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SIMULATION: THE CRITICAL TECHNOLOGY IN DIGITAL TWIN DEVELOPMENT

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ABSTRACT

Digital twins are virtual representations of physical entities and processes. They aid in deriving insights to control entities and processes in the digital world and use those insights to drive actions in the physical world. Simulation is one of the key enabling technologies that lie at the heart of digital twin development, as it provides enhanced visibility into future performance and the ability to identify profit-optimal decisions. This tutorial describes how we envision the digital twins developed in industry and the pivotal role simulation plays in their development. Using supply chain digital twins as an example application, we introduce our digital twin framework that simulation practitioners might find useful when developing their digital twin solutions to understand what did happen, predict what may happen, and determine solutions to fix future problems before they happen. We conclude with simulation research streams that contribute to the use of simulation in digital twin development.

1 INTRODUCTION

Global Market Insights (2020) reports that the digital twin market size exceeded \$5 billion in 2020 and is expected to grow at over 35% compound annual growth rate between 2021 and 2027. McKinsey expects digital twin adoption to unlock \$5.5 trillion – \$12.6 trillion globally by 2030 (McKinsey 2021). While these estimates are vastly different, it is apparent that digital twin will play a paramount role in companies' digital transformation efforts. The Digital Twin Consortium defines digital twins as virtual representations of real-world entities and processes synchronized at a specified frequency and fidelity (Digital Twin Consortium 2020). An example of a real-world entity may be an individual asset such as an industrial machine, an aircraft, or an industrial pump. It may also represent a specific component or sub-system of a machine as well as a collection of sub-systems depending on the complexity of the machine. In each of these cases, the digital twin is called "asset twin" as it approximates the behavior of a physical asset. Digital twins can also represent systems of physical assets such as supply chain networks of suppliers, plants, warehouses, and customers. Namely, a "process twin" can be built to represent a business process flow and capture the interactions of physical assets in the corresponding system. The asset and process twins can be used (i) to predict key performance indicators (KPIs) and gain visibility into the future health of assets and processes, (ii) to assess the impact of operational policy, design, and investment decisions in a virtual environment, and (iii) to stress test assets and processes under consideration and identify best courses of action to take when faced with disruptions. The ability to provide real-world feedback to digital twin models of assets and processes about the effects of their solutions implemented in the physical world is key to achieving these objectives. The adoption of emerging technologies such as Internet of Things (IoT) and cloud has accelerated this closed-loop aspect of digital twin development in a wide variety of industries ranging from aerospace and defense, healthcare, and manufacturing to retail and consumer goods, transportation, and energy and utilities. Digital twins are expected to remain a critical component of digital transformation in the years to come.

Consider an asset twin developed for an industrial machine to predict its health. After the IoT data are collected from the sensors presenting a snapshot of the state the machine is in, the simulation of this asset becomes the centerpiece of the digital twin. The health prediction capability would be of tremendous value in a system with limited resources where it is critical to find zero downtime maintenance plans. Another example is a supply chain digital twin, building on production, transportation, and inventory optimization models together with a stochastic supply chain network simulation to predict intervals of product shortages, understand what may cause these shortages, and identify the best courses of action to take to optimize cost and service under uncertainty. It is important to emphasize that neither of these digital twins is a one-off solution. Each matures over time and drives learning and adaptation as a result of which virtual models are improved and control in the physical world is enhanced. Since it is the only practical technology to model, understand, and optimize complex systems, simulation is THE pivotal component of these digital twins. Empowered by the simulation technology, the digital twins drive decisions that unlock value in businesses.

In addition to simulation, building asset and process twins requires a variety of analytics tools ranging from IoT, statistical modeling, and visual analytics to AI/ML, natural language processing, computer vision, and optimization. However, at the heart of an asset twin often lies a physics-based simulation driven by domain expertise and data. At the foundation of a process digital twin, there is a flexible, data-driven, and scalable process simulation operating under uncertainty, mimicking the operations of the physical system through which thousands of objects may flow, and predicting the future KPIs. Complexity together with uncertainty often invalidates the use of deterministic techniques for developing decision-support solutions and turns stochastic simulation into a critical component of process twins. *This tutorial brings clarity to what a digital twin is and discusses the role of stochastic simulations in the development of process twins*.

The potential of digital twins has been discovered by the simulation community for some time now. As a "hot" topic among researchers, software vendors, and practitioners, "digital twin" has been mentioned in over 50 Winter Simulation Conference (WSC) papers in the last three years. Different aspects of digital twins are covered by considering applications related to manufacturing (Latif et al. 2020; Shao et al. 2019), production logistics (Flores et al. 2021; Li et al. 2020), transportation and logistics (Gyulai et al. 2020; Montevechi et al. 2020), and material handling (Sharotry et al. 2020; Yue 2021). While most applications fall under the umbrella of Industry 4.0, Ye et al. (2021) consider a healthcare system and Pu et al. (2021) focuses on indoor modeling and mapping. Kulkarni et al. (2019), on the other hand, presents an advanced tutorial on the use of digital twins for enterprise adaptation. There are also WSC proceedings papers on the simulation methodologies that would help conquer the technical barriers in digital twin implementation. Example studies include simulation optimization that enables near-real time decision making (Cao et al. 2021; Liu et al. 2021), synchronization for efficient bi-directional data flow (Marquardt et al. 2021; Lugaresi and Matta 2020), and model validation and verification (Sargent 2020). In addition, panels have been held to discuss what a digital twin is for manufacturing research and development (Shao et al. 2019) and how it relates to Modeling and Simulation (Taylor et al. 2021).

This tutorial describes how we envision the digital twins developed in industry. There is also the topic of how a digital twin is built, known as digital thread (Szypulski and Garrett 2021), which is beyond our scope. In the remainder of the tutorial, Section 2 provides background information on digital twin frameworks. Section 3 describes the digital twin development steps. Section 4 applies these contents to a supply chain application and presents a supply chain digital twin framework. Section 5 discusses how simulation research may overcome the process twin development challenges, followed by a conclusion in Section 6.

