How to Leverage Digital Twin for System Design?

Jean-Sébastien Sottet[1][a], Pierre Brimont[1][b], Cedric Pruski[1][c] and Faima Abbasi[1,2][d]
[1]*Luxembourg Institute of Science and Technology, Esch-sur-Alzette, Luxembourg*
[2]*University of Luxembourg, Luxembourg*
{firstname.lastname}@list.lu

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Abstract: Digital Twins (DT) are deeply rooted in digital simulation environments. Today, they are still considered data-driven constructs aimed at supporting simulation, optimization, prediction on a physical system. However, data alone may not completely describe a system. This necessitates additional knowledge, encapsulated within models, which forms the foundation of the Model-Driven Digital Twins (MDDT) paradigm. At the start of a DT life-cycle, or when dealing with a system under construction, models becomes the primary artifact enabling the DT due to the lack of available data. This paper explores the advantages of simultaneously engaging in model-driven system design while preparing its corresponding DT. Using a real-world case study focused on developing a hydrogen valley, we demonstrate the substantial benefits of integrating models at the earliest stages of the DT's design and implementation process. This covers preparing data collection and sensors, and incorporating human knowledge throughout the system lifecycle, enhancing replicability.

1 INTRODUCTION

The term Digital Twin (DT) first emerged from the manufacturing industry in the early 2000 as a digital replicate (i.e., a twin) of a production line or a product. If the notions behind Digital Twin are anchored in the early digital simulation environments, it has only been recently formalized by the original claimed authors of the DT definition (Grieves and Vickers, 2017). DT aims at supporting any simulation (Boschert and Rosen, 2016; Zhang et al., 2022) or prospective scenario, such as predictive maintenance (Liu et al., 2018; Feng et al., 2023), in a digital world. According to (Grieves and Vickers, 2017), a DT is composed of three major elements: (i) a physical entity of the real world, (ii) its counterpart in the virtual world (the twin) and (iii) a bidirectional data exchange connecting those two worlds. In practice, it is hard to achieve this pure bidirectional exchange, and most of the advanced works only consider the realization of a digital shadow. A digital shadow (Becker et al., 2021) is a digital replica of the physical system with few or even no possible feedback actions on the physical system. Ideally, DTs aim at being the exact replica of the physical entity: each action on the physical system is reproduced on the DT. In practice, DTs serve as close approximations of reality (Abdoune et al., 2021), as they are often limited by an incomplete understanding of the system and its context, unforeseen changes, or the absence of high-quality data, among other factors.

Digital Twins are often perceived as entities built exclusively from data, predominantly sourced from sensors. This data, consisting of various measurements taken from the physical system, is aggregated to form the DT, as discussed in works such as (Friederich et al., 2022). Consequently, most existing technological infrastructures, including platforms like FiWare (Foundation,) and Azur DT (Microsoft, 2022), are designed with a strong emphasis on sensors and data management. Those are complemented with machine-learning models for representing the behavior of the system itself, nurtured from the aforementioned data.

However, besides data, models describing the system conveys significant knowledge that is often neglected (Kirchhof et al., 2020; Bibow et al., 2020; Sottet and Pruski, 2023; Sottet et al., 2022).

These models are particularly crucial during the early phases of designing a digital twin because:

- They offer critical system information when data is unavailable, insufficient, or of poor quality,

[a] https://orcid.org/0000-0002-3071-6371
[b] https://orcid.org/0000-0002-0730-7190
[c] https://orcid.org/0000-0002-2103-0431
[d] https://orcid.org/0009-0001-7484-9256

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serving as a foundation for initial design decisions and simulations.

- They assist in defining the boundaries, objectives, and functions of the digital twin, ensuring alignment with the intended real-world counterpart.
- They provide a structured framework for organizing and planning the data collection process, identifying key parameters and sources that need to be monitored.
- They facilitate stakeholder collaboration by allowing experts to contribute their knowledge and perspectives, fostering consensus and reducing misunderstandings through shared viewpoints.
- They enable early prototyping and scenario testing, allowing designers to explore potential configurations, identify risks, and evaluate feasibility before committing resources to implementation.
- They act as a communication tool, translating complex system dynamics into comprehensible representations for diverse teams, including technical and non-technical stakeholders.
- They help anticipate future challenges by integrating predictive elements into the design, allowing for a smoother transition to dynamic and adaptive digital twin systems.

