Smart Water Networks as Cyber-Physical-Socio-Environmental Systems

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***Abstract*—This position paper introduces a novel Cyber-Physical-Socio-Environmental Systems (CPSES) framework for Smart Water Networks (SWN). The proposed framework introduces environmental aspects as a key constituent, which is important for addressing the interconnected challenges of water systems, such as climate change impacts, contamination risk, and sustainability. The CPSES framework dynamically incorporates interactions between physical components (sensors, actuators), cyber systems (control, monitoring, digital twins), social factors (policy, demand management, crisis response), and environmental impacts (emissions, resource availability). The significance of this framework lies in its potential to enable more resilient, sustainable, and secure SWNs by incorporating feedback loops among the CPSES constituents. Key CPSES research challenges are outlined, such as modeling the impacts of climate change, dynamic risk estimation, and ethical and fairness aspects within SWN. A real-world use case on water contamination crisis management demonstrates the framework's practical application and relevance for researchers.**

***Index Terms*—water resources, water pollution, water monitoring, cyber-physical systems, system of systems, environmental factors, social factors, smart water networks**

I. Introduction

WATER systems are crucial for the continuous supply of water, which is vital for everyday human needs, sustainable development, energy production, and industrial and agricultural processes. In particular, Drinking Water Distribution Systems (DWDS) comprise multiple physical subsystems, including infrastructure and processes for collecting, cleaning, disinfecting, and delivering clean water to consumers [1]. These systems may operate in urban or rural environments, distributing water to consumers through networks of pipes, pumps, and tanks. The main operational objective is to ensure the delivery of water in adequate quantities and quality while maintaining a high level of efficiency.

DWDS face multiple challenges, such as aging infrastructure, increased water losses, degrading water quality, the risk of contamination events, increased energy costs, and the threat of cyberattacks [2]. Rapid population growth and urbanization also increase water consumption, which is linked with increased energy usage and water losses. These factors contribute to increased environmental stress [3]. The climate crisis further raises the risk of disrupting water distribution, e.g., through the reduced availability of water for treatment [4], or due to emergencies affecting system operation [5].

Industrial *Cyber-Physical Systems* (CPS) provide a suitable framework for modeling DWDS by integrating infrastructure and processes (the *physical* constituent) with communication and computing capabilities (the *cyber* constituent) for monitoring and control [6]–[8].

In general, CPS provide an abstraction for modeling and analysis, capturing complex dynamics, with feedback control software on the *physical* constituent through actuators for reconfiguration and automation, while sensors in the *physical* constituent communicate data back to the *cyber* constituent for processing, monitoring, and event diagnosis [9], [10].

Various CPS challenges have been investigated in research, focusing on modeling, security, and AI-based decision support. For instance, in [11], the problem of cyber-physical security is studied from a systems and control perspective, and the use of multi-agent AI systems to manage the dynamic CPS environment is studied in [12]. Moreover, in [13], the problem of modeling under missing data and noise was examined, and the proposed dynamic latent variable model was demonstrated in a wastewater treatment case study.

Recently, a scientific policy brief advocated for the need for AI-enhanced CPS to support intelligent decarbonization [14]. Although CPS provides a valuable framework for water systems control and security, they often neglect to account for human and policy-related factors. In addition, environmental dynamics (such as emissions or water losses) are typically treated as constraints or static variables. As a result, industrial CPS research tends to overlook crucial connections between water-related challenges and social or environmental dimensions. Addressing the pressing issues of climate change, the rapid increase in water demand, and the rapid adoption of ICT and AI requires a more comprehensive approach that integrates

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these overlooked aspects.

This paper builds upon CPS research and introduces the *Cyber-Physical-Socio-Environmental Systems* (CPSES) modeling framework, designed specifically for DWDS. By explicitly incorporating environmental factors alongside cyber, physical, and social components, this framework enables a more holistic and adaptive approach to managing water distribution systems. The CPSES model allows for better risk management, climate adaptation, and operational efficiency through the integration of real-time data, advanced modeling, and stakeholder engagement.

The contributions of this position paper are summarized as follows:

1) We propose a new *Cyber-Physical-Socio-Environmental Systems* (CPSES) modeling framework that explicitly integrates social and environmental aspects within DWDS.
2) We map critical interdependencies between environmental, social, and cyber-physical constituents in DWDS, which are required for modeling, optimization, and decision support tools of SWN.
3) We address key CPSES research challenges relevant to DWDS, including understanding policy impacts on water consumption, mitigating extreme weather effects on water quality, ensuring equitable distribution in scarcity, optimizing energy efficiency with renewable sources, and enhancing resilience to threats and faults.
4) We discuss practical aspects relevant to the implementation and demonstrate the conceptual application of the framework in a realistic contamination event management scenario.

The paper is structured as follows: Section II provides background on Smart Water Networks. Section III introduces the foundational concepts and explains the constituents of the framework. Section IV presents the CPSES framework and how it is adapted for DWDS, expanding on each constituent and its dynamics. Section V discusses key aspects of the proposed framework and provides high-level specifications for its practical applications within Digital Twins. Section VI outlines the challenges and future directions of the CPSES framework. Section VII concludes the paper, summarizing key implications and future work. In the Supplementary Material, we demonstrate how the framework applies to a pathogen contamination emergency response case study, and its digital twin.

