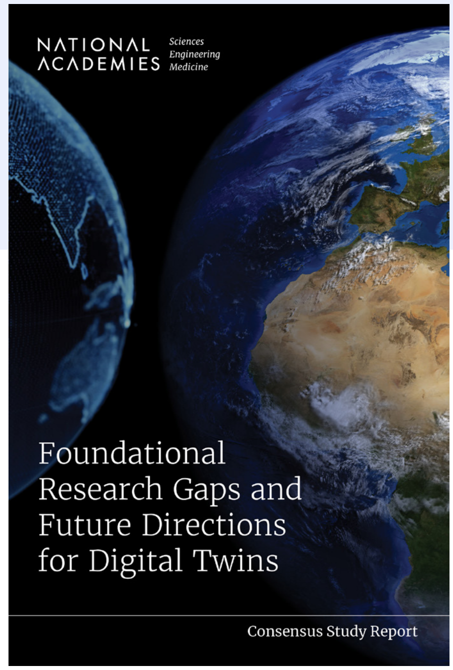
Foundational Research Gaps and Future Directions for Digital Twins



Excitement is growing about the potential of digital twins to transform scientific research, industrial practices, and many aspects of daily life. A digital twin couples computational models with a physical counterpart to create a system that is dynamically updated through bidirectional data flows as conditions change. Going beyond traditional simulation and modeling, digital twins could enable improved medical decision-making at the individual patient level, predictions of future weather and climate conditions over longer timescales, and safer, more efficient engineering processes.

However, many challenges remain before the full potential of digital twins can be realized. There are gaps in the foundational mathematical, statistical, and computational research that underlies digital twin technology, in addition to broader systemic and translational challenges. At the request of the Department of Defense, the Department of Energy, the National Institutes of Health, and the National Science Foundation, this report identifies the key research needed to overcome these challenges and offers practical recommendations to help bring the promise of digital twins to fruition. Learn more and download the report at https://nap.nationalacademies.org/catalog/26894.

WHAT IS A DIGITAL TWIN?

The report uses the following definition of a digital twin:

> A digital twin is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems), is dynamically updated with data from its physical twin, has a predictive capability, and informs decisions that realize value. The bidirectional interaction between the virtual and the physical is central to the digital twin.

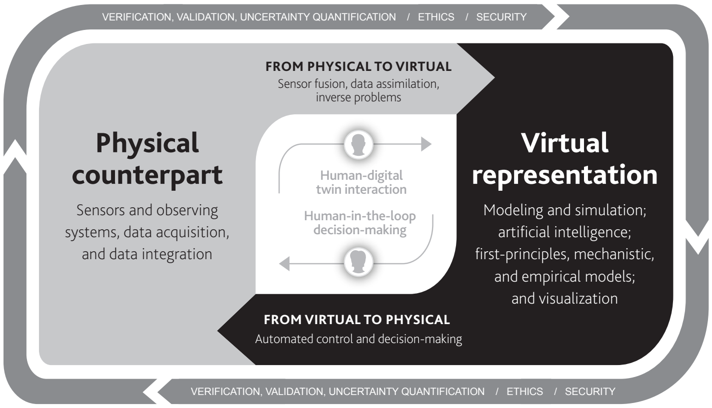


FIGURE 1 Elements of the digital twin ecosystem.

A digital twin is more than just simulation and modeling. The key elements (see Figure 1) that comprise a digital twin include:

- Modeling and simulation to create a **virtual representation** of a physical counterpart.
- Observations from the **physical counterpart** to inform and improve the virtual representation. These data could be acquired from onboard or in situ sensors, remote sensing, automated and visual inspections, operational logs, or imaging.
- **Bidirectional interaction** between the virtual and the physical. Data from the physical counterpart are used to dynamically update the virtual representation, and predictions and simulations from the virtual representation drive changes in the physical counterpart or in its sensor and observing systems. The decision-making involved in these changes may be fully automated, for example, in automated sensor steering, may rely on human interaction, or may include a combination of both.
- **Verification, validation, and uncertainty quantification (VVUQ)** to build confidence and trust in the digital twin and establish boundaries for the use of simulations.

FUTURE APPLICATIONS OF DIGITAL TWINS

With potential applications in biomedical research, atmospheric science, engineering domains, and more, digital twins could lead to improved health, more efficient operations and production strategies, and an improved understanding of scientific processes. Examples include the following sections.

Medicine and Biomedical Research

The digital twin of a cancer patient and tumor could inform clinical decisions such as treatment options and clinical assessments (see Figure 2). Other potential applications in the biomedical realm include digital twins of patients with cardiovascular disease and osteoporosis.

Aircraft Engine

The digital twin of an aircraft engine could be leveraged for tasks such as optimizing fuel efficiency in real time, predicting parts that may soon need replacement for efficient inventory management, and assessing and planning for carbon emission reduction. In this application, the virtual representation could include machine learning models trained on a large database of sensor data and flight logs collected across a fleet of engines. Quantities of interest might include computational estimates of possible blade material degradation.

