Automatic Verification and Validation of Automatically Generated Simulation-Based Digital Twins for Discrete Material Flow Systems

Author: Daniel Fischer

Supervisor: Prof. Christian Schwede

Program: Research Master Data Science

Institution: Hochschule Bielefeld (HSBI)

Submission Date: March 25, 2025

Abstract

This thesis investigates the application of Digital Twins within discrete material flow systems, a key component of Industry 4.0. It reviews the progression from Digital Models and Digital Shadows to fully realized Digital Twins that integrate real-time data, simulation, and control mechanisms. While DTs promise enhanced monitoring, predictive analytics, and operational control in manufacturing, their automated generation poses challenges in terms of accuracy, overfitting, and real-time performance. To address these challenges, this research proposes a data-driven framework for automated verification, validation, and uncertainty quantification of simulation-based DTs. Leveraging object-centric event logs and advanced machine learning techniques, the framework aims to seamlessly integrate digital simulation with real-world data. This approach not only improves decision support in dynamic manufacturing settings but also ensures that the resulting DTs maintain high fidelity and robustness by continuously benchmarking their performance against operational metrics. The framework is evaluated via a comprehensive case study examining its effectiveness in enhancing process efficiency and predictive precision.

Keywords: Digital Twins, Automated VVUQ, Process Mining, Machine Learning, Discrete Material Flow Systems.

Contents

List of Abbreviations

AGDT Automatically Generated Digital Twin. 1

CPS Cyber-Physical System. 1

DES Discrete-Event Simulation. 1

DM Digital Model. 1

DMFS Discrete Material Flow Systems. 1

DS Digital Shadow. 1

DT Digital Twin. 1

IoT Internet of Things. 1

ML Machine Learning. 1

PM Process Mining. 1

PPC Production Planning and Control. 1

SBDT Simulation-Based Digital Twin. 1

V&V Verification and Validation. 1

VVUQ Verification, Validation, and Uncertainty Quantification. 1

Chapter 1

Introduction

1.1 Initial Situation

Digital Twins (DT) are a key technology at the front of the fourth industrial revolution, coined Industry 4.0. The latter term is characterized by the interaction of cyber-physical systems (CPS), the Internet of Things (IoT), and cloud computing to create smart factories with the goal of automation and efficiency (Oztemel & Gursev, 2020). Companies pursue this ideal by trying to remain competitive through the adoption of innovative technologies that promise enhanced productivity and reduced operational costs. One such technology that supports this transformation is the DT. It can be defined as a virtual representation of physical assets enabling real-time monitoring and optimization (Tao et al., 2018). The DT bridges the connection between the two entities with a bi-directional data flow to exchange information and to influence the behaviour of the physical asset (Grieves, 2014). This technology in Industry 4.0 connects the physical and digital worlds through real-time data integration, simulation, and optimization (Judijanto et al., 2024).

Although this field is rapidly evolving, a unified definition of DT has yet to be established due to the diverse requirements and perspectives across different fields. In engineering, the focus might be on the real-time interaction between physical systems and their digital counterparts, whereas in computer science, the emphasis is often on data integration and simulation capabilities. These varying priorities result in multiple interpretations and applications of the term DT. The term was first introduced by Michael Grieves in 2002, defining it as a digital representation of a physical object or system (Grieves, 2014). However, the concept has evolved since then, encompassing a broader range of applications and technologies. Going back through the literature, there are three terms used to describe similar characteristics of DT: Digital Model (DM), Digital Shadow (DS), and Digital Twin (DT), see Figure 1.1 (Jones et al., 2020; Zhang et al., 2021).

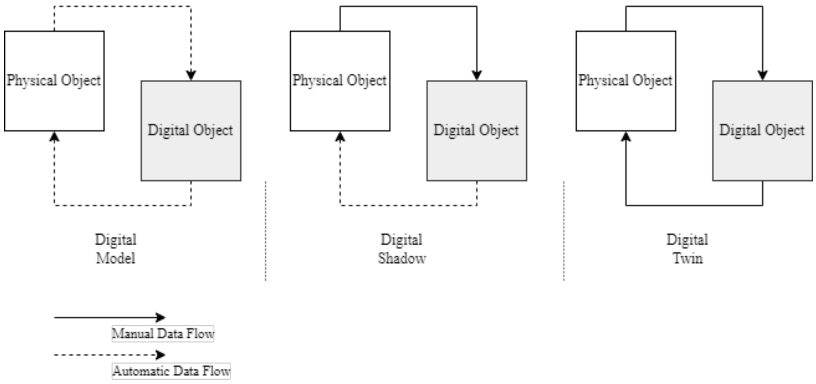

Figure 1.1: Comparison of Digital Shadow (DS), Digital Model (DM) and Digital Twin (DT) as presented by Kritzinger (2018). This distinction is crucial for understanding validation requirements across different digital representation types.

The DM represents the most basic form. It contains manual data connections between physical and digital entities. These connections can be temporarily shifted or even disconnected. There is no control of the digital object over the physical entity. It rather is a simple or complex model *describing* the modelled object. It can not make decisions by itself to influence the physical object. The reason lies in the potential outdated data the digital part possesses or in the fact that it does not contain logic to control the data flow back to the physical part by itself. The control and the obligation to interpret the results is completely in the hands of the modeller. The DS is a more advanced version of the DM. It is a digital representation of the physical object, which is continuously updated with real-time data. The DS can be used for monitoring, analysis and simulation purposes. It can predict the future state of the physical object based on the current state and historical data. However, the DS is not able to influence the physical object. The control is, similar to the DM, still in the hands of the modeller. A DS is frequently used for simulation purposes and is often misclassified as a DT in the literature (Kritzinger et al., 2018; Sepasgozar, 2021). The DT is the most advanced version of the triplet. It is a digital representation of the physical object, which is also continuously updated with real-time data. The DT can be used for monitoring, analysis, and *control* purposes. It can predict the future state of the physical object based on the current state and historical data. The DT can also influence the physical object by sending control signals to it. The control is partially or completely in the hands of the DT. The DT thus *can* serve more purpose than modelling or simulating the physical object. It may serve as an autonomic system, updating itself or by help of the modeller (Kritzinger et al., 2018).

