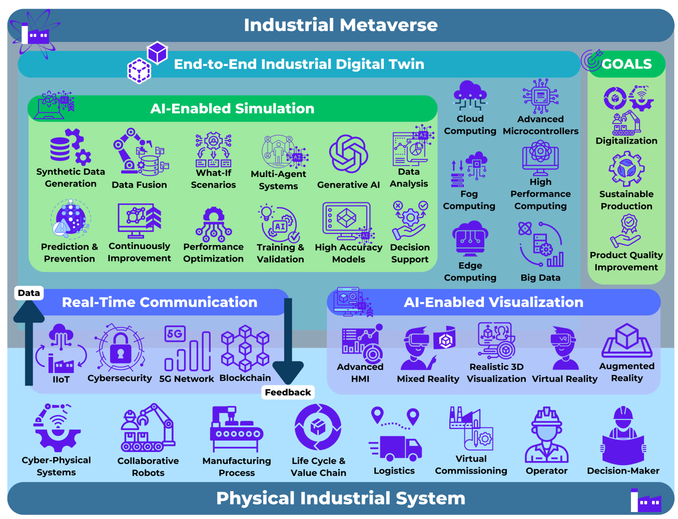

Figure 2. Industrial Metaverse's technological ecosystem.

The intermediate layer is composed of two classes which are responsible for bridging the physical and digital worlds. The "Real-Time Communication" class covers the technologies associated with the real-time transmission of data from the physical assets to the Metaverse DT and for sending feedback and configuration parameters from the Metaverse to the physical assets, thereby highlighting 5G networks and technologies based on IIoT and blockchain, as well as enablers which guarantee cybersecurity in the exchange of data. The "AI-Enabled Visualization" class features AI-powered technologies that support operators and decision-makers, such as advanced human-machine interfaces (HMI), mixed reality, realistic 3D visualization, virtual reality and augmented reality.

The top layer represents the Industrial Metaverse, which has as one of its main "Goals" the complete digitalization of the production chain to improve product quality and achieve more sustainable, optimized, and less wasteful production. As a result of the digitization process, the Industrial Metaverse incorporates the "End-to-End Industrial Digital Twin", which covers all the correlations of existing components in the physical industrial system, which are now digitalized. The end-to-end DT includes elements such as high-performance computing, big data, cloud, fog and edge computing, and advanced microcontrollers to allow handling the high volume of data derived from complex systems that are part of the DT. The key component of the end-to-end DT in the Metaverse is the "AI-Enabled Simulation" component, which includes the simulation aspect and its functionalities. Many of these functionalities were already considered as DT design factors at the advent of I4.0 and are now further enhanced by adopting AI techniques and approaches.

AI-enabled simulation has as its key elements the generation and execution of realistic what-if scenarios, enhanced by the fusion of actual data from physical assets with synthetic data generated by operating high-accuracy simulation models and AI approaches based on machine learning or generative AI. Moreover, considering the symbiotic relationship between simulation and AI, simulation can be continuously improved, just as AI models can be trained and validated, providing constant performance optimization of both. With the high-quality data generated by the simulation and collected in the physical environment, AI is responsible for the data analysis process and can provide predictions and prevent future situations and defects, thereby supporting decision-making. Given the complexity of the end-to-end DT, multi-agent systems (MAS) can act as facilitators in coordinating simulation between the various elements and models that make up the DT.

IV. Discussion and Research Challenges

The effective integration of simulation and AI within DTs presents several ongoing research challenges, which are further compounded by the complexities introduced by the emergence of the Industrial Metaverse. Table I outlines these challenges along with their current degree of maturity and classification in the different types of iteration between simulation and AI, drawing from the existing literature and the inherent requirements of the Industrial Metaverse concept.

Concerning AI to support DT-based simulation, advancements in generative AI models have outstanding potential to create precise simulation models, generate hypothetical scenarios, produce high-quality datasets, and develop more reliable recommendation systems as part of the support for the decision-making process. This process must be further improved through simulation results and AI-powered HMIs that provide a more realistic visualization of simulation models supported by virtual, augmented, and mixed reality and advanced 3D modelling. Advances are also necessary for the development of AI methods that allow accurate simulation models to be built and that bridge the realism gap between the actual system and its DT, allowing the simulated models to be adapted in real-time according to changes in the physical system, and for the DT to autonomously operate on the physical assets.

