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What can we expect from Quantum (Digital) Twins?

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Presenter Information

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Abstract. Digital twins enable the modeling and simulation of real-world entities (objects, processes or systems), resulting in improvements in the associated value chains. The emerging field of quantum computing holds tremendous promise for evolving this virtualization towards Quantum (Digital) Twins (QDT) and ultimately Quantum Twins (QT). The quantum (digital) twin concept is not a contradiction in terms - but instead describes a hybrid approach that can be implemented using the technologies available today by combining classical computing and digital twin concepts with quantum processing. This paper presents the status quo of research and practice on quantum (digital) twins. It also discuses their potential to create competitive advantage through real-time simulation of highly complex, interconnected entities that helps companies better address changes in their environment and differentiate their products and services.
Keywords: Artificial Intelligence, Digital Twin Evolution, Machine Learning, Quantum Computing, Quantum Machine Learning, Quantum Digital Twin, Quantum Twin, Simulation

1 Introduction

1.1 A short summary on the state of classical Digital Twins today

Today, objects, processes or systems in the physical world oftentimes have a digital representation called a digital twin [1]. Factory machine tools, robots used on assembly lines, fully automated warehouses, or building systems collect data about their

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operation and send it to servers, where it can be further processed to understand the current state of operations, identify needed adjustments for optimal performance, and make future improvements [2]. Digital twins are virtualized assets (such as products, machine tools, equipment), processes (such as finance, supply chain or human resources) or systems (such as entire production plants or buildings) that containing data, models, computations, simulations and service interfaces that enable the representation, understanding and prediction of the underlying real-world entity's operational states and behaviors, the prescription of actions based on business logic and objectives, and even augmented reality representation [1–3].

This virtual mirroring allows for rapid access to the properties of the real-world entity and therefore enable simulations regarding design updates, maintenance, correction of issues, or even the interaction with other digital twins. For example, a digital twin of a whole factory floor allows for simulated factory modifications which would be highly expensive if done in the physical realm—especially considering required factory downtime. In addition, the virtual double can act like a digital shadow through all stages of the value chain - design, production, delivery, operation, service, return, recycling, and end of life. The information collected by a digital twin in all of these stages can be further analyzed to develop better future products, processes or systems in less time and at a lower cost [2]. This is possible because these real-world entities can not only be designed virtually, but also tested before physical models or prototypes are built, and with much greater speed. The virtual twin also increases the efficiency of the design, as it can be tested with more configurations than would be possible physically. In sum, a digital twin enables the identification of best-case scenarios and mitigation of worst case outcomes [3]. For example, the use of digital twins in the aeronautics industry greatly helps product quality and design [4]; in power plants, they offer vast new capabilities in operations and analysis [5]; and in new buildings, they increase energy efficiency and optimize the design of the climate control system [2]. In the words of Dirk Hartmann, senior expert for simulation at Siemens Corporate Technology, "The goal of this development is a closed loop that connects the virtual world of product development and production planning with the physical world of production system and product performance" [2].

1.2 Related research directions on Digital Twins

Accenture forecasts the digital twin to be one of five technology trends within the next two years [6]. Accordingly, much research is being done on the topic. For a small selection, refer to [7–10]. Today, digital twins come more and more into everyday use [11] - as discrete components or as assemblies in which multiple digital twins are combined. The assembly can be organized hierarchically (as in a production line digital twin composed of individual manufacturing equipment digital twins, or a factory digital twin composed of multiple production line digital twins), by association (as in a gas pipeline digital twin consisting of gas production and consumption equipment digital twins), or peer-to-peer (as in a digital twin assembly representing a group of equipment performing the same or similar function, and each adding its outcome to the total outcome of the assembly) [1].

The computational intensity connected with creating and operating a digital twin is becoming increasingly high. This is due to data capture methods offering vastly higher resolutions (e.g. sampling rate, sensor resolution or image size), and also due to the ubiquity of the Internet and therefore the means to connect to, collect data from, and update a digital twin. Keeping up with this exponential increase in data and therefore opportunity translates into the requirement for exponential increase in computing power—which is clearly becoming a limiting factor. Therefore, researchers have turned to the previously unavailable capability increase that quantum computing, an emerging technology, might offer. This new direction of research is Quantum (Digital) Twins - a term that denotes how classical digital computing and quantum computing will be initially used together, and how, as the quantum technology evolves, the twin will rely more and more on quantum computing. In this paper, we discuss the potential of quantum computing for implementing digital twins, the benefits of this novel technology, early examples of implementation, and future directions.