II. Background on Smart Water Networks

The adoption of *Information and Communication Technologies* (ICT) in DWDS, augmented by the sensing capabilities of the *Supervisory Control and Data Acquisition System* (SCADA), has significantly enhanced the monitoring and control of physical elements through cyber components [15]. In general, urban water networks, compared to rural networks, are better monitored using advanced technologies. The potential of integrating ICT with smart algorithms to address the multiple challenges of DWDS has fostered the development of *Smart Water Networks* (SWN) [16]–[18], a concept analogous to the Smart Grid in Power Systems [19], [20]. This analogy highlights the use of advanced technologies and data-driven approaches to optimize operations and enhance efficiency.

SWN refers to an integrated DWDS that uses advanced sensing and actuation technologies, communications, data management, and visualizations, along with advanced data analytics and decision support systems. Analytics in SWN are strategically designed to enhance system management. The goals include dealing with events/faults such as pipe bursts and leakages [21], [22], ensuring water quality and mitigating contamination risks [5], [23], [24], reducing energy usage [25], [26], improving cyber-physical security [27], [28], optimizing system efficiency [29], [30], increasing reliability [31], and addressing the consequences of climate change and diminishing water resources, such as through intermittent water supply [32], [33]. At the same time, the widespread adoption of these technologies increases potential security risks, expanding the number of potential attack vectors [34].

It is important to note that the current state of practice in DWDS management is still quite far from the envisioned SWN described in this paper, and significant investments, as well as a cultural shift, would be needed to enable their adoption.

III. Conceptual Foundations and Framework Development

The epistemological foundations for our work are based on Systems Theory [35] and Systems-of-Systems [36], [37]. Systems Theory provides a comprehensive framework for modeling interdependencies between various components within a system, whereas Systems-of-Systems extends this by integrating multiple independent systems, each with its high-level objectives. Through these mechanisms, we identify interconnected components of different systems (constituents) of industrial CPS that interact dynamically, governed by complex relations.

In addition, feedback loops are directly considered, and emerging properties can be identified and explored to provide insights into system behavior and performance. Based on these foundations, we identify multiple constituents that are interrelated with industrial CPS, including human or social dynamics, as well as dynamics interacting with the environment.

To incorporate human dynamics (the *social* constituent) as an essential part of these systems, the concept of *Cyber-Physical-Social Systems* (CPSS) was introduced [38]–[40], expanding the foundational CPS framework. CPSS emphasizes the importance of the *social* constituent, recognizing human dynamics as integral to effective system design and analysis. In CPSS, the *social* constituent, comprising human actors at various levels, interacts with the *cyber* constituent through information exchange and decision enforcement. In addition, this *social* constituent influences the *physical* constituent by affecting its dynamics and making decisions that impact the physical infrastructure.

CPSS have been considered in various application domains, notably in smart cities. Urban environments can leverage the CPSS framework to design innovative services, including environmental monitoring, business, commerce, social activities, and emergency response, thus improving urban functionality and livability [41].

Additionally, social aspects are recognized as crucial in the design and analysis of various industrial systems. In Intelligent Transportation Systems [42], [43], CPSS enables the capture, analysis, and utilization of uncertain, complex, and diverse social behaviors of humans, optimizing control and management performance through model-based, data-driven, or hybrid approaches.

In the context of moving toward a sustainable energy future, the traditional concept of the Smart (Energy) Grid, which previously omitted the *social* constituent, is now considered inadequate for addressing the challenges of modern systems [44]–[46]. The inclusion of CPSS in future energy systems is advocated as a holistic approach that considers environmental, economic, and social factors, as well as human behaviors [44].

Similarly, the manufacturing sector is evolving toward *Industry 4.0* [47], characterized by the interaction between physical, cyber, and social factors, which underlines the comprehensive benefits of CPSS [48]. An extensive literature review on the topic for various infrastructures is available in [49]. A key contribution of that work is the inclusion of the function of humans, rather than just the social aspects in general, as well as the presentation of a virtualized architecture and an integrated framework suitable for optimization. A key differentiation of our work with respect to [49], is the direct consideration of the environmental constituent, specifically within the context of SWN.

Consumers influence the hydraulic dynamics of the system through their consumption patterns and can act as "sensors" by detecting and reporting leaks or quality problems. Furthermore, consumers can push for policy changes, as seen in the *European Right2Water citizen initiative* [50]. In research, the role of consumers has been investigated in various studies [51]–[53] as an independent component. However, there has been limited examination of the human factor as an integral part of the design and operational phases of CPS control.

Moreover, the roles of operators, managers, and policymakers are often not considered within the framework of CPS. *Operators* set the system parameters to meet operational goals, and *Managers* ensure adherence to service standards and legislation. The overall management and governance framework is specified by *Policymakers*, who are becoming more aware of the ethical and societal equity aspects related to water supply, as well as the impact on the environment and citizens' health. For example, the EU Directive 2020/2184 [54] related to drinking water quality was a socially driven process outcome.