In this paper, we argue that Model-Driven Digital Twins (MDDTs) can effectively support the system throughout its entire lifecycle, including the early design phases where traditional data-driven digital twins fall short due to the unavailability of data at the design stage (Friederich et al., 2022). The selected case, consisting in the development of a hydrogen valley in Luxembourg[1], presents a compelling example: since the system is not yet developed, we cannot rely on existing data. Taking this into account, we hypothesize that co-designing the system and its DT, with alignment across the entire lifecycle of both the physical system and its twin starting from the earliest design phases, leads to enhanced consistency, efficiency, and long-term adaptability in Digital Twin implementations. We aim at covering a subset of the different system concerns, encompassing both technological core and environmental, economic, and human aspects. We consider the current system as an open world (system borders in evolution) and not yet operating in runtime mode.

We further propose that this model-driven co-design approach not only ensures alignment between the system and its Digital Twin but also creates opportunities for seamlessly transferring and replicating the methodology across diverse applications and domains.

We propose to develop and illustrate our hypothesis through the creation of a new system and its digital twin: towards a hydrogen value chain in Luxembourg.

The paper is organized as follows: Section 2 introduced our illustrative case study based on a large exploratory project of hydrogen value chain. Section 3 proposes an approach to co-design the system and the twin in our exploratory context. Section 4 discusses the support of MDDT during the system lifecycle (exploitation, evolution, transfer).

2 ILLUSTRATIVE CASE STUDY: HYDROGEN VALUE CHAIN

The complete production and exploitation of hydrogen is a complex task pertaining to many domains: industry, mobility, housing, etc. The relevance and sustainability of hydrogen as a source of energy is currently under study and requires understanding the overall impact (from initial energy provision to market sells).

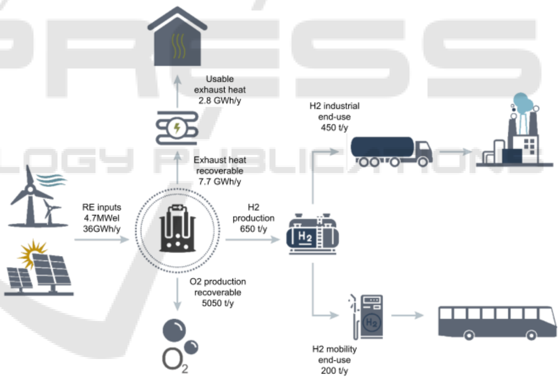

Figure 1: Hydrogen value chain.

The objective of LuxHyVal (see Figure 1) is to evaluate a complete value chain of hydrogen from production to consummation (motivated by the reduction of CO_2 production). The value chain encompasses the following aspects:

- The hydrogen produced will be used both for mobility purposes (e.g. hydrogen fuelling stations) and as an energy source for industry.
- Existing, or short to medium term planned infrastructure green energy production (Windmills and solar panels, on the left-hand side of Figure 1), H_2 pipelines or transportation network.
- Reusing generated heat locally, for, e.g., residential heating or industrial use.

[1]LuxHyVal see: https://www.luxhyval.eu/

To evaluate the optimal implementation of such a value chain, a DT approach is proposed. This DT enables the analysis of various design alternatives and what-if scenarios, providing valuable insights. Furthermore, the DT can be leveraged for scaling up the solution and replicating the hydrogen valley concept across other sites.

The novelty of our approach is to consider the DT from the start of the design of the system and its value chain. When the system and value chain are not (fully) established, and no data is currently available. Therefore, it is necessary to make assumptions about how the value chain will operate and the potential scenarios that may arise. The co-design of the system (system + value chain) and the DT, will rely more on expertise and knowledge about the expected operations than on real-time data collection. This involves various domain experts (e.g., policymakers, mobility specialists, energy producers, public transportation managers, etc.) not only in the system design phase itself but also simultaneously in the design of its Digital Twin. This co-design process can be seen as a virtuous cycle: each stakeholder will be committed to the DT and become deeply involved in its development, enhancing its accuracy and, consequently, the quality of the services it will provide. This approach requires expertise from various domains, notably encompassing models from high-level socio-economic view (e.g, economical viability of the value chain) to very technical issue solving (e.g., how to exploit the green energy production peaks).