The optimization of the simulation process depends on the integration of advanced AI methods to reduce the consumption of computational resources and processing time, as well as allowing the correct choice of hypothetical scenarios, eliminating unpromising hypotheses and permitting the simulation to have a more real-time bias, while also taking advantage of the dynamic distribution of processing between different computational levels such as edge, fog and cloud. Furthermore, MAS can be highly valuable to refine the simulation process, by handling the allocation of tasks and reduction of what-if scenarios across interconnected components. Each agent can be responsible for executing a specific part of the simulation model, allowing the parallelization between coordinated systems that synchronize operations and guarantee data coherence. In this context, efforts are devoted to design lighter but accurate AI and simulation strategies that can run on constrained embedded systems.

Much has already been developed concerning simulation to support AI approaches in DT by running advanced simulation models to generate accurate synthetic data for training AI models and validating them through exhaustive testing. However, this research has yet to focus on defining effective methods that allow for the continuous improvement of AI models.

Several challenges lie ahead in the effective Industrial Metaverse's simulation and AI integration, aimed at enhancing product quality, minimizing waste for sustainable production and aligning with ZDM predictive aspects. As the Industrial Metaverse spans intricate end-to-end systems, standardization methodologies for embedded simulation and AI within DTs are imperative to ensure interoperability between complex systems. Moreover, addressing the complexity of coordinating the simulation across distributed modules in real-time demands the adoption of disruptive technologies like IIoT and MAS.

V. Conclusions

As I4.0 continues to evolve, new paradigms are emerging to elevate industry development standards further. The Industrial Metaverse is at the forefront of expanding the simulation aspect capabilities in DTs and encompassing a series of whole-complex systems connected throughout the entire production chain, underscoring an even more emphasised appreciation for adopting AI as a DT and simulation-enabling technology.

This work focused on understanding and analyzing the different types of iterations that exist between simulation and AI in the context of DT, highlighting the current state of development of these in the literature, whether for supporting simulation in hypothetical scenarios, generating and processing data, analyzing and predicting anomalies, supporting decision-making, optimizing simulation processes, dynamically configuring models, or validating and training them. A representation

Table I
RESEARCH CHALLENGES REGARDING THE INTEGRATION OF SIMULATION AND AI IN DTS AND INDUSTRIAL METAVERSE

Cluster	Research Challenge	Maturity
AI to support DT-based simulation	Generative AI to produce what-if scenarios, parameters and models, accurate datasets and expert recommendations	Low
	Merging simulation models into AI-powered HMI to support decision-making and 3D realistic visualization	Low
	AI to adjust simulation models in real-time and to provide feedback to physical assets	Medium
	AI for improvement of decision-making support systems based on simulation results	Medium
	Decrease the realism gap between the physical system and its simulation model or representation through AI	Medium
AI for optimization of simulation within DT	Employment of AI to optimize what-if simulation and analysis processes by targeting relevant scenarios	Low
	Integration of advanced AI methods to optimize simulation, reducing resource consumption and processing time	Low
	AI for simulation processing distribution amongst distinct computational levels (edge, fog, cloud)	Low
	MAS to optimize what-if simulation by reducing scenarios space and paralelizing their execution	Medium
	Simulations and lightweight AI algorithms for embedded systems and low-performance computing systems	Medium
Simulation to support AI approaches in DT	Definition of effective methods to enable continuous improvement of AI models based on simulation feedback	Low
	Execution of simulation for high-accuracy data generation for AI model training	Medium
	Simulation for exhaustive validation of AI approaches under DTs	High
Effective integration of simulation and AI within the Industrial Metaverse	Collaboration over simulation and AI to increase product quality, reduce waste and enhance sustainable production	Low
	Standardization to embed simulation and AI in end-to-end DTs and ensure interoperability across several systems	Low
	MAS to coordinate distributed and cooperative simulation among distinct systems	Low
	Highly accurate AI-enhanced simulation models for ZDM and predictive manufacture in complex end-to-end DT	Low
	AI to integrate and analyze both simulated and real-time IIoT data from the whole industrial production system	Medium

of the technological ecosystem, as an Industrial Metaverse, was built to represent the main features involved in the digitalization of complex production systems in their complete life cycle and highlight the role of AI-enabled simulation for the completeness of the end-to-end DT. The discussed research challenges help pave the way for developing new lines of research that address the existing gaps in constructing more realistic and optimized simulations, which elevate DTs from simple representations of isolated and discrete CPS to a chain of high-level interconnected manufacturing systems.

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