A comparative analysis of the CPS, CPSS, and CPSES modeling frameworks is provided in Table I. The analysis illustrates that CPS and CPSS frameworks do not directly consider, or only implicitly consider, environmental and sustainability factors. For example, such considerations are implicitly associated with various studies, e.g., on smart cities [41], [55]–[57], and on the smart grid [58]. Notably, [59] combines CPS and water systems toward sustainability through monitoring, sensing, and control for sustainability, without considering social aspects. Overall, there is an emphasis on the technological challenges relevant to modeling, simulation, interoperability, and security. Social aspects have also been explored in research, focusing on human behavior,

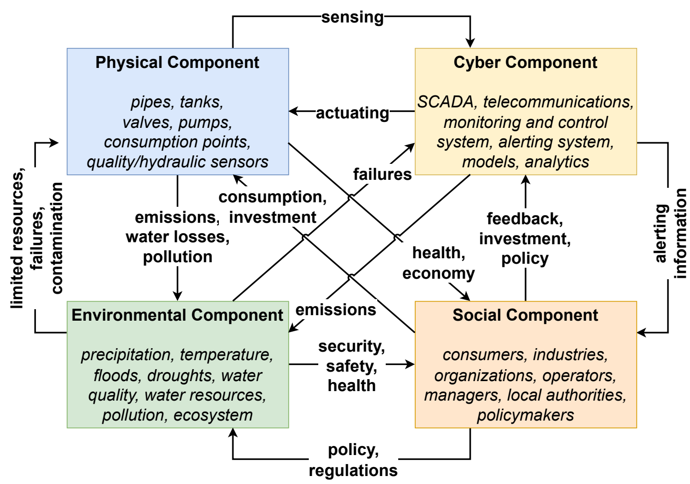

Fig. 1. High-level architecture of main constituents of DWDS as CPSES.

understanding societal impacts, and exploring human-machine collaborations.

Moreover, our study identified that, there is limited access to software tools capable of modeling all the different physical, cyber, social, and environmental dynamics in a unified way, as well as relevant benchmarks and testbeds.

We propose a broader inclusion of environmental dynamics in system planning and execution through the design of conceptual frameworks, as well as models and software tools to capture these dynamics and explore different options. In the following section, we propose such a framework that can be used to design new integrated platforms, supporting interoperability and the exploration of the dynamics of the different constituents.

IV. A Cyber-Physical-Socio-Environmental Systems Architecture for SWN

Figure 1 offers a high-level overview, illustrating how the core constituents (physical, cyber, social, and environmental) map to SWN.

The *Physical* constituent (blue) encompasses infrastructure elements such as pipes, tanks, valves, pumps, and consumption points, along with sensors and actuators. The *Cyber* constituent (yellow) includes the SCADA system, telecommunications, control and alerting algorithms, and advanced analytics methods. The *Social* constituent (orange) consists of stakeholders who impact the other constituents directly or indirectly through information exchange, decision-making, or influencing the system dynamics.

This group includes consumers (citizens and industries), organizations, technical operators, utility managers, local authorities, and policymakers. Finally, the *Environmental* constituent (green) encompasses elements affecting water supply, including aspects of climate change (such as precipitation, temperature, floods, and droughts), water quality, availability of water resources, pollution, and ecosystem impacts.

The directed lines in Fig. 1 indicate the relationships between the different constituents:

TABLE I
COMPARATIVE ANALYSIS OF CPS, CPSS, AND CPSES MODELLING FRAMEWORKS IN DWDS

Characteristic	CPS	CPSS	CPSES
Physical Constituents	*Directly modeled:* Real-time control and monitoring of physical assets (pipes, sensors, actuators).	*Directly modeled:* As in CPS, includes human actions (e.g., water demands, maintenance activities).	*Directly modeled:* As in CPSS, includes environmental effects (e.g., water losses impacting ecosystems).
Cyber Constituents	*Directly modeled:* SCADA, control algorithms, and real-time monitoring.	*Directly modeled:* As in CPS, with feedback loops from social systems (e.g., consumer feedback).	*Directly modeled:* As in CPSS, includes environmental dynamics (e.g., GHG emissions models).
Social Constituents	*Indirectly modeled:* Social behavior is considered constant or periodic (e.g., water demands).	*Directly modeled:* Social behaviors, policies, and human decision-making affect operations.	*Directly modeled:* As in CPSS, includes impacts to public health due to environmental conditions.
Environmental Constituents	*Indirectly modeled:* Typically related to efficiency or availability constraints (e.g., energy use).	*Indirectly modeled:* As in CPS.	*Directly modeled:* Includes climate change, emissions, resource management, and environmental conditions.

The *Physical* constituent provides sensing signals of its states to the *Cyber* constituent, and the *Cyber* constituent returns control actions to regulate the actuators of the *Physical* constituent. The use of actuators in the *Physical* constituent generates *Greenhouse Gas* (GHG) emissions. Together with underground water losses and potential pollution events, this impacts the *Environmental* constituent on a larger scale. Simultaneously, the *Environmental* constituent affects the *Physical* constituent, as there may be limited water resources available, and disruptive natural events (such as floods or fires) may cause failures and water contamination in the *Physical* constituent.