DTs are applied across various sectors, including manufacturing, defense, automotive, service, finance and healthcare (Tao et al., 2018). Manufacturing stands out due to its high potential for process optimization and automation. This thesis focuses on the latter, particularly discrete material flow systems (DMFS). These systems process discrete objects (parts) that move along transportation routes or conveyor lines—either at regular or irregular intervals—integrating both production and logistics operations (Arnold & Furmans, 2005; Schwede & Fischer, 2024). A core simplification in their modeling is the abstraction of material flow as a sequence of discrete events, in accordance to the principles of discrete-event simulation (DES) (Kovacs & Kostal, 2016; Robinson, 2014). DES is particularly well-suited for analyzing complex systems where state changes occur at discrete points in time, such as arrivals, departures, and processing steps (Robinson, 2014).

In hindsight, DM played a crucial role in the design, planning, and control of DMFS, primarily through applications such as material flow simulations, logistic assistance systems, and digital factory implementations (Thiede et al., 2013). However, advancements in both DS and DT have enabled a revolution from isolated, usecase-specific models toward complete digital representations that span the entire lifecycle of DMFS (Abdoune et al., 2023). This transition is largely driven by the increasing demand for predictive capabilities by stakeholders and automated decision support in manufacturing systems, reflecting the cornerstones of Industry 4.0 (Frank et al., 2019). A second driver of DT innovation lies in the widely available data from IoT devices and sensors. Unlocking these potentials in model training and real-time adaption of the DT is crucial for its modelling capabilities (Tao et al., 2018).

In practice, the automated data transfer between the digital model and the physical system is of secondary importance for DMFS management. Unlike in time-critical applications, human decision-makers remain an integral part of the control loop, ensuring that real-time automation is not always necessary (Schwede & Fischer, 2024). Consequently, for this thesis, digital simulations and DTs will be treated as equivalent concepts.

Beyond merely replicating the current state and managing historical data, DTs serve a crucial function in predicting system behavior and evaluating potential modifications. The widespread adoption of DES within digital twins highlights the central role of simulation-based DTss (SBDT) in DMFS (Lugaresi & Matta, 2021). As Schwede and Fischer emphasize, SBDTs provide decision support for optimizing cost and performance in highly competitive manufacturing environments. While current SBDTs are primarily developed and updated manually by domain experts, emerging research explores how machine learning (ML) can enhance predictive accuracy and automate model updates by automatically learning model characteristics, reducing costs and development time.

Thus, the progression from digital models to simulation-based DTs reflects an ongoing shift towards data-driven, predictive, and increasingly automated representations of DMFS, ensuring more informed decision-making throughout the whole system lifecycle (Boschert & Rosen, 2016; Lim et al., 2020).

1.2 Problem

Despite the transformative potential of DT, their implementation can be challenging. The creation and maintenance of accurate DTs require substantial investments in technology and domain knowledge. This investment yields no return if the resulting model fails to accurately represent the modelled entity or delivers incorrect results. Automatic generation may be an elegant solution, but possesses the risk of overfitting or biased predictions (Geman et al., 1992). Manufacturing data used as training data must be preprocessed and cleaned rigourusly. The DT per definition has to be able to perform real-time decision making without excessive time lags (Sepasgozar, 2021). This yields the requirement to extract, transform, clean and load (ETL process, Vassiliadis et al., 2002) data on the fly. ETL needs to happen fully in cache or memory so that inference can happen instantly. All other persistence methods would lead to excessive disk I/O (Mandala, 2024). All these hurdles are challenges to automatic learning (Ribeiro et al., 2016; Zhao et al., 2024). As industries integrate DT into their production processes, establishing trust becomes fundamental as well (Arrieta et al., 2020; Trauer et al., 2022). To gain widespread acceptance under coworkers, stakeholders and investors, the technology must demonstrate accuracy, transparency, and cost-efficiency (Shao et al., 2023; Wright & Davidson, 2020). Without these qualities, organizations will likely fall back to familiar methods, potentially building resistance to technological advancement (Lapointe & Rivard, 2005). If DTs dont live up to the expectations, divestments will follow (Montgomery & Thomas, 1988).

Even if DT learning is successfully performed, questions regarding its correctness, precision, and robustness remain unanswered. These questions are tackled by validation, verification and uncertainty quantification frameworks (VVUQ)

(Sel et al., 2025). Ensuring the validity, reliability, and accuracy of a DT is critical, yet traditional VVUQ approaches rely heavily on manual expert involvement and case-specific reference values (Bitencourt et al., 2023; Hua et al., 2022). This creates inefficiencies, particularly in the context of automated DT generation, where such manual processes conflict with the goal of reducing development effort. Hua et al. even argue that there are no robust and standardized verification and validation methods for DTs. As (Sel et al., 2025) point out, uncertainty quantification is often overseen, but adresses an important aspect of assessing low noise in explanations. One hurdle to standardized VVUQ frameworks is the lack of a clear definition for validity and verification in the context of DTs (Bitencourt et al., 2023).

For discrete material flow systems, these challenges are even more pressing due to their processual nature and stochasticity. Manufacturing processes may fail due to, among other factors, anomalies, resource constraints, software faults or human error (Cheng et al., 2022). VVUQ approaches have to anticipate these risks. When DTs for these systems are generated automatically, conventional validation approaches become problematic, as they negate much of the efficiency gained through automation. This creates a fundamental conflict: While automated DT generation reduces initial development- and updating efforts, it simultaneously increases the complexity of validation and verification, potentially counteracting its intended efficiency gains.

