Architecture of Simulation-Based Representations for Digital Twins

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Abstract. The world faces significant sustainability challenges, from resource consumption to supply chain inefficiencies. A comprehensive simulation-based approach for creating Digital Twins (DTs) is developed to address these issues. This paper contributes to the gradual development of DTs and presents a novel architecture for a simulation tool. The proposed architecture enables the creation of a holistic virtual representation of the system by incorporating linear and circular production models, supporting various scenarios, identifying optimization potential, and making data-driven decisions. Using simulation-based DTs indicates the potential to drive sustainable transformation in the beverage industry and beyond. As the approach progresses, it aims to provide a blueprint for leveraging digital technologies, fostering a more sustainable and resilient future.

Introduction

The world is confronted with unprecedented sustainability hurdles, including climate change, resource depletion, social inequality, and economic instability. There is a desperate need to tackle these intricate and interrelated issues. To combat these problems, the United Nations has established the Sustainable Development Goals (SDGs), a global framework for achieving a more sustainable, equitable, and prosperous future for all [1]. Digital technologies, such as the Internet of Things (IoT), Artificial Intelligence (AI), and simulation, are increasingly recognized as powerful tools for supporting the achievement of the SDGs [2, 3].

In particular, SDG 9 emphasizes promoting inclusive and sustainable industrialization, fostering innovation, and the need for resilient and sustainable infrastructure. By using digital technologies to design, optimize, and manage auch infrastructures and industrial processes, organizations can make data-driven decisions that minimize environmental impact and promote responsible production and consumption, as highlighted in SDG 12 [3, 4]. This aligns with the emerging paradigm of Industry 5.0, which builds upon the technological advancements of Industry 4.0 while placing a strong emphasis on the collaboration between humans and machines to create more sustainable, resilient, and human-centric industrial processes [5, 6].

One promising application of digital technologies for sustainable development is the concept of virtual representations of physical systems that are capable of real-time data to mirror the behavior and performance of their real-world counterparts [7, 8]. By integrating sustainability metrics and indicators into these systems, organizations can assess their operations' environmental impact, identify improvement opportunities, and make informed decisions to reduce their ecological footprint [9].

Manufacturing also encounters critical sustainability concerns, from energy and water consumption to waste generation and supply chain inefficiencies. To address these, the BeverGreen project [10], a collaborative effort involving the beverage industry and academic partners, aims to develop an extensive methodology for creating sustainability systems in this field. Aided by simulation techniques and integrating sustainability metrics, the project seeks to optimize resource efficiency, minimize environmental impact, and promote circular economy principles.

We aim to provide valuable insights and practical guidance for organizations seeking to harness technologies for driving sustainable development and Industry 5.0 principles through examining the intersection of simulation, DTs and sustainability,

1 Digital Twins and Simulation

1.1 Digital Twin Fundamentals

DTs are virtual representations of physical systems that use historical data, real-time data, and different data processing methods to act as a system or part of it. It also allows for simulation, analysis, and optimization of the physical counterpart. The concept of DTs was first introduced by Michael Grieves in 2002 in the context of product lifecycle management (PLM) [11]. Since then, they have evolved to encompass various applications, from manufacturing to healthcare [12]. A key characteristic of DTs is their ability to integrate data from multiple sources, such as sensors, historical data, and domain knowledge, to create an accurate and up-to-date representation of the physical system [13]. Simulation plays a crucial role in developing DTs by enabling the prediction of system behavior under different conditions and scenarios [14].

1.2 Simulation Paradigms for Digital Twins

Several simulation paradigms are employed in developing DTs, each with strengths and limitations. Discrete event simulation (DES) is widely used to model systems where state changes occur at discrete points, such as manufacturing systems and supply chains [15]. Agent-based simulation (ABS) focuses on modeling the behavior and interactions of individual agents within a system, making it suitable for modeling complex adaptive systems [16]. System dynamics (SD) models the feedback loops and nonlinear relationships in complex systems, such as ecosystems and social systems [17]. Hybrid simulation approaches combine multiple paradigms to leverage their strengths and address individual paradigms' limitations [18].