The *Physical* constituent contributes to the *Social* constituent through the reliability of the service provided, as well as by maintaining a high level of public health and supporting an evolving economy. Conversely, the *Social* constituent is the key driver of the *Physical* constituent's dynamics through water consumption and investments in new infrastructure. The *Social* constituent can act as "human sensors," providing feedback (e.g., on leaks using online tools) and driving investments and policies for the *Cyber* constituent. Concurrently, the *Cyber* constituent communicates alerts and other relevant information to the *Social* constituent, aiding in decision-making. The *Social* constituent also influences the *Environmental* constituent through policy-making and regulations.

However, the *Environmental* constituent can dramatically affect the *Social* constituent, especially during extreme events, which can impact security, safety, and overall public health. Likewise, extreme events can cause failures in the *Cyber* constituent, disrupting its operation. Finally, the *Cyber* constituent can affect the *Environmental* constituent through associated GHG and heat emissions, as well as other technology-related pollution (e.g., from rare earth materials, electronic waste, etc.).

Other critical aspects are the cyber-physical security risks, which affect both the cyber and physical domains, and can have direct or indirect implications for the environment and societal stakeholders [11], [60]. For instance, an attack on a state estimation module [61] can trigger a change in the system actuators, causing tank overflows with increased disinfectant concentrations, which can have a severe environmental impact [62].

The following subsections outline the proposed architecture of the CPSES, detailing the distinct constituents and their interrelationships, as illustrated in Fig. 2. Note that the *Social* constituent is segmented into four main categories of stakeholders within the water sector: consumers, utility operators, water management authorities, and policymakers. Practical aspects of how the CPSES modeling framework can be implemented within the context of Digital Twins, are discussed in the next section.

A. Physical Constituent

The *Physical* constituent comprises the DWDS, central to which is the **network** of pipes that deliver water to consumers. The network's flows are affected by water consumption and **water losses**, including leaks. To maintain system pressure and ensure sufficient water quantities for all consumers, even during emergencies, **water storage & disinfection** facilities and **actuators** (such as pumps, valves, and disinfection stations) are essential. Water supply depends on the overall availability and quality of **water resources**. The system's physical characteristics are monitored by **sensors** installed within the infrastructure, measuring consumption volume, flow rates, pressures, water levels in tanks, and water quality (e.g., turbidity, pH, etc.). Portable sensors may also be employed in this context for monitoring flexibility.

The *Physical* constituent is closely interconnected with the *Social* constituent through various stakeholders. *Consumers'* consumption behavior significantly affects the hydraulic dynamics of the system, acting as an uncontrolled disturbance. From the perspective of the water authority, *Operators* are tasked with ensuring the efficient operation of the system. This responsibility includes maintaining, repairing, or upgrading the physical infrastructure. Lastly, *Managers* play a crucial role in decision-making, particularly regarding investments in new technologies and the expansion of the infrastructure. These decisions are made in alignment with the policies established by *Policymakers*.

B. Cyber Constituent

The *Cyber* constituent consists of all the *Information and Operational Technology* (IT/OT) infrastructure, including both

