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Perspectives

Adaptive digital twins for energy-intensive industries and their local communities

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ABSTRACT

Digital Twins (DTs) are high-fidelity virtual models that behave-like, look-like and connect-to a physical system. In this work, the physical systems are operations and processes from energy-intensive industrial plants and their local communities. The creation of DTs demands expertise not just in engineering, but also in computer science, data science, and artificial intelligence. Here, we introduce the Adaptive Digital Twins (ADT) concept, anchored in five attributes inspired by the self-adaptive systems field from software engineering. These attributes are self-learning, self-optimizing, self-evolving, self-monitoring, and self-protection. This new approach merges cutting-edge computing with pragmatic engineering needs. ADTs can enhance decision-making in both the design phase and real-time operation of industrial facilities and allow for versatile 'what-if' scenario simulations. Seven applications within the energy-intensive industries are described where ADTs could be transformative.

1. Introduction

Industry 4.0 and digitalization, underpinned by Digital Twin (DT) technology, are changing the ways engineers design and operate industrial sites. A DT captures the likeness and behavior of a physical system using digital replicas and establishes connections between physical assets and digital models (Yu et al., 2022). Industry 4.0 integrates these technological developments to improve the efficiency and performance of an industrial process. Leading-edge computing technologies (Gill et al., 2022), such as the Internet of Things (IoT), cloud services, edge computing, and artificial intelligence (AI)-driven decision-making tools, can be integrated with DTs to expand and enhance their capabilities.

Domain-specific DT technology complemented with modern computing technologies marks a new digitalization paradigm (Madni et al., 2019). In the manufacturing and process industries, DT technology is anticipated to significantly improve industrial efficiency and productivity through advanced decisions. These include real-time control decisions that affect the operation of the plant and design and retrofit decisions (referred to as design-time decisions in this study) that are planned and implemented as discrete events during plant shutdowns (Burnak et al., 2019). Additionally, they can also help achieve strategic goals, such as accelerating the uptake and utilization of low and net-zero carbon energy technologies and sources (Yu et al., 2022).

To facilitate the uptake of renewable energy, industrial processes need to be considered in the context of their energy sources. Most new and untapped renewable energy sources lend themselves to being distributed (Bañales, 2020), and are hence likely to be in the neighborhood of the industrial site (referred to as the site-edge). Many are also non-dispatchable (e.g., solar PV, wind), so require careful load management and control, whereas other sources (e.g., biomass, hydro) involve fuels and natural energy storage. Around the site-edge, not only are such energy sources often available, but there will also be a community (residential, commercial and/or industrial) with additional and differing energy demands from the site. As a result, the prospect of sharing and balancing demands beyond the site becomes attractive. Consequently, the notion of the DT extends beyond the site limits to include localized energy sources (Nguyen et al., 2022) and neighboring community demand (Perry et al., 2008), essentially forming a microgrid (Bazmohammadi et al., 2022) for both electricity and heat.

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DTs can be classified as real-time (control) or design-time centric. Real-time control and optimization systems require a two-way, secure channel for the DT to receive data and actuate specific actions. In this light, existing control methodologies, like model predictive control, represent a form of DT for a specific operation (Udugama et al., 2021). A site-wide DT, or a system of DTs, is a higher-level concept with greater potential for advanced operational decision-making. However, plant design and thermodynamics physically limit the potential performance gains. Design-time DTs can help alleviate such limitations. Retrofitting, revamping, and replacing assets are common design-time problems that represent capital investment in performance (Klemeš et al., 2020).

In this article, we define the concept of an Adaptive Digital Twin (ADT) technology with a specific focus on the manufacturing, process, and energy industries. The adaptive element embeds the idea that a DT must natively adapt to underlying performance shifts (e.g., concept drift). The concept draws from the software engineering field of self-adaptive systems (Weyns et al., 2023) and includes five self-* attributes that are specialized in the context of the specific problem. ADTs need to combine domain- (e.g., models and methods) and computing-specific knowledge. This fusion of capabilities can unlock new opportunities in optimizing an industrial site's energy productivity and sustainability while ensuring that they operate safely and economically. The concept aligns with both levels 3 and 4 of the maturity model presented by Madni et al. (2019) but adds significantly more detail.

Overall, this study makes the following novel contributions:

- Conceptualizes the interdisciplinary domain of ADTs focusing on sustainability and decarburization outcomes, while leveraging adaptive, intelligent, and cooperative methods.
- Highlights that ADTs offer continuous process improvement via advanced decision-making during the operation and design phases.
- Identifies energy- and emissions-intensive industrial use cases and discusses ADT requirements to assist in their decarburization.
- Outlines the critical adaptive attributes of ADT to form a roadmap to assist in developing an AI-augmented software platform.

2. Two perspectives of digital twins for industrial applications

In considering industrial DTs, one should note that: "all [digital twins] are wrong but some are useful", and "[digital twins] should be made as simple as possible, but no simpler" (adapted from well-known sayings attributed to George Box and Albert Einstein, respectively). The challenge in developing DTs is to ensure outputs add the greatest benefit to well-defined objectives using as little physical measurement, human resource, and computing resources as possible.

Energy-intensive industries operate across multiple time horizons, encompass massive infrastructures that have physical limitations, and mandate top-level safety requirements above all else. Developing and applying DT technology involves two distinct perspectives. In the physical domain, DT technology focuses on the specific application and attempts to virtualise the physical dimensions and performance of assets, processes, and systems. From a computing perspective, DTs leverage advanced computing capabilities to enable seamless integration of the physical and virtual worlds through appropriate abstraction. Both perspectives are essential to achieving the promise of DT technology and are explored in greater detail through the following sections.