1.3 Objective

The thesis thus addresses this contradiction by developing a data-driven framework for automated VVUQ of automatically generated, simulation-based DTs which have been learned from data. The focus lies on DMFS due to their practical relevance and dynamical, processual nature. The endeavor can further be concretized by the following research questions (RQ):

- **RQ1:** How can automated validation and verification processes for DTs be efficiently implemented to maintain both accuracy and computational feasibility?
- **RQ2:** Which data-driven approaches are best suited to identify discrepancies between simulated behavior and real operational data in discrete material flow systems?
- **RQ3:** To what extent does the developed framework improve the quality and reliability of DTs compared to traditional VV methods?

This thesis addresses these questions by proposing that object-centric event logs—the same data structures often used to generate DT in manufacturing—can serve as the foundation for an automated, use case-independent validation and verification framework. Such an approach would maintain the efficiency benefits of automated generation while ensuring the resulting DTs meet necessary standards. The development and monitoring of generic, statistically grounded reference values is a key aspect of this approach. Such key indicators need to have an underlying distribution and have to be quantifiable. The framework will be evaluated using a case study from the discrete material flow domain, providing empirical evidence of its effectiveness in improving model accuracy and efficiency.

1.4 Structure and Methodology

Structure

The thesis is structured into eight chapters. Chapter 2 establishes the theoretical groundwork. It begins with broad, domain-specific concepts and progressively narrowing the focus to the core topics of this thesis: Automated verification and validation (VVUQ) of simulation-based digital twins (SBDTs) in discrete material flow systems. Section 2.1 introduces material flow planning and simulation, outlining the fundamental elements of production systems, including processes, resources, and control mechanisms. It defines key performance indicators (KPIs) that are essential for evaluating both real and simulated systems, thereby providing the practical context in which digital twins operate. Section 2.2 then transitions to the DT concepts. A framework for comparing DTs by Schwede and Fischer (2024) is presented. Particular attention is given to data-driven digital twins and their subset, automatically generated digital twins (AGDTs). The section concludes by contrasting AGDTs with classical simulation models, emphasizing the challenges posed by automatically generated models. Building on this foundation, Section 2.3 presents the principles of process mining (PM) and event log analysis, with a focus on object-centric event logs as a data basis for automated validation. This section demonstrates how PM acts as a bridge between real-world process data and model validation, thus enabling continuous verification of SBDTs. Section 2.4 narrows the focus further to VVUQ in the context of SBDTs, beginning with a historical overview of VVUQ methodologies. It then addresses the specific challenges posed by automatically generated models, such as data dependency and lack of transparency in model creation. The section introduces machine learning-based approaches for VVUQ, particularly classification methods for model deviation detection. It also explores the current state of VVUQ in corporate practice, emphasizing the necessity for continuous and automated validation processes.

Chapter 3 outlines the methodology used to develop the proposed framework. It begins with a classical requirements analysis, deriving functional, technical, and data format requirements from theoretical findings. The chapter elaborates on the data-based validation strategy, machine learning-based validation approach, metrics for model evaluation, and online validation with continuous monitoring.

Chapter 4 presents the framework implementation, starting with the architecture and system setup, followed by detailed descriptions of event log processing, simulation integration, and the machine learning pipeline.

Chapter 5 presents the case study results, evaluating the framework's effectiveness in improving DT quality. It describes the application scenario and data basis, the automatically generated DT, validation experiments, and result interpretation. It concludes with a comparison to manual validation methods.

Chapter 6 discusses the implications of the results and provides recommendations for future research. It evaluates the framework in light of the research questions, examines the significance of verification in automatically generated DT, addresses limitations, and explores implications for research and practice.

Chapter 7 concludes the thesis by summarizing key findings and their implications. It addresses the research questions and hypotheses, discusses the results' significance, acknowledges limitations, and provides recommendations for future work.

Methodology

Methodologically the thesis follows a design science research approach (DSR). This approach is characterized by the development of artifacts to solve practical problems (Hevner et al., 2004; Peffers et al., 2007). Artifacts in the sense of DSR are created objects or constructs which adress the given problem and contribute in direction of both theory and practice. The artifacts are evaluated in a real-world context to demonstrate their effectiveness. The thesis follows DSR by applying the cyclical DSR model, see figure 1.2.

The research paradigm of the thesis can be characterized as deductive-theory critical (Eberhard, 1987). A conceptual VVUQ framework is developed based on existing theoretical foundations, while deriving new requirements thorugh a requirements analysis. The framework is then applied in a case study to evaluate its