1.3 Simulation-Based Digital Twin Development Process

Developing, commissioning, running, and maintaining DTs using simulation typically involves four main stages: conceptual modeling, implementation, verification, and validation [19], and experimentation. Conceptual modeling consists of defining the scope, objectives, and assumptions of DTs, as well as identifying the key components and relationships within the system [20].

Implementation involves translating the model into a computer model using appropriate simulation software and programming languages [21]. Verification and validation ensure that DTs accurately represents the real-world system and produces reliable results. Experimentation involves exploring different scenarios, optimizing system performance, and supporting decision-making.

The concept of Green Digital Twins (GDTs) [22] has recently emerged as a promising approach to address as of SDGs. These expanded DTs with a subclass containing properties and requirements mainly characterized by integrating sustainability-related specifications. A GDT based on this concept requires digital models of resources, processes, domain knowledge, and energy networks, such as energy sources and sinks, as well as models of their relationships as well as a component emission repository, by which emission factors can be used for calculating CO2-equivalents or other metrics. [9]. This enables organizations to assess their operations' environmental impact, identify improvement opportunities, and make data-driven decisions to reduce their ecological footprint [4]. Across economic, environmental, and social dimensions, GDTs facilitates the alignment of business objectives with sustainability goals, promoting responsible production and consumption practices by providing a holistic view of the system's performance.

The emergence of AI has been a significant driver in the development and application of DTs [23]. Its techniques, such as machine learning, enable them to learn from data, adapt to changing conditions, and make autonomous decisions [24]. The integration of AI has opened up new possibilities for optimizing system performance, predicting failures, and enabling predictive maintenance [8]. AI-powered DTs can analyze vast amounts of data in real time, identify patterns and anomalies, and provide actionable insights for improving operational efficiency and reducing downtime. This synergy between AI and DTs is particularly relevant for complex, dynamic systems, where traditional simulation approaches may struggle to capture the full range of system behaviors and interactions.

Addressing these challenges requires collaborative efforts across disciplines to develop robust, scalable, and interoperable platforms. The BeverGreen project aims to address some of these challenges by developing a thorough methodology for creating GDTs in the beverage industry, focusing on integrating sustainability metrics and reducing environmental impact.

2 Methodology

2.1 Overview and Objectives

Our simulation-focused architecture builds on assembling a team of domain experts in production and distribution, software developers, and scientific researchers to develop comprehensive DTs that map a supply chain. Within the BeverGreen project, we aim to digitally interlock linear production chains within companies and circular processes involving multiple actors to provide a foundation for wide-ranging optimization potential. In line with global sustainability goals and resilient economics, the project focuses on critical areas such as energy management, production planning, inventory management, and transport logistics, seeking to identify adaptable parameters that contribute to these objectives [9].