2 DIGITAL TWIN FRAMEWORKS

Market confusion arises as one of the challenges of implementing digital twins. There are limited use cases to learn from and little research on how to define requirements for minimally viable digital twins. Also, it is difficult to determine the technologies to use, ensure outcome delivery, and identify the knowledge and skills gaps to fill. A step towards addressing these difficulties is the use of a framework to facilitate collaboration in multidisciplinary teams tasked with digital twin creation. To help the development of such a digital twin framework, we present the digital twin required characteristics in Section 2.1, the foundational digital twin elements in Section 2.2, and the digital twin capabilities periodic table in Section 2.3.

2.1 Digital Twin Required Characteristics

Although digital twin is a key enabling technology for digital transformation, it comes with challenges of adoption due to limited interoperability, market confusion, and heavy investment required in people and technology. The Digital Twin Consortium was founded in 2020 with the mission to bring multinational corporations, small and large technology innovators, academia, and governments together to collaboratively overcome these challenges and accelerate the development, adoption, and widespread use of the digital twin technology.

According to the Digital Twin Consortium, a digital twin must have the following characteristics, which we refer to as **D**igital **T**win **R**equired **C**haracteristics (DTRCs): (1) a physical representation; (2) a virtual representation; (3) synchronization between physical and digital representations at a pre-specified frequency and fidelity; and (4) ability to learn and adapt that leads to improved virtual models and enhancements in physical representations. It is critical that DTRCs are used for a meaningful business outcome that can be clearly stated and objectively measured. Because of DTRCs 1 and 2, it is often asked whether any simulation model would qualify as a digital twin. A simulation model of a physical asset or process (DTRC 2) would by itself not be sufficient to meet the requirements of a digital twin. DTRCs 3 and 4 are what distinguish a traditionally one-off simulation model from a digital twin solution. Synchronization (DTRC 3) and learning (DTRC 4) are essential since digital twins evolve over the lifecycles of products and processes. Ideally, they transform businesses by accelerating holistic understanding, optimal decision making, and effective controls. They build on a combination of real-time and historical data to represent past and present and predict future. Furthermore, digital twins are motivated by outcomes, tailored to use cases, powered by integration, and guided by domain knowledge and implementation in IT/OT systems.

2.2 Digital Twin Foundational Elements

There are four foundational elements of digital twin development to meet the DTRCs: (1) data; (2) domain; (3) advanced analytics; and (4) outcomes. If a simulation practitioner is asked about the differentiators of the digital twin under development, we recommend answering this question with respect to these four elements.

2.2.1 Data

This foundational element includes data of all types: engineering and design data, experts' opinions, historical data, reliability reports, data from EAM (Enterprise Asset Management), PLM (Product Lifecycle Management), and MES (Manufacturing Execution Systems), sensor IoT data, texts, images, videos, and audio. These datasets also reflect the disruptions that occurred and the real outcomes associated with the decisions implemented in previous time periods. They are used for describing the system's configuration and state (i.e., descriptive analytics) and for capturing the uncertainty in the input processes (i.e., stochastic input modeling). The granularity of the input data and the unit of time assumed by the digital twin are chosen to match the speed of making decisions. Within the context of plant twins, Biller and Biller (2021) discuss aligning data collection with the simulation models supporting decisions from strategic to tactical and operational. They describe the types of data needed to validate simulations and predict the plant KPIs.

The collection of data is followed by a search for stochastic input-model characterizations that adequately capture the inputs' distributional characteristics. The representation of uncertainty in input processes (i.e., stochastic input modeling) is a problem that has been well studied by the simulation community. There are several tutorials presented at the WSCs over the years for representing, fitting, and generating multivariate time-series input processes ranging from being independent and identically distributed to having arbitrary marginal distributions and complex dependence structures. We refer the interested reader to Law (2016) for selecting input probability distributions and Pasupathy and Nagaraj (2015) for dependence modeling. At the foundation of developing input models with arbitrary marginal distributions and dependence structures lies a transformation-based method that reduces the input-modeling problem to finding a suitable multivariate normal distribution. This distribution is chosen to match the distributional characteristics of the input processes whose dependence structures are captured by pair-wise correlations. In the case of using alternate measures of dependence, the approach becomes finding a suitable multivariate uniform distribution, i.e., a copula function (Biller and Corlu 2012). More recently, several researchers have investigated the use of neural networks to mimic the characteristics embedded in large simulation input datasets; see Wang et al. (2020) for an example study utilizing generative neural networks. While building on AI to automate input modeling to drive simulations with complex dependence structures is a novel idea, it is critical to have the ability to conduct sensitivity analysis and to account for the input model uncertainty in the presence of limited data.

2.2.2 Domain

The domain element combines subject matter expertise with physics-based modeling to build asset twins. A physics-based model captures the effects of governing laws of nature on operating the asset. If the asset were a pump and the objective were to predict its health, then motor current, pressure, and flow rate discharge would be among the primary model parameters to consider. Furthermore, there is a physical relationship among these parameters. Building a physics-based model accounting for that relationship would be the first step towards creating an asset twin. Integrating this model with data-driven analytics (i.e., a hybrid model) would be the next step to improve accuracy, lower cost, and scale the operationalization of the asset twin. Subject matter expertise also plays a critical role in process twin development. Often, production operations optimization projects require interdisciplinary teams whose expertise is critical to develop simulation models and understand constraints of performance optimization. In this case, examples of domain expertise would extend to plant maintenance, material analysis, design limits, and operational constraints.

2.2.3 Advanced Analytics

Developing digital twins requires an integrated use of advanced analytics tools ranging from IoT, streaming and sensor analytics, and statistical modeling to computer vision, AI/ML, simulation, and optimization. A significant number of companies have been building on this integration in their digital twin development.