2.1. Physical system perspective

Mathematical models, i.e., sets of equations and data that describe

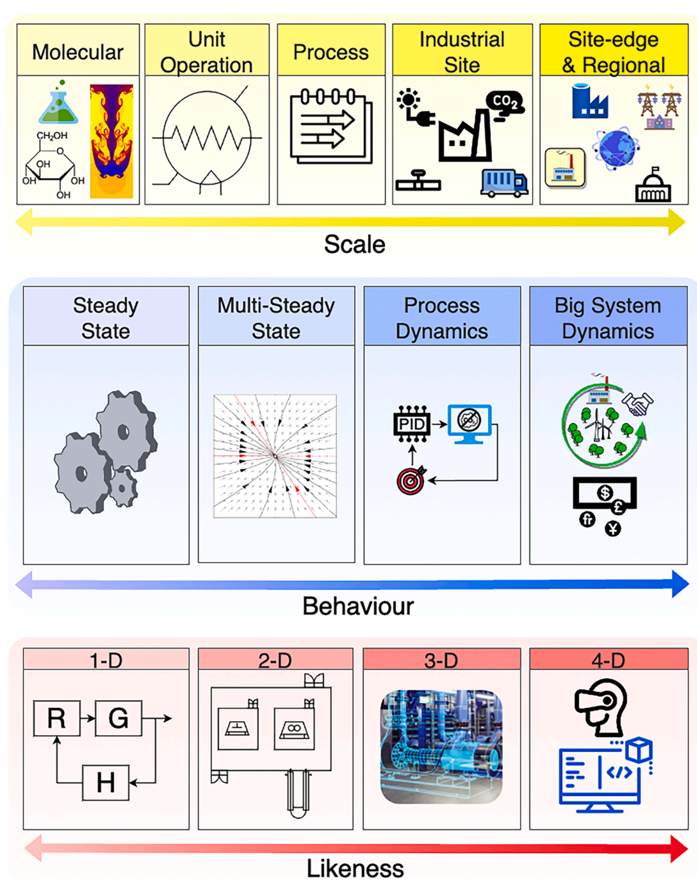

Fig. 1. A physical system perspective on digital twin technology.

the behavior of physical systems and processes, are essential for digital twinning energy-intensive industries throughout the design, build and operation stages. DTs need to span multiple spatial and temporal *scales* to capture critical interactions and information in terms of *likeness* and behavior to improve decision-making. The framework in Fig. 1 builds on the review of Yu et al. (2022) by adding a fourth level of the looks-like and behaves-like dimensions.

(1) **Scale**, describing the physical size of the modelled system.

Using a fractal approach, a DT often views the physical application as a system-of-systems(-of-systems). The modelling ranges from a molecular level involving chemical or biochemical reactions to unit operations, plants, sites and communities. A collection of unit operations tasked with specific production goals (e.g., producing butter, cheese or milk powder) is viewed as a process. An entire industrial site comprises a collection of processes with potentially one or more products, as well as utility services, such as boilers, heat pumps and refrigeration. Sites are often located within a specific context where the site-edge includes other industrial players, commercial entities, and cities.

(2) **Likeness**, capturing the spatial layout and physical dimensions and appearance of an industrial system.

A 1-D diagram is a linear representation of a process, showing primarily the order of unit operations (e.g., a block-flow diagram). Next, 2-D diagrams capture the detailed layout of an industrial plant (e.g., process flow diagrams, piping and instrumentation diagrams, and plot plans). 3-D representations enable full modelling of pipe network topology and process equipment location (e.g., digital isometrics), which can be used to assess, among others, proximity constraints. The final level, 4-D, represents an additional immersive dimension where interaction between the 3-D model and the user is made possible through technologies such as virtual reality, augmented reality, and mixed reality.

(3) **Behavior**, describing the relationship between inputs and outputs over time.

behavior modelling can also span multiple scales. At a basic level, behavior captures static representations of a system at a stable operating point or a design specification. Next, time-varying models attempt to discretise operations into multiple, event-driven, distinct modes or states. Full process dynamics include state transition dynamics, process capacitance, and the effect of disturbances. At the final level of fidelity, big system dynamics include not just internal process dynamics but also the interaction between processes and site-edge variations (e.g., supply dynamics of renewable energy).

Cross-cutting all three physical dimensions is physical **safety**. These two aspects must be considered and embedded into DTs of site operations. For example, behavioral models must include a comprehension of operational limits while likeness models can warn of incompatible site layouts where particular operations must be physically separated.

2.2. Computing system perspective

From a computing system perspective, DT technology, as illustrated in Fig. 2, encompasses three distinct dimensions: *connectivity* that links ongoing operations and historical data with domain-specific models, *control and autonomy* for improved decision-making across all time-scales, and the specific roles and allowance for *human-in-the-loop* interventions. Cross-cutting all three dimensions is the need to protect the

