Digital Twins for Cyber-Biophysical Systems: Challenges and Lessons Learned

Istvan David^{*}[®], Pascal Archambault^{*}, Quentin Wolak^{*}, Cong Vinh Vu^{*}, Timothé Lalonde[†], Kashif Riaz[†], Eugene Syriani^{*}[®], Houari Sahraoui^{*}[®] ^{*}DIRO, Université de Montréal, Canada – {firstname.lastname}@umontreal.ca [†]Ferme d'Hiver Technologies, Canada – {tlalonde,kriaz}@fermedhiver.ca

Abstract—Digital twinning is gaining popularity in domains outside of traditional engineered systems, including cyberphysical systems (CPS) with biological modalities, or cyberbiophysical systems (CBPS) in short. While digital twinning has well-established practices in CPS settings, it raises special challenges in the context of CBPS. In this paper, we identify such challenges and lessons learned through an industry case of a digital twin for CBPS in controlled environment agriculture.

Index Terms—controlled environment agriculture, industry, model-driven, report, simulation

I. INTRODUCTION

Digital twins are virtual representations of physical assets [1], mirroring their prevalent state with high fidelity. The tight coupling with its physical counterpart allows the digital twin to provide a proxy interface for advanced computeraided services, such as monitoring, predictive analytics, and automated decision-making. Digital twinning is especially popular in engineering domains where models of the underlying system are accessible or can be efficiently constructed, like cyber-physical systems (CPS) [2] and smart production assemblies [3]. Model-driven engineering (MDE) [4] is particularly well-positioned in this realm and provides digital twinning endeavors with mature techniques for the creation and management of heterogeneous models [5], [6], and using models at runtime [7], [8] to capture the prevalent state of the physical twin. Thanks to its beneficial properties that enable an overall higher digital maturity, digital twinning is gaining popularity in a wide array of domains, including cyber-physical systems with biological modalities, or cyberbiophysical systems (CBPS) in short. Pertinent examples of CBPS can be encountered in smart agriculture [9] and precision healthcare [10], where biotic (living) and abiotic (nonliving) components are integrated and operated in unison.

Due to their biotic components, CBPS are characterized by a high degree of uncertainty and stochastic attributes [11]. These traits substantially limit the understandability and modeling of CBPS and coupled with the lack of clear guidelines, render the digital twinning of CBPS exceedingly more challenging than the digital twinning of traditional CPS.

To help the MDE community mitigate the risk of their prospective biophysical digital twinning endeavors, we report our experiences from an ongoing industry collaboration, outlining challenges and lessons learned from a computer scientist's point of view. Our work is situated within a specific case of Controlled Environment Agriculture (CEA) [12]. CEA is the technique of growing crops in an isolated and artificially controlled environment. Controlled environments allow for better planning and execution of the growth strategy, substantially reducing the associated risks, costs, and waste. Digital twinning has become a technique of particular interest in CEA for the optimal control of the environment.

The main contribution of this paper is the list of challenges and lessons learned from a project on the digital twinning of an industry-scale CBPS. Through the specific case of CEA, we ground our findings in real requirements. Nevertheless, our observations can be extended to the broader domain of CBPS.

II. BACKGROUND

In this section, we present some background concepts, the partner organization, and the twinned system.

A. Digital Twins

The goal of the digital twin is to allow reasoning about the prevalent state of the physical twin without having to observe or query it directly. In essence, the digital twin is a proxy for digital services to the physical twin. Examples of such digital services include visualization and monitoring, decision support for human stakeholders, and automated control and re-configuration of the system.

At the core of a digital twin, models of the physical twin keep track of its prevalent state [13]. These models are maintained by the continuous processing of real-time sensor data originating from the physical twin and constitute the foundations of the services provided by the digital twin.

Such services are often enabled by simulators [14]. Simulators are programs that encode a probabilistic mechanism on a computer and enact its changes over a sufficiently long period of time [15]. In this paper, we present a digital twin with advanced simulation aspects that supports the decision-making process of domain experts through quantitative and qualitative what-if analyses and real-time predictive capabilities.

The control of the physical twin is achieved in an automated fashion through the actuators of the system. However, some safety-critical settings, such as CEA, might limit the autonomy of the digital twin and prohibit automated actuation.

B. Partner organization

Ferme d'Hiver [16] (transl. "Winter Farm"), is a Montrealbased start-up targeting the production of off-season, highnutrition fruit, and vegetables by CEA techniques, without the use of chemical pesticides. The mission of Ferme d'Hiver is to improve the food autonomy of Canada, and within it, the province of Quebec. Food imports in Canada were reported to comprise about 8.2% of the total import merchandise [17] of CA\$614 billion [18] in 2021, amounting to CA\$53.63 billion. These figures, coupled with the steadily increasing population of Canada by over 300 000 annually since the 1960s, pose serious threats to the sustainability of Canadian food autonomy. Four-season climate challenges sustainable food autonomy as it prevents year-round open-air farming. This problem is vastly exacerbated in Quebec with dry cold Winters and humid hot Summers spanning an average temperature range of 40°C. CEA alleviates these problems through resourceand cost-efficient solutions to produce vegetables and fruit in a closed environment by artificial lighting and managed environmental conditions. In this context, Ferme d'Hiver aims to optimize the yield and energy consumption of its operations by integrating various cutting-edge technologies to automate its production system and by recovering the heat produced by vertical farming lights to heat adjacent greenhouses.

C. Controlled Environment Agriculture

Increasingly unpredictable environmental conditions challenge traditional agriculture. In four-season climate areas, temperature, precipitation, and sunlight differ significantly season by season. Large-scale disruptions, such as climate change and the steady growth of the global population further exacerbate this issue [19]. To address these challenges, CEA [12] isolates crops from natural environmental conditions throughout the plant development cycle. CEA constitutes a pertinent example of CBPS in which environmental conditions are controlled through highly configurable light, irrigation, and HVAC systems. To enable optimal growing conditions, expert domain knowledge is used to properly orchestrate these systems.

Thanks to automation, CEA achieves better yield and quality than traditional farming settings. Unfortunately, the improved output comes at the expense of higher energy consumption [20]. Consequently, the cost factors of CEA settings are sensitive to changes in the artificial environmental conditions and human control might easily result in disadvantageous configurations. Computer-aided support is in high demand, positioning CEA as a prime candidate for digital twinning.

CEA is chiefly associated with vertical farming, the agricultural practice of growing plants using often soilless platforms stacked vertically, with the purpose of reducing crop yield per unit area of land [21]. The vertical farming environment at Ferme d'Hiver is composed of 11 aisles, each split into two sections, with 22 walls of vertically stacked soilless containers for the plants. Each section has a dedicated lighting and irrigation system (defining a plantation zone) spanning its entire height that provides photosynthetically active radiation (PAR) to the canopy and meets its irrigation needs. The ventilation of the stacked plants is handled by a central HVAC system that condenses the water evaporated from plant canopies to be reused for irrigation purposes. The HVAC system is also connected to a system of vertical and horizontal plenums for uniform distribution of the conditioned air next to the plants.

D. CEA production room

The physical twin is the *production room* of Ferme d'Hiver. It is composed of physical and biological components.

Physical components. Physical components are organized by subsystems. The *lighting* subsystem is responsible for adapting the light conditions in the room and triggering photosynthesis in the plants. The *irrigation* subsystem is responsible for providing the plants with water and nutrients required for their growth. Plants are primarily irrigated by drip irrigation, where water is periodically dripped on the plant substrate through appropriately situated pipes, tubes, and valves. The *HVAC* subsystem ensures proper air temperature and humidity in the room as the lights, temperature, and humidity change.

Each subsystem provides a set of sensors and actuators which we use to support the interaction between the digital twin and the production room. The *lighting* system is equipped with sensors to measure the temperature of its LED components and photosynthetic photon flux density, a commonly used metric by biologists to quantify photosynthesis-related phenomena [22]. The irrigation system is equipped with sensors to measure the soil temperature, water content and electrical conductivity (EC), the irrigation solution (pH, electrical conductivity, flow rate), and the current capacity of the water storage tanks. The *HVAC* system is equipped with sensors to measure the temperature and flow rate of air flowing through the fans, and the liquids flowing through the pumps.