One approach is to implement a robust federation of models (Golra et al., 2016), ensuring that the different models are properly interconnected. Model federation provides several key advantages. First, it enables the integration of diverse domain-specific models, allowing each to retain its own structure and semantics while contributing to a unified representation of the system. This approach reduces the need for extensive re-engineering or restructuring of individual models, preserving domain expertise and ensuring scalability. Second, federating models supports modularity, making it easier to update or replace specific components without disrupting the entire system. Third, a federation of models promotes collaboration among stakeholders by providing a shared framework where different disciplines can contribute their models while maintaining control over their specific areas.

Co-designing the system and its twin enables optimizing the value chain's operation, planning future investments, and enhancing both professional and public understanding of its benefits. Ultimately, a similar approach could be used for preparing the transfer of local experience to larger initiatives and in different countries.

3 DESIGNING MDDT FOR EXPLORATORY SYSTEMS

In this section, we describe the envisioned design approach of an MDDT in our specific context. We propose a progressive design of system models from requirement up to detailed specification and execution on a given DT platform. This is represented in Figure 2, by first establishing requirement models, then deriving an architecture that is progressively refined (and made executable) to the full system architecture reunifying non-functional and functional requirements.

Those design models will be the core of the MDDT. Our stance is to blur the distinction between the DT and design models; In line with (Wagg et al., 2020), the primary goal is to leverage these models to establish an operational Digital Twin from the outset, even when minimal or no data is available. The models in the MDDT can be used at the run-time (Bordeleau et al., 2020) both for simulation (including early simulation during the design phase) and monitoring. The other goal is to ensure that the design models retain comprehensive information about the system once it is operational. It also preserves the design rationale within the MDDT and prevents unwanted behavior. Due to this strong interconnection between the system and the twin through design models, one additional step (see Figure 2 DT support infrastructure) consists in designing the support infrastructure for data collection connected to the DT.

3.1 Early System Design: Identifying the Stakeholders and High Level Architectural View

In the context of the Hydrogen valley, building the corresponding DT starts by identifying all the key players involved and the limits of the considered system. In our case, for example, we are not considering the private hydrogen cars due to very low market penetration. Our approach consists in providing a high level architectural views including the actors and their roles, the value chain (value modelling), the goal and principles and high level (business) services. Subsequently, we also consider the main services or technical components to be developed (or existing one to be adapted, like public transportation migration to hydrogen). This first architectural description is a composition of different viewpoints inspired by Enterprise Architecture (e.g., (Greefhorst et al., 2011)) on one side and Manufacturing / System Architecture (e.g., (Benkamoun et al., 2014)) on the other side. The context in which the system is developed, notably all the related elements, must be considered as well. Ideally, the context, should be identified to provide insights into how the system could operate in practice within its environment. As no data can be inferred from a non-operational system, relying on model-driven approaches is paramount.

3.2 Executable Model Architecture

Exploring and assessing the hydrogen value chain is one of the core question of hydrogen implementation. Ideally, we should evaluate the potential development of hydrogen before the system is put into production. This preliminary phase must address numerous uncertainties, as there is limited exploitable data to confirm that a green hydrogen power plant could effectively integrate into our specific context. As a result, we adopt a design approach that is progressively refined through models that can be executed and/or simulate the system's behavior early in the design phase (Dahmann et al., 2017). This approach necessitates understanding external context elements that could impact the system, such as meteorology, market demand, urban development, etc. Additionally, we must manage design-time uncertainty (Famelis and Chechik, 2019) by making assumptions about system content and behavior, using partial models to handle these uncertainties (Bandyszak et al., 2021). In our case study, we can integrate the early design of the hydrogen production system, incorporating estimations with error margins, with projected future demand for public transportation to calibrate the plant size and required input energy. Additionally, by providing information about typical weather patterns for specific times of the year, we can ensure that green energy production aligns with demand, optimizing the system's efficiency and reliability.