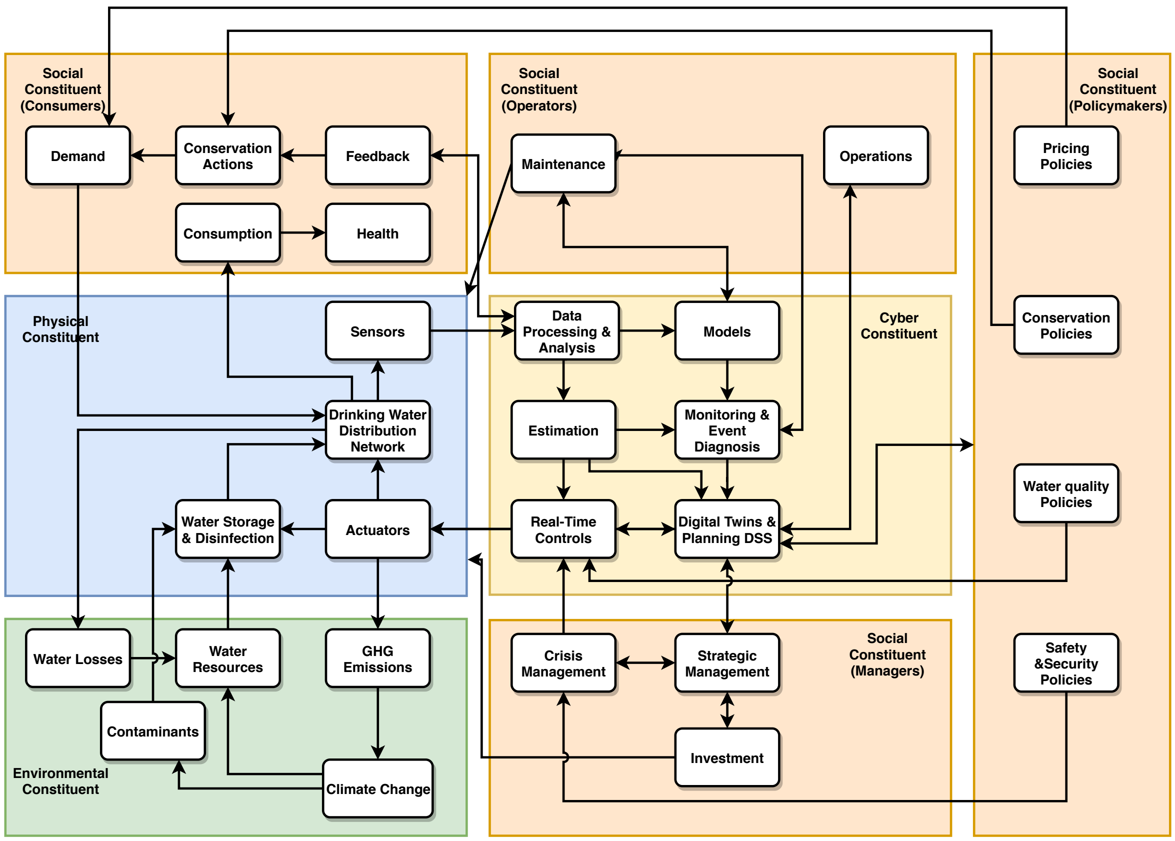

Fig. 2. An outline of the proposed CPSES Architecture for SWN.

hardware and software, necessary to monitor, operate, control, and manage the *Physical* constituent. Additionally, it serves as an interface with social stakeholders. The main software modules of the *Cyber* constituent are described in the following paragraphs. Notably, the integration of advanced computing paradigms, such as Artificial Intelligence (AI) and Machine Learning (ML) methods, will enable automation across the various modules and decision support tools.

The **Data Processing and Analysis** module is responsible for receiving measurements from sensors, processing, and storing data for use by other modules. Data can be semantically annotated depending on their type. This module also checks data quality, identifying issues such as missing data. Besides physical sensor information, this module incorporates information from the *Social* constituent, such as consumer feedback about system operations, including reports of pressure drops, abnormal water quality, or leaks. Data pre-processing can be incorporated in this module [63].

The **Models** module comprises mathematical and computational representations of the physical system and its dynamics. For example, DWDS topology is modeled using *Geographic Information Systems* (GIS) and is mathematically characterized using Differential-Algebraic Equations for hydraulics and Partial Differential Equations for water quality [5]. Alongside first-principle models, AI/ML data-driven models are also utilized. It is important to note that hydraulic dynamics drive water quality dynamics, which are associated with uncertainties. This module can include models of various faults affecting the dynamics and requires updates when the physical system undergoes changes, such as upgrades or maintenance, possibly through online learning.

The **Estimator** module utilizes models of the physical system and the latest sensor data to estimate unmeasured consumptions and hydraulic and water quality state dynamics in real time. These state estimates are crucial for diagnosis and control. The estimations are fed to the **Monitoring and Diagnosis** module. Leveraging sensor data, consumer reports, state estimates, and models, this module is tasked with detecting, isolating, and identifying faults in the Smart Water Network. These may include leaks, actuator/sensor faults, contamination events, and cyber-physical attacks.

The **Digital Twin & Planning** module is a virtual representation of the physical system that assists stakeholders, primarily *Operators*, and secondarily *Managers* and *Policymakers*, in decision-making. For short-term decisions, it uses recent sensor data, state estimates, and nominal computational models to create an updated, calibrated system model (a Digital Twin) for simulation and optimization. For long-term planning, it offers tools to evaluate different policies and investment decisions by exploring various future scenarios, e.g., under different climatic conditions. Lastly, the **Real-time Control** module, controlling actuators such as pumps, valves, and disinfection systems, is guided by the high-level control decisions of *Operators* using the outputs of the **Digital Twin** and **Estimation** modules. Additional details regarding the Digital Twin are provided in the next section.

C. Environmental Constituent

The dynamics of the *Environmental* constituent are closely linked with those of the *Physical* constituent. The increased use of pumps, which leads to higher energy consumption, results in greater **GHG emissions**, thereby contributing to climate change. Conversely, **climate change** significantly affects the availability and quality of **water resources**. This, in turn, impacts the water supply and quality within the distribution network. Additionally, increased **water losses** from the network diminish the overall availability of water resources, necessitating the use of more clean water to satisfy demand. Moreover, water quality degradation, caused by **contaminants** due to floods or high temperatures, can affect water quality, and subsequently, the health of Consumers.

D. Social Constituent

The *Social* constituent in SWN comprises four primary stakeholder groups: (i) *Consumers*; (ii) *Operators*; (iii) *Managers*; and (iv) *Policymakers*. Each group plays distinct roles and holds different responsibilities within the system. *Consumers* directly influence water demand and usage patterns. *Operators* are responsible for the day-to-day management and operational efficiency of the system. *Managers* make strategic decisions regarding system upgrades and investments. *Policymakers* set the regulatory framework and policies guiding the system's operations. These stakeholders interact with the *Cyber*, *Physical*, and *Environmental* constituents in various ways, shaping the system's overall functionality and effectiveness. A more detailed analysis follows.