2 Quantum Computing in a Nutshell

Quantum computing exploits quantum mechanical phenomena for information processing. The basic building block of a quantum computer is a quantum bit, or qubit, which can represent 0, 1 or a combination of both in an infinite number of values, not just 0 and 1 as classical bits [12, 13]. Qubits are implemented as physical systems (using trapped ions, superconducting circuits or photonic devices) and are abstracted as mathematical models [14, 15]. The quantum nature of qubits can be beneficial in many computer applications that are hard to solve with classical technology - for example, modeling the electronic structure of molecules, molecular synthesis, computational biology, bioinformatics, secure communication, highly specialized sensors, and machine learning [13–17]. At present, the major drawbacks of quantum computing are that the number of qubits in physical implementations is small - too small to show a significant benefit over classical supercomputers available today, and the resulting systems are prone to computational errors leading to computational failure [14, 15]. In fact, today's available quantum computing implementations are characterized as Noisy Intermediate-Scale Quantum (NISQ) systems [15] and require algorithms that combine quantum and classical computing to alleviate the drawbacks [14]. Major companies, such as Google, IBM and Honeywell, provide access to their proprietary implementations of quantum computers, with modest numbers of qubits so far (10-53), through cloud services [15].

This new computing paradigm offers the potential for great computational power but also requires a different kind of thinking than in the domain of classical digital computing. The latter may explain why quantum computing has still not yet received widespread attention in mainstream computer science. As of this writing, major obstacles for a broader engagement with the topic likely are as follows: 1) quantum mechanical phenomena such as superposition, entanglement, tunneling, decoherence, or the uncertainty principle appear to be weird, abstract or unintuitive, and hard to accept for they cannot be observed in our daily macroscopic environments; 2) the mathematical tools used to model these phenomena are complex (no pun intended) and again rather abstract; and 3) to the uninitiated, the mathematical notation used in the quantum computing literature appears even more abstract and needs getting used to. Acknowledging these difficulties, this section provides a brief introduction to the basic terminology of- and fundamental concepts behind quantum computing.

To begin with, we recall that a quantum mechanical system (QM system) is characterized by a state vector $|\psi>$ in a Hilbert space $\mathbb{H}$ over $\mathbb{C}$. The temporal evolution of such a system is governed by the Schrödinger equation and its observable physical properties (such as position, momentum, or energy) correspond to Hermitian operators. A measurement of an observable property of a QM system collapses its state to an eigenvector of the respective operator. This is to say that a measurement of a quantum variable results in an eigenvalue of the operator under consideration and the state "jumps" to the corresponding eigenvector. Which of the eigenvalues and corresponding eigenvectors this will be depends on certain probabilities encoded in the state vector. The crucial question as to why this kind of mathematics describes the behavior of nature on one of its most fundamental levels still awaits conclusive answers; for now, the empirically undeniable success of this linear algebraic framework has to be attributed to "the unreasonable effectiveness of mathematics in the natural sciences" [18].

3 Digital Twins in the era of Quantum Computing

3.1 Digital Twins and Cyber-physical Systems

The idea of connecting the physical and virtual world - so-called Cyber-physical Systems - is not new and has been discussed under the terms Internet of Things (IoT) and Machine-to-Machine (M2M) communication for a while. The general idea of M2M is ubiquitous communication among devices (machines) in order to enable automated operations among them [19]. The evolution of this concept leads to the vision of IoT as a set of connection among everyday objects. Cyber-physical Systems are increasingly connecting physical devices and software components in all areas through computer networks to often highly complex, heterogeneous systems. As a result, the next level of digitalization on an industry level is enabled, allowing new frameworks, business models, and technical innovations, such as "Industry 4.0", Smart Factories [20], as well as information technology ecosystems where cyber-physical systems cooperate to reach a common goal.

Steinmetz et al. [21] understand Digital Twins as a major concept to realize Cyberphysical Systems and propose an architecture using Digital Twins to connect the physical world with end-user applications. The concept can go as far as building a digital twin of a whole factory. The Digital Twin contains all information of the physical object and provides a virtual representation of it. Qi et al. [20] define a five-dimension digital twin model containing (1) a physical entity, (2) a virtual model, (3) digital twin data, (4) digital twin services, and (5) connections of those four parts.