2.2 Simulation-Focused Approach for DTs

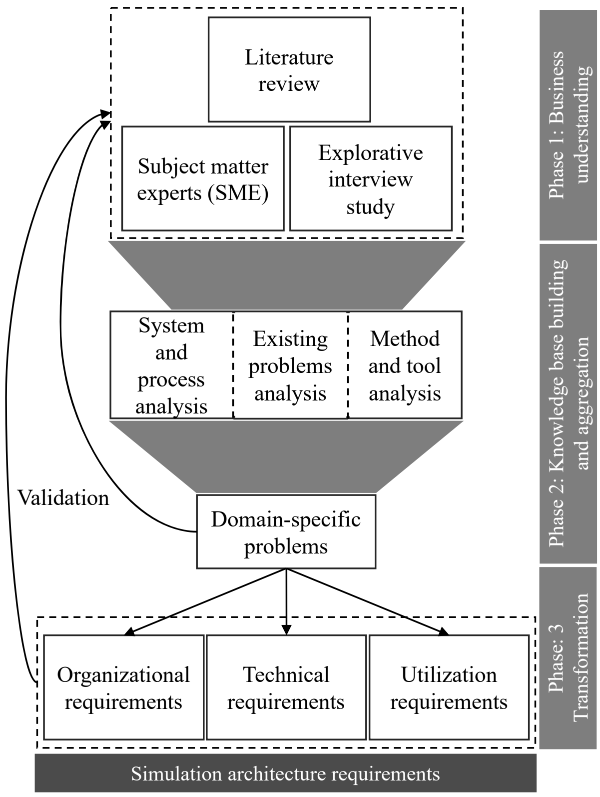

Figure 1: Determinational Approach for Architectural Requirements

Our simulation-focused approach (Figure 1) consists of business understanding, an initial phase that aims to identify sources for generating a comprehensive knowledge foundation. Starting with a literature review, an explorative interview study including all relevant partners along the supply chain (manufacturers, intermediate trade and retail, associational partners), aided by exchange with several subject matter experts (SME) within the team, we created a multi-layered and multi-perspective glimpse of general systematic and procedural conditions as well as challenges along the supply chain.

Based on insights gained in phase 1, we conducted further analysis in a second phase, knowledge base building and aggregation. We dissected the system's production, distribution, and circulation behavior and their systemic interactions. On a process level, we investigated necessary conditions and movement patterns of products and resources within the manufacturing company and also between partners of the supply chain. Problems regarding efficiency and sustainability were identified and specified regarding their origin in existing processes and, if possible, analyzed and concretized.

Simultaneously, methods and tools that might contribute to overcoming existing challenges were viewed to reduce identified black boxes in the relevant processes and simulate future scenarios. Based on the dissection, domain-specific problems could be described and validated by synchronizing them with the initially detected sources of business understanding.

Phase three, Transformation, mainly addressed characterizing specific requirements resulting from challenges. Given the standards and conditions, organizational requirements that refer to diverse demands along the supply chain were identified. At the same time, necessary organizational conditions must be ensured for the successful development of comprehensive DTs.

The DT being developed must meet a range of technical requirements and functionalities, including the ability to map relationships between machines, resources, and products, the utilization of domain knowledge, rules, and indicators, connectivity to various data sources and simulations, visualization capabilities, integration of data analysis apps, and forecasting capabilities.

Utilized, individual interests and aims regarding the usage of a DT were specified, including the essential provision of sensible user interfaces and high data security standards. Furthermore, requirements that software developers need as a foundation for building were emphasized.

However, the availability of data to develop and use DTs is heavily restricted due to varying levels of digitalization and interests among supply chain partners, including limitations in transferability between different systems. Alongside efforts to access data and form a basis for their functionality, simulation models will initially generate data and test various scenarios for energy utilization, routing, and product launching [3].

2.3 Model and Simulation Approach

The simulation approach has been selected to address data black boxes, gain well-founded knowledge about processes and their reciprocal influence, and identify optimization potential within individual steps [18]. To capture the system's behavior, we have chosen a multi-method simulation approach [25].

A meta-model will be developed to understand system behavior and dynamics more thoroughly, as well as global dependencies between system inputs and outputs. Individual process chains will also be analyzed to create a foundation for developing discrete event simulation models [15]. Both methods need to be combined to achieve the overall goal of representing an entire supply chain. Given the high complexity of the system and the need to examine emergent behavior, agent-based methods will also be incorporated into the modeling process [16].

2.4 Data Collection and Analysis Methods

Data generation and connection are crucial aspects of the project. The team will work on establishing a robust data infrastructure that enables the integration of data from various sources, including sensors, historical records, and domain expertise. Advanced data analysis techniques, such as machine learning and data mining, can extract valuable insights from the collected data [23]. The resulting dataset can inform and validate the simulation models, ensuring their accuracy and reliability in representing the real-world system [19].

Our methodology combines state-of-the-art DT technologies, simulation paradigms, and data analysis techniques to develop a comprehensive and sustainable approach for optimizing supply chain operations and processes in the beverage industry. By addressing the challenges associated with data availability, model integration, and system complexity, the project aims to demonstrate the potential of DTs in driving progress towards the United Nations SDGs [2].