1) Consumer Stakeholder: The term *Consumers* refers to all entities (humans, industries, etc.) that request drinking water. **Demand** is characterized by a complex socio-economic function, influencing consumption patterns. For instance, demand can be affected by factors such as water pricing or the **conservation actions** adopted by consumers, which may be driven by policies. Additionally, consumers may provide direct or indirect feedback to water authorities regarding faults or other events, thereby enhancing the system's early warning capabilities by acting as "sensors." Concurrently, information communicated by the *Cyber* constituent to consumers, such as comparisons of their consumption with similar consumer profiles, can influence their conservation behaviors. Critically, consumer health can be affected by the *Environmental* constituent.

2) Operator Stakeholder: Operators play a crucial role in managing **maintenance** and **operations** within a water authority. Their responsibilities include making decisions on the best ways to control the system, such as opening, closing, or regulating valves and pumps to ensure efficient system operation. For this process, Operators interact with the system through the *Cyber* constituent. In SWN, they may utilize *Digital Twins* to determine the most effective actions for optimizing operations. Maintenance activities, involving interaction with the *Physical* constituent, might include disconnecting parts of the network or replacing infrastructure elements. Such maintenance actions are often guided by the *Monitoring and Event Diagnosis* module. After completing maintenance tasks, Operators update the system's model (e.g., the GIS) to reflect physical changes, such as new pipes, sensors, or actuators, and to incorporate new fault types into the model.

3) Manager Stakeholder: Managers are responsible for making decisions that affect the entire water organization. This role encompasses **strategic management**, often informed by insights gained from **Digital Twins and planning** tools within the *Cyber* constituent. Their decisions involve resource allocation and **investments** in both the *Physical* and *Cyber* constituents. Effective strategic management must align with the various **policies** established by *Policymakers*. Additionally, Managers are tasked with **crisis management**, where they make crucial decisions and coordinate with external stakeholders, such as First Responders (FR) during emergencies (e.g., contamination events, earthquakes, or floods).

4) Policymaker Stakeholder: The role of the *Policymakers* is to establish high-level policies that broadly affect all other stakeholders within the system. For example, **pricing policies** pertain to the cost of water for different consumer categories, such as offering lower tariffs for large families. Meanwhile, **conservation policies** aim to incentivize sustainable demand behavior among consumers, such as the installation of water-saving fixtures. **Water quality policies** play a crucial role in setting safety standards for chemical and biological components in drinking water, which are monitored and controlled through the *Cyber* constituent. Lastly, **safety and security policies** address the management of risks associated with uncertainties in water resources, climate change, and unforeseen events like accidents or malicious attacks. An example of this is the *Water Safety Plans* (WSP) proposed by the World Health Organization [64].

V. Towards a CPSES Digital Twin: Discussion and Practical Applications

In this section, we discuss practical aspects of the application of the framework and provide a reference architecture for future implementations. Various measurement data, models, and analytics are required to capture the dynamics between the different constituents. As a result, the connection with legacy systems (such as GIS and SCADA), as well as the integration with more advanced technologies (such as IoT Platforms, Data Spaces, and Digital Twins), is critical. This is also aligned with the Smart Water Networks Forum's (SWAN) reference architecture [65], which considers the physical, sensing and control, communication, data management, and analytics layers as enablers of Smart Water Networks.

A Digital Twin of the physical DWDS is a virtual (computational) representation that is continuously updated with real-time data, such as pressure and flow rate measurements [66], [67]. This real-time data integration allows for a deeper understanding of the system's behavior and enables more informed decision-making in DWDS management. Digital Twins can be used for a variety of purposes, including monitoring network conditions, locating leaks, optimizing pressures and disinfectant dosage, and more. They can also be used to simulate the impacts of different scenarios, such as changes in demand or water main breaks, which can help water

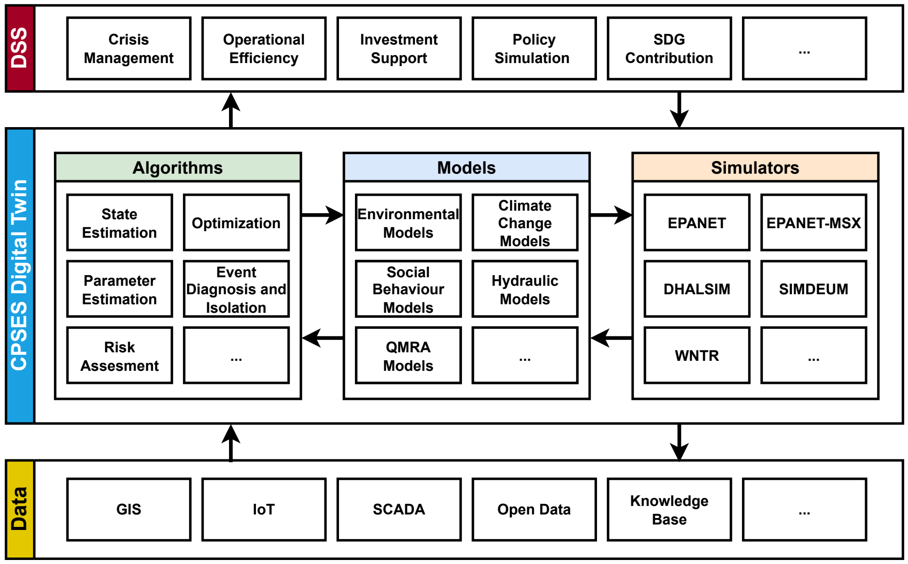

Fig. 3. A Digital Twin according to the CPSES framework. The Data layer provides access to various types of data and knowledge. The DSS layer includes different Decision Support Systems that require the Digital Twin to operate. The main elements of the Digital Twin include the mathematical/computational models, the simulators, and the supporting algorithms.

utilities plan for future events and improve their response to emergencies [68], [69].