Biological components. The production room is populated with plants that are ready to produce the crop. The plants are grown in specially designed pots contained commercially available substrates (apprx. 1.5 liters/plant). About 50 000 plants are present in the production room at any point, mounting up to 3 tons of thermal mass, contributing substantial inertia to the system. The plant canopy in the room releases a significant amount of moisture into the air through the process of evapotranspiration [23]. Consequently, biological components have a measurable impact on the physical properties of the room, especially temperature and humidity.

The impact of the plant on the production room varies during the lifecycle of the plant. Along its production cycle, the plant goes through stages of vegetation (rooting and leaf development) and regeneration (flowering and fruiting). The conditions required to induce each stage as well as their length vary widely according to the plant cultivar and environmental conditions—light quality, light duration, and temperature and could be enforced by stressing the plant. These periods of stress affect the energy balance of the plant, as the plant may conserve the energy to produce fruits or release it to cool down. Inducing each stage through stressing the plant requires daily manual observation of the plant and the production room, and subsequent adjustments by agronomists and the farmers.

E. Motivation for digital twinning

The digital twinning of the production room is motivated by the complexity of control decisions that are not feasible without computer-aided means. While domain experts can rely on their expertise in smaller-scale operations, these efforts do not scale at the size of the production room.

Operative use cases of the digital twin focus on the optimization of production. One such optimization is the improvement of the yield-to-energy consumption ratio. In this case, the optimization objective is the maximization of the mass of produced crop and minimization of energy consumption by hardware elements. Another optimization scenario is concerned with the right timing of harvest. Producing and maintaining crop consumes energy from the plant. Optimally scheduled harvest maximizes the energy retention of the plant by relieving it from its produce. In support of a typical precision farming scenario, the digital twin is also used to stimulate plant growth at a pace that produces a predetermined amount of crop over a period of time. In our settings, 50 grams of strawberries need to be produced on a weekly basis throughout the production lifecycle. The precision demand of such a scenario vastly exceeds human reasoning capabilities.

Strategic use cases include technical decision-making support for improvements to the room and surrounding facilities. Based on an expected output of crop, the simulators of the digital twin will support engineers in dimensioning the equipment to be acquired for newly erected production rooms. To optimize the input and output factors of the overall supply chain the company is situated within, the digital twin will be used for what-if analyses to set quality gates for their plant suppliers. As a cross-cutting concern, in support of decisionmaking services, the digital twin is leveraged as a safe and economic proxy for the real environment in the training of AI agents. In such scenarios, large quantities of data can be generated, e.g., for deep learning purposes, or a continuous data stream can be generated, e.g., for reinforcement learning.

III. REQUIREMENTS FOR DIGITAL TWINS OF CBPS

Here, we elicit requirements for the digital twin to be developed. To contextualize the requirements and understand their relationships, we construct a conceptual reference framework and map requirements onto it, as shown in Fig. 1.

Conceptual reference framework

We obtained the framework by the case-based generalization approach of Wieringa and Daneva [24]. First, we analyzed the requirements that emerged in our project. Second, we decomposed the requirements architecturally. Third, we generalized the requirements to architecturally similar cases. Finally, we organized evidence by the conceptual reference framework. The framework provides the following components.

- **Production room:** The physical twin. It includes biological and physical entities, as well as human staff members who interact with the production room.
- **Physics and Biology models:** Responsible for capturing the prevalent state of physical and biological components.

Populated either by real-time data from the Production room or by the outputs of the simulators.

- **A, B:** Data stream from the physical and biological components of the production room, respectively.
- **Inferred:** The physical and biological models are partially populated by data from the production room (via A and B streams), and partially inferred, implementing a soft sensing functionality. Soft sensors are virtual sensors that provide a real-time sensing signal by accurate predictions [25] and by that, can serve as a cost-efficient replacement for more expensive hardware sensors.
- **C:** Information flow between the physical and biological models to support inference.
- **Physics simulator, Biology simulator:** Computer-aided reasoning machinery. They perform analysis based on the models and universal rules of physics and biology.
- **D**, **E**: Control and information flow from the simulators to their respective models.
- **GUI/API** User-facing endpoint. Graphical user interfaces (GUI) for human stakeholders and application programming interfaces (API) for computer-aided agents.

Actuation: Responsible for controlling the production room.

F, G: Information stream to the user-facing services used by humans, machines, and actuation services.

- H: User interactions with the system.
- **I:** Control feedback to the production room. It can be fully automated or can feature a human in the loop.
- A. Data and information gathering needs to be ensured (R1)

The ability to process real-time data is a distinguishing feature of digital twins. Real-time data stream processing requires specialized infrastructure that ensures low-latency data ingestion, persistence, and access. At the same time, such data infrastructures need to exhibit flexibility to allow for channeling data streams of newly deployed sensors to the digital twin. Commonly used solutions have been developed in Internet-of-Things (IoT) settings, e.g., under the Eclipse IoT umbrella project [26]. However, acquiring, operating, and maintaining advanced IoT frameworks may not be within reach for every organization with digital twinning ambitions. This is typical for companies with a core business in domains characterized by limited digital capabilities, such as agriculture. Such companies typically resort to vendor-specific solutions with limited flexibility and APIs, resulting in vertical siloes imposed by vendors, from sensors to end-user software. Siloed settings, in turn, hinder digital twinning efforts as they prevent easy integration of systems. A direct link to sensor data readings and reliable manual data collection procedures are crucial requirements for digital twinning.

Implications. Digital twins aiming to address instances of this requirement need to augment the **production room** with proper data capabilities and facilitate data links **A** and **B**.

B. Models and simulators need to be constructed (R2)

MDE helps manage the accidental complexity of the problem at hand by elevating the level of reasoning to higher levels



Fig. 1: Requirements (R1-R3) contextualized within the conceptual reference framework

of abstraction. Explicit modeling of the relevant aspect of the system allows for narrowing the cognitive gap between the problem and the expert's reasoning process. This is especially desirable in complex CBPS settings, such as CEA. Simulation makes use of these models for analysis and optimization.

However, modeling and simulation based techniques come at the cost of the increased complexity of developing models and simulators. Due to the inherent complexity of CBPS, one modeling formalism is not sufficient to capture every relevant aspect of the system. Techniques such as multi-paradigm modeling [6] and co-simulation [27] promote domain-specific modeling and simulation concerns, while distributed simulation [28] allows for reasoning on resource-constrained devices often present in IoT and edge infrastructures. However, their application requires coordination between models and simulators of different concepts, units, timescales, etc.

Implications. Digital twins aiming to address this requirement must employ advanced engineering techniques to deliver **models** and **simulators**, and their data links **C**, **D**, and **E**.

C. Actuation autonomy needs to be flexible (R3)

While one of the distinguishing features of a digital twin is the automated actuation of the production room, trust, and safety challenges limit this ability in digital twins of CBPS. Biological modalities of the production room are often artifacts of *living* organisms, e.g., plants, animals, or humans. In such cases, particular safety requirements apply which, in turn, often demand verifiable and provable safety guarantees from the system. In the absence of such guarantees, operators of the digital twin need to gain trust in the system by gradually giving it more actuation autonomy. During its lifecycle, the digital twin exhibits various levels of actuation autonomy, including human-actuated digital twin, followed by digital twin with human oversight, and finally, reaching full autonomy.

Implications. Digital twins aiming to address this challenge need to support various levels of **actuation** autonomy, along with its data links **G** and **I**. In particular, the data links need to account for the two extremes of the autonomy scale and produce (i) humanly comprehensible actuation instructions, and (ii) API-level instructions for actuation components.