Earth Systems

In this as-yet aspirational application, a collection of high-fidelity, high-resolution physics models and associated surrogate models, collectively representing coupled atmospheric, oceanic, terrestrial, and cryospheric physics, could be used to create large-scale atmospheric, climate, and sustainability digital twins. These digital twins could potentially provide predictive insights such as future global mean temperature or extreme precipitation events and help support decisions related to policy-making, deployment of new observing systems, and emergency preparedness.

THE NEED FOR AN INTEGRATED RESEARCH AGENDA

In general, interest and enthusiasm around digital twin solutions currently outweighs evidence of their success. Separating the aspirational from the actual would strengthen the credibility of digital twin research and help to identify the critical knowledge gaps that remain. Realizing the potential of digital twins will require an integrated research agenda that includes

Digital Twin of a Cancer Patient and Tumor

This example of a digital twin demonstrates the dynamic bidirectional interaction between the real world patient and digital twin to inform clinical decisions regarding interventions including treatments and clinical assessments, which in turn informs the digital twin.

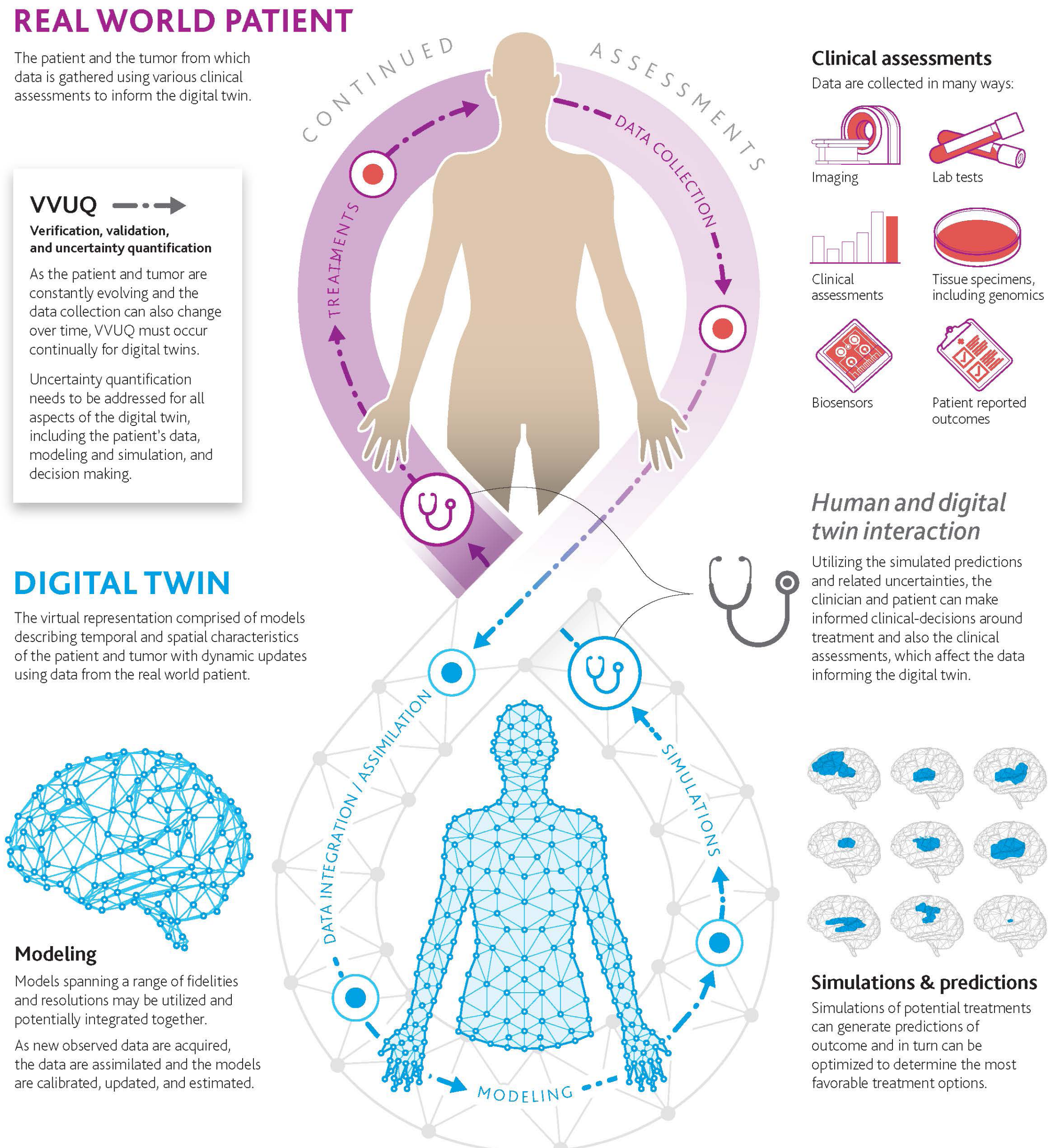


FIGURE 2 An example of a digital twin for a cancer patient and tumor.

foundational needs in basic mathematical, statistical, and computational research that span multiple domains, as well as domain-specific research. The report calls for **federal agencies to launch new crosscutting programs to advance mathematical, statistical, and computational foundations for digital twins,** recommending specific actions for each of the report's sponsoring agencies**. As new digital twin–focused efforts are created and**

launched, federal agencies should identify opportunities for cross-agency interactions and facilitate cross-community collaborations.

