

Perspective

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AI-enabled environmental digital twins: a new paradigm for predictive environmental research

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Abstract

Environmental systems are often characterized by strong dynamics, multiscale coupling, nonlinear responses, and high uncertainty. These features limit conventional approaches based on trial-and-error experimentation and static modeling. While artificial intelligence (AI) has greatly enhanced environmental data analysis and prediction, complex environmental systems further require dynamic coupling among data, models, physical processes, and decision feedback. Digital twins dynamically connect physical systems and virtual representations through real-time data exchange, modeling, analytics, and feedback to enable dynamic understanding, prediction, and intervention. This Perspective examines the core concepts, technical architectures, and maturity levels of AI-enabled environmental digital twins, with particular attention to their conceptual boundaries and physical-virtual integration. It also highlights emerging applications across environmentally relevant energy systems, water environment management, and natural environmental systems. The reviewed studies span different levels of physical-virtual integration, from offline digital models and one-way digital shadows to a smaller number of bidirectionally coupled digital twins. We identify three critical challenges: limited bidirectional coupling, insufficient representation of microscale processes, and a lack of standardized architectures and fit-for-purpose evaluation frameworks. We further discuss emerging opportunities in environmental equipment development and predictive digital toxicology, where AI-enabled digital twins may support virtual experimentation, adaptive equipment optimization, dynamic risk assessment, and personalized environmental exposure prediction. The integration of AI with environmental digital twins may enable adaptive learning, uncertainty-aware prediction, intelligent decision-making, and predictive environmental management, thereby accelerating the transition from passive monitoring toward predictive, adaptive, and model-driven environmental science.

Keywords: Environmental digital twins, Artificial intelligence, Physical-virtual coupling, Real-time data integration, Predictive environmental research

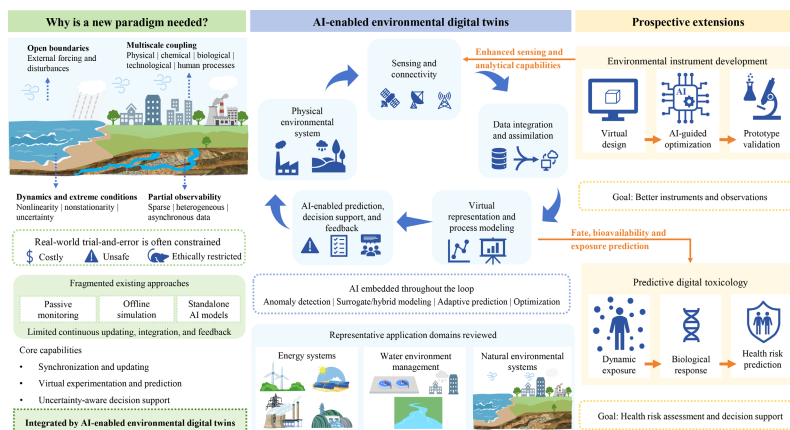
Highlights

- AI enhances state updating, prediction, uncertainty assessment, and decision-making in environmental digital twins.
- Applications span environmentally relevant energy systems, water environment management, and natural environmental systems.
- Current implementations range from digital models and shadows to bidirectionally coupled digital twins.
- Limited feedback, microscale representation, and standardized validation remain key barriers.
- Environmental equipment development and predictive digital toxicology extend the digital-twin framework.

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Graphical abstract



Introduction

Environmental science is increasingly confronted with a class of real-world challenges that are intrinsically difficult to probe through trial-and-error. These problems usually arise in extreme and high-risk environments, as well as complex and uncertainty-driven systems. Examples include nuclear facility operation^[1–3], renewable energy equipment management^[4], toxic effects of mixed pollutant exposures^[5,6], and processes occurring in natural environmental systems such as the atmosphere, watersheds, coastal zones, and subsurface environments. Such systems are typically open-boundary, multiscale, partially observable, nonlinear, and uncertainty-driven^[3,7]. Their behavior is shaped by coupled physical, chemical, biological, technological, and human processes, making mechanistic understanding, dynamic prediction, and timely intervention particularly challenging^[8]. Under these conditions, conventional experimental paradigms based on field or laboratory trial-and-error are fundamentally constrained. Experiments are often prohibitively costly, operationally unsafe^[9], or ethically infeasible. For example, destructive corrosion testing cannot be performed on operational nuclear pipelines, and systematic human experiments are infeasible for assessing long-term health risks of mixed chemical exposures^[10]. In addition, ethical restrictions on in vivo experimentation are becoming increasingly stringent^[11]. These non-experimentable regimes therefore represent a critical bottleneck for advancing mechanistic understanding, dynamic prediction, and precise intervention in environmental systems.

Existing studies have attempted to address these challenges through approaches such as online monitoring, offline modeling, simulation-based analysis, AI-based prediction, and experiment-based optimization^[3,12]. However, these methods remain limited in their ability to support adaptive understanding, intelligent prediction, and real-time control of complex environmental systems. For instance, online technologies, e.g., video surveillance, are often restricted to passive recording and post-event analysis^[13]. Offline models and simulations can elucidate underlying mechanisms but cannot interact continuously with dynamic systems or calibrate against real-world conditions^[7,8]. Moreover, conventional models often struggle to assimilate heterogeneous environmental data and capture highly nonlinear system behaviors under evolving conditions^[14]. Standalone AI models can learn complex patterns from data, but may lack physical consistency, uncertainty awareness, and decision feedback. Physical trial-and-error in research and development (R&D) and optimization, including three-dimensional (3D)

printing and catalyst synthesis, is costly and time-consuming^[15,16]. In this context, digital twins integrate physical models, real-time sensing, data assimilation, and AI-assisted analytics within a continuously updated physical–virtual framework^[3]. This integration supports model updating, state tracking, virtual experimentation, and, at higher levels of maturity, feedback-informed decision-making^[8,17,18]. AI further enhances these functions by learning from heterogeneous data, accelerating complex simulations, detecting anomalies, and supporting uncertainty-aware prediction and optimization^[14]. Accordingly, we use the term AI-enabled environmental digital twins to describe systems in which AI is functionally embedded within the observation–model updating–prediction–decision loop rather than applied as an isolated prediction tool. Together, these capabilities support a shift from passive monitoring and costly trial-and-error toward predictive and adaptive environmental research^[7].

Despite this conceptual promise, current environmental digital-twin implementations remain fragmented across disciplines and uneven in physical–virtual integration and operational maturity^[19]. Here, we clarify the conceptual boundaries, enabling AI functions, and evaluation criteria of AI-enabled environmental digital twins. We then critically examine representative applications across environmentally relevant energy systems, water environment management, and natural environmental systems, and synthesize their current levels of integration and technological maturity. Finally, we discuss the broader challenges and development priorities of environmental digital twins, and further highlight two prospective application directions: environmental monitoring equipment development and predictive digital toxicology.

Concepts, architecture, and principles of AI-enabled environmental digital twins

Digital twins are dynamic virtual representations of physical systems that are continuously updated through bidirectional data exchange, enabling real-time state estimation as well as prediction and optimization of system behavior^[18,20,21]. A typical architecture comprises a physical system, a virtual model, and a data connectivity and integration layer^[17,20,22], corresponding to system operation, model representation, and data interaction. The physical system provides real-time operational states, the virtual model represents and simulates system behavior, and the data layer enables real-time data acquisition, transmission, and feedback^[23,24].

Because the terms digital model, digital shadow, and digital twin represent different levels of physical–virtual integration, this Perspective distinguishes them according to the direction and continuity of data exchange and the presence of a systematic feedback pathway (Table 1). Digital models involve no automatic physical–virtual data exchange, digital shadows support automatic one-way updating from the physical system to the virtual representation, and digital twins require recurrent bidirectional interaction and feedback.

Definition of AI-enabled environmental digital twins

In this Perspective, an AI-enabled environmental digital twin is defined as a dynamically synchronized virtual representation of a natural or environmentally relevant engineered system in which AI methods are functionally embedded in the twinning workflow to support data integration, process modeling, prediction, uncertainty assessment, decision-making, or feedback[26,27].