IV. DEVELOPING A DIGITAL TWIN FOR CEA

Here, we discuss the digital twin we are developing for the vertical farming of strawberries in a controlled environment.

A. Approach

We approach the system subject to twinning as a cyberphysical system with biological modalities and maintain a systems engineer's point of view. MDE is central to the design and implementation of the digital twin. We rely on different modeling formalisms, make extensive use of model-based analysis and simulation, and generate code from models.

Following the principles of multi-paradigm modeling (MPM) [6], we model every relevant aspect of the system at the most appropriate level(s) of abstraction, using the most appropriate formalism(s). We use the Discrete Event System Specification (DEVS) formalism [29] to model the appliances in the room. DEVS is a compositional formalism that allows for hierarchically composed simulators, a trait that, in turn, allows for reasoning at different levels of abstraction. We use continuous biology formalisms to model the growth of the crop, captured via differential equations, implemented in Simulink's Causal Block Diagram language. Finally, we use continuous physics formalisms to model the energy balance between the previous two models, captured via differential equations and a solver in Matlab and Python.

We integrate these models by explicitly modeling the orchestration of simulators via DEVS. We use process models to describe the schedule of treatments the crop requires. We use state-of-the-art code generators as we operationalize Simulink and Matlab models as Functional Mockup Units (FMU). Each FMU contains a model and its solver, encoded as C executables with XML interfaces. Additional details on the simulators are available in previous work [30].

B. Real-time monitoring

A cohort of 50000 plants may produce multiple batches of fruits that are regularly harvested over time (13-28 weeks) and may be subjected to successive vegetative and regenerative growth and development processes. To schedule interactions such as treatments and harvesting—experts need to access aggregated information about the plants. In addition, Ferme d'Hiver has multiple geographically distanced sites that require coordinated oversight. Real-time monitoring provides experts with the ability to observe the production room and make better and faster decisions.

As shown in Fig. 2a, the requirement of real-time monitoring necessitates establishing a direct data link with the production room (A and B), and the *physics* and *biology*



Fig. 2: Digital twinning concerns as instances of the conceptual framework

models to be readily available to persist sensor data in an intermediate model from which the GUI is populated (F). The physics model captures the prevalent state of the physical environment, i.e., the production room. Similarly, the biology model captures the prevalent state of the plants in the production room. From a multiplicity point of view, the solitary biology model represents all the plants in the production room in an aggregated view. Both models follow runtime model principles [31], i.e., they are designed with the intent to be able to handle frequent updates. In monitoring scenarios, the physics model is updated continuously with real-time sensor data from the production room, and the *biology model* is updated by manually gathered data. Manual data collection includes non-destructive measurements, e.g., counting individual organs (e.g., leaves, stems), and destructive measurements, e.g., measuring root length, root density, or the weight of individual organs and their chemical concentrations.

C. Real-time inference

The *physics* and *biology models* allow for inferring metrics that might not be directly observable. These metrics often carry crucial information for domain experts and help formulate appropriate intervention strategies. For example, an agronomy expert might want to reason about the physiological properties of the plant by assessing how much water is currently absorbed by the plants. However, there are no sensors to directly measure this metric at the facility. In a closed environment agriculture setting, the amount of water in the environment is practically constant and most of its states can be measured by physical sensors. Real-time inference provides experts the ability to enrich their reasoning process with information that would be infeasible to directly observe.

Architecturally, this service is identical to *Real-time monitoring* (Fig. 2a), but in addition, it makes use of *inferred* values in the *physics* and *biology models*. The data link between the production room and the runtime models (A and B) is still the primary source of information, but performant inplace analyses provide additional inferred information. This mechanism is known as soft sensing [25]. The inference is carried out over the overall biophysical model, necessitating information flow between the two models (C).

D. What-if analysis

Ferme d'Hiver aims to optimize the yield (kilograms of crop produced) and the energy consumption of its operations (kilowatt-hours of electricity consumed). Both metrics are evaluated over the 13-week production cycle. However, experts have to make decisions about the configuration frequently and from the beginning of the production cycle. Here, a configuration means the entirety of the settings of each actuator. Due to the lack of predictive models, experts have to rely on heuristics when choosing configurations. Previous experience is used as the starting point to find the approximate configurations for the given production cycle. Additionally, the agronomy expert might carry out small-scale trial-and-error experiments, which refine their knowledge about the effect of specific settings on crop yield. Finally, the yield is assessed on a weekly basis to evaluate the progress of the production cycle. What-if analysis provides capabilities to predict the values of yield and energy consumption based on the settings of the equipment provided by the experts. Additionally, it provides experts with interfaces for experimenting with input configurations and output values.

As shown in Fig. 2b, this service does not require direct input from the production room. However, it requires the appropriate simulators to carry out what-if simulations. The *physics simulator* is tasked with, e.g., calculating energy consumption. The *biology simulator* is tasked with, e.g., calculating the crop yield. The simulators use the same models that are used in *Real-time monitoring* and *Real-time inference* to capture direct and inferred data from the production room. However, instead of real-time data, models are populated by synthetic values from the simulators (D and E), based on the simulation scenario specified by the expert (H). Two simulation components are used to calculate various metrics of physical and biological nature.

E. Environment for training AI/ML agents

Exact solutions are intractable in CBPS due to their vast complexity. Machine learning (ML) techniques can alleviate the problems of manually designing models [32]. Specifically, in CEA, ML techniques can be used to infer patterns of the complex underlying heterogeneous systems and automate the recognition of optimal configurations in specific situations in the production room. However, these techniques require vast amounts of data, which is often not feasible to collect from the real system, e.g., due to various functional and extra-functional considerations, such as the efficiency of data collection sourced from biotic components, and safety of concerns of biotic components (here, the crop) during data collection. In CBPS, the impact of stimuli takes a substantially longer time to manifest, rendering real-time data collection ineffective. Furthermore, biological entities impose higher safety standards. Digital twins are prime candidates to establish safe ML environments thanks to their ability to generate training data and automatically label it [33], [34].

Architecturally, this service is identical to that of *What-if analysis* (Fig. 2b). The main difference is the end-point of information stream F. While in *What-if analysis*, the end-point is a user interface for the human stakeholder, in *AI/ML agent training*, the end-point is an API for the learning agent. Depending on the machine learning approach, the API needs to support different interaction protocols. For example, deep learning [35] scenarios require vast amounts of data generated in one batch for off-line processing, while reinforcement learning [36] requires smaller amounts of data generated in an interactive fashion. The success of this service relies on the proper calibration of the digital twin and its ability to act as a virtual experimental device [37].

F. Configuration space exploration

As explained in What-if analysis, our aim is to optimize the yield and the energy consumption of its operations. During the day-to-day operation, the room is configured by the agronomy expert and the engineer, concerned with yield and energy consumption, respectively. Both experts make configuration decisions that aim to generate the most optimal outcome for their purposes. In a number of negotiation steps, the agronomy expert and the engineer agree on a configuration that is acceptable for yield production and is feasible with the current equipment. However, assessing the optimality of their choices is not feasible as neither expert has a complete view of the overall CBPS. It is the union of the two views that provides a holistic image of the production room. During the negotiation, the experts explore the space of configurations in a joint effort, while optimizing for their own goals. A joint effort is required because the two metrics are strongly interleaved. While a higher amount of yield generates a higher amount of revenue, it also consumes more energy. Additionally, plants have an optimal level of yield. While forcing the plant to produce more crop is possible, it will cost more energy and reduce the energy efficiency of the plant. Thus, optimal configurations must find a trade-off between high yield and low energy consumption.