3 Use Case and Results

3.1 Project BeverGreen

BeverGreen focuses on leveraging digital technologies to address the specific challenges faced by the beverage industry, such as resource efficiency, reusable bottle circulation scheduling, and energy efficiency. Global issues, including rising energy and raw material costs, limited resources, climate protection initiatives, and new resilience requirements for supply chains exacerbate these challenges. To tackle these challenges, it aims to develop an assistance system that maps existing data structures to domain-specific ontologies containing relevant information, forming the basis for GDTs.

An assistance system is the starting point for linking internal and external datasets, such as life cycle assessment databases and CO2 equivalents (CO2e). By integrating these datasets, the project seeks to create a holistic view of the beverage industry's environmental impact and identify opportunities for optimization. The development of GDTs, in combination with machine learning methods, is a crucial objective of the BeverGreen project, aiming to identify and realize energy and resource savings in exemplary application scenarios.

3.2 Explanation of the Simulation-Based Digital Twin Architecture

Two primary areas are focused on: closed application circles in production and circular value creation networks. In brewing processes, DTs are being developed to optimize resource consumption, minimize waste, and improve overall efficiency. Creating simulation-based representations of brewing processes enables stakeholders to simulate various scenarios, test optimization strategies, and make data-driven decisions to reduce the environmental footprint of their products.

Within logistics, the project addresses challenges associated with reusable bottle circulation scheduling. DTs of this circuit aims to optimize the flow of reusable bottles, minimize transportation costs, and reduce the overall environmental impact of distribution. Co-opting real-time data and advanced analytics seeks to create a more efficient and sustainable logistics network for the beverage industry.

BeverGreen's use cases demonstrate the potential of DTs and machine learning in driving the sustainable Transformation of the beverage industry. The project aims to serve as a beacon for other industries seeking to optimize their operations and reduce their environmental impact by addressing specific challenges related to resource efficiency, energy consumption, and circular value creation. The insights gained from this project will contribute to developing best practices and guidelines for implementing digital technologies in pursuit of sustainability goals.

3.3 Architecture

The proposed architecture for simulation-based representations is an integral part of this development and is illustrated in Figure 2. It aims to provide a comprehensive framework for integrating various data sources, enabling semantic linking, and facilitating holistic DTs.

3.3.1 Data Sources and Mapping

The first step in the architecture is to identify and connect all relevant data sources across the supply chain that provide the necessary data for the desired functionalities. As shown in Figure 2, this includes data from Enterprise Resource Planning (ERP), Manufacturing Execution Systems (MES), Supervisory Control and Data Acquisition (SCADA) systems, and other databases, which are crucial for depicting production and distribution processes at all relevant operational system levels within and across partners.

For BeverGreen, specific data sources may include brewery production data, inventory levels, energy consumption metrics, and transportation logistics information. Additionally, environmental data sources, such as emission data, weather data, traffic data, economic and political data, and state or institutional regulations, must be incorporated to increase sustainability along the entire supply chain. In the context of the beverage industry, this may involve integrating data on carbon footprints, water usage, and waste generation throughout the production and distribution processes.

To integrate these diverse datasets, a Federated Database Systems (FDBSs) will be established, which connects to the various data sources through Application Programming Interfacess (APIs) and serves as the essential basis for the simulation. The FDBS leverages technologies such as data lakes, data warehouses, and ETL (Extract, Transform, Load) processes to enable robust data integration from heterogeneous sources in a predefined ontology. A data pipeline will be set up to prepare data for use in simulation models and feed data analysis workflows. These analytical processes, such as machine learning algorithms for optimization and data mining techniques for identifying patterns and anomalies, can be embedded at this stage to enhance the data processing capabilities.

In the context of collaborative data warehousing initiatives. To facilitate simulation objectives and develop company-wide DTs, the industry strictly uses anonymized or aggregated data to protect sensitive information.