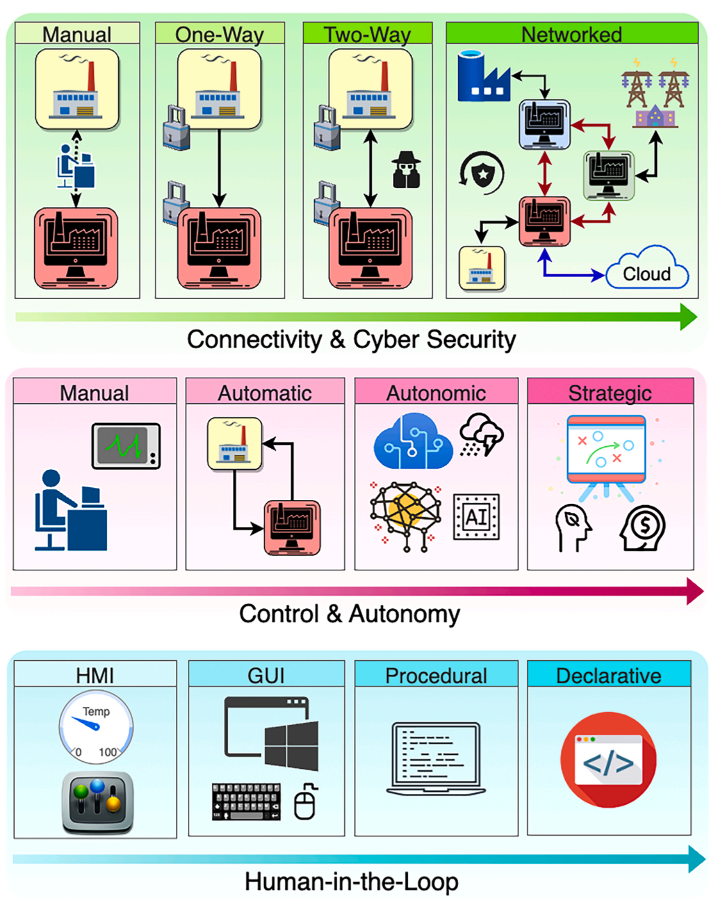

Fig. 2. A computing-specific perspective on digital twin technology.

data and integrity of the DT platform through *cybersecurity*.

(1) **Connectivity**, describing the capacity for secure information flow between the physical and digital twins and other DTs.

Basic DTs, or *digital models*, may only include a manual information flow in one direction. Automating this information flow from the physical to the digital models leads to a new level of DT called a *digital shadow*. Once robustness is verified, a two-way communicating DT could act as a *digital manager*, directly affecting physical operations and decisions. At a higher level, a network of DTs will exchange information among themselves, essentially forming an *Internet of Digital Twins* (IoDT).

(2) **Control and Autonomy**, specify the capacity of a DT for taking independent and well-informed actions without compromising security and safety.

Manual control relies completely on trained human operators to decide how to set key manipulated variables by, for example, physically adjusting manual control valves. Automatic control can determine and actuate decisions in a pre-programmed or non-adaptive manner without interaction with external computing resources. Feedback, feedforward, and model predictive control are widespread throughout all energy-intensive industries, successfully providing process control. Autonomic differs from automatic control in that the controller can detect changes, learn from, and adapt to dynamic environmental changes, and evolve as the environment around it changes. The transition from automatic to autonomic control needs to leverage artificial intelligence (AI) using smart retraining triggers such as concept drift. The final level of control and autonomy is strategic control, which is geared towards achieving higher-level objectives such as minimising both operational costs and greenhouse gas emissions.

(3) **Human-in-the-loop**, describing the need for human decision-making to ensure the safety of specific actions.

Human-Machine Interface (HMI) is the method an operator interacts with industrial operations. The operator views a simple abstraction of the physical system (e.g., process flow diagram with measurements), which facilitates the basic exchange of information. More sophisticated Graphical User Interfaces (GUI) are often reserved for applications requiring higher levels of likeness fidelity, e.g., Computer-Aided Design (CAD) software to assist in decision-making. Existing applications of such DTs include operator training simulations. The next step is the procedural explanation of instructions the system needs to perform as defined by the human-in-the-loop. This will be followed eventually by an abstraction layer that can automatically define and implement plans based on human-in-the-loop specified declarative goals. As such, a DT facilitates switching from how-to-do to what-to-achieve from a whole-of-systems perspective.

Cross-cutting all three computing-system dimensions is **cybersecurity**. Increasing levels of connectivity and autonomy with less human verification exposes an industrial site to malicious cyber-attacks. As a result, cybersecurity needs to be built in at every level to minimize and mitigate vulnerabilities. An authentication framework (e.g., Open Authentication or human-in-the-loop) is needed to validate individual decisions and verify the scope of actions taken.

3. The adaptive digital twin concept for energy-intensive industries

The vision of a new Adaptive Digital Twin (ADT) concept fuses state-of-the-art knowledge and methods from the engineering and computing domains. In the considered context, ADT technology aims to assist and optimize decision-making for industrial sites to achieve a set of high-level objectives within specified constraints. Key to this concept is the additional dimension of adaptivity. This dimension means the DT will be able to respond to uncertainty—such as changes in process behavior, external conditions, and strategic goals—and imagine future developments.

ADTs are, therefore, high-fidelity virtual models that behave-like, look-like, connect-to, and adapt-with a physical system. In the DT literature, the concept of adaptivity is present; however, the scope is narrow (e.g., control applications). This section generalizes the concepts and lays out a complete adaptivity framework for understanding, developing, and applying ADTs across both design and operations. Research, development, and implementation is needed to operationalize ADTs in industrial practice.

3.1. Self-adaptive systems meets digital twins

Adaptivity in DT technology can be achieved through the implementation of at least one self-* attribute. These attributes are inspired by the field of self-adaptive systems in computing technology and are redefined for their application to energy-intensive industries.

- **Self-learning**, entailing a real-time system analysis that uses first-principles models, AI methods, and hybrid models of the two, to build and update data-informed DTs automatically. As underlying performance characteristics of the physical system change with time, self-learning detects this concept drift and triggers retraining of the learned model. This attribute forms the foundation of the ADT concept and is a prerequisite to achieving any of the other four attributes.
- **Self-optimizing**, enabling operational and tactical decision-making to optimize production via process control, planning and scheduling, and energy trading. Such optimization often requires either a digital shadow or a digital manager level of connectivity.
- **Self-evolving**, emphasizing the need to optimally decide how to retrofit, revamp and retire process and utility system assets. These are discrete decisions for an industrial site.
- **Self-monitoring**, including an asset-monitoring system, often using advanced statistical or AI methods to detect and predict failures and disruptions. These predictions can then form the basis of proactive maintenance planning and other human-in-the-loop decisions.
- **Self-protecting**, recognizing the increased vulnerability of digital systems to cyber-attacks due to cloud-based computing and the proliferation of IoT and smart assets. ADTs need built-in security features to block and counteract malicious attacks. Beyond robust software design, self-protecting represents an authentication process to limit the scope of changes and allow for human-in-the-loop approval. Finally, ADTs need to reflectively protect the industrial site against cascade failures that could be triggered by adaptive systems that implement any of the above self-* properties.