This requirement makes use of the overall architecture, as shown in Fig. 2c. An exhaustive search for the best possible configuration is not feasible due to the large number of combinations the experts can choose from when configuring the production room. Therefore, an intelligent search approach is required. For this purpose, we rely on design space exploration (DSE) [38]. In a DSE approach, an underlying design is modified in a sequence of steps, and in each step, the newly obtained design is evaluated with respect to a set of metrics. The design space is the closed set of every possible variation of the original design that can be reached from the original design by applying a sequence of the permitted change operations. In our case, the design is the configuration of the room; thus, we refer to this approach as configuration space exploration. Change operations capture the actions of the experts, e.g., increasing the temperature of the room by 1°C, turning the fans of the HVAC to 100%, extending the duration of a day, or increasing the light intensity. Although the search space is theoretically infinite, agronomy experts and engineers can prune the search space by setting reasonable metric boundaries for the room and plants. The exploration process is guided by heuristics to converge to optimal solutions rapidly. We implemented the typical DSE heuristics in our digital twin, including hill climbing, simulated annealing, depth-first, and breadth-first search. The search is governed by one or more objective functions. In our case, at least two objective functions are considered. The first objective is always minimizing energy consumption. The other objectives aim at maximizing crop yield and differ depending on the plant growth phase.

V. CHALLENGES IN DIGITAL TWINNING OF CBPS

In this section, we elaborate on the challenges we faced during our project.

Unique influencing factors

We identified a set of factors characteristic of BPS that gave rise to the challenges we faced. The notion of system *state* is hard to characterize in CBPS due to the exclusively continuous nature of biological systems. Although discretization is still possible, it comes at the cost of elevated information loss as compared to traditional physical or cyber-physical systems. *Causal relationships* are challenging to identify in CBPS due to the limited understanding of biological entities. Finally, *time scales* significantly differ from those in physical engineering settings. Observing the effects of a particular treatment is hardly ever instantaneous as effects might take weeks to manifest. This exacerbates the challenge of establishing causal relationships and limits the applicability of traditional, causal modeling formalisms, such as Simulink [39] and DEVS [29].

A. Data and information gathering needs to be ensured (R1)

Challenge 1: Data is a critical enabler for both design and operation. The construction of digital twins, especially their simulation models requires readily available historical data. This is especially crucial in the calibration phase of simulators. We faced substantial challenges in this regard, especially because of the lack of systematic data collection methods, which is expected in companies in less digitalized domains, such as agriculture. As for the operation, all but one service (with the exception of *AI/ML agent training*) rely on data emerging from the production room.

We recommend making it a priority to obtain data of acceptable quality at the onset of the project to accelerate the development of digital twins. Ensuring data early on helps avoid the pitfalls of uncalibrated digital twins.

Challenge 2: Automated data collection runs through siloed subsystems. The sensors are part of larger, vendorspecific vertical silos, including a building automation and control (BAC) system, and a plant physiology support system. Both systems define end-to-end vertical solutions from hardware to user-facing functionality. However, they do not provide APIs for integration scenarios. To provide a bettermanaged interface for data-intensive services a central data repository was deployed on the premises prior to our project. Due to vendor-imposed constraints, sensor readings are carried out in the order of minutes, which results in substantially fewer readings compared to traditional CPS settings.

We recommend advocating for open APIs and relying on IoT frameworks that provide flexible foundations for many digital twinning scenarios, such as Eclipse Ditto [40]. In many cases, vertically integrated siloes are developed by high-tech suppliers who can open up their APIs.

Challenge 3: Large amount of data is collected manually. Manually collected data leads to an error-prone and costly process that is also slow, especially compared to sensor readings. Manually collected physiological data of plants includes metrics such as yield, plant size, flower color, and traces of diseases. In our setting, staff members collect observations in digital sheets, which are subsequently uploaded to the system in a batch fashion. While the quality and quantity of data are not comparable to those in traditional CPS, the slower rate of change of plants permits a slower data gathering process. Such practices align well with grower companies that might not have advanced data governance in place.

We found success in maintaining a consultant's point of view and advocating for accelerator technologies with high return-on-investment, such as computer vision. The digital evolution of Ferme d'Hiver has resulted in gradually increasing automation in collecting physiological data.

Challenge 4: Intrusive and destructive measurements are unavoidable. Testing the properties of plants is often achieved by intrusive measurements and destructive procedures that are irreversible. For example, measuring the root length of plants is achieved by removing the plant from the soil and measuring its longest root, while measuring the weight of the various plant organs requires the plant's dissection.

As the plant is turned to waste, it cannot be used for longitudinal measurements in which long-term treatment-effect relationships are investigated. In effect, testing properties that require destructive measurements, inhibits testing properties that require longitudinal measurements. In addition, there are ethical concerns when working with biological entities [41], although this is less of a concern in the case of plants.

We recommend avoiding destructive measurements as much as possible and relying on inferred properties and meaningful approximations instead of directly observing them. For example, in our project, the water level of a plant is approximated and calculated from the overall amount of water in the system and measurable water levels. The reliability of such approximations needs to be verified before using them in critical optimization and control scenarios.

Challenge 5: Interference with operation creates noise. Human staff is in frequent interactions with the physical twin. The impact of these interactions on the system ranges from negligible (i.e., safe to omit in the model) to severe (i.e., might render models invalid unless explicitly represented in the models). We consider activities, such as measurement and regular oversight negligible interference. However, typical to CEA settings, the biotic subsystem is continuously modified as ripe strawberries need to be harvested.

We recommend integration with planning systems at partner companies that contain information about the work schedules of staff and planned interactions to be factored into simulations. However, acquiring such data might be problematic from accuracy, confidentiality, and legal points of view. In the lack of such data, simulators might have to be calibrated on data that inherently features noise.

B. Models and simulators need to be constructed (R2)

Challenge 6: Tool-independent modeling languages are missing. The lack of modeling languages to support conceptualization and design activities is one of the major blockers of efficient collaboration. While there exist domainspecific modeling tools for agriculture (e.g., APSIM [42] and L-system [43]), modeling languages are tied to these tools. Furthermore, "modeling" is often interpreted as mere mathematical formulation of basic physical and biological principles, e.g., through differential equations. Such low-level formal systems do not help narrow the cognitive gap between experts and the problems at hand as much as MDE does.

We recommend taking a proactive standpoint and evangelizing MDE principles early on. The ability to use modeling languages is especially crucial in the phase of developing runtime models and simulators of digital twins, but benefits can be observed as early as the conceptualization phase.

Challenge 7: Gap between stakeholders is wider than that in CPS. Biology and engineering domains are drastically different domains. The resulting disparate vocabularies and the previously discussed lack of tool-independent modeling languages render the elicitation of expert knowledge challenging. MDE researchers are particularly well-positioned to facilitate mutual understanding and collaboration. We recommend adopting advanced modeling and reasoning techniques for bridging the gap between distant domains, such as introducing domain-specific modeling languages (DSML) [44] and ontological reasoning [45]. Both techniques have been successfully applied in traditional CPS and suggest improved returns on investment settings with distanced domains, such as CBPS subject to digital twinning. Furthermore, we advocate introducing open-ended and non-time-boxed socialization activities between modeling experts and domain experts based on the SECI model [46]. We dedicated a researcher with a computer science background to regular open-ended work discussions with the agronomy expert. Instead of eliciting domain knowledge directly into simulation schemes, the researcher spent multiple weeks with the expert mapping his knowledge. Eventually, the researcher developed his own tacit knowledge which he was able to externalize as simulation models.

Challenge 8: Factual knowledge and untested hypotheses are often not clearly separated. Due to the highly empirical nature of knowledge creation, hypothesis testing is the typical way to build knowledge. We found that often, factual knowledge (tested and proven hypotheses) and untested claims are not clearly separated. Invalid assumptions hinder the creation of faithful models and might render models unusable.

We recommend separating tested and untested hypotheses in collaboration with experts. We organized workshops with the experts to elicit a map of concepts using the i^* concept modeling language [47]. By that, we were able to isolate knowledge that is rooted in well-tested facts (mostly on the engineering side) from that rooted in weaker empirical evidence (mostly on the agronomy side).