This definition establishes three boundaries. First, the physical system must have explicit environmental relevance. Engineered systems are included only when their operation is directly coupled to environmental conditions, environmental safety, pollutant or resource flows, ecological or health risks, or low-carbon outcomes; generic industrial asset twins without such connections are outside the scope of this Perspective. Second, the virtual representation must maintain a dynamic connection with the physical system rather than operate solely as an offline model or simulation[25,28]. Feedback may be automated or human-mediated, but must link virtual predictions or decisions to physical or management actions, with the resulting responses used to update the virtual representation. This distinguishes a digital twin from a one-way digital shadow. Third, AI must contribute to one or more functional stages of the twinning process rather than act as a standalone prediction tool. AI can enhance the predictive, adaptive, and decision-support capabilities of a digital twin, but it cannot replace physical–virtual coupling[26]. A conventional digital twin may therefore operate without AI, whereas the use of AI alone does not constitute a digital twin[7]. AI enablement should therefore be regarded as a functional enhancement of a digital twin rather than as a separate level of physical–virtual integration[18,29].

Core architecture of AI-enabled environmental digital twins

An AI-enabled environmental digital twin can be organized into five functionally connected layers: the physical environmental system, the sensing and connectivity layer, the data integration and assimilation layer, the virtual representation and process-modeling layer, and the AI-enabled prediction, decision, and feedback layer[3,26].

The physical layer may represent a natural system, such as the atmosphere, a watershed, a coastal zone, or an ecosystem, or an environmentally relevant engineered system, such as a wastewater-treatment facility, renewable-energy installation, or pollution-control process. The sensing and connectivity layer acquires and transmits observations from sensors, remote sensing, monitoring networks, operational databases, and Internet of Things devices[19,27]. The data integration and assimilation layer preprocesses, aligns, combines, and assimilates heterogeneous observations and model outputs[26,27,30]. The virtual representation and process-modeling layer describes system states and processes through physics-based, data-driven, or hybrid models[30]. The AI-enabled prediction, decision, and feedback layer converts the synchronized virtual state into forecasts, warnings, management alternatives, and operational recommendations[26].

Together, these layers form an iterative physical-data-model-decision-feedback workflow rather than an isolated collection of digital technologies[22]. Figure 1 illustrates this architecture and the flow of information between its components.

Functional roles of AI within the digital-twin architecture

Within the digital-twin architecture, AI contributes at three interconnected functional levels: state perception and dynamic updating, model prediction and credibility assessment, and decision optimization and feedback[14,31]. At these levels, AI transforms observations and model outputs into updated system states, forecasts, uncertainty estimates, and decision-relevant actions.

These functional levels are implemented through combinations of statistical algorithms, machine-learning architectures, physics-informed models, optimization methods, and control strategies. Table 2 links each digital-twin function to its practical role, representative technical categories, commonly used methods, and implementation frameworks.

At the state-perception level, AI-assisted data assimilation updates unobserved states and uncertain parameters by integrating observations with model predictions[30], while anomaly-detection methods identify deviations associated with sensor faults, unusual events, operational failures, or model drift. Together, these functions improve physical–virtual synchronization and support early warning[27,43].

At the level of model prediction and credibility assessment, AI-based surrogate models provide computationally efficient approximations of high-fidelity simulations or observed system behavior, enabling near-real-time forecasting, rapid scenario evaluation, and repeated execution during optimization[30]. Physics-informed and hybrid models combine the mechanistic interpretability and physical consistency of physics-based models with the computational speed and flexibility of AI, thereby improving the reliability and

Table 1 Distinction between digital models, digital shadows, and digital twins according to the automation and direction of data exchange and the presence of feedback[22,25]

Category	Core feature	Classification in this Perspective
Digital model	No automatic data exchange between the physical system and its virtual representation; data are updated manually or used offline	A digital representation used for simulation, analysis, or prediction; it does not meet the physical–virtual coupling criterion for a digital twin.
Digital shadow	Automatic one-way data flow from the physical system to the virtual representation, enabling continuous or periodic virtual updating.	A one-way coupled system that supports monitoring, state estimation, or prediction but lacks a systematic virtual-to-physical return pathway.
Digital twin	Recurrent bidirectional data exchange between the physical and virtual systems, with dynamic updating and an implemented feedback pathway.	A bidirectionally coupled system in which virtual predictions or decisions inform physical actions and the resulting physical responses support subsequent model updating.

Note: Classification is based on the demonstrated direction, continuity, and recurrence of physical–virtual data exchange and on whether a systematic feedback pathway is implemented.

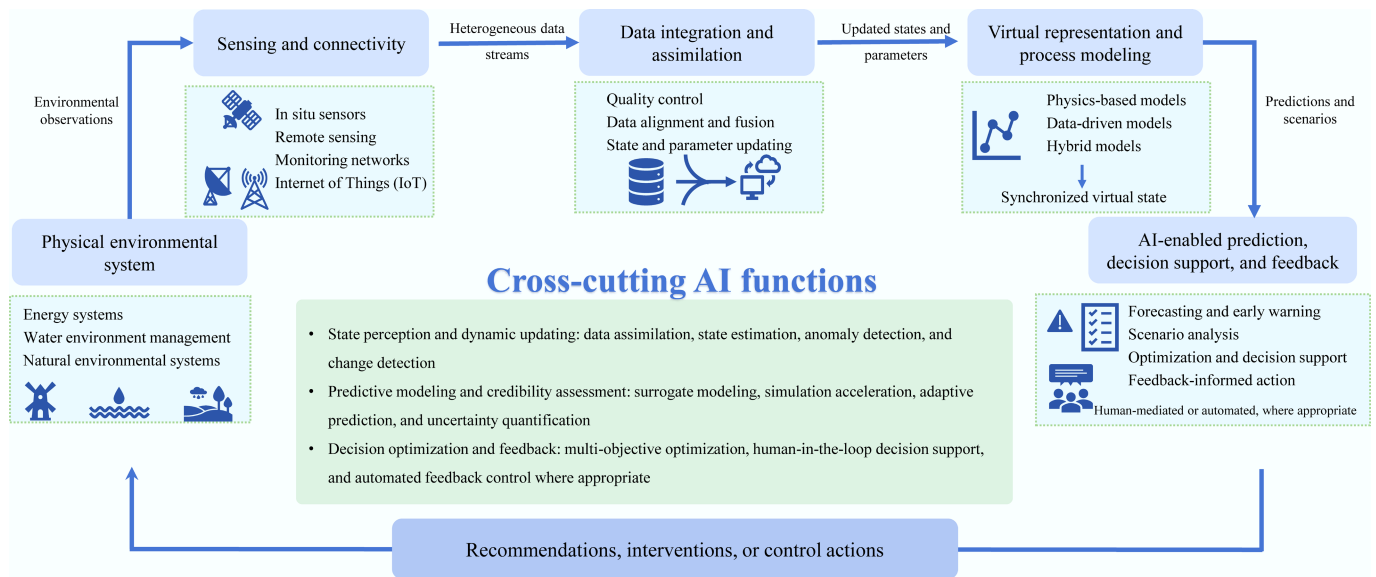


Fig. 1 Architecture and functional roles of AI-enabled environmental digital twins. The framework integrates physical environmental systems, sensing and connectivity, data assimilation, virtual representation and process modeling, and AI-enabled prediction and feedback. AI functions are embedded across the loop to support state updating, prediction, uncertainty assessment, optimization, and decision support.