At this stage, we only have models representing the system, but we can simulate scenarios close to "what if" analyses typically performed by a digital twin. The goal of this proto-digital twin (i.e., the system is not yet in fully running) is to experiment and quickly identify problematic designs ("fail fast") while exploring alternative designs before the system is implemented. This proactive approach allows us to refine and optimize the system's design, reducing the risk of costly adjustments after deployment.

3.3 System Architecture and Deployment

In the traditional modelling approach (Roques, 2016), the last layer consists in preparing the deployment of the system on its targeted platform (see Figure 2 Full System Architecture). It integrates both non-functional (hardware/software support) and functional requirements, offering a comprehensive and detailed architecture. This includes the intricate design of each system component.

3.4 Preparing Support for Digital Twining

Beyond this traditional design approach, we can already prepare the Digital Twin. The data to be collected, particularly the data needed to enable the DT for its intended purposes (e.g., predictive maintenance, value optimization, etc.), can be directly associated with specific model components. Similarly, the operations to be performed back on the system (e.g., actuators) can be directly connected to model elements (see lower layer of Figure 2). In terms of implementation of such a support, we can rely on the MontiThing approach (Kirchhof et al., 2021) that annotates the architectural models with the data to be collected by IoT sensors and action to be performed thanks to actuators. We can extend this approach to non-IoT data sources (any system log, external observation, databases for contextual data, etc.).

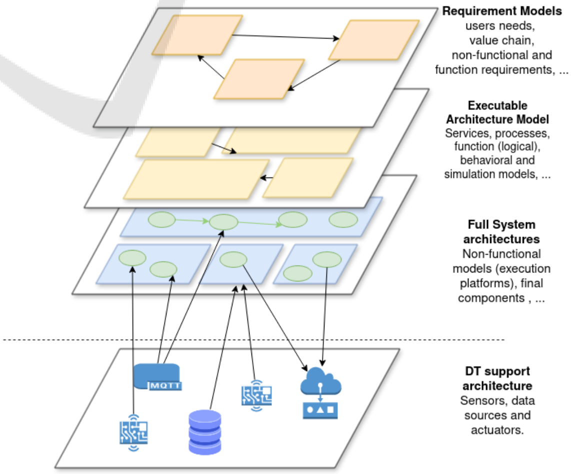

Figure 2: Design layers of Model-Driven Digital Twin.

4 MDDT DURING SYSTEM LIFECYCLE

In this section, we describe how the MDDT and the system are co-evolving together beyond the design phase. The overall lifecycle is given in Figure 3. It shows the successive steps starting from the design phase (see Section 3) to the operationalization and enhancement of the system. We did not mention the decommissioning and recycling of the system, which is currently out of the scope of our study. The typical process is organized as follows: the two first step **Require** and **Model** in Figure 3 corresponds to the first modelling layer of Figure 2. The **Execute** phase, uses the executable or simulated models. The two middle layers in Figure 2 are used in order to explore design choices and evaluate the system before it is in production. A system and its DT support are deployed at the beginning of the **Align** step of Figure 3. This step allows for a progressive alignment of the MDDT to the system, keeping it up to date according to integration of operational data. Finally, the **Exploit** phase takes place when the MDDT reaches an acceptable level of fidelity to the system in operation: this level can be related to a margin of error in the frame of the sensor's known errors margin.

When it reached this level of maturity, the MDDT can deliver its different services: monitoring, prediction, enhancement of the system, etc. After that, it is possible to enter a new cycle, by extending the system (**Extend** phase in Figure 3) or to **Export** the system in another context (e.g., another country with other electricity production profile). In our approach, the extension is systemically made under a modelling approach (i.e., **Model** phase). In the following subsections, we will focus on the phase that occurs after the design: DT alignment and exploitation/operationalization, extension and transferability.