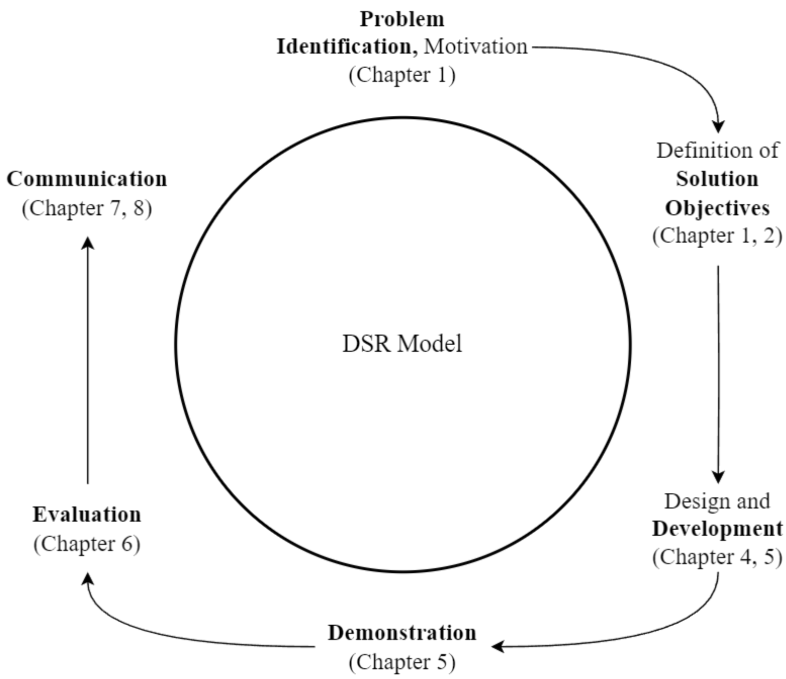

Figure 1.2: The cyclical design science research model. The model consists of six steps. The problem identification (1) refers to the research gap in automated VVUQ of SBDT. Defining the solution objectives (2) specifies the research gap by formulating questions and hypotheses based on the theoretical foundations. The design and development (3) phase includes the development of the framework. The demonstration (4) phase shows the application of the framework in a case study. The evaluation (5) phase assesses the effectiveness of the framework. The communication (6) phase concludes the research by presenting the results.

effectiveness. The research is critical in the sense that it aims to improve the efficiency and effectiveness of VVUQ for automatically generated DTs. Elements of empirical research are included through the case study and the data-driven approach.

Chapter 2

Theoretical Foundation

The following chapter provides a theoretical foundation for the research conducted in this thesis. It introduces the basic concepts of material flow planning and simulation, digital twins, process mining, and verification, validation, and uncertainty quantification (VVUQ). The relevance of these concepts in the context of simulation-based digital twins and their application in corporate practice will also be discussed.

2.1 Discrete Material Flow Systems and Simulation

This section begins with an introduction of the underlying concepts of Discrete Material Flow Systems (DMFS) and Simulation Based Digital Twins (SBDT).

2.1.1 Basic Concepts

Discrete material flow systems cannot be fully understood without first clarifying the principles of Discrete Event Simulation (DES) for Discrete Event Systems. In DES, a system changes its state through *events* that occur at specific, discrete time instances; it is assumed that no changes occur between two successive events. Consequently, the state of the system is completely defined by the values of its descriptive variables at each event occurrence (Varga, 2001). The time at which an event occurs is typically marked by a timestamp, and the scientific observation of such systems is conducted by analyzing the discrete *sequence* of events over time (Robinson, 2014).

Simulation, in this context, refers to the process of imitating the operation of a Discrete Event System over time—often through multiple event sequences. This imitation is captured in a model, and the core activities in a simulation involve constructing and experimenting with this model. A high-quality simulation abstracts the essential features of the system, which requires the modeller to have a sound a priori understanding of what “essential” means in the given context. Although the model can later be refined, its quality is primarily measured by its ability to predict outcomes and offer a diverse range of scenarios (Maria, 1997).

In the context of DMFS, their simulation describes the imitation of material flow systems by breaking down continuous flows into discrete events. Such material flow systems can be characterized as “systems processing discrete objects (parts) that move at regular or irregular intervals along transportation routes or conveyor lines, comprising production and logistic systems” (Arnold & Furmans, 2006; Schwede & Fischer, 2024). These systems form the backbone of material flow planning and control structures. The central idea of material flow planning and control is to ensure that material requirements—both in terms of quantity and timing—are met during transportation and storage across the various stages of the supply chain (“Der Materialfluss im Zuliefernetzwerk — integrierte und prozessorientierte Planung und Steuerung”, 2007). Importantly, the time horizon of interest spans from order placement up to delivery. To summarize, DMFS are often simulated using DES, which abstracts the continuous flow of materials into discrete events. The simulation is carried out using a model. The simulation and modeller are embedded in the context of material flow planning and control, which aims to ensure that material requirements are met across the supply chain. Successfully performed material flow planning and control induce high quality data for simulation and modelling purposes.

2.1.2 Comparing DMFS

Because the simulation of DMFS often involves (discrete) event simulation, events in DMFS need to be further differentiated to be comparable. (Arnold & Furmans, 2006) propose to differentiate DMFS into static and dynamic components.

Static components describe the possible states of the system. Possible states can be the set of possible processes given a part or resource, for example. Dynamic components define the concrete material flow for a certain part or order. Static components include parts, resources and processes (Schwede & Fischer, 2024). Parts are transformed by processes using resources sometimes based on orders. Transformation can have an impact on physical properties of the parts (transformation model), spatial position (transition model), the quality of the parts (quality model) and takes time (time model) and uses resources (resource model). Resources have a capacity of handling parts in parallel (resource capacity model) and processes have a predecessor-successors relationship (process model). Dynamic components are used to define the concrete dynamic material flow within the DMFS. There are four components: Order generation, order control, resource control and supply control. Order generation defines the load the system must process. Order control defines how parts are processed, sometimes referred to as routing rules (Milde & Reinhart, 2019). Resource control defines how resources decide to handle processing requests, also sometimes referred to as priority rules. Supply control describes how supply parts are provided (Milde & Reinhart, 2019; Schwede & Fischer, 2024). See the latter source for a more detailed description of the components.

2.1.3 Production Planning and Control

Successful companies use production planning and control frameworks to describe and optimize their DMFS. After establishing a theoretical foundation and simulation approaches for DMFS, this section thus focusses on Production Planning and Control (PPC) as a critical factor influencing the quality and quantity of data generated by Discrete Event Simulation. PPC is the structured approach to planning, scheduling, controlling and managing all aspects of the manufacturing process. It involves the coordination of resources, processes, and orders to meet production goals. PPC is essential for optimizing production processes, reducing costs, and improving quality. The main functions of PPC include production planning, production scheduling, and production control. Production planning involves determining the production capacity, production goals, and production processes. Production scheduling involves creating a detailed schedule for production activities. Production control involves monitoring and controlling production activities to ensure that production goals are met (Kiran, 2019). Scheduling is usually the last step performed before execution of the plan (Pinedo & Pinedo, 2012).