Table 2 Functional roles, representative methods, and implementation platforms supporting AI-enabled environmental digital twins

Function within AI-enabled DTs	Practical role in the DT	Technical category	Representative method	Representative framework/platform	Ref.
Data assimilation and state estimation	Updates system states and parameters to maintain physical–virtual synchronization.	Sequential/ensemble; variational; ML-assisted DA	Kalman filter; ensemble Kalman filter; particle filter; 3D-Var/4D-Var; ensemble data assimilation	OpenDA; DART; MATLAB	[32]
Anomaly and change detection	Detects faults, abnormal states, regime shifts, and model drift.	Statistical/one-class; neural reconstruction/sequence models	PCA; one-class SVM; LSTM; Isolation Forest; Transformer; autoencoder/VAE	scikit-learn; PyTorch; TensorFlow/Keras	[33–35]
Surrogate modeling and simulation acceleration	Accelerates process simulation, prediction, scenario evaluation, and optimization.	Physics-informed/hybrid; neural operators; general data-driven surrogates	PINNs; hybrid physics–ML; DeepONet; FNO; GPR; random forest; XGBoost	DeepXDE; PyTorch; TensorFlow; scikit-learn	[36–38]
Adaptive prediction	Updates models to maintain performance under changing environmental and operational conditions.	Online/continual learning; transfer/domain adaptation; drift-aware updating	Incremental learning; adaptive ensembles; transfer learning; concept-drift detection; domain adaptation	River; TensorFlow/Keras; PyTorch	[39]
Uncertainty quantification	Quantifies uncertainty for calibrated prediction and risk-informed decisions.	Sampling/sensitivity; probabilistic/Bayesian/ensemble	Monte Carlo bootstrap; Sobol analysis; Gaussian processes; deep ensembles; Bayesian inference	SALib; Pyro; GPyTorch;	[40]
Decision optimization	Identifies strategies under multiple objectives, constraints, and uncertainties.	Evolutionary/swarm; Bayesian/surrogate-based optimization	GA; PSO; MOPSO; NSGA-II; Bayesian optimization; multi-objective optimization	DEAP; pymoo; BoTorch; MATLAB	[38]
Feedback control	Implements control actions and returns physical responses for model updating.	Model-based and learning-based control	MPC; reinforcement learning; fuzzy/neuro-fuzzy control; PID; adaptive critic	MATLAB/Simulink; Stable-Baselines3; Gymnasium	[41,42]

Note: The methods and frameworks listed are representative rather than exhaustive. Individual methods may support multiple digital-twin functions, and the listed platforms do not necessarily correspond to every reviewed case.

Abbreviations: DT, Digital Twin; DA, Data Assimilation; DART, Data Assimilation Research Testbed; PCA, Principal Component Analysis; SVM, Support Vector Machine; LSTM, Long Short-Term Memory; VAE, Variational Autoencoder; PINNs, Physics-informed Neural Networks; ML, Machine Learning; DeepONet, Deep Operator Network; FNO, Fourier Neural Operator; GPR, Gaussian Process Regression; XGBoost, eXtreme Gradient Boosting; SALib, Sensitivity Analysis Library; GPyTorch, Gaussian Process PyTorch; GA, Genetic Algorithm; PSO, Particle Swarm Optimization; MOPSO, Multi-Objective Particle Swarm Optimization; NSGA-II, Non-dominated Sorting Genetic Algorithm II; DEAP, Distributed Evolutionary Algorithms in Python; MPC, Model Predictive Control; PID, Proportional–Integral–Derivative.

efficiency of data-driven predictions^[30,44]. Adaptive methods update model parameters or representations as new observations become available or environmental conditions change, thereby reducing model drift. Uncertainty-quantification methods characterize uncertainties arising from observations, parameters, model structure, and future scenarios through confidence intervals, probability distributions, or sensitivity estimates^[28].

At the level of decision optimization and feedback, AI-supported optimization repeatedly evaluates updated system states and predicted trajectories to search large decision spaces and identify management or control strategies under multiple objectives and constraints^[30]. Controllers or decision-support interfaces then translate these strategies into operational recommendations, human-mediated interventions, or automatically implemented actions^[25,45].

The resulting physical response is subsequently observed and returned to the virtual model for further updating, completing the information and decision loop. AI extends the functional capabilities of a dynamically coupled digital twin toward adaptive prediction, uncertainty-aware decision support, and feedback optimization^[20].

Conceptual boundaries, operational maturity, and evaluation

Physical–virtual coupling and AI enablement should be evaluated as two related but distinct dimensions. The former reflects the automation, direction, and feedback of data exchange, whereas the latter reflects the extent to which AI supports state updating, prediction, uncertainty assessment, decision-making, or control. A system may therefore use advanced AI while remaining an offline model, whereas a dynamically synchronized digital twin may employ only limited AI functionality^[17,18].

Digital-twin maturity should be assessed according to the demonstrated level of physical–virtual integration and operational implementation, whereas performance should be evaluated in a fit-for-purpose manner across predictive validity, operational reliability, model credibility, and system-level functionality^[46–48]. Evaluation should be conducted at both the module and system levels, because improvements in an individual sensing, prediction, or optimization module do not by themselves demonstrate the maturity or effectiveness of the complete digital twin^[30,49]. Specific validation and reporting requirements are discussed in Section 5. Accordingly, the applications reviewed in Section 3 are classified according to their demonstrated level of physical–virtual integration and operational implementation; systems limited to offline simulation, one-way monitoring, or standalone AI prediction are not described as fully bidirectionally coupled digital twins.

Digital-twin-related applications and maturity levels in environmental research

In recent years, digital-twin-related research has been increasingly explored in environmental science^[7]. Applications of digital twins have evolved from proof-of-concept studies and localized demonstrations to scenario-driven implementations for system optimization, state awareness, and decision support. AI and machine learning (ML) have played an increasingly important role in this transition by enhancing data assimilation, anomaly detection, predictive inference, and system optimization.

The application domains reviewed in this section were selected according to three criteria. First, methodological representativeness requires each domain to demonstrate one or more key technical functions of AI-enabled digital twins, such as surrogate modeling, data assimilation, state reconstruction, anomaly detection, uncertainty quantification, forecasting, or operational optimization. Second, environmental relevance requires that system dynamics either be directly influenced by environmental variables or that system operation have consequential effects on pollutant discharge, resource consumption, environmental safety, or low-carbon transition. Third, cross-domain transferability requires that the underlying methods and integration strategies have potential relevance to other environmental systems, including air-quality forecasting, water-quality prediction, hazard assessment, and ecosystem monitoring.

Accordingly, this section focuses on three complementary domains: energy systems, water environment management, and natural environmental systems (Fig. 2). Energy systems combine selected nuclear and renewable-energy applications because both are closely coupled with environmental conditions and outcomes. Renewable-energy operation is directly constrained by meteorological and