Even though Digital Twins have demonstrated their effectiveness in addressing challenges in the physical system, there is still a need for integrating cyber, social, and environmental aspects, compatible with the proposed CPSES modeling framework. As a result, CPSES Digital Twins need to go a step further by modeling the different constituents and their interdependencies to enable the exploration of different what-if scenarios.

A. Modeling

CPSES Digital Twins should include mathematical and computational models spanning various domains. Hydraulic and water quality dynamics are required for modeling flows, pressures, as well as substance transport and reaction dynamics, using EPANET/EPANET-MSX and their toolkits [70]–[73]. Environmental models quantify greenhouse gas emissions, based on pump energy consumption and water losses [74]–[76]. Cybersecurity models can estimate the behavior of the system under potential attacks, using the *Digital Hydraulic Simulator* (DHALSIM) [77], [78]. Emergency response optimization models provide situational awareness and suggest actions to mitigate the impacts of events, such as using the *Water Network Tool for Resilience* (WNTR) [79]. Quantitative Microbial Risk Assessment (QMRA) can be used to assess public health risks by linking pathogen exposure, dose-response functions, and risk characterization [80].

Another critical aspect highlighted by the CPSES framework is societal dynamics. Consumer behavior and behavioral economics can be modeled to simulate consumer response to financial and conservation policies, price and income elasticity [81], [82], as well as stochastic consumer behavior through the *SIMulation of water Demand, and End-Use Model* (SIMDEUM) [83]. During a water contamination crisis, disinformation, such as fake news, may spread among the population, affecting demand dynamics and, in turn, the overall system dynamics (e.g., causing a drop in system pressure due to the simultaneous opening of all water taps). For this reason, tools integrated with Digital Twins to detect fake news during crisis management are of great importance [84], [85].

Mapping and modeling the interconnections between the different elements of the framework require synergies between different scientific domains (such as engineering, computer science, economics, social sciences, and environmental science) and different stakeholders (citizens, volunteers, operators, managers, and policymakers). To achieve this, social science frameworks can be utilized, such as the *Communities of Practice* (CoP) framework, a multi-stakeholder, participatory, and co-creation approach [86], as well as through choice experiments [87].

B. Proposed CPSES Digital Twin Architecture

A high-level overview of the Digital Twin, which is aligned with the proposed CPSES framework, is depicted in Fig. 3. The south-bound *Data Layer* comprises different data sources, such as GIS, IoT, SCADA, Open Data, other Data Spaces, knowledge bases, and others. The CPSES Digital Twin is composed of the Models, the Simulators, and the Algorithms Modules. The Models Module consists of the mathematical and computational models that describe the different dynamics of the CPSES.

The Simulator Module links the models with simulation engines capable of executing various experiments and evaluating multiple scenarios. Finally, the Algorithms Module includes all the methods needed for estimating the states (as points and/or as boundaries), optimization, parameter estimation, event diagnosis, risk assessment, etc. The CPSES can communicate with Decision Support Systems (DSS), which fully utilize the CPSES framework. Examples of such DSS include Crisis Management, Operational Efficiency, Investment Support, Policy Simulation, Sustainable Development Goals (SDG) contribution, and others.

A use case where the CPSES framework was applied in the context of pathogen contamination emergency response, is provided in the Supplementary Material.

C. Investment and Scalability

Beyond the Digital Twin, the CPSES framework requires investments in infrastructure (for sensors, actuators, communication systems, etc.), software (for developing innovative or acquiring existing software, customizing it to specific needs, data management, etc.), and maintenance.

However, the potential benefits can be substantial, measured through various performance indicators linked, among others, to the UN Sustainable Development Goals (SDGs) and the International Water Association (IWA) [88]. These performance indicators will also facilitate benchmarking between water providers across various aspects, including efficiency, resilience, and sustainability.

Lastly, we note that the CPSES framework is adaptable to other industrial CPS domains. For example, even though the main emphasis is on urban DWDS, CPSES can be adapted to rural DWDS and wastewater systems.

VI. Challenges and Future Directions

The proposed architecture opens up research questions spanning various disciplines, including water engineering, ML, control systems, social sciences, and economics. In the following paragraphs, we introduce several new challenges that highlight the opportunities presented by adopting this holistic framework across different research areas. Addressing these challenges necessitates interdisciplinary approaches, calling for the exchange of knowledge among experts from diverse scientific fields. This requirement for cross-disciplinary collaboration presents a significant challenge in itself, underscoring the complexity and integrated nature of CPSES.