Challenge 9: Manual model construction is not feasible. Due to the complexity of systems subject to digital twinning, manual model construction is inefficient and often not feasible. The process of constructing models is hindered by the blackbox nature of biological systems, a source of substantial accidental complexity. Empirical models are often used to approximate the transfer function of biological systems by input-output characteristics. However, trial-and-error experiments required for such empirical models are costly and often suffer from repeatability and generalizability issues.

We recommend the automation of model construction. We found success with automated simulator construction by ML [48], [49], but other techniques—e.g., statistical inference [50]—are readily available as well.

Challenge 10: Reusability of models is challenged by the extensive variety of genera. Developing models for one genus comes with elevated threats to external validity and with the expectation that the developed model will not work for different plant species and cultivars. For example, in our project, strawberry models were particularly hard to obtain. Alternative crop growth models have been proposed, e.g., for tomatoes [51], but the majority of principles are crop-specific. We recommend developing domain ontologies to organize and share knowledge [52]. The open-world assumption of ontologies allows for integrating new knowledge when it becomes available. Under more traditional closed-world assumptions, modeling frames [53] could be considered to explicitly capture the validity conditions of models.

C. Actuation autonomy needs to be flexible (R3)

Challenge 11: The lack of explainability limits autonomy potential. Safety concerns related to biological entities limit

the autonomy of digital twins. By gradually gaining trust in their safety and efficiency, operators can give increasingly more autonomy to digital twins. In line with the observations of Bradshaw et al. [54], we observed that the explainability of the digital twin's behavior is paramount in improving stakeholder trust and accelerating convergence to higher autonomy. We suggest researchers investigate the broader context of explainability, recently researched in great detail in ML and AI [55]. We see the involvement of the human in the configuration space exploration process as a promising aid of understanding, underlining the need for human-machine cooperative techniques recommended by Bradshaw et al. [54].

Challenge 12: Full autonomy is hard to achieve. While domain experts were reluctant to commit to fully autonomous actuation, they were permissive in specific cases. These services tend to have no direct safety impact on the biotic subsystem. For example, automated hazard detection and actuation appeared as an early tentative candidate feature.

We recommend seeking partial autonomy scenarios in collaboration with decision-makers. Such efforts improve the acceptance of the digital twin. For example, stakeholders are likely to re-evaluate safety concerns when the digital twin demonstrates utility in hazardous situations. Identifying such negative scenarios allowed us to elicit additional usage scenarios in which the digital twin could operate autonomously. We recommend breaking down the working of the digital twin into usage scenarios and linking those scenarios with conceptual autonomy levels. However, such roadmapping exercises should be carried out carefully and should consider that perceived levels of autonomy are specific to the particular context [54].

Challenge 13: Fidelity considerations of conventional CPS do not apply. In our setting, fidelity concerns were substantially impacted by the delays in sensor data and manual data. At best, our real-time data stream consisted of sensor samplings in the order of magnitude of minutes. Such limitations in fidelity might have severe impacts on the actuation performance of the digital twin. Although such limitations would be unacceptable for the majority of CPS (e.g., in the control of a production line), we found slower sensing works well for biophysical settings. This is due to the relatively slow rate of change of biological entities. However, accuracy and precision issues still limit reasoning about the physical twin. We advocate surveying the fidelity characteristics of CBPS to better scope the capabilities of digital twins. We recommend encoding such knowledge in domain ontologies for automated reasoning in digital twinning scenarios.

VI. LESSONS LEARNED

In this section, we summarize some lessons learned about modeling activities and associated processes.

A. Modeling aspects

From domain-specific to domain-augmented languages. We observed that the lack of effective modeling languages motivated domain experts to craft their own *informal* DSLs to communicate ideas. For example, a graphical language rooted in causal block diagram semantics [56] and augmented with domain-specific visual elements was regularly used by an engineering expert to communicate simulation scenarios Ferme d'Hiver wished to support with the digital twin. Due to the lack of formal abstract syntax and semantics, these languages cannot be considered domain-specific languages per se, but it is important to recognize that they were sufficient in communicating elaborate concepts and ideas and serve as an excellent starting point for DSL engineering.

We encourage supporting complex digitalization endeavors in such heterogeneous settings with proper engineering support for DSL prototyping and maintenance. Such mechanisms aid the externalization of domain knowledge, and in turn, accelerate the development process of digital twins. Furthermore, these languages can serve as the visual front-end of digital twin dashboards to interact with the deployed digital twin.

Collaborative model-based reasoning is a crucial enabler. Reflecting the bipartite nature of CBPS, optimality criteria of configurations tend to comprise cyber-physical and biological KPIs. We observed that such complex optimization scenarios are approached in a collaborative fashion. Engineers and agronomy experts express their configuration preferences and try to communicate through boundary objects [57], i.e., shared units of understanding, such as energy concepts.

We recommend automating such reasoning mechanisms, e.g., by facilitating design-space exploration [58] with multiple views on the design space and collaborative mechanisms [59].

Data-driven techniques offer limited upside for inferring parts of the digital twin (e.g., simulators or models) based on historical often provide limited upside. Safety considerations force experts to over-dimension their safety margins and ensure safe configurations as much as the system permits. Furthermore, systems in production context are configured based on what is known to provide adequate results to the best of the operator's knowledge, allowing little to no possibility to test alternative configurations. Thus, historical data is biased towards these safe settings, and data outside of safe settings cannot be obtained. However, historical data might still be useful for calibration purposes.

B. Process aspects (CI/CD, DevOps)

Instrumentation of the physical twin is to be addressed early on. The instrumentation of the physical twin might not be suitable for digital twinning, severely limiting the digital twin in fulfilling the goals of stakeholders. Although we started working with an already instrumented system, we identified its limitations early on and started working in an inclusive cooperation on planning improvements and acquiring sensors and actuators. As a result, the IoT infrastructure has substantially evolved. In some cases, corporate procurement policies might pose problems, further necessitating an early treatment of such issues.

Testability and calibration are challenged by safety considerations (of crops) limiting interactions with the physical twin. Since simulators need to be calibrated for a specific environment and need to be regularly re-calibrated to maintain a proper frame of validity [53], establishing testbeds for validation and testing purposes does not mitigate the need for interacting with the physical twin.

Frequent refactorings necessitate proper test coverage. We implemented the digital twin in Python, mostly relying on open-source libraries and frameworks. Due to the functional and architectural impacts of newly encountered requirements, refactorings were frequent throughout the entirety of the development. We observed more architectural changes in the early stages of the development and fewer as we reached the delivery phase of the development cycle. Proper test coverage proved to be crucial in maintaining the pace of development and the ability to react to changing needs.

Early and frequent user acceptance testing is crucial in ensuring rapid convergence to actual business goals. Even though the users of the digital twin are not technical users, they are still considered power users with a high digital aptitude and the ability to tell useful digital facilities from less useful ones. Thus, user acceptance testing can generate value from the early stages of development until late in the maintenance and continuous improvement phase.

Deployment and operation might require active support. Since a digital twinning project might be the first advanced digital endeavor at a company primarily focusing on biological and biophysical systems, deployment becomes an issue. Architectural choices might be suboptimal for digital twinning. We observed that security and availability considerations render even relatively trivial decisions problematic—e.g., deciding between on-premises and cloud environments. Compatibility with existing production systems and compliance with internal standards are additional aspects to be considered when preparing for the deployment of a digital twin.

VII. RELATED WORK

While digital twinning of engineered systems has welldocumented applications, digital twinning of biological systems is still in an early phase.