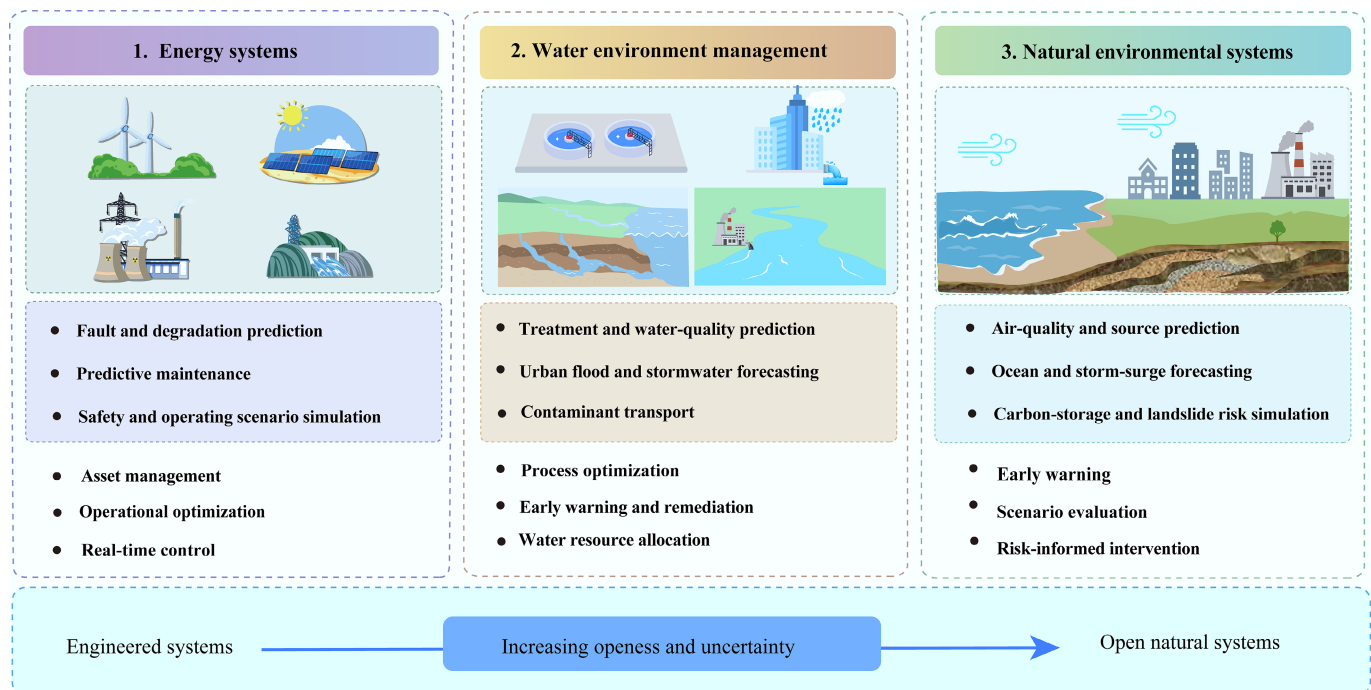


Fig. 2 Representative application domains of AI-enabled environmental digital twins. Current applications span energy systems, water environment management, and natural environmental systems, covering monitoring, prediction, optimization, and risk assessment under increasing system complexity and uncertainty. Icons representing industry, smart cities, wastewater treatment, and drainage systems were obtained from Flaticon under valid licenses, and were created by smashingstocks, Magnific, and Icon home.

hydrological inputs^[4,50], whereas the safety and operation of nuclear-energy infrastructure have important implications for resource use, cooling-water impacts, radioactive-release risks, and low-carbon transition. These two settings also provide contrasting but methodologically informative contexts for safety-critical monitoring, environmental-input forecasting, predictive maintenance, and coordinated optimization^[3,51]. Water environment management is included to represent engineered environmental systems in which monitoring, prediction, and operational decisions are directly associated with pollutant removal, water-quality protection, resource consumption, and receiving-environment impacts^[52]. Natural environmental systems extend the discussion beyond engineered facilities to spatially distributed, partially observed, and less directly controllable processes, including atmospheric pollution, marine and coastal hazards, and geological risks. The representative cases are systematically compared in [Supplementary Tables S1–S3](#) according to their application tasks, AI/DT functions, data sources and system scales, validation evidence, principal limitations, and demonstrated levels of physical–virtual integration.

Environmentally relevant energy systems

Although nuclear and renewable-energy systems differ substantially in their operating conditions and risk profiles, they share several core requirements for AI-enabled digital twins, including reliable state estimation, rapid prediction, predictive maintenance, scenario evaluation, and operational optimization. Nuclear applications operate within safety-critical and tightly regulated infrastructures^[53]. They therefore require stringent verification of abnormal-state predictions and intervention strategies^[3]. By contrast, renewable-energy systems involve distributed assets, multi-agent interactions, and strong dependence on stochastic meteorological and hydrological inputs^[50]. These differences shape how similar AI-enabled digital-twin functions are implemented in the two fields.

A first common function is AI-assisted virtual sensing for state perception. In both nuclear and renewable-energy systems, direct measurements may be limited by harsh operating conditions, sensor failure, physical inaccessibility, or incomplete spatial coverage. In a scaled AP1000 hot-leg case, a computational fluid dynamics (CFD)-trained DeepONet reconstructed pressure, velocity, and turbulence fields from limited inlet information and produced predictions approximately 1,481 times faster than a conventional finite-volume solver^[54]. Similarly, in a real-time wind-turbine implementation, an AI-based module estimated wind speed with a reported accuracy of 91.73% and reduced reconstruction error by more than 20% relative to the study baseline^[55]. These cases show that virtual sensing can improve system observability, supporting safety assessment and inspection planning in nuclear systems and real-time monitoring and condition assessment in wind-energy systems.

A second common function is predictive inference and scenario evaluation. In nuclear systems, a physics-informed neural network for primary-loop coolant prediction reduced the prediction error by 28.02% relative to the study baseline^[36]. Transformer-based models combined with Bayesian inference have also been used to forecast multiple accident-related parameters while quantifying predictive uncertainty^[33]. In addition, an operator-learning model predicted neutron-flux distributions with an R^2 greater than 0.99 and approximately 1,500-fold computational acceleration, enabling faster comparison of emergency-response options^[37]. In renewable-energy systems, forecasts of renewable generation and system loads support scenario-based operational evaluation under uncertain supply and demand conditions. For example, a digital-twin-enabled deep-learning framework evaluated day-ahead scheduling strategies for

an integrated electricity–gas–heat–electric-vehicle–thermal-storage system under load and renewable-energy uncertainties, reducing the average daily additional operating cost by 63.5% relative to conventional forecast-based methods^[56]. Across the two domains, AI-based predictive models enable more timely evaluation of possible system states and operating strategies. However, nuclear applications emphasize safety-critical transients, uncertainty-aware accident prediction, and emergency-response assessment, whereas renewable-energy applications focus on generation and load uncertainties, scenario-based scheduling, and coordinated operation across multiple energy carriers.

A third common function is the translation of predicted system states into maintenance and operational decisions. In nuclear systems, reconstructed thermal-hydraulic variables can reveal operating conditions associated with erosion, fatigue, and corrosion, thereby supporting degradation assessment and inspection planning. More broadly, nuclear-energy digital twins combine real-time monitoring and system-behavior prediction with condition-based maintenance and maintenance-schedule optimization, with the intended goals of improving safety and reducing unnecessary downtime^[53]. An advanced gas-cooled reactor proof-of-concept also integrated multiphysics models to simulate irradiation- and mass-loss-induced changes in graphite properties over the reactor operating life, supporting lifetime assessment and safety-informed maintenance^[1]. Renewable-energy digital twins apply similar functions to asset health management. For example, a digital twin for a 10-MW floating offshore wind-turbine drivetrain combined online measurements with dynamic and stochastic fatigue models to estimate component damage and remaining useful life under normal, faulty, and overload conditions, with uncertainty quantified using Monte Carlo simulations^[57]. Together, these examples show how predicted degradation and health states can be translated into inspection planning, maintenance scheduling, and asset-life management in nuclear and renewable-energy systems.

Overall, energy-system applications follow a perception–prediction–decision chain, although their operational maturity remains constrained by stringent safety requirements in nuclear systems and by system-level coordination challenges in distributed renewable-energy systems.

Water environment management

Water-environment applications span a gradient from bounded and directly controllable treatment facilities to spatially distributed and partially observable surface-water and subsurface systems^[48,52,58]. Along this gradient, the principal functions of AI-enabled digital twins shift from process-state estimation and operational optimization toward event forecasting, scenario evaluation, and coordinated management.

In wastewater treatment systems, digital twin applications have shifted from unit-level modeling and offline simulation toward operational optimization, energy management, and predictive maintenance^[34,35]. This transition is driven by highly variable influent conditions, strong process nonlinearity, and increasing demands for energy efficiency and carbon reduction^[38,41]. Mechanistic models are combined with operational data and AI-based soft sensors or surrogate models for process monitoring, effluent-quality prediction, and optimization of variables such as aeration and sludge recirculation^[59]. At the equipment level, an AI-assisted membrane bioreactor (MBR) control module reduced blower energy consumption from 0.12–0.15 kWh·t^{−1} to 0.06–0.12 kWh·t^{−1} relative to Proportional–integral–derivative (PID) control, while a Long Short-Term Memory (LSTM) model predicted membrane fouling with mean

absolute percentage error (MAPE) $< 6.45\%$, $R^2 > 0.87$, supporting proactive cleaning decisions^[38]. More integrated frameworks have linked online state modeling with control and risk assessment. An online digital-twin adaptive critic design combined an LSTM-based digital model with an action-critic controller and achieved lower dissolved-oxygen and nitrate-nitrogen tracking errors than PID control in Benchmark simulation model No. 1 (BSM1) simulations under three weather conditions^[41]. At the system level, an integrated framework combining the Internet of Things (IoT), hydraulic simulation, and an Adaptive Neuro-Fuzzy Inference System (ANFIS) achieved control-path latencies of approximately 9.51–11.01 s and a diagnostic precision of 89.3%, while its worst-case latency under blockchain-secured operation remained below 18 s^[35].