Each of the adaptive attributes would benefit from applying a common MAPE-K (Monitoring-Analysis-Planning-Execution supported by accumulating Knowledge) system design pattern. Fig. 3 illustrates how an ADT might be applied to an industrial site and shows the potential interactions between the five self-* attributes.

3.2. System architecture, hosting, and deployment

The ADT concept requires a multi-tiered system architecture where the view (e.g., user interface), control (e.g., feedback), and analysis are abstracted to operate and compute independently in “containers” wherein each software process is encapsulated individually. Through containerization, processes can be distributed across hardware pools, hence resource allocations can be scaled beyond what is achievable through a local installation (e.g., installation on a laptop). Performance can thus be guaranteed in the face of scaling complexity as additional

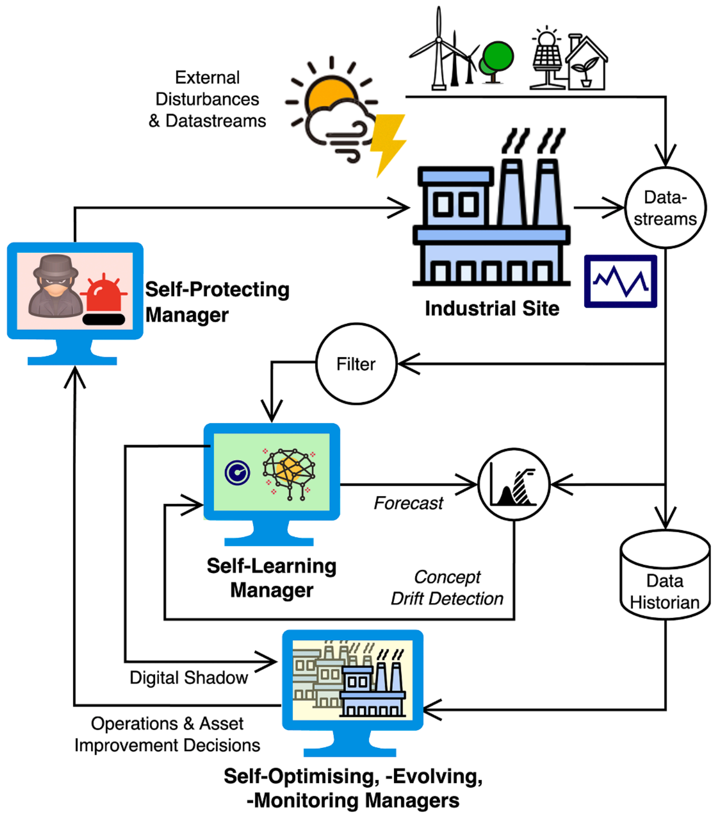

Fig. 3. Interactions and dataflow within site-based adaptive digital twins comprising the five self-* attributes.

containers can be quickly deployed in response to dynamic loads. Furthermore, containerization allows for greater flexibility of deployment as each process operates within a layer of encapsulation, abstracting inconsistencies in Operating System and hardware environments. This is achievable without compromising data sovereignty as computational processing takes place within an isolated environment, greatly reducing the potential for unauthorized access.

The emergence of DT Cloud Service Providers (DT-CSPs), such as Microsoft Azure (azure.microsoft.com), offers consistent frameworks for data processing and system design as a hosting service. DT-CSPs can offer standardized Application Programming Interfaces (APIs) through which application-specific DTs can be produced within a generalizable framework. Hosted services and edging-computing methodologies have the inherent advantage of being able to massively scale computation capacity to enable multiscale DTs and ADTs. Furthermore, the integration of site-edge processing ensures that sensitive data can remain fully within the control of the relevant stakeholders, with model structures abstracting away proprietary information prior to wider cloud processing. This allows for greater access to cloud computing resources while reducing the exposure of sensitive data to cyber-attacks.

Development of DTs with common API calls and data structures can further promote strategic collaboration between an industrial site, its neighbors at the site-edge and other sites that they have an interest in (e.g., other sites owned by the same company). Enabling DTs to communicate with each other and other external databases through standardised APIs facilitates area-wide integration between multiple sites. Industry stakeholders could then optimize operation across multiple sites. Energy producers can likewise benefit from a standardized approach through communicated models that capture the energy profiles of a given site while abstracting away sensitive data specific to the operational state of the site in question.

However, the knowledge of specific behaviors internal to each system could be kept hidden while still gaining benefits based on improved collaboration between DT owners. For example, the design, scheduling, and operation of multiple plants and sites could be synchronized at a wider area level to reflect dynamics in resource availability, processing capacity, and environmental goals. Such collaboration can naturally be extended to the management of energy supply infrastructure across a heterogeneous pool of consumers, with knowledge of abstracted energy requirements and trends.

Fig. 4 encapsulates the notion of DT communication as an Internet of DTs with cooperation leading to emergent outcomes for energy producers, consumers, and prosumers (both produce and consume electricity).

4. Application to energy-intensive industries

Industrial sites comprise complex systems whose behavior is intrinsically difficult to model and control; they have distinct properties that arise from dynamic, non-linear, non-convex, and non-continuous characteristics. To make the transition to net-zero-carbon, their energy systems will become more integrated and even more complex to model, control and optimize.