Lockheed Martin maximizes uptime by using AI, IoT, and advanced analytics to predict when parts will fail, keeping more aircraft airborne for vital missions worldwide (Isbill 2022). US Gypsum – a world-wide industry leader in wallboard production – uses predictive analytics to estimate product quality for the line operators in real time (Reed 2022). US Gypsum deploys optimization models so that its production lines are operated in an ideal setting with real-time adjustments as needed. Siemens combines plant simulation and IoT capabilities to improve production efficiency and quality by replaying history and conducting bottleneck and what-if analyses (Siemens 2020). The role of simulation is critical in the delivery of these outcomes. Furthermore, simulation complements composite AI – introduced by Gartner in 2021 – by bringing in the additional benefits of explainability, uncertainty quantification, and risk management.

Because simulation can be viewed as a big data generation program, performance prediction and scenario analyses can be accelerated by integrating simulation with machine learning and optimization. A code-based description of such an integration is available in Biller et al. (2019) within the context of clinical trial enrollment planning. Furthermore, simulation has been increasingly used as an environment to enable on-policy training of reinforcement learning agents (U.S. Patent and Trademark Office 2021).

2.2.4 Outcomes

All digital twins are expected to (1) provide situation awareness, thereby enable decision making with more information, and (2) automate the identification of the response to operate an asset and/or a process at their optimal settings. Examples of target outcomes include performance monitoring, data accuracy enhancement, increased turnover, decreased storage, increased production, cash and service improvement, and improved resilience. Nevertheless, this is not a comprehensive list. Isbill (2022) and Reed (2022) also report downtime reduction and product yield improvement. It is critical that digital twins are motivated by outcomes and tailored to use cases; the target outcome is the key driver in the design of any digital twin.

2.3 Digital Twin Capabilities Periodic Table

Building on its 250+ members, the Digital Twin Consortium published the **D**igital **T**win **C**apabilities **P**eriodic **T**able (DTCPT) in Figure 1, demonstrating the different ways in which the term "digital twin" can be interpreted. This tabulation of the digital twin capabilities uses six categories highlighted in different

1 Data Acquis. & Data Ingestion	9 Synthetic Data Generation	17 Enterprise Syst. Integration	23 Edge AI and Intelligence	29 Prediction		39 Basic Visualization	45 Dashboards
2 Data Streaming	10 Ontology Management	18 Eng. System Integration	24 Command and Control	30 Machine Learning ML		40 Advanced Visualization	46 Continuous Intelligence
3 Data Transformation	11 DT Model Repository	19 OT/IoT System Integration	25 Orchestration	31 Artificial Intelligence AI	35 Prescriptive Suggestion	41 Real-Time Monitoring	47 Business Intelligence
4 Data Contextualize.	12 DT Instance Repository	20 Digital Twin Integration	26 Alerts and Notifications	32 Federated Learning	36 Business Rules	42 Entity Relationship V.	48 BPM and Workflow
5 Batch Processing	13 Temporal Data Store	21 Collab Platform Integration	27 Reporting	33 Simulation	37 Dstb. Ledger & Smart Contracts	43 Augmented Reality AR	49 Gaming Engine Vis.
6 Real-Time Processing	14 Data Storage & Archive Service	22 API Services	28 Data Analysis and Analytics	34 Mathematical Analytics	38 Composition	44 Virtual Reality VR	50 3D Rendering
7 Data PubSub Push	15 Simulation Model Repos.	52 Device Management	54 Event Logging	56 Data Encryption	58 Security	60 Safety	51 Gamification
8 Data Aggregation	16 AI Model Repository	53 System Monitoring	55 Data Governance	57 Device Security	59 Privacy	61 Reliability	62 Resilience

Figure 1: Digital twin capabilities periodic table (DTCPT) (Schalkwyk 2022).

colors (Schalkwyk 2022): (1) “data services” connecting physical to virtual with the data collected from equipment sensors and control systems; (2) “integration” enabling digital twin communication; (3) “intelligence” representing the services associated with developing and deploying industrial digital twin solutions; (4) “user experience ” interacting with digital twins and visualizing their data; (5) “management” representing ecosystem control; and (6) trustworthiness handling security, privacy, safety, reliability and resilience. Each of these six categories is composed of capabilities with similar characteristics and applications. The main idea of DTCPT is to use these capabilities to meet the DTRCs. However, every digital twin solution does not require the use of every capability in DTCPT. Although it is critical for a company on a journey of digital transformation to hit a high percentage of the boxes in Figure 1 by offering either core functionality or a solution together with third-party integration, this percentage would vary from one use case to another based on complexity and resource availability.

DTRCs and DTCPT apply to both asset twins and process twins. However, our tutorial focuses on process twins and discusses the role of simulation in process twin development. In DTCPT, simulation appears as a core functionality in two categories: data services and intelligence. The “data services” category includes the “simulation model repository” and “synthetic data generation” capabilities, while the “intelligence” category includes the “simulation” capability. This is because simulation can be viewed as a big system-data generation program, and it enables learning about physical assets and processes and making decisions with more information. Section 4 presents an alternative table of composable elements but customized to supply chains by building on the DTRCs (Section 2.1), the four foundational elements (Section 2.2), and our own experience of building supply chain digital twins with stochastic discrete-event simulations at the centerpiece.