4.1 Alignment and Exploitation

Once we have reached a first deployment of the system, we can officially talk about Digital twin: but the design models of the previous phases should already behave as close as possible to a real DT. In practice, it will be necessary to refactor the DT models (keeping in mind that the system may only be partially operational), some model flexibility (Sottet and Biri, 2016) will be necessary to ensure that both the DT and the physical system could operate together at any time, even if they are not fully aligned. The **Align** phase will consist in a progressive convergence of the twin and the system based on the feedback from sensed data. It will consist in analyzing the drifts (David and Bork, 2023) that could occur between system and data. The drift can show some valid discrepancy (i.e., the MDDT is not aligned with the system) or invalid due to a sensor defect (Abbasi et al., 2024).

In the **Exploit** phase, the MDDT could monitor the system according to data collection support connected to its models. The MDDT relies largely on models at run time, the models being the representation of the run-time events, keeping an image of the state of the system. The complete usefulness of MDDT as a decision-support tool could occur once this stage is reached: notably providing realistic simulation of potential future event (what if scenario), prediction of error, optimization of the system, etc.

Ultimately, this progressive alignment all along the exploitation will hopefully enhance the accuracy of the MDDT models. but could also foster for a hybrid approach of model-driven and data-driven, e.g., by replacing a function by a learned model (Sottet et al., 2022).

4.2 Extending the System

Once the system and the MDDT are aligned, after one or more iteration(s) of the previous cycle, the system can be expanded (represented in Figure 3 with progressive extensions of considered system in the center of the cycles). In our example, we first design the Hydrogen production (without considering green energy) and try to assess the quantity for the direct consumers (public transportation, factories) as well as the potential return on investment. This first cycle is representative of the initial design of a MDDT along its system. As represented in blue in Figure 3, the two first steps are purely models (see Section 3) then the systems and the MDDT are co-existing and co-evolving in the green part.

We can extend the initial hydrogen producer-consumer, in a second cycle (middle of Figure 3), with the indirect beneficiary of the Hydrogen production (public heating network and recoverable O_2 production); and similarly evaluate the global value and return on investment. This cycle is completely green, meaning that from that point on, MDDT and the system are co-existing. Nevertheless, during the **Model** and **Execute** phases, the MDDT works in a hybrid mode: one part is aligned with the current system and the other part is under study (similar to design phase). We then have to rely on the models to assess if the system is sustainable (i.e., from business to technical perspectives) and for its implementation.

Finally, as illustrated in Figure 3, the final visible cycle involves integrating green energy production to evaluate whether the demand can be met with the current energy output. This step also includes planning for future installations of photovoltaic fields and windmills to ensure sustainable energy supply. This last case illustrates a different hybrid approach, as the country already has existing photovoltaic panels and windmills. Here, since the extension infrastructure is already in place, the objective is to derive and integrate models of the existing green energy production system. The way the system is extended, is indeed a co-evolution between the system and the MDDT, like in the Mertens et al. approach (Mertens and Denil, 2023): we ensure a continuum between design and operation of the system.

4.3 MDDT for System Transferability

The LuxHyVal tends to be an experimental and feasibility prototype that aims at being transferred to different countries. Modelling the context under which our system behaves is key. In the project, it is important to have some entry points in external factors (and related data sources) that influences the Hydrogen marker like e.g., transportation need/demand, public subventions, size of industry that could work with hydrogen, etc. Such contextual models should appear in the early modelling phase. The internal elements should also be adapted to the target country (e.g., availability of green energy production). The context model of the new country (e.g., local energy production) will be used to project the prototype in a different set-up. For instance, the market penetration of Hydrogen will be less if the country has no plan to facilitate the conversation of transportation into hydrogen. Finally, the proposed MDDT can be used as a decision-making system at a high level of management: country deciders, policymakers, etc.

As summary, our idea is to be able to use the MDDT as the simulation environment to assess under which conditions the overall system could be transferred in a different context. To perform the transfer we can rely on the same approach, thanks to executable models, ideally refined after a first cycle of implementation.