Treatment plants generally have well-defined boundaries and concentrated monitoring and control variables. Urban stormwater systems, by contrast, couple drainage infrastructure with spatially distributed rainfall, terrain, surface runoff, and receiving-water conditions^[48]. In these systems, digital twins integrate rainfall observations, drainage-network states, terrain data, and hydraulic models to support flood forecasting and the evaluation of drainage or blue-green infrastructure interventions^[42]. A representative experimental platform combined physical-virtual interaction, two-dimensional hydrodynamic simulation, deep-learning-based rapid prediction, and multi-objective pump scheduling to coordinate municipal drainage with changing river and lake levels. Urban flood-control decisions must therefore account for local runoff, drainage capacity, receiving-water backflow, and operating costs^[42,48].

At the watershed scale, system boundaries become more open, and management decisions extend beyond individual infrastructure operators. River-reservoir twins are being explored for algal-bloom mitigation, accidental contaminant containment, flood coordination, and adaptive water-quality management^[60]. At Wadi Dayqah Dam, an optimized variational autoencoder was used to construct a time-varying three-dimensional representation of reservoir water quality from 31,322 measurements, while explainable AI revealed approximately 37% variation in indicator weights across locations, depths, and sampling periods^[61]. This case illustrates how AI can improve reservoir-scale state reconstruction and water-quality assessment. In these open systems, the key challenge is not only forecasting environmental change but also converting forecasts into safe and accountable interventions involving reservoirs, gates, and other controllable infrastructure, often across multiple administrative jurisdictions^[58,60].

Groundwater systems present an even greater challenge because subsurface states are inferred indirectly from sparse observations and often evolve over long timescales^[62]. Applications therefore emphasize state reconstruction, contaminant-transport prediction, and the comparison of remediation scenarios rather than real-time operational control. At the Bemidji petroleum-contaminated site, a multiphase, multicomponent, multi-microbial, and non-isothermal model reproduced long-term field observations and was used to compare natural source-zone depletion with active remediation^[62,63]. At a multi-contaminant groundwater site in Suzhou, a machine-learning surrogate was coupled with ensemble-based data assimilation to reconstruct hydraulic heterogeneity and identify contaminant sources from sparse observations. The framework identified three contaminant sources within eight iterations and improved computational efficiency by 85.6%, demonstrating the value of AI-assisted surrogate modeling for rapid state and parameter updating^[32]. The central difficulty in this domain is the reliable characterization of subsurface states under sparse observations, geological heterogeneity, coupled transport-reaction processes, and decadal management horizons^[62].

At broader management scales, digital-twin schemes integrate hydrological forecasting, early warning, scenario rehearsal, and plan selection to support flood and drought management, reservoir release, sluice and pump operation, and water-resource allocation^[58]. Overall, as system boundaries expand from treatment facilities to watersheds and groundwater systems, AI functions shift from process control and operational optimization toward state reconstruction, event forecasting, and scenario evaluation, while direct feedback and operational validation become progressively more limited.

Natural environmental systems

Natural environmental systems extend digital twin applications beyond engineered facilities with relatively clear boundaries and controllable operating conditions. Atmospheric, ocean-coastal, and geological systems are open, multiscale, and only partially observable. Their evolution is governed by interactions among physical processes, environmental disturbances, and human activities. Accordingly, digital twins of natural environments place greater emphasis on multisource data assimilation, dynamic state reconstruction, process-based prediction, and uncertainty-aware decision support than on direct physical control. Across atmospheric, marine-coastal, and geological applications, this common functional chain links multisource observation and state updating with prediction, risk assessment, and human-mediated management responses. At a broader scale, Earth digital twins represent an emerging framework for integrating satellite observations, in situ measurements, Earth system models, and data-driven methods to continuously update environmental states and evaluate future natural and anthropogenic scenarios^[7,30].

In atmospheric systems, digital twins integrate multisource observations and predictive models to reconstruct pollutant fields and support human-mediated decisions. One atmospheric twin fused satellite, meteorological, and ground-monitoring data for district-scale PM_{2.5} estimation and policy recommendation across three cities^[64]. A field-connected twin in Elizabeth, New Jersey, combined real-time sensor data with spatiotemporal modeling to provide hourly air-quality maps, short-term forecasts, and a public decision-support dashboard^[65]. Beyond forecasting, atmospheric digital twins are also being explored for pollution-source inversion. A data-assimilation subsystem for an urban-atmosphere twin used adjoint-based sensitivity operators to reconstruct distributed NO emissions from synthetic Weather Research and Forecasting model coupled with Chemistry (WRF-Chem) observations in a Novosibirsk scenario^[66]. A simulation-based framework further combined reduced-order wind-field estimation, Bayesian source inversion, plume prediction, and pedestrian-flow optimization to support emergency evacuation planning in a campus-scale built environment^[67]. Overall, current applications remain largely at the methodological demonstration or project-development stage, with limited validation using long-term real-world observations.

Marine and coastal digital twins similarly combine satellite observations, buoys, tide gauges, hydrographic surveys, and numerical models to reconstruct ocean and coastal states. A representative example is the coastal-ocean digital twin prototype developed for the Wadden Sea, which downscaled large-scale ocean products by incorporating local bathymetry, seabed sediments, meteorological forcing, river discharge, and in situ observations used for model validation. The resulting high-resolution model reconstructed sea level, currents, waves, salinity, temperature, and suspended sediment at spatial resolutions of approximately 200–600 m, providing a process-based foundation for pollutant-transport analysis and extreme-water-level assessment^[68]. At Annapolis in the Chesapeake

Bay, an ensemble of random forest, eXtreme Gradient Boosting (XGBoost), gradient-boosting, and LSTM models integrated real-time monitoring data to predict short-term coastal water levels and flood-threshold exceedance under compound flooding conditions. Six-year validation yielded a root mean square error (RMSE) of 0.043 ft and an R^2 of 0.997; however, the single-site validation and strong sensitivity to recent water-level conditions limit the generalizability of the reported performance^[69]. Although the Wadden Sea prototype currently relies mainly on historical simulations rather than a fully operational real-time connection, it illustrates how regional observations and models can improve the representation of nearshore processes that are insufficiently resolved by large-scale ocean twins. Building on such hydrodynamic state reconstruction, coupled wind-wave-current digital twins have been proposed to support storm-surge forecasting, coastal inundation warnings, and the evaluation of alternative protection measures^[70].

In geological systems, digital twins are particularly valuable because subsurface states cannot be observed directly. For geological CO₂ storage, time-lapse seismic and well data can be combined with reservoir models to update estimates of CO₂ saturation and pressure and quantify uncertainty. A simulation-based digital shadow demonstrated multimodal state reconstruction, while a subsequent control-oriented prototype used the inferred pressure distribution to adjust CO₂ injection rate and reduce cap-rock fracturing risk^[71,72]. Landslide digital twins can transform static hazard assessment into dynamic stability forecasting and operational early warning. One study used rainfall, pore-water-pressure observations, and slope-performance records to update model parameters and predict changes in factor of safety and failure probability^[73]. A later operational system further integrated real-time monitoring and weather forecasts to provide rolling three-day stability forecasts and automatically issue alerts when thresholds were exceeded^[74]. Overall, natural-environment applications emphasize state reconstruction, forecasting, and warning-oriented decision support, but most remain at the digital-model, digital-shadow, or human-supervised stage because direct control and intervention-response validation are limited.