3 DIGITAL TWIN DEVELOPMENT

There are three primary functions to perform during the development of digital twins (Figure 2): (1) offline model development; (2) real-time synchronization; (3) online learning. The offline model development represents the first phase of the digital twin development. Its output is a digital representation of the physical system, built and validated by using a static dataset representing the history of the system. The validated model is used to predict future KPIs and provide insights about how to optimize the system performance. Next comes the second phase of the digital twin development where the capabilities of monitoring the system and tracking the past are in place and the model is calibrated by using the most recent data reflecting

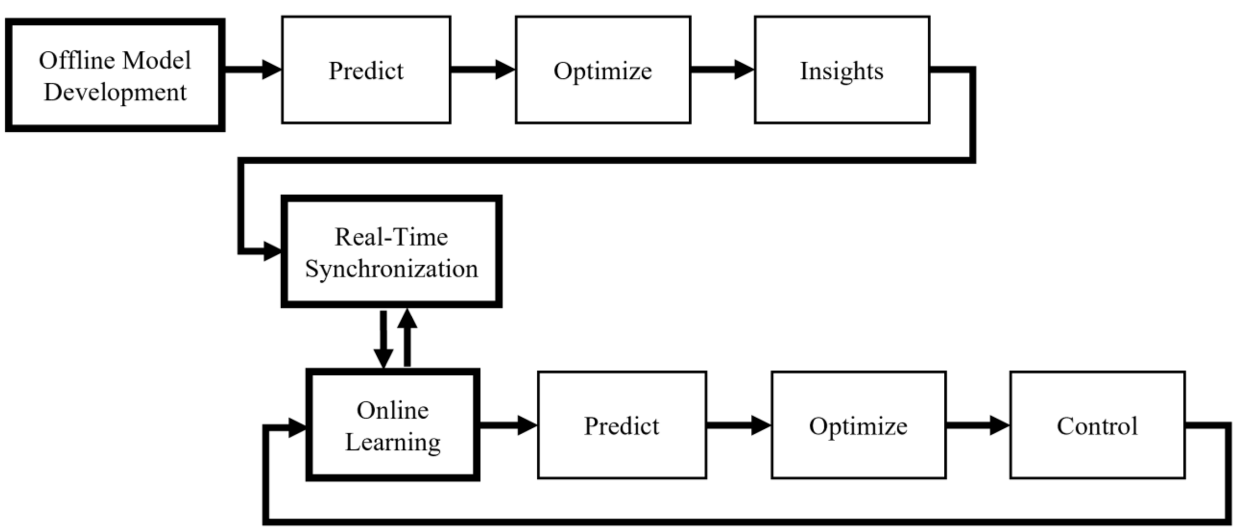

Figure 2: Key digital twin development functions.

the state of the system at that point in time. Using the calibrated model, the future KPIs are predicted; actions to optimize performance are identified and implemented in the physical system to enhance control in real time. Thus, learnings obtained from this phase of the development are not just insights; they establish a closed loop between physical and digital representations. Next, we describe each of these three primary functions in detail.

3.1 Offline Model Development

This function – illustrated in Figure 3 for a supply chain – develops digital representations by building on domain expertise, assumptions, and historical data with analytics techniques such as statistical and stochastic process modeling, AI/ML, simulation, and optimization. After the validation of the twin, the practitioner experiments with it via an integrated use of simulation and ML and derives insights about how to improve performance. However, the learning here is offline, i.e., no new datasets flow into the analysis.

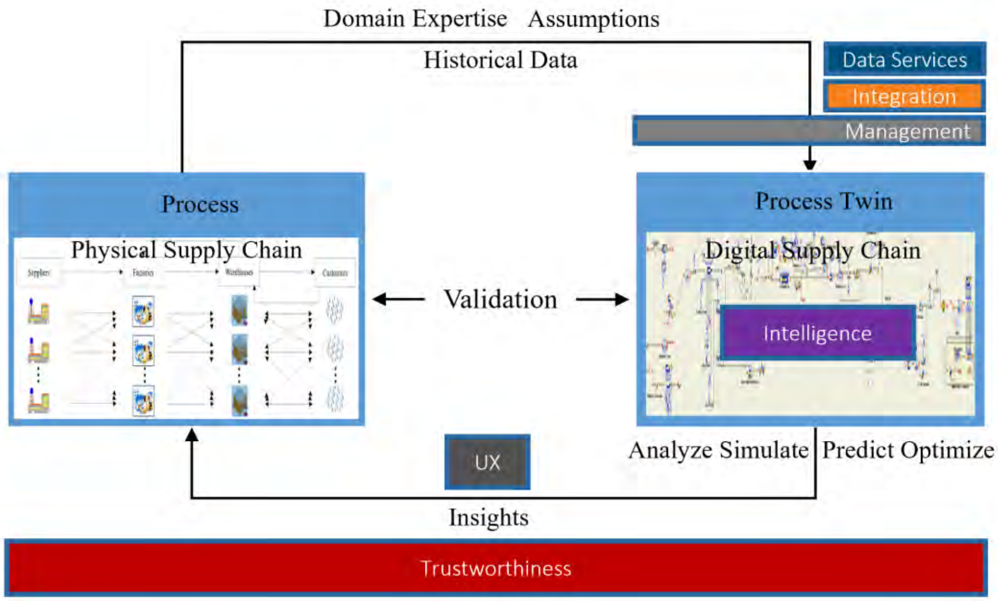

Figure 3: Offline model development with DTCPT categories.

Traditionally, a one-off project falls under the umbrella of offline model development. If the virtual representation of the physical system is developed by using a stochastic simulation, then offline model creation overlaps with the development of a stochastic dynamic system simulation for which WSC offers tutorials. We refer the reader to White and Ingalls (2020) for the basics of simulation with focus on discrete-event simulation, Sargent (2020) for verification and validation, Sanchez et al. (2021) for the design of simulation experiments, and Eckman and Henderson (2018) for first ranking and then selecting the best courses of action to take to improve performance. Also, Figure 4 illustrates a cookbook recipe for a supply chain simulation project and describes how modular tasks come together for end-to-end offline learning. We further refer the reader to Sturrock (2020) for tips on simulation project excellence. However, it is important to recognize that the resulting solution would not yet qualify as a digital twin. What qualifies a solution as a digital twin is its online learning component enabled by the real-time synchronization function.