The integration of PPC with simulation models is crucial because it directly affects the data quality used in DES of DMFS. Effective PPC processes anticipate anomalies in the production cycle, allowing for adjustments that maintain system efficiency and reliability. If successful, these adjustments yield high-quality data that enhance the accuracy of simulation outcomes. (Kiran, 2019).

2.1.4 Relevant KPIs and Metrics

Up to this point, DES for SBDT of DMFS has been introduced, outlining the key factors that contribute to a robust simulation. A model differentiation framework proposed by Schwede and Fischer has been briefly presented to facilitate comparison of SBDT. Furthermore, the critical role of PPC in generating high-quality data for simulation has been discussed. These discussions ignored up till now that, even when SBDT are integrated within well-functioning PPC processes, various SBDT models remain prone to errors and inherent trade-offs that must be addressed by the modeller (Tao et al., 2018).

The goal conflict of the modeller when developing SBDT can be described by the following conflict triangle (Balci, 2012; Robinson, 2014):

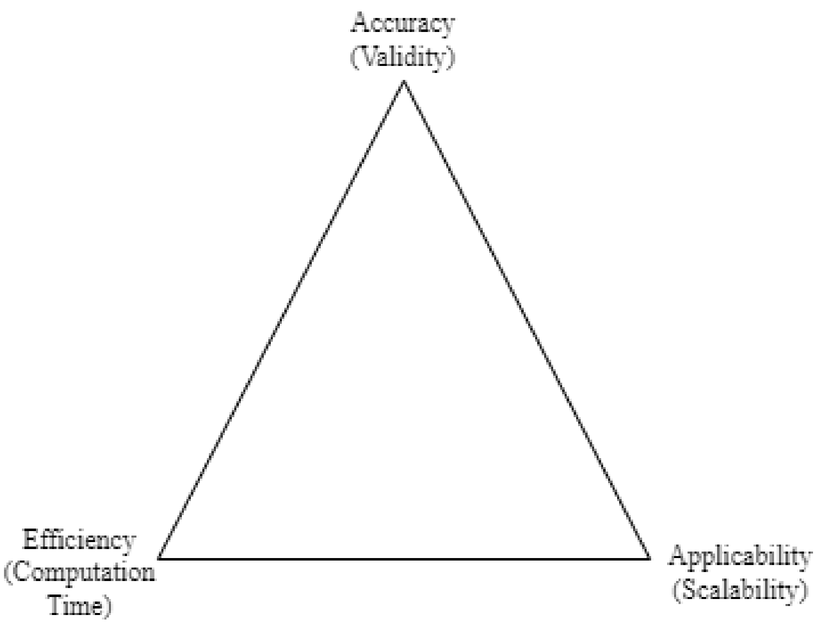

Figure 2.1: The goal conflict of the modeller when developing SBDT. Aiming for higher accuracy (validity) often leads to higher computational costs (efficiency) and reduced scalability (applicability). Reaching more efficiency often leads to reduced accuracy and scalability. Aiming for higher scalability often leads to reduced accuracy and efficiency.

Focusing one of the three dimensions—accuracy (validity), efficiency (computation time), and applicability (scalability)—often leads to trade-offs in the other two dimensions. Oftentimes the data itself is not sufficient to make a decision on which trade-off to make. Limited data points may hinder the modeller from reaching high validity. System architecture may block the system from reaching good scalability. Hardware limitations may hinder the modeller from reaching high efficiency. At other times, corporate management may have a preference for one of the dimensions.

One solution to balance and quantify these goals can be achieved by defining a set of KPIs. Some may already be available through PPC, some may be calculated from DES data or the DES itself. Optimally, the data warehouse provides relevant views (Cui et al., 2020). Because the SBDT in theory mirrors the DMFS, the KPIs gathered from PPC and the DES should yield identical values. Deviations between the KPIs of the SBDT and the DMFS may indicate errors in the SBDT or anomalies in the DFMS. The following KPIs are relevant for the evaluation of SBDT:

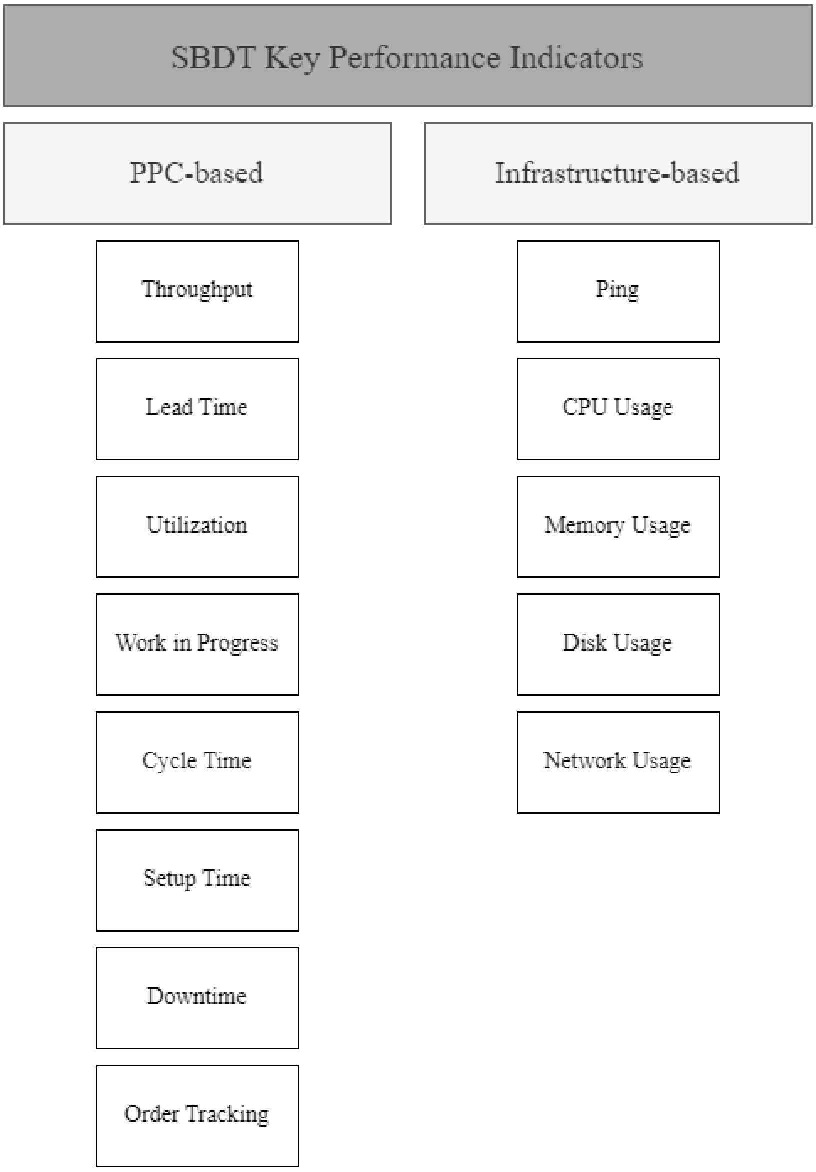

Figure 2.2: SBDT KPIs differentiated by PPC-based and Infrastructure-based indicators.

The PPC related KPIs may be provided by above mentioned data warehouse, because they are highly relevant in the context of production scheduling and -control. Throughput measures the number of produced parts at the last station in a specified period. It is an indicator for the productivity of the manufacturing sytem (Imseitif et al., 2019). Lead time is the cumulative time a part travels through the system from start to sink. It is an indicator for the efficiency of the manufacturing system (Pfeiffer et al., 2016). Cycle time measures the same amount like lead time but focusses only on the active production process, excluding transports and waiting times (Griffin, 1993). Setup time measures the time needed to prepare a machine for a new task. It is an indicator for the flexibility of the manufacturing system (Allahverdi & Soroush, 2008). In the given usecase, we aggregate the setup time for all setup processes. All KPIs presented so far can be calculated dynamically when new data has been sent. Later on, they may serve as an alert system for the modeller to detect deviations between the SBDT and the DMFS, see section 2.4.

The infrastructure related KPIs are derived by sensors from the executing system of the SBDT. Ping time measures the time needed to send a signal from one point to another. It is an indicator for the latency of the infrastructure (Wu et al., 2021). SBDT need to enforce real-time control over the physical entity. The latency thus needs to be as low as possible. In this scenario, one point (sender) is represented by the physical entity and its sensors. The receiving point runs the SBDT. It is advantageous to run the SBDT on Edge to minmize latency- and transmission costs (Li et al., 2018). CPU-, memory-, disk- and network usage metrics are indicators for the load of the infrastructure. They are important to detect bottlenecks in the infrastructure (Li et al., 2018). The first indicator is usually measured in percent of the maximum CPU capacity. The latter three indicators are usually measured in bytes or bits per second (Granelli et al., 2021).

2.2 Digital Twin: Definition and Concepts

The latter section gave a short intrduction into DFMS, DES, its metrics and the corporate processes accompanying the SBDT. Now, we shed light on the DT itself. For a short introduction to the topic, see chapter 1.

Like introduced in the predecessing chapter, DT inherent the highest order of modelling fidelity compared to DM or DS. There are different definitions of DT present in the literature (Boschert & Rosen, 2016; Demkovich et al., 2018; Glaessgen & Stargel, 2012; Grieves, 2014; Kritzinger et al., 2018; Negri et al., 2017; Tao et al., 2018; Zehnder & Riemer, 2018; Zheng et al., 2019). Each of them highlights different aspects of the DT. This thesis uliziles the definition by (Grieves, 2014) which highlughts the cinceptual elements of the twin and its lifecylce focus:

> The digital twin concept (...) contains three main parts: A) Physical products in real space, (B) virtual products in virtual space and (C) the two-way connections of data and information that tie the virtual and real products together. (Grieves, 2014)

2.2.1 Types of Digital Twins

2.2.2 Data-Driven Digital Twins

2.2.3 Automatically Generated Digital Twins

2.2.4 Definitions and Differences from Classical Simulation Literature

2.3 Process Mining and Event Logs

2.3.1 Core Concepts

2.3.2 Object-Centric Event Logs as a Data Basis

2.3.3 Process Mining as Enabling Technology

2.4 VVUQ in the Context of Simulation-Based Digital Twins

2.4.1 Historical Development of VVUQ Concepts

2.4.2 Requirements of VVUQ for Automatically Generated Models

2.4.3 Theoretical Argumentation for Merging Verification, Validation and Uncertainty Quantification

2.4.4 Machine Learning-Based Approaches

2.4.5 VVUQ in the Context of Digital Twins

2.4.6 VVUQ in Corporate Practice

Chapter 3

Framework Design

Chapter 4

Implementation

Chapter 5

Testing

5.1 Application Scenario and Data Basis

5.2 Automatically Generated Digital Twin

5.3 Validation Experiments

5.4 Results and Interpretation

5.5 Comparison with Manual Validation Methods

Chapter 6

Discussion

6.1 Evaluation of the Developed Framework

6.2 Significance of Verification in Automatically Generated Digital Twins

6.3 Limitations of Automated Validation

6.4 Implications for Research and Practice

Chapter 7

Conclusion and Outlook

7.1 Summary of the Key Findings

7.2 Methodological and Theoretical Insights

7.3 Outlook

7.4 Recommendations for Practical Application

Bibliography

Abdoune, F., Nouiri, M., Cardin, O., & Castagna, P. (2023). Digital twin lifecycle: Core challenges and open issues. In T. Borangiu, D. Trentesaux, & P. Leitão (Eds.), *Service oriented, holonic and multi-agent manufacturing systems for industry of the future: Proceedings of sohoma 2022* (pp. 157–167). Springer International Publishing. https://doi.org/10.1007/978-3-031-19647-3_14

Allahverdi, A., & Soroush, H. M. (2008). The significance of reducing setup times/setup costs. *European journal of operational research*, *187*(3), 978–984.