The next generation of sites will need to harness a range of emerging, market-available and currently-installed energy technology and identify when, where, and how to apply and operate these technologies to maximize strategic-level objectives. Improving decision-making across all time horizons is possible through the ADT concept, which can facilitate industrial sites to transition affordably, resiliently, and rapidly.

This section focuses on seven applications for ADT in energy-intensive industries (Fig. 5) with example use cases. These applications span multiple time horizons and involve a significant amount of interdependence. Additional research is needed in all seven applications to prove the optimal value proposition of ADTs.

4.1. Process control

Effective process control is crucial for energy-intensive industries to

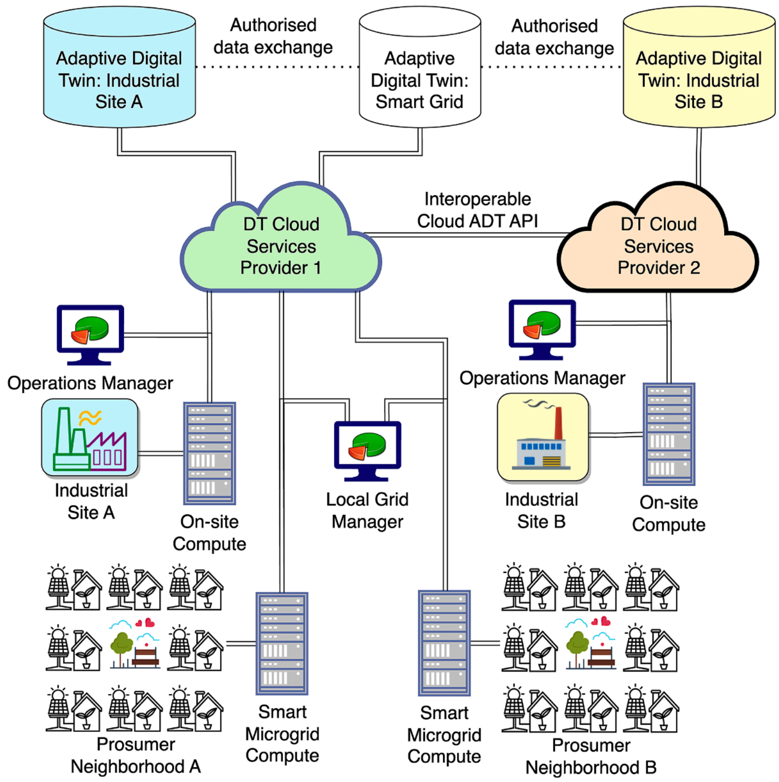

Fig. 4. Cooperative energy planning with networked digital twins hosted through a DT-CSP.

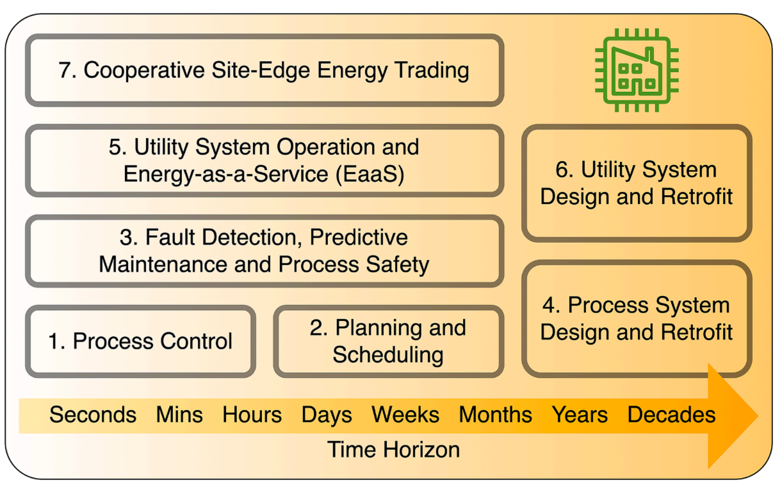

Fig. 5. Increasing goal time horizon of digital twin applications to critical energy-intensive operations.

maintain process variables at their optimal levels, ensuring stable and efficient production while optimizing production indicators, including product quality, throughput, raw material efficiency, energy consumption, cost, and environmental impact (Meng et al., 2018). However, traditional process control theories and algorithms have limitations, necessitating the adoption of new technologies to drive advancements in this field. The integration of digitalization technology into mainstream operations holds the potential for significant process control improvements, and this is where ADTs come into play.

ADTs offer a transformative approach to process control through self-learning and self-optimizing attributes. With the capability to continuously analyze real-time performance and learn from historical data, ADTs enhance process control by adapting to changing conditions and performance models and optimizing control decisions based on strategic production objectives. By utilizing dynamic models driven by AI algorithms, ADTs can predict disruption and implement efficient set-points as well as control internal parameters to account for various factors, including energy consumption and environmental impact. This is achieved through a higher layer adaptive layer that controls goals and real-time operation decisions to reach objectives across multiple outcomes.

To illustrate the potential of ADTs in process control, consider the real-world example of an Organic Rankine Cycle (ORC) geothermal power (Proctor et al., 2015). This plant faced challenges with feedback control due to delays in the opening of wellhead valves caused by an extensive pipeline network. This delay resulted in significant emissions of geothermal water and CO_2 vapour into the atmosphere, impacting the plant's sustainability and efficiency.

To address this issue, a set-point feed-forward control scheme was developed using detailed dynamic models of both the ORC plant and the pipeline network. The feed-forward control scheme, integrated into the plant's operations through a deployed DT, exhibited a remarkable improvement in response time, reducing it by a factor of four to six. Additionally, the control scheme significantly reduced the emission of CO_2 and water from geothermal fluid into the atmosphere, enhancing the plant's sustainability and aligning it with environmental goals.