5 CONCLUSION

We have proposed an approach to design and operationalize new systems relying on model-based approach to build both proto-digital twin (i.e., models of the system under design) and (real) digital twins. The goal of the proto-digital twin is to assist in the design of a not yet established system through its Digital Twin, even when the system is not completely established. It helps to design prospective cases, notably in our situation where the full value chain is not known a priori. It also helps to identify new concerns of interest that have indirect impact on the system. This approach facilitates the involvement of stakeholders, enabling the early capture of their knowledge that can be seamlessly integrated into the proto-digital twin. The proposed MDDT approach is blurring the distinction between design-time and run-time, on which the different stakeholder can play with like a real DT. The proposed approach mainly helps to:

- provide feedback on the system feasibility (i.e., value chain) as early as possible,
- prepare the data collection to directly feed the MDDT
- ensure the co-evolution and consistency of MDDT's models and the system.
- reduce the usual initial alignment effort between the system and the twin prior to the development of decision-support functions.
- support extensions of the system scope with a hybrid approach: a model representing an actual part of the system associated to a pure modeled part (i.e., proto-digital twin) corresponding to the extension.
- rely on context models to prepare the transfer of a similar system into a different context (i.e., a different country).
- operate the transfer based on a similar approach as MDDT extension.

This approach is a preliminary work, proposing a methodology to support our case study. Because of this, the next step of our work will focus on providing the landscape of models and languages to be used (e.g., value chain modelling, SysML, etc.). This will also comprise a deeper search on the models used to represent the context (i.e., the external influencing factors), notably understanding where to put the limit of such open-world DT. Then, we will design or select an execution language to operate the models. This will ensure that we can simulate, even at higher level of abstraction, the behavior of the overall hydrogen value chain. We will also provide a way to control the alignment between the MDDT and the system: providing analysis of the drift (Abbasi et al., 2024). It is important to understand if the system is in bad health (e.g., sensors malfunctions) or if the MDDT's models are no longer reflecting the system. Our ultimate goal is to be able to support the co-existence of the system and its design rational all along its lifecycle, supported by the operational notion of MDDT presented in this article.

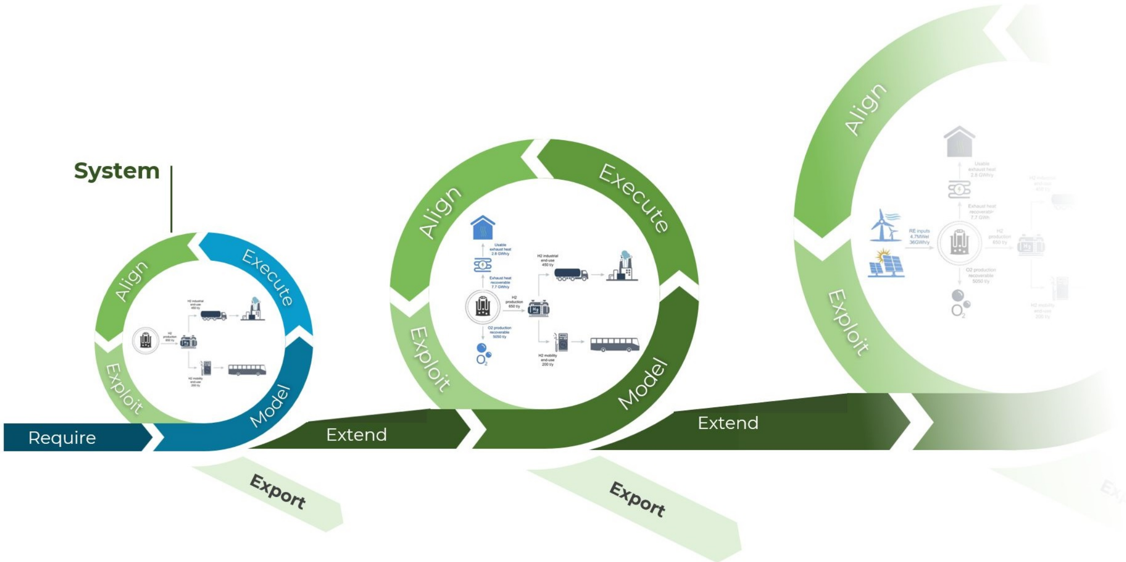

Figure 3: Design and operation cycles of MDDT.

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