Taken together, the reviewed domains provide complementary and methodologically representative cases spanning different forms and levels of digital-twin development, rather than equally mature implementations or an exhaustive taxonomy of environmental digital-twin applications. Wastewater-treatment systems currently provide comparatively strong evidence of operational implementation^[49,52]. Renewable-energy systems have also progressed toward operational deployment in asset monitoring, predictive maintenance, environmental-input forecasting, remote diagnostics, and localized control^[4,75,76]. Nuclear applications remain at intermediate or safety-constrained stages, with many implementations confined to component-level, proof-of-concept, or human-supervised settings^[3]. Urban-stormwater and watershed applications also occupy intermediate stages, whereas groundwater, atmospheric, marine-coastal, and geological applications remain predominantly emerging^[48,58]. Across all domains, maturity depends not only on the performance of individual AI or modeling modules, but also on continuous physical-virtual synchronization, operational validation, decision implementation, and feedback^[46,51].

Accordingly, reported improvements in prediction accuracy, computational speed, energy use, downtime, or operating cost should be interpreted as evidence of performance gains for specific modules under defined baselines, scales, datasets, and validation conditions, rather than as general evidence of the maturity or effectiveness of the complete digital-twin system (Supplementary Tables S1–S3). The reviewed studies span offline digital models, one-way

digital shadows, DT-enabling AI modules, human-supervised decision-support systems, and a smaller number of bidirectionally coupled experimental or operational twins. These categories represent different levels of physical-virtual integration and operational implementation rather than equivalent levels of digital-twin maturity.

Key gaps and core challenges

Despite recent progress in digital twins across selected environment-related domains, several critical knowledge gaps remain:

i) Most reported environmental digital-twin initiatives remain at the level of digital shadows or human-supervised decision-support systems, with predominantly unidirectional information flow from the physical system to the virtual representation^[35]. Observational data are used to update models for state reconstruction or scenario simulation, but rarely feed back to the physical system for real-time control^[50,75]. This limitation arises from persistent mismatches between observation, modeling, AI-assisted analysis, and decision-making, including temporal lags, scale inconsistencies, and operational constraints. As a result, many current initiatives remain decision-support tools rather than fully bidirectionally coupled, adaptive environmental digital twins capable of timely intervention.

ii) Complex environmental behavior is often governed by microscale processes and mechanisms operating under extreme conditions, including pollutant transformation pathways, biochemical interactions, and system responses to climatic or disturbance extremes. However, these processes typically occur at spatiotemporal scales that are difficult to observe continuously. They range from nanoscale reactions to transient events, or occur under extreme conditions such as high temperature, high pressure, or strong radiation. This leads to a persistent lack of reliable data for model development and validation^[54,77].

iii) Environmental digital twins currently lack standardized system architectures, benchmark datasets, and trustworthy evaluation frameworks, partly because environmental systems have open boundaries, strong spatiotemporal heterogeneity, and uncontrollable disturbances^[13,78]. As a result, existing studies rely on heterogeneous data sources, model structures, and evaluation metrics, hindering comparability and reproducibility across applications^[40,48]. Validation is also frequently treated as a one-time activity, although changing observations, environmental states, data distributions, and model structures may progressively reduce digital-twin fidelity^[13,33,48,79]. Common requirements for independent validation, post-deployment performance monitoring, uncertainty reporting, latency, reproducibility, and applicability boundaries remain insufficiently standardized^[48,49]. More importantly, under extreme events or low-probability, high-impact conditions, the uncertainty, interpretability, and applicability of AI-enhanced predictions remain difficult to assess^[34,80,81]. Consequently, many environmental digital twins remain case-specific, with limited reliability and transferability in risk assessment and policy decision-making. These key gaps and corresponding research priorities are summarized in Fig. 3.

Outlook

Building upon the identified gaps, enabling robust environmental applications requires digital twins to move beyond simply increasing model complexity toward developing fit-for-purpose and adaptive environmental digital twin systems. Rather than pursuing full physical replication, environmental digital twins should balance model fidelity,

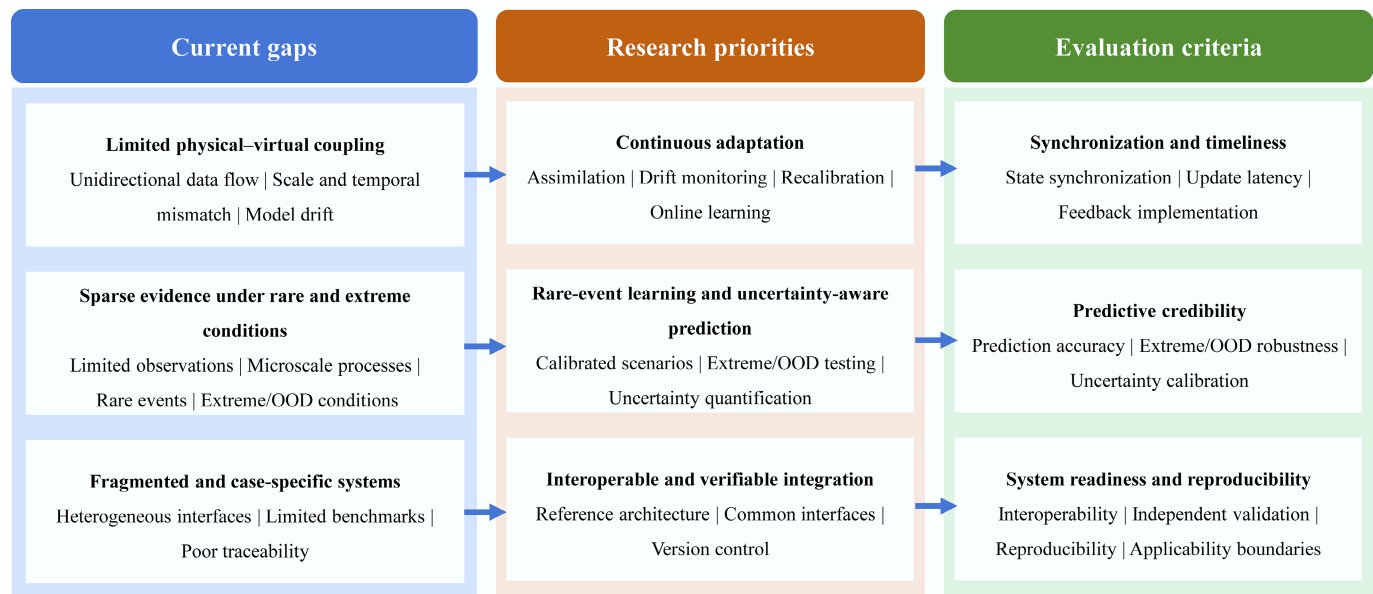


Fig. 3 Key challenges, research priorities, and operational evaluation criteria for AI-enabled environmental digital twins. Major challenges include limited physical–virtual coupling, insufficient learning under rare and extreme conditions, and fragmented system integration. Future development requires continuous adaptation, uncertainty-aware prediction, interoperability, and reproducible evaluation. OOD, Out-of-Distribution.

computational efficiency, operational robustness and adaptive learning capacity^[43]. Three interconnected tasks should be prioritized: continuous adaptation, learning under rare and extreme conditions, and interoperable and verifiable system integration.

First, continuous adaptation should be developed as a lifecycle capability rather than a one-time model update. This requires modeling frameworks that support continuous updating, where newly acquired observations are assimilated through data assimilation or online learning to enable dynamic calibration of system states. At the same time, processes that are difficult to observe or explicitly represent can be approximated using machine-learning-based surrogate models or parameterization strategies embedded within the overall system architecture^[30,40,82]. During operation, changes in observation quality, environmental states, data distributions, model structures, and decision tasks should be monitored. Such monitoring can detect model drift and trigger recalibration, retraining, or model replacement^[33,48]. Model assessment, parameter calibration, uncertainty quantification, and verification and validation should be integrated throughout the digital-twin lifecycle^[47].