The example showcases the potential benefits of a DT, which an ADT would bring to process control. The capabilities of ADTs go beyond mere feed-forward control. The multi-tiered architecture enables comprehensive decision-making aligned with strategic objectives. By continuously monitoring and analyzing real-time data, ADTs can make self-learning adjustments and self-optimize control strategies over time to achieve higher levels of efficiency, sustainability, and profitability.

4.2. Planning and scheduling

Effective planning and scheduling are paramount for ensuring operational efficiency in energy-intensive industries. Whether this involves batch sub-unit scheduling, equipment and operating line swapping, or whole-of-plant operation planning, the ultimate goal is to maintain high throughput and consistent quality despite process disturbances or variations.

Traditionally, industries have relied on manual scheduling methods, such as utilizing planning boards or spreadsheets. However, these approaches have their limitations, often resulting in scheduling inefficiencies and reduced production rates due to risk-aversion and large buffers to avoid processing conflicts. On the other hand, some industries have experimented with automated planning and scheduling based on resource models of the entire plant. While automation offers benefits, over-simplification of constraints and a lack of tools to transform top-level objectives into production plans have limited its effectiveness.

To overcome these challenges, the integration of ADT technology emerges as a transformative solution. Self-optimizing ADTs can seamlessly combine production data (e.g., temperature, worker allocation) with external information, such as market trends and environmental conditions to adapt to changes and update production schedules automatically. This enhanced situational awareness also enables proactive responses to disturbances and opportunities, facilitating adaptively optimized decision-making on resource allocation.

As a practical example, consider the challenges faced in scheduling operations at industrial cream cheese plants where batch fermentation times often vary, making it difficult to predetermine the exact batch duration at the outset. To address this complexity and achieve continuous operation while adhering to various constraints, a sophisticated scheduling framework has been proposed, leveraging adaptive modelling and real-time updates (Ebrahimpour et al., 2022).

The framework incorporates an artificial neural network model to predict dynamic pH values, which estimates the time required for each batch to reach the desired pH level and enables dynamic adjustments to the schedule based on real-time data. By accounting for filling, draining, and cleaning constraints, and considering the varying batch durations, the proposed framework enhances continuous production while maintaining consistent product quality.

ADTs, through their self-* attributes described in Section 3.1 can enhance the above example by:

- *Continuous improvement and learning:* ADTs continuously learn from historical data and production outcomes, leading to continuous performance improvement in their predictions and decision-making, optimizing scheduling efficiency.
- *Resource* optimization *and conflict resolution:* ADTs consider various resource constraints, such as equipment availability and worker shifts, to optimize the allocation of resources across different batches, and identify potential scheduling conflicts and propose contingency plans to resolve them proactively.
- *Proactive decision-making:* By analyzing real-time data and predicting batch durations, ADTs can anticipate potential scheduling bottlenecks and disruptions. The ADT-driven scheduling framework enables proactive decision-making, allowing the plant to take pre-emptive actions to maintain smooth operations.
- *Alignment with sustainability goals:* ADTs consider environmental impact factors, such as energy consumption and waste generation, in their scheduling decisions. By optimizing resource usage and reducing production downtime, the ADT contributes to the plant's sustainability efforts.

4.3. Fault detection, predictive maintenance and process safety

Semi and non-continuous production processes face numerous challenges to maintain reliability and keep production rates high for long periods while ensuring product quality, high energy efficiency and low environmental impact. Fault detection is essential for assuring the safety of both personnel and equipment and providing essential information for predictive maintenance management. Predictive maintenance helps energy-intensive industries expand the whole-of-plant life span and reduce maintenance costs.

In the future, industrial sites could make use of ADTs to analyze abnormalities (to detect faults) and combine the fault-detection information to establish a predictive maintenance schedule. An ADT with a self-healing attribute could anticipate faults in a predictive fashion, potentially avoiding (or delaying) unplanned plant shutdowns.

For example, the importance of environmental safety in operating a wastewater treatment plant has been investigated by Liu et al. (2023). First, they developed a DT-based fault detection method to ensure a wastewater treatment plant operates within the environmental safety factors. Second, they constructed a data-driven modelling and diagnosis concept called a sliding window convolutional autoencoder (SW-CAE) and multi-block information convolutional autoencoder (MBI-CAE)). The Benchmark Simulation Model No. 1, which is a generic model of a wastewater treatment plant, provides a point of comparison and helps facilitate the training of a data-driven model. The DT could then help identify potential faults and performance drifts in practice, providing an early warning.

4.4. Process system design and retrofit

Process retrofitting, revamping, and retiring can be informed through self-evolving analysis that focuses on optimizing and upgrading the individual production processes, equipment, and systems used on energy-intensive industrial sites (Akpomiemie and Smith, 2018). These are discrete, design-time-type decisions that can only happen once or twice per year for industrial sites. As a virtual replica of the industrial processes, equipment, and systems, an ADT can provide the analysis tools to develop process change concepts and test these concepts through the application of digital shadows based on historical data including spatial layout. This approach provides significant insight into the effectiveness and spatial feasibility of the process change plan and its impact on energy efficiency, potential risks, and more accurate cost savings results.

Trained digital models of the existing processes can capture as a baseline the performance characteristics, for example, energy consumption, moisture content and powder quality in spray drying for milk powder production. ADTs can then simulate different retrofitting scenarios, such as the installation of a new heat pump or process technology, virtually testing and analyzing the selection and placement of retrofitting technologies and equipment. In a similar use case, as ADTs learn the underlying model of the process, they can also detect subtle drifts in performance caused by common mechanisms such as fouling or equipment degradation. The degradation in performance indicates both the need to retrain the digital model of the process and consider revamping or restoring performance through appropriate measures (e.

g., cleaning).