3.2 Quantum (Digital) Twins today

Quantum computing holds a lot of promise for digital twin applications. Quantum simulation and quantum machine learning can be used to build a Quantum (Digital) Twin (QDT) and eventually a full Quantum Twin (QT). We posit that the quantum (digital) twin concept is not a contradiction in terms - but instead describes a hybrid approach that can be implemented using the technologies available today and combines classical computing and digital twin concepts with quantum processing. As the quantum computing field evolves, quantum twins that use quantum-only approaches will likely become possible as well.

So far, a variety of quantum algorithms for machine learning have been developed, using both classical data (encoded as quantum states) and quantum data. In addition, researchers have proposed that deep quantum learning networks can be built using specialpurpose quantum information processors (such as quantum annealers and programmable photonic circuits) that are easier to build and operate than general-purpose quantum computers [16]. While possible quantum machine learning speedups seem to be very promising, this advantage is affected by the limitations of the algorithms, the hardware, and of the data used in these applications [16, 17].

Villalba-Diez et al. [22] focus on the new possibilities for manufacturing process control that arise from Industry 4.0 using the data delivered by a network of sensors connected to workstations. Real-time monitoring of each parameter determines whether the values provided by the sensor are within the normal operating range. However, in interaction with a large number of parameters, deterministic analysis becomes intractable and we enter the realm of "uncertain knowledge". While Bayesian decision networks are an established method to control the effects of conditional probabilities in such systems, detecting whether a manufacturing process is out of range requires significant computation time. As a consequence, triggering the alarm will be delayed, or false positives might be introduced. The JIDOKA principle - an important factor in lean management as well as in quality assurance - describes the ability of a machine, a plant or an entire system to shut itself down in the event of errors, quality and production problems. This motivates Villalba-Diez et al. to investigate QDTs - their hypothesis is that the internal sensor network of a computer numerical control machine can be modelled with quantum simulations having a higher performance than decision networks. They confirm their hypothesis by implementing a QDT that enables the integration of quantum computing and Industry 4.0. This QDT simulates the complex sensor network and enables real-time JIDOKA in manufacturing processes thanks to its high processing performance.

Khan et al. [23] investigate the requirements of digital twin-driven autonomous maintenance and they see the QDT as having the potential for significant performance gains that will enable real-time simulations. The authors recognize a limitation of classical computing to test different simulations in each digital twin. Quantum computing could meet such requirements and make real-time machine learning (almost) infinitely possible. Kahn et al. consider a QDT would be a complex and accurate simulation of the real world, which utilizes data from other digital twin models and simulates millions of variables interacting with each other. Thus, future digital twin platforms can leverage the computational power of quantum devices to simulate different scenarios in a short time and drive the autonomous decisions on the most optimal strategy [23].

The quantum (digital) twin concept has been mentioned in the context of chemical and oil and gas industries as well. In addition to its smart room collaboration environments, Total has developed a digital twin of a refinery – a QDT as a virtual plant. This 3D model serves as the single source of truth throughout the life of this plant [24, p. 32]. Papile [25] sees QDTs as an opportunity to preserve and enhance the value of plants by enabling sustainable earnings and providing for clean, safe and economical chemical and energy production. A digital quantum twin for chemical goods can be used to defend against infringements such as the "depreciation or erosion of intellectual assets".

Harvey [26] proposes QDT as a solution for autonomous buildings that add the business logic to the complex systems of equipment, interconnections, and control interfaces. He argues that QDT combines behaviors, (computed) properties, actors, and information flows with a new AI technology based on neural nets. From an implementation perspective, a modelling tool for QDT is proposed that can be used by integrator, manufacturer, engineer, and service provider to realize the vision of completely autonomous buildings [27].

In the context of transportation (road, rail, and air) Gordon [28] sees QDT as a gamechanging technology to overcome the obstacles of today's traffic management tools. Ubiquitous, real-time data (e.g., traffic state, weather) combined with multi-dimensional modeling functionalities based on quantum computing and AI can help to early identify and react on disruptions. First possible use case for route optimization of bus fleet as well as adaptive re-planning and reallocation of delivery assets have been realized in practice.