Modelling Climate Change: Climate change significantly affects the availability of water resources, making it crucial to model its impact on both the quality and quantity of these resources, as well as the changing frequency of extreme events like floods and droughts [89], [90]. By modeling various climate change scenarios and their associated uncertainties, such as changes in temperatures, precipitation patterns, and sea-level rise, this information becomes invaluable for the long-term planning processes of *Managers* and informs the development of new policies. Concurrently, the operation of DWDS also influences climate change, evident through GHG emissions and potential environmental impacts from water losses. Therefore, incorporating energy efficiency and sustainability into the design and operation of DWDS represents a significant challenge.

System Evolution and Deep Uncertainties: DWDS are constantly evolving. The geospatial distribution of consumers changes over time, and concurrently, the *Physical* constituent undergoes aging and requires replacement over periods spanning decades. Additionally, technological advancements in sensing and actuator technologies, ICT, and AI are leading to the generation of large volumes of data. Societal priorities also evolve, influencing policies in ways that are challenging to predict over the long term. Consequently, a critical challenge is managing these deep uncertainties in a manner that ensures system designs are flexible [91], technology adoption is reconfigurable and not limited to specific protocols, and models can be continuously updated through incremental learning [92]–[94].

Human-System Interaction: Recent technological advances in AI have given rise to Large Language Models (LLMs). LLMs (such as Meta's Llama [95]) are statistical models pre-trained on massive amounts of diverse text data (e.g., websites and code). They are capable of generating text and enabling applications such as question-answering. In the context of CPSES and particularly within the *Social* constituent, these models can provide a means of interacting with stakeholders. Consumer feedback can also be actionable data for AI/ML models [96].

Water Quality and Dynamic Risk Estimation: Currently, water quality and risk are managed through sparse, periodic sampling. Samples are analyzed in laboratories with significant latency (typically days). At the same time, regulations and risk assessment studies only consider a small fraction of contaminants. For some potentially dangerous substances (e.g., disinfection by-products), there are no widely available technologies for real-time monitoring, nor are there clear indications of their health impacts. Advancements in sensor technologies and the integration of ML for creating models of water quality and its health impacts represent a critical step towards CPSES. By incorporating a real-time, data-driven approach, it is possible to design models for dynamic and continuous risk assessment.

Fusing Multi-Modal Data: "Modality" refers to how information is experienced or occurs—for instance, visual observation, auditory signals, or textural sensations. Multimodal learning [97] extends beyond traditional data fusion methods [98], aiming to build models capable of processing and correlating information from various modalities. In SWN, rich interactions between the physical, cyber, and socio-environmental constituents generate a diverse array of data. This includes time-series data from various sensors in the *Physical* constituent, billing records, telephone interactions, and even social media. The challenge lies in how to effectively collect, represent, and fuse these different data types to enhance the system's ability to make informed decisions and predictions.

Ethics and Faireness: The continuous integration of *Physical* constituents (sensors and actuators) with *Cyber* constituents (controls, communications, and AI-enabled automation), alongside human interaction, raises significant ethical issues [99], [100]. Decision-making processes must be unbiased and promote equitable water distribution, especially in times of scarcity (e.g., due to droughts). Additionally, the proliferation of SWN risks widening the digital divide, disproportionately impacting low-income or marginalized communities.

Modeling Consumer Demand: Modeling consumer demand is a pivotal aspect of smart water network management. Consumption is often viewed as a diurnal time series. ML techniques are employed to analyze the vast data collected from diverse consumption patterns, thereby refining models and enhancing predictive accuracy. In reality, consumption is influenced by a complex interplay of factors, including pricing policies, conservation perceptions, demographics, and socioeconomic status. Insights from social studies, particularly in psychology and behavioral economics, are instrumental in unraveling the key determinants of consumption behavior, ultimately aiding in more informed decision-making.

VII. Conclusions

This paper has introduced a comprehensive modeling framework for conceptualizing Smart Water Networks (SWN) as Cyber-Physical-Socio-Environmental Systems (CPSES). CPSES integrates the complex interactions between the cyber and physical constituents, along with societal stakeholders, while considering critical interdependencies with the environment and the implications of climate change.

The framework provides a holistic approach to understanding the complex dynamics and risks of SWN, aiming to guide future software and decision support tools. Through the adoption of tools built using the CPSES reference framework (such as Digital Twins), stakeholders will be able to manage SWN more efficiently and resiliently. By incorporating real-time data analytics, enhanced sensor networks, and advanced modeling techniques, the CPSES framework supports more effective monitoring, control, and management of water resources. The integration of societal and environmental aspects will improve not only operational efficiency but also resilience during emergencies. Furthermore, the adoption of the framework will provide actionable insights to industry professionals and policymakers for future investments as well as strategic decisions toward adaptability, security, and sustainability, considering the challenges of climate change, urbanization, and other cyber-physical threats.

CPSES emphasizes the need for multidisciplinary collaboration, extending beyond the technical and engineering dimensions to include social sciences, economics, and environmental science. Through these synergies, we can foster the evolution of future smart water distribution systems that are more sustainable, efficient, resilient, and equitable. Future research should focus on refining the computational models within the CPSES framework to better capture the dynamics and interdependencies, further understand the security challenges, and integrate advanced technologies. Furthermore, open tools should be designed to support the development of Digital Twins, which incorporate the different CPSES models and interdependencies with water data spaces.

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