However, guaranteeing data security across DTs functions and layers utilized by various supply chain partners is a formidable challenge that must be addressed. Numerous studies have investigated security risks and proposed several approaches to tackle these issues, both from a technological standpoint; security protocols are paramount in terms of security management and procedures [26]. Our project team will evaluate different measures to identify and implement effective security solutions while establishing a robust user and access rights management system.

3.3.2 Simulation Models and Data Routes

The prepared simulation data is used to parameterize linear and circular production models via an API, enabling the initiation of multiple simulation runs and experiments, as depicted in Figure 2. In BeverGreen, linear production models may represent brewing processes, while circular production models may encompass reusable bottle circulation and recycling processes.

To validate and verify the initial results and, more importantly, the underlying simulation model, validation techniques such as historical data validation, face validity, and sensitivity analysis are applied. These techniques involve comparing simulation results with existing real-life data in the FDBS, ensuring that the model accurately depicts the real-world system. For example, the simulated energy consumption and resource utilization in the brewing process can be compared against historical data to validate the model's accuracy.

Furthermore, the resilient simulation results that emerge later must be imported back into the FDBS to continuously feed the knowledge base with

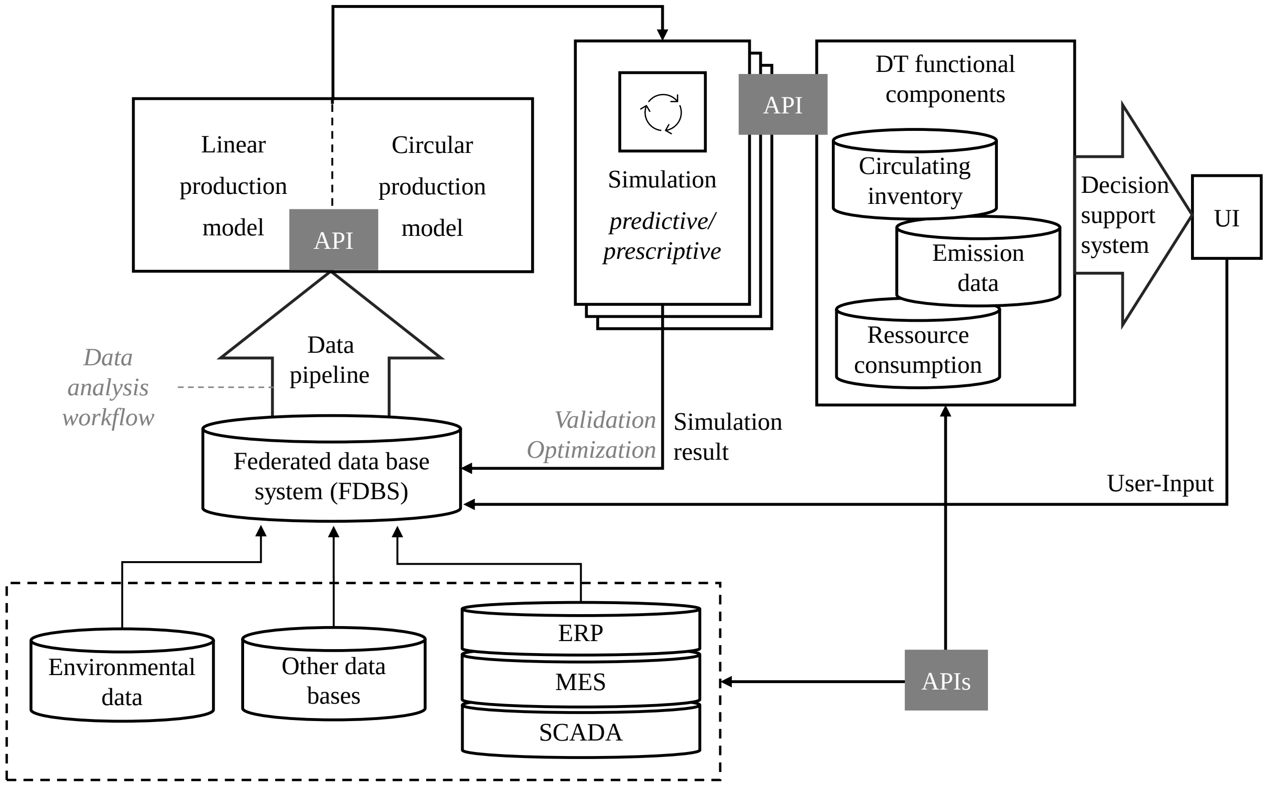

Figure 2: Architecture of a Simulation-based DT

new findings. The resulting feedback loop and simulation-assisted exploration of What-If analysis allows decision-makers to anticipate the impact of potential changes or disruptions on the supply chain, which guides iterative improvement of simulation models and hence DTs overall.

Another API is set up to incorporate the results of various simulation runs and experiments into the DTs functional components, e.g. circulating inventory, resource consumption, and emission data. Specifically, simulation results provide synthetic data to understand assumed relationships between machines, resources, and products, such as indicators and rules for circulating inventory, consumption, or emissions. For instance, the simulation may reveal correlations between production time, energy consumption, and peak electricity usage, which can be used to optimize the sheduling of brewing processes for sustainability. All results are merged with data retrieved by the DTs using a multi-connective data mapping assistant, ensuring a comprehensive and up-to-date representation of the system.

3.3.3 Decision Support and User Interface

Enriched with synthetic data, DTs will provide a rich backend for decision support systems of various individual stages along supply chains. In order to offer options designed to detect patterns, predict future trends, and provide actionable insights to support data-driven decision-making. The decision support is realized via a User Interface (UI), as illustrated in Figure 2, and enables stakeholders to access decision-specific elements.