Gradoni and Di Renzo [29] propose using QDTs for an ad-hoc and ongoing optimization of wireless networks (eg. 5G, 6G), achieving optimal communication performance during changing conditions of the network as a whole. As the optimization dimensions (degrees of freedom) grow very large, the advantages of QDTs become apparent. They state that quantum computing has already been adopted to plan wireless communications networks (5G).

The European Space Agency (ESA) even goes so far as to propose a digital twin for planet Earth and suggest that quantum computing will help manage its complexity. Today's challenges and threats—like climate change, as well as human-caused resource scarcity and impact on the ecosystem—require constant observations, accessible monitoring information from a multitude of sources, as well as up-to-date interpretations and calculations. Using specialized digital twins of the planet, forecasts and visualizations can be produced in different areas of interest [30]. For example, a digital twin of Antarctica is already helping analyze ice sheet data and understand how these ice sheets melt under different scenarios. A digital twin for global food systems can simulate agricultural activities within the context of different ecosystems with different crops, water sources and irrigation management systems. And a digital twin for forests can combine high-quality satellite observations with local measurements for each forest, then model and simulate the global forest system in order to provide a better understanding of its structure and functioning [31]. Insightful simulations based on latest data can be created and used, perhaps most importantly, in convincing political decision making and influencing policies for sustainable development. As data quantities can become very large, technologies like artificial intelligence methods, as well as quantum computing, will need to be employed in analysis and even storage and collection of the digital twin data [30]. ESA has already launched activities around creating a quantum capability for solving geoscience problems in collaboration with the European Organization for Nuclear Research (CERN), which has embarked on its own quantum technology initiative as well [30, 31].

4 Implications and estimates on the impact of Quantum (Digital) Twins

The evolving research results and practical applications of quantum computing in the area of digital twins suggest that we are likely to see a phase transition from digital twins to hybrid quantum (digital) twins to quantum twins. This phased transition will be moderated by developments in several areas, as explained below.

Current real-world applications of quantum computing are relatively small - the maximum computing power available through current cloud services is in the range of 50 qubits. As quantum processing power will increase, more realistic applications will be implemented, including complex "twin"simulations of real-world objects, processes and systems.

At present, even if enough quantum processing power can be made available, it is still classified as NISQ - subject to errors and noise limiting the number of computations that can be completed reliably, irrespective of how many qubits are employed. Future development of error-correcting mechanisms and fault-tolerant quantum computing systems will be essential for fully exploiting the available increased processing power for real-world applications. Ultimately, the increase in computing power and fault tolerance will support the long-term vision of quantum twins.

In the near to mid-term, one way to overcome these challenges could be to develop special-purpose quantum computers - for example, for neural networks or other machine learning algorithm processing - rather than general purpose quantum computers. Existing research shows that these specialized quantum computers can be easier to develop, scale, and control for errors. Such developments could support hybrid quantum (digital) twins where some aspects of the digital twin are managed by classical algorithms, while others employ the specialized quantum capability.

Current use-cases are much more aligned with the mid-term quantum computing and quantum (digital) twins expectations. For example, a quantum (digital) twin factory is still too big (from a modeling perspective) for the available qubit-size, and the benefits of using quantum computing in this instance are likely to be small. On the other hand, some applications - such as wireless communication network modeling - require much more simulations that can take advantage of quantum (digital) twins.

In the future, with the emergence of better, more reliable quantum computers - general-purpose or specialized circuits - it will be possible to run simulations of highly complex, interconnected real-world objects, processes and systems - such as complex machines, factories or supply chains - in real time - compared to weeks as with classical digital technologies. In addition, the amount of entities and variables that can be included in the simulation will increase - significantly above and beyond what current classical digital twin simulations can handle, thus increasing the fidelity of the simulation models and the usefulness of the results. Companies that invest in technology to build quantum (digital) twins (and ultimately evolve them towards quantum twins) will enjoy competitive advantage from being able to discover (or even anticipate) issues, plan, react and recover much quicker than their competitors, and thus differentiate themselves through better products or services. For example, quantum (digital) twins can enable companies to understand the impact of market changes and select the right response better and quicker. However, competitors who do not have access to the speed and complexity of processing offered by quantum (digital) twins will not be able to react in time - even if they invest in other types of traditional analysis tools and technologies.