Pylianidis et al. [60] review 28 case studies of digital twins in agriculture, but note that most solutions never made it past the prototype stage. Digital twins that are eventually deployed in real settings focus on the monitoring aspects of the greenhouse or farm, rather than providing computer-aided decision support or control. In addition, the sampled digital twins did not attempt the twinning of biological entities. This is in stark contrast with our approach, in which the biophysical model captures the prevalent state of the plants. Similar to our setting, Chaux et al. [20] developed a digital twin of a greenhouse with environment control and crop treatment strategies. However, the digital twin has been implemented in a miniature-scale prototype greenhouse and has not been deployed in a real setting. In contrast, our work was situated in a real industry context. This allowed us to assess the imperfections of real industry settings that challenge or even limit the development of digital twins for CBPS. Alves et al. [61] developed a digital twin for farmers to understand the state of their farms with respect to resource and equipment

utilization. The twin is able to collect data from a soil sensor and display the information on a dashboard. However, no computer-aided decision-making or reasoning is provided by the digital twin, limiting the insights expert stakeholders can gain from it. Skobelev et al. [62] note that current digital twins of plants are not adequate for decision-making support as agricultural models fail to capture the variability of plant growth dynamics within different environments. To address this issue, they propose modeling the phases of plant development and their relations and using this underlying model to support decision-making. The approach is operationalized as a digital twin. However, it focuses only on biological entities and does not support reasoning about physical counterparts.

In the broader sense of biological systems, digital twinning has been a topic of particular interest in healthcare. Most of these works emphasize modeling and computational challenges that translate to other biological systems as well. Gerach et al. [10] developed a complex physics-based model of the heart with the intent of creating a heart digital twin and highlighting the need for complex mechanistic models to build such systems. To speed up the computation required to detect heart diseases, Martinez-Velazquez et al. [63] propose an edge-computing architecture for digital twins. Biancolini et al. [64] find a trade-off between computational complexity and real-time constraints in the context of modeling and simulation of blood vessels by fluid dynamics. The challenges and solutions outlined in the healthcare domain translate well to general biophysical digital twinning cases and align with our experiences gained in the CEA domain.

Digital twinning has enjoyed more rapid and widespread adoption in engineered systems, such as cyber-physical systems [65], and is recognized as key enablers to modern industry practices [66]. Similar to our simulation-based approach but situated in Industry 4.0 settings, Schluse et al. [37] define experimentable digital twins (EDT) that allow for what-if analysis of the physical system through simulation. Eisenberg et al. [67] use such EDT in support of reactive planning by model-based optimization. The EDT, in their case, is used for simulating how the physical system would look at a specific point in time, under specific plans. Similar avenues have been explored by Barat et al. [68] who use digital twins as a risk-free experimentation aid for complex techno-socioeconomic systems. Nonetheless, challenges in building faithful physical models have been demonstrated in numerous cases. Govindasamy et al. [69] note that the effort needed to integrate physical simulations for complex systems is enormous if carried out manually and recommend automation. However, testing causality, one of the key challenges in BPS, has been shown to be feasible in CPS by Somers et al. [70].

VIII. CONCLUSION

In this paper, we reported the challenges and lessons learned from a real, industry-scale digital twinning project in the biophysical domain, through a specific case of controlled environment agriculture. In addition, we discussed some lessons learned related to modeling activities and associated processes.

The main conclusion of our project is that the digital capabilities in sectors associated with CBPS-such as CEA and vertical farming-are moderate compared to sectors associated with CPS, such as automotive, and avionics. The relative underdevelopment of digital capabilities is manifested in lacking equipment, resources, and expert manpower, particularly from modeling, systems engineering, and data management perspectives. However, CEA and similar sectors are experiencing a rapid digital transformation [71], [72], indicating elevated future interest in advanced digital capabilities, such as digital twinning. To be able to efficiently support these sectors, the modeling community must take a proactive role, evangelize solutions with a proven track record in CPS, and aid partner organizations in their digital transformation journey. To this end, our paper supports researchers and practitioners with high-value-added industry takeaways.

The challenges we collectively overcame during the reported digital twinning endeavor impacted Ferme d'Hiver at technical and strategic levels. The data quality requirements imposed by the digital twin were addressed by improving data collection and management capabilities at the company. These efforts included improving the low-level sensor infrastructure, adopting solutions that are not tied into vertical technological siloes, and identifying advanced analytics scenarios based on improved data quality and quantity. At a strategic level, this project also helped the company to develop efficient ways to cooperate with (current and prospective) academic partners, and leverage synergies more efficiently. Eventually, the company launched internal research initiatives augmenting our research, fostering a true multi-disciplinary research setting.

The digital twin is currently in use through human actuation due to the elevated safety concerns pertaining to biological components. A human-actuated digital twin is different from what some authors call a "Digital Shadow" [13]: our digital twin provides actuation instructions, but the actuation is carried out by human stakeholders who can confirm that safety criteria are met. Throughout the project, we have been gradually shifting towards more autonomous digital twins. We achieved this by frequent prototyping and by keeping key stakeholders involved. We are continuously working on the digital twin for calibration and execution time optimization. Currently, the digital twin is at the prototype stage fully used in the experimentation lab of the farm.

Future work will focus on developing advanced digital capabilities built on top of the digital twin. Specifically, human-guided design-space exploration and human-machine collaborative optimization will be researched in the near future. We plan to map our conceptual framework onto well-established standards for digital twins in traditional manufacturing domains, such as ISO 23247-1:2021 [73], [74].

ACKNOWLEDGEMENT

This work was partially supported by the NSERC, IVADO, and Mitacs. The authors would like to thank Marie-José Montpetit and Maximilien Gaudette for their comments on early versions of this work.

REFERENCES

- A. Rasheed, O. San, and T. Kvamsdal, "Digital twin: Values, challenges and enablers from a modeling perspective," *IEEE Access*, vol. 8, pp. 21 980–22 012, 2020.
- [2] J. C. Kirchhof, J. Michael, B. Rumpe, S. Varga, and A. Wortmann, "Model-driven digital twin construction: synthesizing the integration of cyber-physical systems with their information systems," in *Proceedings* of the 23rd ACM/IEEE International Conference on Model Driven Engineering Languages and Systems, 2020, pp. 90–101.
- [3] F. Tao, H. Zhang, A. Liu, and A. Y. Nee, "Digital twin in industry: State-of-the-art," *IEEE Transactions on Industrial Informatics*, vol. 15, no. 4, pp. 2405–2415, 2018.
- [4] D. C. Schmidt, "Model-driven engineering," Computer-IEEE Computer Society, vol. 39, no. 2, p. 25, 2006.
- [5] M. Dalibor, N. Jansen, B. Rumpe, D. Schmalzing, L. Wachtmeister, M. Wimmer, and A. Wortmann, "A cross-domain systematic mapping study on software engineering for digital twins," *J. Syst. Softw.*, vol. 193, p. 111361, 2022. [Online]. Available: https://doi.org/10.1016/j.jss. 2022.111361
- [6] P. J. Mosterman and H. Vangheluwe, "Computer automated multiparadigm modeling: An introduction," *Simul.*, vol. 80, no. 9, pp. 433– 450, 2004.
- [7] M. Szvetits and U. Zdun, "Systematic literature review of the objectives, techniques, kinds, and architectures of models at runtime," *Softw. Syst. Model.*, vol. 15, no. 1, pp. 31–69, 2016.
- [8] I. David, I. Ráth, and D. Varró, "Foundations for streaming model transformations by complex event processing," *Softw. Syst. Model.*, vol. 17, no. 1, pp. 135–162, 2016.
- [9] T. Defraeye, C. Shrivastava, T. Berry, P. Verboven, D. Onwude, S. Schudel, A. Bühlmann, P. Cronje, and R. M. Rossi, "Digital twins are coming: Will we need them in supply chains of fresh horticultural produce?" *Trends in Food Science & Technology*, vol. 109, pp. 245–258, 2021.
- [10] T. Gerach, S. Schuler, J. Fröhlich, L. Lindner, E. Kovacheva, R. Moss, E. M. Wülfers, G. Seemann, C. Wieners, and A. Loewe, "Electromechanical whole-heart digital twins: A fully coupled multi-physics approach," *Mathematics*, vol. 9, no. 11, 2021.
- [11] G. Bellocchi, M. Rivington, M. Donatelli, and K. Matthews, "Validation of biophysical models: issues and methodologies. a review," *Agron. Sustain. Dev.*, vol. 30, no. 1, pp. 109–130, 2010.
- [12] K. C. Ting, T. Lin, and P. C. Davidson, *Integrated Urban Controlled Environment Agriculture Systems*. Springer Singapore, 2016.
- [13] W. Kritzinger, M. Karner, G. Traar, J. Henjes, and W. Sihn, "Digital twin in manufacturing: A categorical literature review and classification," *IFAC-PapersOnLine*, vol. 51, no. 11, pp. 1016–1022, 2018.
- [14] S. Boschert and R. Rosen, "Digital twin-the simulation aspect," in *Mechatronic futures.* Springer, 2016, pp. 59–74.
- [15] S. M. Ross, *Simulation (5. ed.)*, ser. Statistical modeling and decision science. Academic Press, 2012.
- [16] "Ferme d'Hiver Official Website," https://winterfarm.com/, retrieved: June 27, 2023.
- [17] Trading Economics, "Canada Food Imports," https://tradingeconomics. com/canada/food-imports-percent-of-merchandise-imports-wb-data. html, retrieved: April 5, 2023.
- [18] K. Jiang, "Highlights of Canada's Merchandise Trade Performance in 2021," https://www.international.gc.ca/trade-commerce/ economist-economiste/analysis-analyse/merchandise_trade-commerce_ marchandises-2021.aspx?lang=eng, retrieved: April 5, 2023.
- [19] V. Masson-Delmotte *et al.*, "Climate change 2021: the physical science basis," *Contribution of working group I to the sixth assessment report of the intergovernmental panel on climate change*, p. 2, 2021.
- [20] J. D. Chaux, D. Sanchez-Londono, and G. Barbieri, "A digital twin architecture to optimize productivity within controlled environment agriculture," *Applied Sciences*, vol. 11, no. 19, 2021.
- [21] A. M. Beacham, L. H. Vickers, and J. M. Monaghan, "Vertical farming: a summary of approaches to growing skywards," *The Journal of Horticultural Science and Biotechnology*, vol. 94, no. 3, pp. 277–283, 2019.
- [22] D. O. Hall and K. Rao, *Studies in biology: Photosynthesis*, 6th ed., ser. Studies in biology. Cambridge, England: Cambridge University Press, Jun. 1999.