3.2 Real-Time Synchronization

A critical aspect of digital twin development is the synchronization of the real-world entity and its twin via the use of streaming data in real time. Specifically, the IoT data collected from the sensors present a snapshot reflecting the system state at that point in time. The use of this data to hot start the simulation is what primarily distinguishes a simulation developed as part of the digital twin effort from that created in a one-off simulation project. This distinguishing feature is evident in the hospital digital twin developed by Akbay et al. (2011), where the snapshots of the system are taken several times each day and fed into the model to hot start the supporting simulation with the current state of the hospital.

It is important to revise the previously developed stochastic models with the most recently collected historical data and combine them with experts' opinions when available. This can be done by integrating Bayesian methodology with simulation input modeling (Corlu et al. 2020). Additionally, real-time synchronization may require re-calibration of the simulation. This is especially important when the model includes parameters that are not fully known but still included in the model by relying on limited data and/or information. Morgan et al. (2022) describes the bias that may arise in the simulation outputs in such a case as input model bias and introduces a method that recalibrates the parameters of parametric input models to reduce the bias in the simulation outputs. It is critical to perform this re-calibration task on a periodic basis.

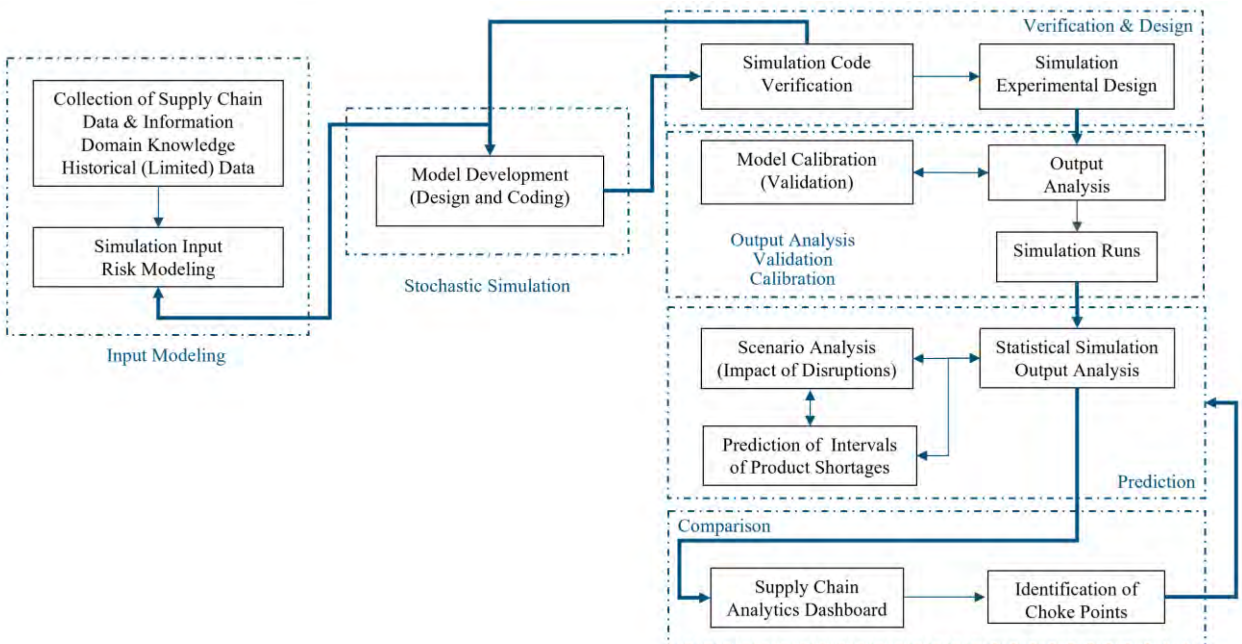

Figure 4: A cookbook recipe for a supply chain network simulation project.

3.3 Online Learning

The real-time synchronization is followed by online learning, which involves system monitoring and tracking the past, predicts the system performance and finds the best course of action to take via optimization. At this phase of the development, the digital twin is expected to provide enhanced visibility into the future and enable playing operational what-if games. Simulation plays the key role in equipping a digital twin with these capabilities.

Figure 5 illustrates an instance of learning from a supply chain digital twin. First, the supply chain network is simulated to predict intervals of product shortages. The distinction between the prediction capability in the offline model development and the prediction capability here is that the latter builds on hot starting the simulation with a calibrated model whose parameters and input risk profiles are updated with the most recent data at a specific frequency of synchronization. Then, the temporal study of the fill rate traces the source of the shortages to a manufacturing facility with high levels of inventory and utilization. This is followed by the investigation of the best course of action to take to address the capacity limitation in that facility. We consider the situation visualized in Biller (2021) and assume three candidate solutions for solving this problem: (A) purchasing a flexible machine that can perform multiple tasks; (B) allowing weekend production; and (C) adding a third shift. The supply chain digital twin can be used to select which one (or a combination) of these actions to take. Figure 5 shows an example risk profile of the supply chain fill rate for each solution and suggests the purchase of a flexible machine (Solution A). This is expected to not only maximize the supply chain fill rate but also reduce the risk exposure. This action can now be implemented in the physical system, resulting in a closed feedback loop between physical and digital environments. The action itself – control – can be implemented either in an automated manner as a closed loop decision or in a manner augmented by human intervention and based on a decisioning logic.