The emerging decision support capabilities of DTs are propelled by enabling synoptic comparison of results after processing the vast amounts of data generated by simulation models and integrated data sources. It also has to be able to visualize the wealth of information generated within a DT. Adapted to the use cases and needs of different applications or roles within the beverage industry, the UI serves as a hub for user access to DT functional components.

4 Discussion and Outlook

The proposed architecture offers a robust framework for integrating diverse data sources, ontologies, and supporting the creation of a comprehensive DT. By incorporating simulation models, data mapping, and user interfaces, this architecture supports the gradual development of DTs, promoting data-driven decision-making and process optimization in the BeverGreen project and the broader beverage industry.

The modular nature of the architecture, with its microservices-based data integration and flexible simulation modeling approach, allows for adaptation to different supply chain structures and sustainability challenges beyond the beverage sector. Adapting and enhancing the architecture to industry-specific data sources, simulation models, and key performance indicators (KPIs) provides a tailored solution that supports sustainable development across sectors.

The simulation component is pivotal in developing and continuously improving DTs by enabling organizations to explore various scenarios, test optimization strategies, and make informed decisions to enhance sustainability performance. The seamless integration of simulation models allows for the continuous refinement of the virtual representation based on real-world feedback, making it an increasingly powerful tool for driving sustainable innovation and decision-making as it evolves and incorporates new data sources and simulation results.

Based on the current state of understanding, the following procedure includes modeling production chains and logistics within the beverage industry at the meta and process level as a basis for running simulations. In this particular process, we address the connection between models to describe the supply chain comprehensively and to tackle overall aims in terms of emissions, circulating inventory, and resource consumption further.

However, the proposed architecture faces obstacles in ensuring data security when integrating sources from multiple partners along the supply chain. This requires careful consideration of specialized solutions and robust security management, where various techniques have been suggested to solve existing challenges with technological or security management measures and procedures to overcome these hurdles. Our project team will consider the framework's scalability and generalizability to other industries and supply chain structures. It may require further investigation and validation to ensure its effectiveness in supporting adequate data security.

As the BeverGreen project progresses and demonstrates the value of simulation-based GDTs in driving sustainable development, it will serve as a blueprint for other industries seeking to harness the power of digital technologies to optimize their operations and reduce environmental impact. By sharing best practices, lessons learned, and the technical architecture developed within the project, we aim to accelerate the adoption of DTs including GDTs across various sectors, moving closer to Industry 5.0 and sustainable production.

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