Second, learning under rare and extreme conditions should be strengthened. Models trained primarily under routine conditions may become unreliable precisely when predictive support is most needed. In addition, addressing the scarcity of extreme-condition and fault data can be facilitated by digital-twin-oriented virtual environments and calibrated simulation platforms, where system dynamics are manipulated to generate representative rare-event datasets for AI training, uncertainty analysis, and predictive modeling^[2,41,83]. However, simulated scenarios should be calibrated against available observations where possible and should complement, rather than be treated as equivalent to, field evidence. Robustness should be evaluated separately under extreme and out-of-distribution conditions, and any performance degradation relative to routine conditions should be explicitly reported. Uncertainty should be reported through probabilistic outputs or prediction intervals. Contributions from observational errors, environmental variability, model parameters, and model structure should be distinguished where feasible^[40,81]. The reliability of uncertainty estimates

should also be evaluated, for example by comparing nominal and empirical coverage rates^[33].

Third, interoperable and verifiable system integration is required to transform isolated sensing, modeling, prediction, and optimization modules into operational environmental digital twins. This requires a unified architecture with clearly defined data and model interfaces for integrating heterogeneous observations, models, and computational components^[48,49]. These interfaces should connect in situ monitoring and remote sensing with model initialization, updating, and execution^[4,84]. Where feedback is intended, the architecture should also specify how decisions are implemented and how the resulting system responses update the virtual representation.

Evaluation and validation should be treated as continual and fit-for-purpose processes rather than one-time assessments^[13,49]. At the module level, sensing, state estimation, surrogate modeling, and prediction components should be evaluated against defined baselines and independent validation data^[33,47,48]. Reports should specify the task setting, system scale, data quality, computational cost, and deployment conditions. At the complete-system level, evaluation should address physical–virtual synchronization, data and model interoperability, feedback implementation, human oversight, update and decision latency, reproducibility, and operational robustness^[13,49]. For time-sensitive applications, end-to-end latency should be evaluated against the time available for the intended decision rather than reported only as an isolated computational metric.

Reproducibility requires versioned records of data, preprocessing procedures, models, software configurations, and update histories, together with sufficient reporting of performance metrics, uncertainty treatment, deployment conditions, and decision-use processes^[48,79]. Studies should clearly distinguish offline validation, experimental-platform testing, pilot deployment, and continuous operational implementation. They should also specify the spatial, temporal, environmental-state, and decision contexts within which the system has been validated^[13]. Evaluation thresholds should reflect the intended use and associated consequences of model failure^[40,43,84]. Shared benchmark datasets, reference architectures, and

standardized reporting templates would further improve cross-study comparison.

Building on these priorities, in applications such as nuclear system safety, pollution events, and extreme climate risks, digital twins should function as human-machine collaborative tools rather than fully autonomous decision makers. The system provides multi-scenario simulations and associated uncertainties. These outputs help assess potential outcomes and support adaptive risk assessment. Final decisions remain with human operators, who consider operational and societal constraints^[43,85]. At larger scales, emerging initiatives such as Destination Earth point toward integrated, multi-scale systems that couple environmental processes with human activities^[27,86], enabling interactive, scenario-based analyses under deep uncertainty^[28,87]. Together, these developments highlight the potential for environmental digital twins to evolve from case-specific applications into generalizable, scalable, and adaptive infrastructures for predictive environmental research^[88].

In addition to technical advances, the application scope of environmental digital twins can be further expanded. Building on the system-level applications reviewed above, the future development of AI-enabled environmental digital twins may extend toward both ends of the environmental information and decision chain. At the upstream end, advanced environmental sensing and analytical equipment determines the quality, resolution, and continuity of the real-world data used to initialize, calibrate, validate, and update environmental digital twins. At the downstream end, predictive digital toxicology can translate simulated environmental fate and exposure into biological effects and human or ecological health risks.

i) Environmental equipment development

At the upstream end of this framework, advanced environmental equipment provides the physical interface through which real-world environmental conditions are converted into data for environmental digital twins. Digital twins can also be applied to the equipment itself, enabling a mutually reinforcing relationship between environmental sensing and model-driven equipment development. Digital twins offer a pathway to enhance the development efficiency of advanced environmental equipment. As demands for sensitivity, resolution, and operational robustness continue to increase, the cost-effective fabrication of high-performance components remains a key challenge, particularly for systems such as mass spectrometry (MS) inlets and microfluidic sensors. These precision devices impose stringent requirements on fluid transport efficiency, structural stability, and signal reliability, making conventional "fabrication-testing-iteration" workflows time-consuming and costly. Although advances in rapid microfabrication technologies, e.g., 3D printing, have accelerated customized production, they mainly shorten the fabrication step but do not eliminate the need for iterative design optimization and performance validation^[89].

Digital twins provide a complementary solution by integrating fluid dynamics, structural mechanics, manufacturing processes, and AI-assisted optimization within a unified virtual environment^[15,90]. This enables pre-evaluation of complex flow pathways and functional structures at the design stage, reducing reliance on multiple rounds of physical prototyping. Moreover, computational-fluid-dynamics-based digital twins can support the optimization of flow channel configurations in gas monitoring systems and MS components. This reduces vortex formation and dead volumes, thereby improving transport efficiency and analytical stability. During manufacturing, digital twins can further couple in situ monitoring data with multiphysics models to identify potential defects in real time, providing a data-driven basis for quality control^[91,92]. AI algorithms may further identify nonlinear relationships among structural

parameters, operating conditions, manufacturing variables, and equipment performance, thereby supporting multi-objective optimization of sensitivity, stability, response time, and production cost.

When combined with rapid fabrication methods, such as 3D printing, digital twins may form a closed design-manufacturing-testing loop, in which virtual simulations guide component design, physical prototypes validate model predictions, and experimental feedback updates the digital model. Together, these capabilities point toward a shift from iterative prototyping to predictive, model-driven design. These advances can improve both the development of environmental instruments and the reliability of the observations they generate. Improved detection and characterization of pollutants, transformation products, and environmental conditions can, in turn, provide more robust inputs for simulating pollutant occurrence, transport, transformation, fate, and bioavailability. These simulations provide an important basis for subsequent exposure and toxicological assessment.

ii) Predictive digital toxicology

A further promising extension lies in environmental toxicology (Fig. 4), where increasing constraints on animal testing and the growing demand for alternative toxicity assessment are driving methodological shifts^[11,93,94]. In response to these challenges, computational approaches, ranging from Quantitative Structure-Activity Relationship (QSAR) models to AI-assisted predictive toxicology, have been widely adopted as substitutes or complements to experimental testing, enabling rapid screening of chemical risks for regulatory and risk assessment purposes^[95,96]. These approaches have greatly advanced toxicity prediction and chemical prioritization. However, many of them remain constrained by a structure-centric or task-specific paradigm, in which toxicity is often inferred as a static function of molecular structure or predefined toxicity endpoints^[97]. As a result, they often oversimplify real-world environmental systems by focusing on single compounds and fixed toxicity endpoints. They neglect critical factors such as environmental conditions and mixture interactions, as well as dynamic processes including transport, transformation, and bioavailability^[95,98]. In addition, their applicability is limited to specific chemical domains^[99,100] and they remain insufficient for predicting chronic, population-level, or ecosystem-scale effects^[95,97].

To address these limitations, digital twins offer a transformative conceptual framework that can extend traditional computational modeling by integrating population-level exposomics with human-relevant biological platforms and predictive modeling^[101]. When connected with environmental monitoring and process-based digital twins, this framework can link the time-varying occurrence, transport, transformation, and bioavailability of pollutants with external exposure, internal dose, and biological responses. AI can facilitate these connections through multi-source data integration, pattern recognition, surrogate modeling, and continuous model updating. Digital twins are not merely another toxicity prediction model; rather, they could provide a closed-loop framework that connects exposure dynamics, biological mechanisms, AI-assisted prediction, and experimental validation. In this sense, digital twins can serve as a system-level framework for applying AI more effectively in environmental toxicology.