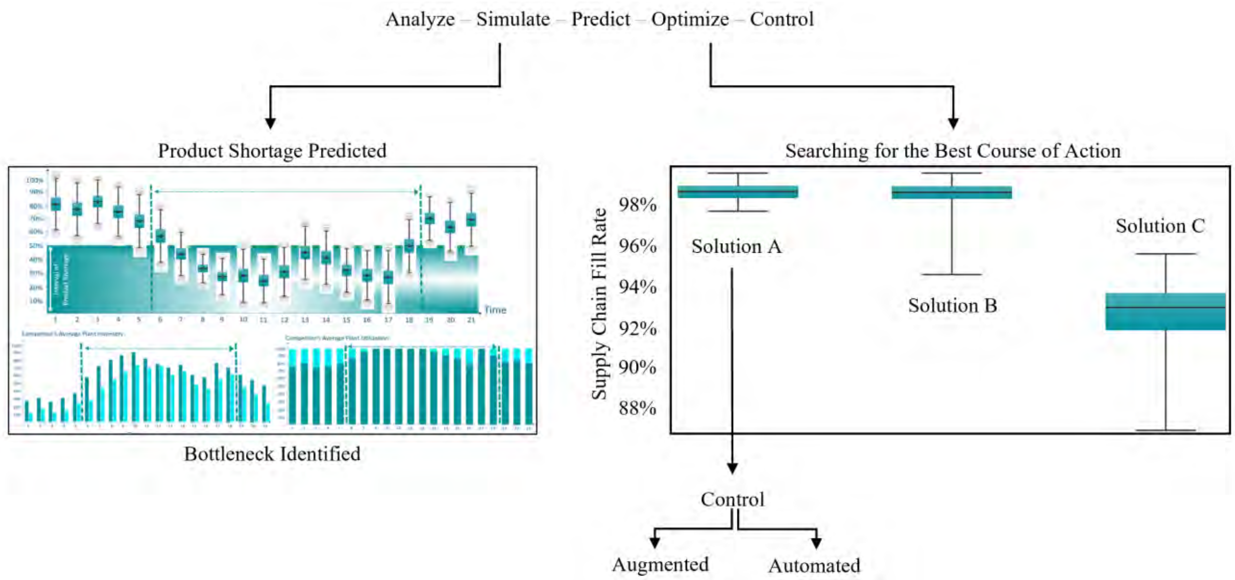

Figure 5: Online learning: Analyze – simulate – predict – optimize – control.

4 A SUPPLY CHAIN DIGITAL TWIN

Supply chain complexity, market uncertainty, and operational risk affect inventory holding and logistics costs and make it difficult to determine profit-optimal decisions. Thus, managing supply chain network operations is a key challenge for many companies. The creation of digital twins of supply chains, however, makes it possible to overcome this challenge and enables profit-optimal decisions under uncertainty. The focus of this section is on a supply chain digital twin development effort. The target outcome is to gain visibility into the future of the supply chain operations, predict supply chain cost and service level, and identify the delivery, inventory, and production plans that optimize cost and service.

4.1 Revisiting the Digital Twin Definition

We ask whether our supply chain digital twin has all the DTRCs defined in Section 2.1:

1) The supply chain network is the physical representation.
2) Supply chain network simulation is the virtual representation.
3) Hot starting the simulation calibrated by updating the model parameters and the input risk profiles with the most recent data at a set frequency synchronizes physical and digital representations of the supply chain network. The frequency needs to be established based in part on the timeline of making decisions to achieve the desired outcomes and in part on the requirements of learning and adaptation.

4) Learning in the virtual world informs the management of the supply chain in the real world. The effect of the supply chain management decisions – captured by the real outcomes, disruptions occurred, collected IoT data, and evolving assumptions and experts' opinions – are fed into the digital world in the form of new input data and/or an adapting supply chain business flow. This leads to a closed feedback loop between the physical supply chain and its digital twin.

Thus, we conclude that our supply chain digital twin possesses all the DTRCs. It is important for simulation practitioners to ask the same question as part of their digital twin development effort and characterize 1) the physical representation, 2) the virtual representation, 3) the synchronization between physical and digital representations, and 4) the details of learning and adaptation over time. Doing so would clarify the gaps between physical and digital representations and lead to plans that would effectively fill those gaps.

4.2 Supply Chain Digital Twin Framework

Figure 6 presents the framework that we find beneficial in our supply chain digital twin development. Every time a simulation practitioner attempts to build a new digital twin, she should not be developing it from scratch. Instead, she should modularize the development effort so that learning from one use case is transferred to the other, as a result of which development time is reduced and scalability is attained.

With this goal in mind, we structure the supply chain digital twin development around the four foundational elements – domain, data, advanced analytics, and outcomes – introduced in Section 2.2. We assign several categories to each foundational element (see the leftmost column of Figure 6) and seven sub-categories to each category, placed horizontally to the right of the leftmost column and highlighted in blue. Additionally, we display the sub-categories required for developing the supply chain digital twin in purple. Thus, Figure 6 can be viewed as the DTCPT for supply chains reflecting our first-hand experience in building supply chain twin solutions.