An example is the recent retrofit design study of Lincoln et al. (2022). As part of the study, they present a comprehensive method for process retrofit, integration and electrification. The method is demonstrated using a milk evaporator case study. Process integration is applied to generate multiple possible retrofit designs before creating digital shadows of the retrofitted process design to more accurately determine impact.

4.5. Utility system operation and energy-as-a-service (EaaS)

In energy-intensive processing plants, the efficient operation of utility systems is of utmost importance to achieve cost-effectiveness and sustainability in energy usage while minimising emissions. Significant operational savings can often be achieved by strategically redistributing steam generation and consumption within the utility system, without the need for additional equipment or major capital investments. The utility system's dynamic response can be effectively achieved using simple Proportional-Integral-Derivative (PID) controls, which make static models sufficient for finding optimal setpoints. However, the discrete nature of utility systems, where equipment can be switched in and out of service, steam flows are redistributed, and zero-flow conditions are common, should be modelled with suitable fidelity levels by combining data, industrial expertise, and process simulator software for effective optimization (Currie et al., 2013). In addition, hot water loops, thermal storage and heat pumps in utility systems are growing in popularity as a means for electrification; however, they too need suitable simulation to ensure they are practical to operate (Chang et al., 2023).

The integration of ADTs in utility system operation opens new horizons:

- *Transitioning to Renewable Energy Sources*: As part of the global energy transition towards decarburization, utility systems in processing plants are actively transitioning from non-renewable sources, such as coal boilers, to more sustainable and renewable alternatives, including biomass boilers and heat pumps.
- *Unlocking Energy-as-a-Service (EaaS) solutions with ADTs*: Integrating ADTs into utility system operation offers Energy-as-a-Service (EaaS) solutions. ADTs, equipped with advanced AI and real-time data analysis capabilities, revolutionize the way plants manage their energy usage and make critical decisions regarding energy sources.
- *Dynamic Decision-Making for Cost-Effective Energy Usage*: For instance, in a processing plant equipped with both biomass boilers and heat pumps for heating, ADTs can identify the most cost-effective energy source by continuously analyzing the relative prices of biomass and electricity in real time.

Consider an example of a steam utility systems optimization. Currie et al. (2013) proposed a mixed integer modelling strategy to approximate a rigorous simulator model, using regressions from literature, industrial experience, and process-specific knowledge. The efficiency of this modelling design is demonstrated through two case studies: a hypothetical three-header model with cogeneration and a four-header refinery utility system. By developing and utilizing a free Matlab optimization toolbox (OPTI Toolbox) for constructing and solving linear, nonlinear, continuous, and discrete optimization problems, the authors showed that a 2 % savings was achieved by switching off inefficient turbines and importing electricity for a real-world example.

While the above example demonstrates efficiency, integrating ADTs can further enhance the optimization of steam utility systems in the following aspects:

- *Real-Time Data Integration:* ADTs can continuously collect and analyze real-time data from the utility systems. This real-time data integration enables ADTs to make more accurate and informed decisions regarding energy usage.
- *Market Intelligence:* ADTs equipped with AI capabilities can access and analyze market trends and electricity prices, allowing them to dynamically identify the most cost-effective energy sources and optimize the operation of the steam utility systems and minimize operational costs.
- *Adaptive Decision-Making:* ADTs adaptively adjust control setpoints and operational parameters based on the evolving plant conditions and energy demand. This dynamic decision-making ensures that the utility systems respond optimally to fluctuations in production requirements and external factors, further improving efficiency.

4.6. Utility system design and retrofit

While electrically driven alternatives, such as electrode boilers, are an established technology, they convert electricity to heat with slightly less than 100 % efficiency. In contrast, a heat pump can produce many times more Watts of heat than Watts of electricity consumed (2–6 times as much, or 200–600 % is typical), making heat pumps much more efficient than electrode boilers (Arpagaus et al., 2018). However, unlike a boiler, the performance of a heat pump is often closely tied to the flow rates and temperatures of the process and utility streams that it pumps heat from and to, which may vary substantially, depending on the process. Performance also depends on the design and structure of the heat pump, especially for large temperature lifts (Adamson et al., 2022). Fossil-fuel boilers may be directly replaced by biomass or electric boilers. Heat pumps (and/or electric boilers), on the other hand, can be applied either as a centralized system or in a distributed way as localized utility systems. Hence, identifying how to fit heat pumps into a site and how to make the best use of them (i.e., which processing and/or utility streams to place them between) is challenging and increases exponentially in possibilities as the number of process streams and units involved increases (Schlosser et al., 2020).

Fuel switching to green energy from solar, wind, or biomass or from agricultural waste are two key solutions being adopted by industries to decarbonize their processes. However, the success of fuel switching depends on the availability and cost of renewable energy sources. ADTs can be used to maximize the use of renewable energy and minimize non-renewable energy sources to reduce emissions while maintaining a reliable supply. ADTs can be used to model the fusion between asset and network ADTs combined with market and price data streams, enabling industries to manage risk effectively. Long-term asset investment can be scheduled based on long-term pricing trends, reducing uncertainty and optimizing investments. Additionally, ADTs can also be used to prolong the lifespan of finite fossil fuel resources.