- [23] L. S. Pereira, A. Perrier, R. G. Allen, and I. Alves, "Evapotranspiration: Concepts and future trends," *Journal of Irrigation and Drainage Engineering*, vol. 125, no. 2, pp. 45–51, 1999.
- [24] R. J. Wieringa and M. Daneva, "Six strategies for generalizing software engineering theories," *Sci. Comput. Program.*, vol. 101, pp. 136–152, 2015.
- [25] B. Lin, B. Recke, J. K. H. Knudsen, and S. B. Jørgensen, "A systematic approach for soft sensor development," *Comput. Chem. Eng.*, vol. 31, no. 5-6, pp. 419–425, 2007.
- [26] Eclipse, "Eclipse IoT Official Website," https://iot.eclipse.org/, retrieved: April 5, 2023.
- [27] C. Gomes, C. Thule, D. Broman, P. G. Larsen, and H. Vangheluwe, "Co-simulation: A survey," ACM Comput. Surv., vol. 51, no. 3, pp. 49:1– 49:33, 2018.
- [28] E. Syriani, H. Vangheluwe, and A. A. Mallah, "Modelling and simulation-based design of a distributed devs simulator," in *Winter Simulation Conference 2011, WSC'11, Phoenix, AZ, USA, December 11-14, 2011.* IEEE, 2011, pp. 3007–3021.
- [29] B. P. Zeigler, A. Muzy, and E. Kofman, *Theory of modeling and simulation: discrete event & iterative system computational foundations*. Academic press, 2018.
- [30] P. Archambault, I. David, E. Syriani, and H. Sahraoui, "Co-Simulation For Controlled Environment Agriculture," in 2023 Annual Modeling and Simulation Conference (ANNSIM). SCS, 2023.
- [31] G. Blair, N. Bencomo, and R. B. France, "Models run.time," *Computer*, vol. 42, no. 10, pp. 22–27, 2009.
- [32] I. David and E. Syriani, "DEVS Model Construction as a Reinforcement Learning Problem," in 2022 Annual Modeling and Simulation Conference (ANNSIM). IEEE, 2022.
- [33] K. Alexopoulos, N. Nikolakis, and G. Chryssolouris, "Digital twindriven supervised machine learning for the development of artificial intelligence applications in manufacturing," *International Journal of Computer Integrated Manufacturing*, vol. 33, no. 5, pp. 429–439, 2020.
- [34] M. Matulis and C. Harvey, "A robot arm digital twin utilising reinforcement learning," *Computers & Graphics*, vol. 95, pp. 106–114, 2021.
- [35] Y. LeCun, Y. Bengio, and G. E. Hinton, "Deep learning," *Nat.*, vol. 521, no. 7553, pp. 436–444, 2015.
- [36] R. S. Sutton and A. G. Barto, *Reinforcement learning: An introduction*. MIT press, 2018.
- [37] M. Schluse, M. Priggemeyer, L. Atorf, and J. Rossmann, "Experimentable digital twins - streamlining simulation-based systems engineering for industry 4.0," *IEEE Trans. Ind. Informatics*, vol. 14, no. 4, pp. 1722–1731, 2018.
- [38] M. Palesi and T. Givargis, "Multi-objective design space exploration using genetic algorithms," in *Proceedings of the Tenth International Symposium on Hardware/Software Codesign, CODES 2002, Estes Park, Colorado, USA, 2002.* ACM, 2002, pp. 67–72.
- [39] J. B. Dabney and T. L. Harman, *Mastering simulink*. Pearson/Prentice Hall Upper Saddle River, 2004, vol. 230.
- [40] Eclipse, "Eclipse Ditto Official Website," https://www.eclipse.org/ditto/, retrieved: April 5, 2023.
- [41] Association for Computing Machinery, "ACM Code of Ethics and Professional Conduct," https://www.acm.org/code-of-ethics, retrieved: April 5, 2023.
- [42] B. Keating, P. Carberry, G. Hammer, M. Probert, M. Robertson, D. Holzworth, N. Huth, J. Hargreaves, H. Meinke, Z. Hochman, G. McLean, K. Verburg, V. Snow, J. Dimes, M. Silburn, E. Wang, S. Brown, K. Bristow, S. Asseng, S. Chapman, R. McCown, D. Freebairn, and C. Smith, "An overview of apsim, a model designed for farming systems simulation," *European Journal of Agronomy*, vol. 18, no. 3, pp. 267–288, 2003, modelling Cropping Systems: Science, Software and Applications.
- [43] F. Boudon, C. Pradal, T. Cokelaer, P. Prusinkiewicz, and C. Godin, "Lpy: An 1-system simulation framework for modeling plant architecture development based on a dynamic language," *Frontiers in Plant Science*, vol. 3, 2012.
- [44] M. Fowler, *Domain-Specific Languages*, ser. The Addison-Wesley signature series. Addison-Wesley, 2011.
- [45] K. Vanherpen, J. Denil, I. David, P. D. Meulenaere, P. J. Mosterman, M. Törngren, A. Qamar, and H. Vangheluwe, "Ontological reasoning for consistency in the design of cyber-physical systems," in *1st International Workshop on Cyber-Physical Production Systems, CPPSCPSWeek 2016, Vienna, Austria, 2016.* IEEE, 2016, pp. 1–8.
- [46] I. Nonaka and H. Takeuchi, "The knowledge-creating company," Harvard Business Review, vol. 85, no. 7/8, p. 162, 2007.