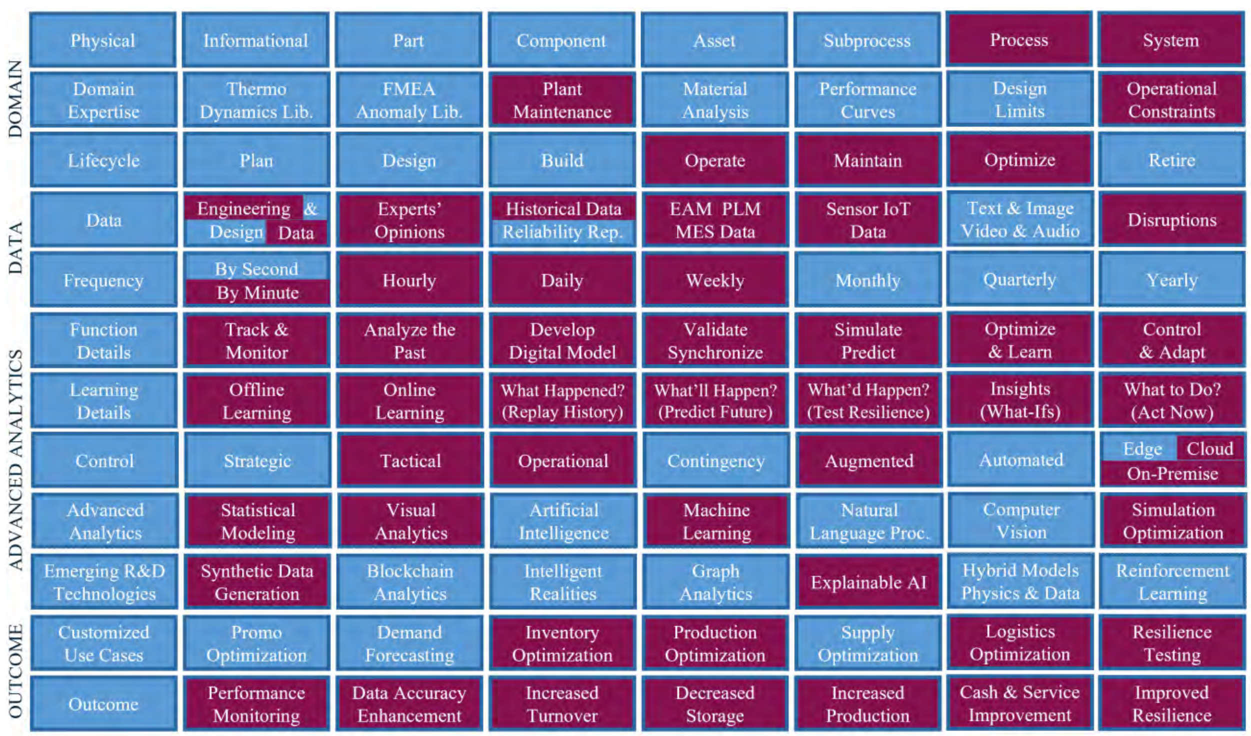

Figure 6: A supply chain digital twin framework.

First, supply chain digital twin is identified as a type of process twin requiring a systems modeling approach. Then, the development begins with the description of the supply chain flow logic, which is obtained by combining the supply chain network configuration with all necessary pieces of information and data that often include supply contracts and supplier data, initial inventory, production plan, customer demand, transportation details, inventory control policies, supply chain cost parameters, and characterization of disruptive events. Production plans, details of transportation, and inventory control policies are generally obtained from solutions of deterministic optimization problems – possibly with different units of time – and brought together in the supply chain network simulation to predict how they will jointly perform in delivering high service levels with minimal costs. However, the details of data collection and definition are dependent on the types of decisions that the supply chain digital twin will support. They are further affected by the speed of making decisions. The "Frequency" category in Figure 6 refers to the data collection frequency that is to be aligned with the speed at which decisions are made. The "Data" category, on the other hand, indicates the potential sources from which the supply chain input data may be collected.

The next steps of development are (i) representing the risk in the supply chain inputs, (ii) designing the experiments where the levers, which could be changed during a scenario analysis, are specified, and (iii) mimicking the flow of all entities through the supply chain network with a scalable, data-driven, and flexible dynamic supply chain network simulation. The analytics tools utilized for performing these steps are indicated as statistical modeling, visual analytics, optimization, simulation, and machine learning in the "Advanced Analytics" category of Figure 6. The execution of the simulation generates vast amounts of data representative of how the supply chain may perform in the future. By taking advantage of statistical modeling and visual analytics, the risk profile for the supply chain's service level is illustrated on the first row and the risk profile for the total cost on the second row of the rightmost block of Figure 7. As indicated by this figure, the supply chain digital twin can be used for several purposes. It can be used to predict KPIs and gain visibility into the future of supply chain operations. It can be used to assess the impact of decisions in a virtual environment. The digital twin can be further used for stress-testing the supply chain. It is important to emphasize that the objective here would not be the prediction of the probabilities of disruptive events. The occurrence of these events is enforced within the simulation and the best courses of action to take – when confronted with these disruptions – are identified through an integrated use of simulation and optimization. We denote this capability of the supply chain digital twin as "Resilience Testing" in Figure 6. Furthermore, we summarize the digital twin development details discussed in Section 3 for generic process twins under the "Function Details" and "Learning Details" categories of Figure 6. The "Customized Use Cases" category is, on the other hand, specific to the problems that often arise in supply chain management. The framework ends with the outcomes often realized by supply chain digital twin solutions.

5 SIMULATION RESEARCH TO SUPPORT PROCESS TWIN DEVELOPMENT

We discuss several research streams that may contribute to using simulation in digital twin development.

5.1 Synthetic Data Generation

An innovative approach to overcome the multivariate input-modeling challenges of large-scale stochastic simulations with correlated input processes is to use Generative Adversarial Networks (GANs) to generate high-fidelity synthetic data. Montevechi et al. (2021) has shown that GAN input models can generate synthetic samples with an average accuracy exceeding 97% while preserving the pairwise correlations among the variables of low-dimensional input processes. It remains to be seen how well GAN-based input models would perform with increasing dimensions and asymmetric dependence structures of the multivariate input processes. It is important to note the need for sufficiently large input datasets to follow this approach. Furthermore, it is crucial to investigate how well the approach would support what-if games.

5.2 Zone of Confidence

One of the digital twin development challenges stems from the inputs that are uncertain due to lack of information and/or errors of measurement and estimation. The situation of lacking full information about business process flows and characterizations of their input distributions is known as the input-uncertainty problem in the simulation community. This is an important problem to consider because uncertainties in the inputs will propagate to simulated output performance measures. In the presence of limited historical input data, it is even possible for the contribution of the input uncertainty to the KPI's variance to dominate the contribution of the stochastic uncertainty.

There exists a well-established body of methodological work (Corlu et al. 2020), which can be utilized to account for this additional layer of input uncertainty in the KPI predictions. The best practice is to decompose the simulation output variance into components due to stochastic uncertainty and input uncertainty to better assess the accuracy of the KPI predictions and identify the largest sources of input uncertainty. Biller et al. (2019) is an example industrial application following this practice in manufacturing simulations. Such characterization of the input uncertainty in stochastic simulations ideally leads to effective data collection schemas (Parmar et al. 2021). We caution that the probabilistic models of input uncertainty are revised over the lifecycle of the digital twins, especially as uncertainty is realized over time.