We believe that applying quantum technology to evolve digital twin applications in companies is not a question of if, but when - with both innovative first movers and savvy fast followers likely to harness the benefits. There is an opportunity to create sustainable competitive advantage by being at the forefront of quantum technology adoption, learning and adaptation though company-specific algorithms, applications and models for quantum (digital) twins that create path dependencies and dynamic capabilities that will be difficult to imitate by others. This is extremely important in today's VUCA (Volatility, Uncertainty, Complexity, and Ambiguity) business environment [32].

It is important to understand that a major advantage of quantum systems come from their native stochastic nature. Most systems for which we desire a digital twin, exhibit some degree of non-determinism or stochasticity (e.g. traffic systems [33], financial systems [34], or 5G core network components [35])—even if theory suggests that the behavior of a system should be deterministic, the interplay of various imperfections of real-world systems can induce randomness. Hence, a fundamental requirement for digital twins is the generation of samples from probability distributions. For simple univariate distributions, this problem is well understood. However, except for simple cases (e.g. multivariate Gaussians), sampling from high-dimensional distributions is a hard computational problem. When the underlying variables are discrete, only a handful of methods is known, i.e., inversion sampling, Markov chain Monte Carlo (MCMC), and perturb-and-MAP (PAM) [36]. Each of these methods corresponds to a hard computational problem: inversion sampling has to traverse an exponentially large state space, MCMC can suffer from an exponentially long mixing time [37], and PAM has to solve the NP-hard maximum a posterior (MAP) prediction problem. Let us explain how quantum computers can alleviate this computational burden: Starting in some initial quantum state, e.g., $|0\rangle$, a unitary evolution via some operator U takes place which drives the quantum system to its final state $|\psi\rangle$. Clearly, the n-qubit state $|\psi\rangle$ cannot be accessed directly. Instead, measurements in the computational basis allow us to sample binary vectors of length n according to the probability amplitudes which are encoded in $|\psi\rangle$. Thus, the output of a quantum computation is a sample from a discrete probability distribution. Simple mappings can be found, which allow us to encode any high-dimensional state space into binary strings as long as n is large enough. Finally, whenever an appropriate unitary operator U can be identified, quantum computing allows us to overcome the computational burden of sampling algorithms. Nevertheless, finding U which corresponds to a quantum gate circuit of polynomial length is an open problem at the time of writing.

5 Outlook and Further Research

At present, the research into quantum (digital) twins is in it's infancy—if that. Because of the highly diverse data models involved, one can not yet speak of the quantum computing approach for digital twins. Instead, each individual type and category of digital twin requires their own algorithms and models, and thus their own individual quantum computing approach. In addition, current applications are, at most, a hybrid approach between traditional and quantum computing.

The current state of quantum computing is a second limiting factor. As long as quantum computig systems remain small, and large-scale algorithms stay theoretical, no advantages can be gained from quantum applications. This, in turn, limits the available resources for research into these areas. With the increasing availability of quantum computing devices and cloud services with increasing processing power, we will see increasing adoption of quantum computing approaches. Once sufficient amounts of data can be processed, and computational requirements of quantum successes surpass existing high-performance classical computing, real-world applications of quantum (digital) twins will come into focus.

As mentioned above, any high-dimensional discrete state space can be encoded into the bit strings that can be measured on an n-qubit system. This, however, requires that n, i.e. the number of available qubits, is large enough. In late 2021, IBM announced released quantum processors with the Eagle architecture which allow for $n = 127$. The current D-Wave Advantage 4.1 system, is equipped with more than 5000, but only $n \sim 170$ can be used when all dimensions interact with each other. We may hence say that at the time of writing, between 100 and 200 qubits are available. However, quantum twins of large systems can require thousands or even hundreds of thousands qubits, depending on state space size of the underlying probability distribution. Inspecting vendor roadmaps shows that systems of such size should not be expected before 2026—which is already an optimistic extrapolation, given the technical difficulties of manipulating large quantum systems in a coherent manner.

Future research can shed light on the development of quantum hardware and software, the combinations of classical and quantum algorithms for a variety of hybrid quantum (digital) twin applications with increasing levels of complexity, and the feasibility of quantum twins. In addition, we hope researchers will investigate and document the business benefits of adopting quantum (digital) twins. In the end, we expect any company digital twin will benefit from the move into the quantum world as, if done right, it promises computations and especially simulations of never seen complexities and levels of detail, as well as competitive advantage above and beyond what classical computing technology can offer.

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