4.7. Cooperative site-edge and community energy trading

In energy-intensive industries, the main source of greenhouse gas emissions is energy generation, typically directly in the production of heat. However, the potential for renewable energy sources to provide this heat, either directly or indirectly, can be enhanced through effective and cooperative energy planning and management. By exploiting the energy sources themselves, such management systems look to balance loads through appropriate energy storage mechanisms to meet the fluctuating and distributed demands of the processes. Through careful application of such techniques, significant decarbonisation, or even near carbon neutrality, can be achieved by virtually eliminating the need for fossil fuels, even as backups (Pilpola et al., 2019). It should be highlighted that even though there are many similarities between elasticity and load balancing used in self-adaptive systems and cloud computing (Billimoria, 2021; Carvallo and Cooper, 2015), applying these techniques to electricity distribution comes with significant costs and complexities; for example, transmission line impedance and losses across long physical distances restricts matching supply and demand at will

(Gan et al., 2020).

The need for cooperation becomes apparent when the many different entities that are responsible for the smooth operation of the highly complex and interconnected electricity system are considered. For example, different organizations are responsible for power generation and transmission. Further, with the increasing contribution of locally generated renewable energy, and the priority of local consumption of this energy, recursive or fractal microgrids (Apperley, 2019) operate at the edge of the backbone networks with capabilities and fluctuating demands of feeding back energy, or requiring power from, their parent (micro) grid. This implies high levels of local and hierarchical autonomy, as well as sophisticated inter-node communications within the area network. Decisions made at one point not only need to ensure operational continuity and effectiveness locally but also anticipate and accommodate changes in other domains of the whole network. As was pointed out in the Introduction, considerations need to extend well beyond the site boundary, to exploit the variations in demand, and the available energy sources, across the neighboring community.

Current DT advancements focus on real-time monitoring of energy systems with an increasing capability of AI-augmented modelling and forecasting of supply and demand. This is underpinned by distributed real-time sensing used to communicate load and generation information back to the provider. Smart load actuation can also be utilized by defining some demands as flexible or discretionary, which enables the provider to control them based on centralized planning. For instance, water heating or EV charging can be discretionary in timing, which allows the provider to minimize energy spikes and thus eliminate the need for fossil fuel backup energy sources (Buresh et al., 2020).

Given the high levels of autonomy required, and the need for real-time distributed sensing, control and actuation, edge and fog computing are playing an increasing role in supporting ADT in this domain. AI-augmented and game-theoretic levels of autonomy and self-awareness that can provide adaptation guarantees under uncertainty are increasingly required to ensure the sustainable and optimal operation of such mission-critical and highly networked systems. Each unit needs to have its own DT, or at the very least a surrogate model, and all neighboring and hierarchically connected units need to be fully aware of the actions and responses of those twins, enabling the collective confirmation that the proposed adaptation will indeed behave as planned.

5. Whole-of-system digital twins versus over-engineering

So far, the discussion has effectively segregated real-time vs design-time ADT applications. Developing application-specific ADTs enables an engineer to simplify or ignore less relevant aspects that are secondary or lower effects, e.g., design-time analysis often ignores process dynamics, while process control analysis ignores the generation of utility. However, this approach also can miss opportunities or issues with recommended decisions (solutions) from an ADT.

A unified approach to both real-time and design-time DT development across the physical and time scales under a single framework and platform, can facilitate the exchange of relevant information and result in more accurate predictions and solutions. For example, a unit operation level ADT instance would benefit planning and scheduling ADT instances. From a software perspective, such a definition of ADT parts lends itself towards software containerization and cloud computing, making it more practical to solve and use. Similarly, developing relevant data exchange between an ADT of utility systems operations and an ADT for cooperative site-edge energy trading unlocks new variables to consider optimizing for strategic-level goals.

There is, however, a hidden danger. Connecting all application-specific ADTs in a single multiscale ADT can become cumbersome, or even impossible, to solve. Increasing complexity can lead to unnecessary over-engineering. Note, Figs. 1 and 2 show arrows in both directions where the most appropriate level of DT should be selected for the specific application. This approach stands in contrast to many computing-perspective studies on DTs, e.g., (Chen et al., 2021), that propose maturity models for DTs. Maturity models implicitly suggest that the use of more "mature", or newer, technologies lead to improved results. This, too, can lead to ADT over-engineering. While increasing the capability and complexity of DTs can be useful, there are often diminishing returns of the actual gains achieved. Striking a balance between investing in human and computing resources, model accuracy, computational time, useful outputs, and financial benefit is crucial for achieving optimal results.

Effective solutions in energy-intensive industries require collaboration between the industry and computing experts. Clear goals and requirements need to be defined early. Given the applications and goals, the project team needs to decide on the minimum viable ADT fidelities (Figs. 1 and 2), the appropriate adaptive attributes (Fig. 3), and how it might exchange data and energy beyond the site's limits (Fig. 4). By working with the client closely, it is possible to strike an appropriate balance and develop a fit-for-purpose ADT.

6. Conclusions

Adaptive Digital Twins have massive transformational potential to enhance both decision-making and design across energy-intensive industries. These innovative digital twins offer high-fidelity virtual representations of physical assets and systems and encapsulate behave-like, look-like and connect-to attributes. As the landscape of digital twin technology evolves, the integration of advanced software techniques derived from self-adaptive systems, encompassing self-learning, self-optimizing, self-evolving, self-monitoring, and self-protection capabilities, will significantly broaden the scope and adaptability of Adaptive Digital Twins.

This evolution positions Adaptive Digital Twins to not only play a pivotal role in future operational decision-making, such as process control, planning and scheduling, maintenance and reliability, and energy purchasing and trading, but also extends its influence on both greenfield and retrofit design situations. Applications such as process upgrades, enhanced process integration, and retrofits aimed at energy and emissions reduction will benefit from the application of Adaptive Digital Twins. In essence, the incorporation of adaptive digital twin technology with self-adaptive systems represents an innovative and highly beneficial development in digital twin technology. Research, development, and innovation is needed to bring the framework, and an associated software platform, described in this article to become part of industrial practice as part of Industry 4.0.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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