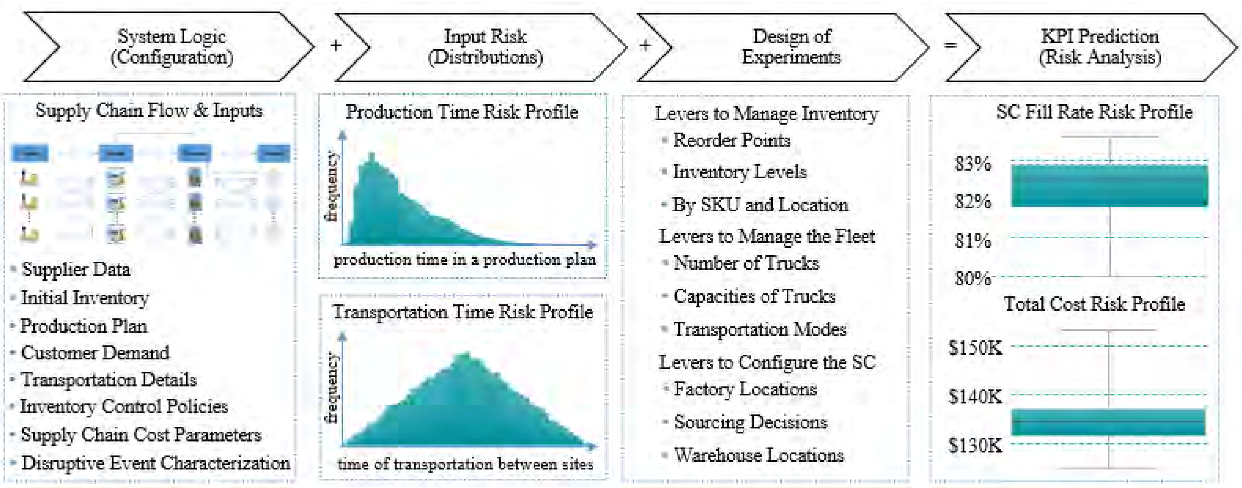

Figure 7: Integration of descriptive, predictive and prescriptive analytics for supply chain digital twins.

5.3 Fast Sensitivity Analysis

Sensitivity analysis (SA) studies how KPIs are affected by inputs, enabling simulation practitioners to better understand system performance, quantify risk, and indicate where input change or management may be desirable. Thus, after running experiments with the calibrated digital twin model, SA becomes a critical component of online learning to answer the what-if questions asked by the simulation practitioners. SA would also quantify the change in the expected system performance for given adjustments in the inputs when the experts' opinions are used for input modeling during the offline model development.

SA methods can be grouped into two categories: global and local. Global sensitivity analysis deals with the case when the input either naturally varies within its range or a distribution is imposed due to the lack of information about its value. The global sensitivity measures attempt to discern the inputs that drive the output uncertainty across their entire ranges. The measures of local sensitivity, on the other hand, focus on the influence of the inputs near a nominal setting. In the context of a digital twin, global sensitivity better fits into the stage of offline model development, while local sensitivity analysis is more applicable for online learning after recalibration when there is confidence in the nominal values chosen for the simulation input parameters. Since both the performance measure and the input are naturally stochastic for process twins, the local sensitivity measure makes the most sense when it is defined as a partial derivative of the property of the performance measure with respect to the input property. Jiang et al. (2021a, 2021b) propose a new family of sensitivity measures that quantifies the directional derivative of an output property to an input property along the changing direction of the input parameters from the nominal setting. The appropriate point and error estimators of this local sensitivity measure can be obtained without requiring any additional simulation effort beyond the nominal experiment. This is especially advantageous for a large-scale digital twin that is expensive to run. Jiang et al. (2021a) demonstrate the use of this approach for a clinical trial enrollment simulation digital twin.

5.4 Simulation and Optimization

The problem of maximizing or minimizing the expected value of a performance measure of a digital twin when the decision variables are discrete is known as "discrete optimization via simulation (DOvS)" in the simulation community. There exist well-established solution methods like ranking and selection (R&S), locally convergent random search, ordinal optimization, and globally convergent Bayesian optimization. In particular, the collection known as R&S returns a selection with statistical confidence and is available in several commercial software packages. However, as an exhaustive search tool, R&S is only applicable to problems with a relatively small number of feasible solutions for simulations that are expensive to run, in particular when computational resources are limited. Intense theoretical and practical interest in R&S has led to many studies tackling this limitation from different angles. Two examples we see as the most relevant to the digital twin development are Plausible Screening (PS) (Eckman et al. 2022) and Parallel Adaptive Survivor Selection (PASS) (Pei et al. 2022). The PS framework solves the problem from the front end by returning a subset of solutions from which a final selection is made. More specifically, it initially measures the discrepancy between the simulation-generated observations and the space of performance functions having certain known properties. Then, it removes with confidence those solutions having low plausible acceptability. In other words, PS exploits domain knowledge and powerful optimization methods to avoid simulation. PASS is, on the other hand, specifically engineered to exploit parallel computing environments for problems with a very large number of feasible solutions by combining parallel R&S with adaptive learning. Instead of using a classical pairwise comparison to find a "good selection", the PASS paradigm adaptively "learns" a standard, the best system performance found so far, while controlling the expected false elimination rate. The computational resources are well balanced between simulation and comparison such that R&S can scale to very large numbers of systems on a parallel computing platform.

6 CONCLUSION

This tutorial describes how we envision digital twins developed in industry and the role of simulation in process twins. We present a framework that builds on digital twin required characteristics, four foundational elements of digital twin development, and our experience of building supply chain digital twins. We conclude with a description of how several simulation research streams may enhance process twin creation.

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