- [47] D. Amyot, S. Ghanavati, J. Horkoff, G. Mussbacher, L. Peyton, and E. Yu, "Evaluating goal models within the goal-oriented requirement language," *International Journal of Intelligent Systems*, vol. 25, no. 8, pp. 841–877, 2010. [Online]. Available: https: //onlinelibrary.wiley.com/doi/abs/10.1002/int.20433
- [48] I. David, J. Galasso, and E. Syriani, "Inference of Simulation Models in Digital Twins by Reinforcement Learning," in *Proceedings of the 24th* ACM/IEEE Intl. Conference on Model Driven Engineering Languages and Systems: Companion Proceedings. ACM, 2021, pp. 221–224.
- [49] I. David and E. Syriani, Automated Inference of Simulators in Digital Twins. CRC Press, 2023, to appear.
- [50] F. Hartig, J. M. Calabrese, B. Reineking, T. Wiegand, and A. Huth, "Statistical inference for stochastic simulation models - Theory and application," *Ecology Letters*, vol. 14, no. 8, pp. 816–827, 2011.
- [51] B. Vanthoor, P. de Visser, C. Stanghellini, and E. van Henten, "A methodology for model-based greenhouse design: Part 2, description and validation of a tomato yield model," *Biosystems Engineering*, vol. 110, no. 4, pp. 378–395, 2011.
- [52] B. Barroca, T. Kühne, and H. Vangheluwe, "Integrating language and ontology engineering," in *Proceedings of the 8th Workshop* on Multi-Paradigm Modeling co-located with the 17th International Conference on Model Driven Engineering Languages and Systems, MPMMODELS 2014, Valencia, Spain, September 30, 2014, ser. CEUR Workshop Proceedings, vol. 1237. CEUR-WS.org, 2014, pp. 77–86. [Online]. Available: https://ceur-ws.org/Vol-1237/paper8.pdf
- [53] J. Denil, S. Klikovits, P. J. Mosterman, A. Vallecillo, and H. Vangheluwe, "The experiment model and validity frame in m&s," in *Proceedings of the Symposium on Theory of Modeling & Simulation, Virginia Beach, VA, USA, April 23 - 26, 2017.* ACM, 2017, pp. 10:1–10:12.
- [54] J. M. Bradshaw, R. R. Hoffman, D. D. Woods, and M. Johnson, "The seven deadly myths of "autonomous systems"," *IEEE Intell. Syst.*, vol. 28, no. 3, pp. 54–61, 2013.
- [55] N. Burkart and M. F. Huber, "A survey on the explainability of supervised machine learning," J. Artif. Intell. Res., vol. 70, pp. 245– 317, 2021.
- [56] B. Denckla and P. J. Mosterman, "Formalizing causal block diagrams for modeling a class of hybrid dynamic systems," in 44th IEEE IEEE Conference on Decision and Control and 8th European Control Conference Control, CDC/ECC 2005, Seville, Spain, 12-15 December, 2005. IEEE, 2005, pp. 4193–4198.
- [57] A. S. Islind, T. Lindroth, J. Lundin, and G. Steineck, "Co-designing a digital platform with boundary objects: bringing together heterogeneous users in healthcare," *Health and Technology*, vol. 9, no. 4, pp. 425–438, 2019.
- [58] H. Abdeen, D. Varró, H. A. Sahraoui, A. S. Nagy, C. Debreceni, Á. Hegedüs, and Á. Horváth, "Multi-objective optimization in rulebased design space exploration," in ACM/IEEE International Conference on Automated Software Engineering, ASE '14, Vasteras, Sweden, 2014. ACM, 2014, pp. 289–300.
- [59] I. David, K. Aslam, I. Malavolta, and P. Lago, "Collaborative model-driven software engineering - A systematic survey of practices and needs in industry," *J. Syst. Softw.*, vol. 199, p. 111626, 2023. [Online]. Available: https://doi.org/10.1016/j.jss.2023.111626
- [60] C. Pylianidis, S. A. Osinga, and I. N. Athanasiadis, "Introducing digital twins to agriculture," *Comput. Electron. Agric.*, vol. 184, p. 105942, 2021.
- [61] R. G. Alves, G. Souza, R. F. Maia, A. L. H. Tran, C. Kamienski, J. Soininen, P. T. Aquino, and F. Lima, "A digital twin for smart farming," in *IEEE Global Humanitarian Technology Conference, GHTC* 2019, Seattle, WA, USA, October 17-20, 2019. IEEE, 2019, pp. 1–4.
- [62] P. Skobelev, V. Laryukhin, E. Simonova, O. Goryanin, V. Yalovenko, and O. Yalovenko, "Developing a smart cyber-physical system based on digital twins of plants," in 2020 Fourth World Conference on Smart Trends in Systems, Security and Sustainability, 2020, pp. 522–527.
- [63] R. Martinez-Velazquez, R. Gamez, and A. El Saddik, "Cardio twin: A digital twin of the human heart running on the edge," in 2019 IEEE International Symposium on Medical Measurements and Applications (MeMeA), 2019, pp. 1–6.
- [64] M. E. Biancolini, K. Capellini, E. Costa, C. Groth, and S. Celi, "Fast interactive cfd evaluation of hemodynamics assisted by rbf mesh morphing and reduced order models: the case of ataa modelling," *International Journal on Interactive Design and Manufacturing (IJIDeM)*, vol. 14, no. 4, pp. 1227–1238, 2020.

- [65] P. Carreira, V. Amaral, and H. Vangheluwe, Eds., Foundations of Multi-Paradigm Modelling for Cyber-Physical Systems. Springer International Publishing, 2020.
- [66] S. Braun, M. Dalibor, N. Jansen, M. Jarke, I. Koren, C. Quix, B. Rumpe, M. Wimmer, and A. Wortmann, *Engineering Digital Twins and Digital Shadows as Key Enablers for Industry 4.0.* Springer Berlin Heidelberg, 2023, pp. 3–31.
- [67] M. Eisenberg, D. Lehner, R. Sindelár, and M. Wimmer, "Towards reactive planning with digital twins and model-driven optimization," in *Leveraging Applications of Formal Methods, Verification and Validation. Practice - 11th International Symposium, ISoLA 2022, Rhodes, Greece, October 22-30, 2022, Proceedings, Part IV*, ser. LNCS, vol. 13704. Springer, 2022, pp. 54–70.
- [68] S. Barat, V. Kulkarni, T. Clark, and B. Barn, "Digital twin as risk-free experimentation aid for techno-socio-economic systems," in *Proceedings* of the 25th International Conference on Model Driven Engineering Languages and Systems, MODELS 2022, Montreal, Quebec, Canada, October 23-28, 2022. ACM, 2022, pp. 66–75.
- [69] H. S. Govindasamy, R. Jayaraman, B. Taspinar, D. Lehner, and M. Wimmer, "Air quality management: An exemplar for model-driven digital twin engineering," in ACM/IEEE International Conference on Model Driven Engineering Languages and Systems Companion, MODELS 2021 Companion, Fukuoka, Japan, October 10-15, 2021. IEEE, 2021, pp. 229–232.
- [70] R. J. Somers, A. G. Clark, N. Walkinshaw, and R. M. Hierons, "Reliable counterparts: efficiently testing causal relationships in digital twins," in *Proceedings of the 25th International Conference on Model Driven En*gineering Languages and Systems: Companion Proceedings, MODELS 2022, Montreal, Quebec, Canada, October 23-28, 2022. ACM, 2022, pp. 468–472.
- [71] M. A. Dayroğlu and U. Turker, "Digital transformation for sustainable future - agriculture 4.0: A review," pp. 373–399, 2021.
- [72] L. Hrustek, "Sustainability driven by agriculture through digital transformation," *Sustainability*, vol. 12, no. 20, 2020. [Online]. Available: https://www.mdpi.com/2071-1050/12/20/8596
- [73] International Organization for Standardization, "ISO 23247-1:2021 Automation systems and integration Digital twin framework for manufacturing Part 1: Overview and general principles," https://www.iso.org/standard/75066.html, retrieved: April 5, 2023.
- [74] G. Shao, "Use case scenarios for digital twin implementation based on ISO 23247," Tech. Rep., May 2021. [Online]. Available: https://doi.org/10.6028/nist.ams.400-2