Arnold, D., & Furmans, K. (2005). *Materialfluss in logistiksystemen* (4th ed.). Springer-Verlag. https://doi.org/10.1007/b139029

Arnold, D., & Furmans, K. (Eds.). (2006). *Materialfluss in logistiksystemen* (5th ed.). Springer Berlin Heidelberg.

Arrieta, A. B., Díaz-Rodríguez, N., Del Ser, J., Bennetot, A., Tabik, S., Barbado, A., García, S., Gil-López, S., Molina, D., Benjamins, R., et al. (2020). Explainable artificial intelligence (xai): Concepts, taxonomies, opportunities and challenges toward responsible ai. *Information fusion*, *58*, 82–115.

Balci, O. (2012). A life cycle for modeling and simulation. *Simulation*, *88*(7), 870–883.

Bitencourt, L., Silva, M., & Costa, J. (2023). Building trust in digital twin through verification and validation. *Proceedings of the 2023 International Conference on Digital Twin Technologies*, 55–63. https://doi.org/10.1000/bitencourt.2023.001

Boschert, S., & Rosen, R. (2016). Digital twin—the simulation aspect. *Mechatronic futures: Challenges and solutions for mechatronic systems and their designers*, 59–74.

Cheng, X., Chaw, J. K., Goh, K. M., Ting, T. T., Sahrani, S., Ahmad, M. N., Abdul Kadir, R., & Ang, M. C. (2022). Systematic literature review on visual analytics of predictive maintenance in the manufacturing industry. *Sensors*, *22*(17), 6321.

Cui, Y., Kara, S., & Chan, K. C. (2020). Manufacturing big data ecosystem: A systematic literature review. *Robotics and computer-integrated Manufacturing*, *62*, 101861.

Demkovich, N., Yablochnikov, E., & Abaev, G. (2018). *Multiscale modeling and simulation for industrial cyber-physical systems*. https://doi.org/10.1109/ICPHYS.2018.8387674

Der materialfluss im zuliefernetzwerk — integrierte und prozessorientierte planung und steuerung. (2007). In *Logistik in der automobilindustrie: Innovatives supply chain management für wettbewerbsfähige zulieferstrukturen* (pp. 73–100). Springer Berlin Heidelberg. https://doi.org/10.1007/978-3-540-68114-4_4

Eberhard, K. (1987). *Einführung in die erkenntnis-und wissenschaftstheorie: Geschichte und praxis der konkurrierenden erkenntniswege*. Kohlhammer.

Frank, A. G., Dalenogare, L. S., & Ayala, N. F. (2019). Industry 4.0 technologies: Implementation patterns in manufacturing companies. *International Journal of Production Economics*, *210*, 15–26. https://doi.org/10.1016/j.ijpe.2019.01.004

Geman, S., Bienenstock, E., & Doursat, R. (1992). Neural networks and the bias/variance dilemma. *Neural Computation*, *4*(1), 1–58. https://doi.org/10.1162/neco.1992.4.1.1

Glaessgen, E., & Stargel, D. (2012). The digital twin paradigm for future NASA and U.S. air force vehicles. *53rd AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics and Materials Conference*. https://doi.org/10.2514/6.2012-1818

Granelli, F., Capraro, R., Lorandi, M., & Casari, P. (2021). Evaluating a digital twin of an iot resource slice: An emulation study using the eliot platform. *IEEE Networking Letters*, *3*(3), 147–151.

Grieves, M. (2014). *Digital twin: Manufacturing excellence through virtual factory replication* (tech. rep.) (White Paper).

Griffin, A. (1993). Metrics for measuring product development cycle time. *Journal of Product Innovation Management: An International Publication of the Product Development & Management Association*, *10*(2), 112–125.

Hevner, A. R., March, S. T., Park, J., & Ram, S. (2004). Design science in information systems research. *MIS quarterly*, 75–105.

Hua, E. Y., Lazarova-Molnar, S., & Francis, D. P. (2022). Validation of digital twins: Challenges and opportunities. *2022 Winter Simulation Conference (WSC)*, 2900–2911. https://doi.org/10.1109/WSC57314.2022.10015420

Imseitif, J., Tang, H., & Smith, M. (2019). Throughput analysis of manufacturing systems with buffers considering reliability and cycle time using des and doe. *Procedia Manufacturing*, *39*, 814–823.

Jones, D., Snider, C., Nassehi, A., Yon, J., & Hicks, B. (2020). Characterising the digital twin: A systematic literature review. *CIRP Journal of Manufacturing Science and Technology*, *29*, 36–52. https://doi.org/10.1016/j.cirpj.2020.02.002

Judijanto, L., Qadriah, L., Prabowo, I. A., Widyatmoko, W., & Sabila, P. C. (2024). Trends in digital twin technology for industry 4.0: A bibliometric study. *The Eastasouth Journal of Information System and Computer Science*, *2*(02), 92–104.

Kiran, D. (2019). *Production planning and control: A comprehensive approach*. Butterworth-heinemann.

Kovacs, G., & Kostal, P. (2016). Mathematical description of material flow. *Materials science and technology*, *1*.

Kritzinger, W., Karner, M., Traar, G., Henjes, J., & Sihn, W. (2018). Digital twin in manufacturing: A categorical literature review and classification. *IFAC-PapersOnLine*, *51*(11), 1016–1022. https://doi.org/10.1016/j.ifacol.2018.08.474

Lapointe, L., & Rivard, S. (2005). A multilevel model of resistance to information technology implementation. *MIS quarterly*, 461–491.

Li, H., Ota, K., & Dong, M. (2018). Learning iot in edge: Deep learning for the internet of things with edge computing. *IEEE network*, *32*(1), 96–101.