Medical digital-twin research and adjacent in silico approaches provide methodological precedents through virtual individuals and populations for longitudinal model updating, individualized simulation, and population-level testing (Supplementary Table S4)^[102–105]. These studies are treated as precedents rather than equally mature digital-twin implementations because they span different levels of physical-virtual integration. Virtual populations have already

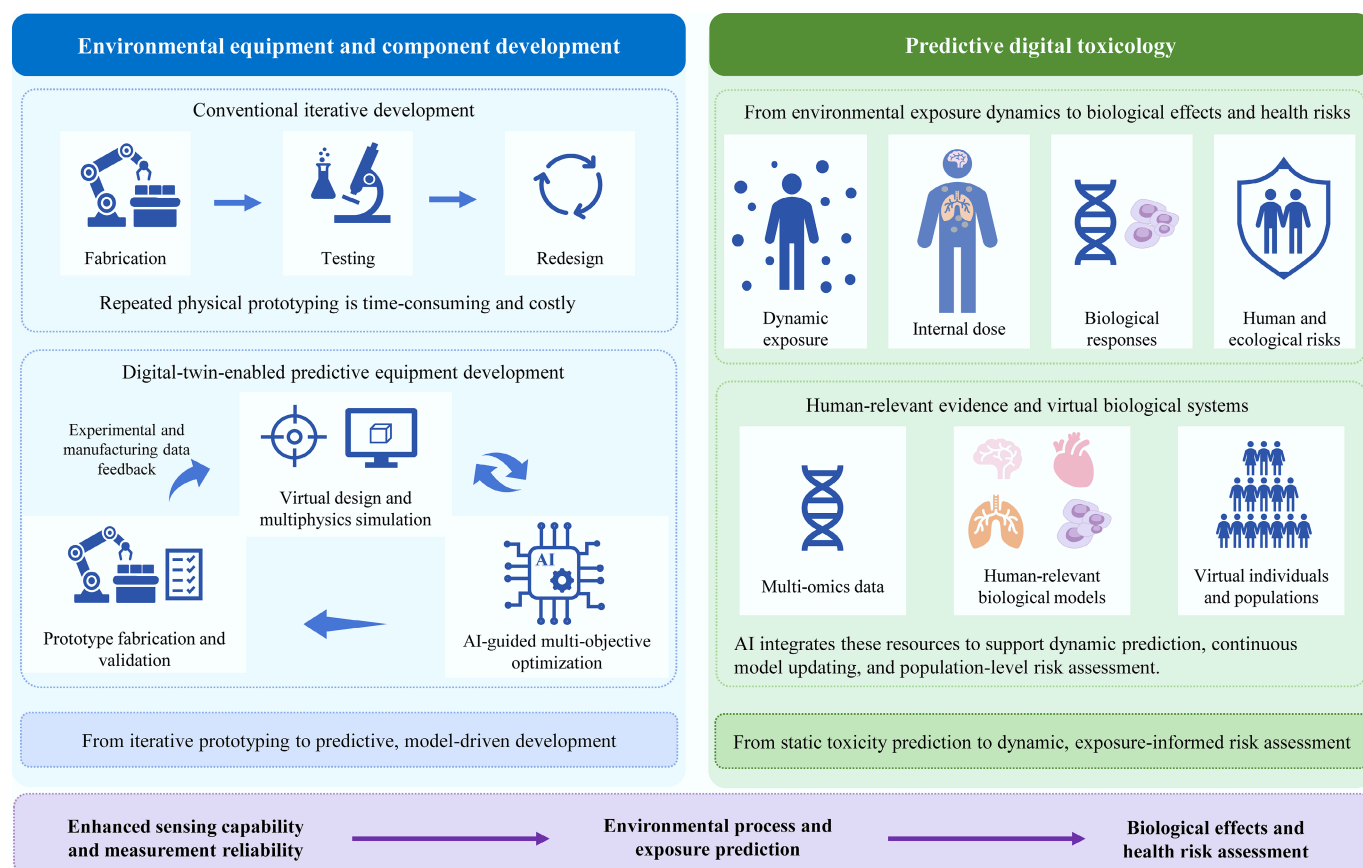


Fig. 4 Prospective extensions of AI-enabled environmental digital twins across the environmental information and decision chain. Two emerging directions are highlighted: digital-twin-assisted environmental equipment development for improved sensing capability and predictive digital toxicology for exposure-informed health-risk assessment.

enabled large-scale cardiac drug safety testing in synthetic cohorts^[44,102,106] and provide a methodological foundation for extension to environmental health. Building on this, digital twins can integrate multi-omics data with patient-derived organoids (PDOs) to simulate individual responses under diverse exposure scenarios. When coupled with spatially and temporally resolved exposure fields generated by environmental digital twins, these virtual biological systems could simulate how different individuals or populations respond to long-term, low-dose, and combined exposure to environmental pollutants. This approach captures inter-individual variability in responses to complex chemical mixtures and enables more dynamic, personalized risk assessment, shifting beyond population-averaged evaluations. However, environmental digital twins face key challenges, including the extreme complexity of chemical mixtures, sparse longitudinal exposure data, and the lack of quantitative Adverse Outcome Pathways (qAOPs)^[107,108]. The interpretability, transferability, and validation of AI-assisted toxicological predictions also remain important challenges. A staged development pathway is therefore needed: near-term validation using priority pollutants with well-characterized mechanisms, mid-term extension to defined mixtures, and long-term development of multi-organ or whole-body toxicological digital twins integrating multi-scale exposome data.

By linking environmental process and exposure predictions with biological-response models, predictive digital toxicology could support biological-effect and health-risk assessment, exposure reduction, and environmental intervention. Renewed environmental and biological monitoring could then update the digital twin and

support an iterative observation–prediction–assessment–intervention process.

Conclusion

Taken together, AI enablement and physical–virtual coupling should be treated as related but distinct dimensions of environmental digital twins. AI strengthens state estimation, prediction, uncertainty assessment, and optimization, whereas digital-twin maturity depends on sustained physical–virtual synchronization and implemented feedback. Current maturity remains uneven, and validated system-level feedback is still uncommon (Table 1 and Supplementary Tables S1–S3). Future progress requires continuous updating, fit-for-purpose and transparent evaluation, interoperable architectures, and reliable feedback under changing and extreme conditions. Advanced environmental equipment supplies the observations needed to update virtual representations, system-level twins translate these data into predictions and decisions, and predictive digital toxicology extends this chain toward exposure and health-risk assessment. Integrating these layers may shift environmental research from passive monitoring and isolated prediction toward a traceable, adaptive, and decision-oriented paradigm.

Electronic supplementary information

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Author disclosure requirements for AI usage

During the preparation of this work, the authors used ChatGPT (accessed in August 2026) for writing assistance, language refinement, and preliminary visual ideation. The tool was used to improve language clarity, grammar, readability, and editorial consistency, and to explore possible figure layouts during the initial design stage. All final figures were independently redesigned and assembled by the authors using Microsoft PowerPoint and Adobe Illustrator. No AI-generated image was directly incorporated into the final figures. Five licensed icons obtained from Flaticon were used and are acknowledged in the relevant figure captions. The authors reviewed and edited all AI-assisted content, verified its scientific accuracy, and take full responsibility for the integrity, originality, and final presentation of the manuscript. No AI tool is credited as an author.

Author contributions

The authors confirm their contributions to the paper as follows: Dawei Lu conceived the idea, developed the core framework, supervised the work, and reviewed and revised the manuscript. Yuyao Qin wrote the original draft, collected and reviewed the literature, and prepared the figures. Yuehan Wu, Yifei Liu, Yuming Huang, Huixuan Yi, Xiangyu Li, Xiao Zhang, Lijun Song, Yongfeng Lin, and Guibin Jiang contributed to reviewing and editing the manuscript. All authors read and approved the final manuscript.

Data availability

Data sharing is not applicable to this *Perspective*, as no datasets were generated or analyzed during the preparation of this article.

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Declarations

Competing interests

The authors declare no competing interests.

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