Lim, K. Y. H., Zheng, P., & Chen, C.-H. (2020). A state-of-the-art survey of digital twin: Techniques, engineering product lifecycle management and business innovation perspectives. *Journal of Intelligent Manufacturing*, *31*(6), 1313–1337.

Lugaresi, G., & Matta, A. (2021). Automated digital twins generation for manufacturing systems: A case study. *IFAC-PapersOnLine*, *54*(1), 749–754. https://doi.org/10.1016/j.ifacol.2021.08.087

Mandala, N. R. (2024). Etl in big data architectures: Challenges and solutions. *International Journal of Science and Research (IJSR)*, *13*(10), 1061–1068. https://doi.org/10.21275/SR241014054151

Maria, A. (1997). Introduction to modeling and simulation. *Proceedings of the 29th conference on Winter simulation*, 7–13.

Milde, M., & Reinhart, G. (2019). Automated model development and parametrization of material flow simulations. *2019 Winter Simulation Conference (WSC)*, 2166–2177. https://doi.org/10.1109/WSC40007.2019.9004702

Montgomery, C. A., & Thomas, A. R. (1988). Divestment: Motives and gains. *Strategic Management Journal*, 93–97.

Negri, E., Fumagalli, L., & Macchi, M. (2017). A review of the roles of digital twin in cps-based production systems. *Procedia Manufacturing*, *11*, 939–948. https://doi.org/10.1016/j.promfg.2017.07.198

Oztemel, E., & Gursev, S. (2020). Literature review of industry 4.0 and related technologies. *Journal of intelligent manufacturing*, *31*(1), 127–182.

Peffers, K., Tuunanen, T., Rothenberger, M. A., & Chatterjee, S. (2007). A design science research methodology for information systems research. *Journal of management information systems*, *24*(3), 45–77.

Pfeiffer, A., Gyulai, D., Kádár, B., & Monostori, L. (2016). Manufacturing lead time estimation with the combination of simulation and statistical learning methods. *Procedia Cirp*, *41*, 75–80.

Pinedo, M. L., & Pinedo, M. L. (2012). Design and implementation of scheduling systems: Basic concepts. *Scheduling: theory, algorithms, and systems*, 459–483.

Ribeiro, M. T., Singh, S., & Guestrin, C. (2016). " why should i trust you?" explaining the predictions of any classifier. *Proceedings of the 22nd ACM SIGKDD international conference on knowledge discovery and data mining*, 1135–1144.

Robinson, S. (2014). *Simulation: The practice of model development and use*. Bloomsbury Publishing.

Schwede, C., & Fischer, D. (2024). Learning simulation-based digital twins for discrete material flow systems: A review. *2024 Winter Simulation Conference (WSC)*, 3070–3081.

Sel, K., Hawkins-Daarud, A., Chaudhuri, A., Osman, D., Bahai, A., Paydarfar, D., Willcox, K., Chung, C., & Jafari, R. (2025). Survey and perspective on verification, validation, and uncertainty quantification of digital twins for precision medicine. *npj Digital Medicine*, *8*(1), 40.

Sepasgozar, S. M. (2021). Differentiating digital twin from digital shadow: Elucidating a paradigm shift to expedite a smart, sustainable built environment. *Buildings*, *11*(4), 151.

Shao, G., Hightower, J., & Schindel, W. (2023). Credibility consideration for digital twins in manufacturing. *Manufacturing Letters*, *35*, 24–28. https://doi.org/10.1016/j.mfglet.2022.11.009

Tao, F., Cheng, J., Qi, Q., Zhang, M., Zhang, H., & Sui, F. (2018). Digital twin-driven product design, manufacturing and service with big data. *The International Journal of Advanced Manufacturing Technology*, *94*(9-12), 3563–3576. https://doi.org/10.1007/s00170-017-0233-1

Thiede, S., Seow, Y., Andersson, J., & Johansson, B. (2013). Environmental aspects in manufacturing system modelling and simulation—state of the art and research perspectives. *CIRP Journal of Manufacturing Science and Technology*, *6*(1), 78–87. https://doi.org/10.1016/j.cirpj.2012.10.002

Trauer, J., Schweigert-Recksiek, S., Schenk, T., Baudisch, T., Mörtl, M., & Zimmermann, M. (2022). A digital twin trust framework for industrial application. *Proceedings of the Design Society*, *2*, 293–302.

Varga, A. (2001). Discrete event simulation system. *Proc. of the European Simulation Multiconference (ESM'2001)*, *17*.

Vassiliadis, P., Simitsis, A., & Skiadopoulos, S. (2002). Conceptual modeling for etl processes. *Proceedings of the 5th ACM international workshop on Data Warehousing and OLAP*, 14–21.

Wright, L., & Davidson, S. (2020). How to tell the difference between a model and a digital twin. *Advanced Modeling and Simulation in Engineering Sciences*, *7*(1), 13. https://doi.org/10.1186/s40323-020-00147-4

Wu, Y., Zhang, K., & Zhang, Y. (2021). Digital twin networks: A survey. *IEEE Internet of Things Journal*, *8*(18), 13789–13804.

Zehnder, P., & Riemer, D. (2018). Representing industrial data streams in digital twins using semantic labeling. *2018 IEEE International Conference on Big Data (Big Data)*, 4223–4226.

Zhang, L., Zhou, L., & Horn, B. K. (2021). Building a right digital twin with model engineering. *Journal of Manufacturing Systems*, *59*, 151–164. https://doi.org/10.1016/j.jmsy.2021.02.009

Zhao, Y. F., Xie, J., & Sun, L. (2024). On the data quality and imbalance in machine learning-based design and manufacturing—a systematic review. *Engineering*.

Zheng, Y., Yang, S., & Cheng, H. (2019). An application framework of digital twin and its case study. *Journal of ambient intelligence and humanized computing*, *10*, 1141–1153.