THE NEED FOR COMPUTATIONAL RESOURCES FOR VIRTUAL REPRESENTATIONS

The report notes that the digital twin virtual representation should be fit for purpose, meaning that the virtual representation—model types, fidelity, resolution, parameterization, and quantities of interest—be chosen, and in many cases dynamically adapted, to fit the particular decision task, the available computational resources, and the acceptable cost. For example, the intended use of a digital twin will determine the frequency at which data are collected from the physical counterpart and used to update the virtual representation. The digital twin for an intensive care unit may require updates from sensor data that are acquired in close to real time, while the digital twin for an ambulatory care system may be updated with electronic health record data on a more sporadic basis.

Although different applications of digital twins drive different requirements for modeling fidelity, precision, and accuracy, many potential applications are currently intractable—meaning that the digital twins and their underlying models are so complex they cannot be solved in a timely manner with existing computational resources. With current computational capabilities, there may be a gap between the scale of the virtual representation and the scale needed to draw predictive insights and support decision-making.

The report recommends that, **in crafting research programs to advance the foundations and applications of digital twins, federal agencies should create mechanisms to provide digital twin researchers with computational resources recognizing the large existing gap between simulated and actionable scales and the differing levels of maturity of high-performance computing across communities.**

Algorithmic advances would reduce computational and data requirements, helping close the gap between simulated and actionable scales, and are an important complement to increased computing resources. Particular opportunities are in hybrid modeling—which leverages the best of data-driven, machine learning, and model-driven formulations—and surrogate modeling approaches.

STRENGTHENING VERIFICATION, VALIDATION, AND UNCERTAINTY QUANTIFICATION

Given the potential use of digital twins in critical decision-making for engineering, medical, and scientific applications, VVUQ should be deeply embedded in the design, creation, and deployment of digital twins to establish trust in the virtual representation and give measures of the quality of predictions. However, despite the growing use of artificial intelligence, machine learning, and empirical modeling in engineering and scientific applications, there is no standard process for reporting VVUQ and little consideration of confidence in modeling outputs. The report recommends that **federal agencies should ensure that VVUQ is an integral part of new digital twin programs.**

Developing robust VVUQ processes for digital twins remains a challenge. Some elements of digital twin VVUQ processes are shared with those developed for other computational models, but there are also key differences. VVUQ for digital twins should be a continual process that adapts to changes in the physical counterpart and its virtual representation, in data inputs, and in the prediction or decision tasks at hand. Research priorities include continual verification, continual validation, VVUQ in extrapolatory conditions, and scalable algorithms for complex multi-scale, multi-physics, and multi-code digital twin software efforts.

SYSTEMIC AND TRANSLATIONAL INVESTMENTS

In addition to foundational research needs, there are also research needs and opportunities that cut across domains and use cases.

Evolution and Sustainability of Digital Twins

Over time, each digital twin will likely need to meet new needs for decision support, incorporate updated models, or adapt to new data sources to maintain accuracy. Meeting these evolving needs will require investments to sustain the digital twin that parallel investments made to sustain and maintain the physical counterpart, as well as workflows and design processes that accommodate revisions. **Federal agencies should each conduct an assessment for their major use cases of digital twin needs to maintain and sustain data, software, sensors, and virtual models beyond their initial creation.**

Collaboration Between Domains

Although many digital twin challenges are specific to a particular field of study or application, others cut across domains and use cases, such as advancing broad modeling techniques or solving data curation issues. Different domains may have varying levels of maturity in the development of digital twin components—for example, the Earth system science community is a leader in data assimilation, many engineering fields have developed ways to integrate VVUQ into simulation-based decision-making, and the medical community has led human-centered decision-making. Cross-domain collaboration would help translate the advances made within disciplinary communities to benefit all disciplines. **Federal agencies should identify targeted areas relevant to their individual or collective missions where collaborations with industry would advance research and translation.**

Models and Data Collaborations

The international climate research community has a history of sharing models and exchanging data that has proven beneficial to furthering climate modeling capabilities. A greater level of coordination would also benefit the maturation and adoption of digital twins in other domains. **In defining new digital twin research efforts, federal agencies should (1) establish forums to facilitate good practices for collaborative exchange of data and models across disciplines and domains, while addressing the growing privacy and ethics demands of digital twins; (2) foster collaborative exchange of data and models; and (3) explicitly consider the role for collaboration and coordination with international bodies.**

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FOR MORE INFORMATION
This Consensus Study Report Highlights was prepared by the National Academies' Board on Mathematical Sciences and Analytics, Computer Science and Telecommunications Board, Board on Life Sciences, and Board on Atmospheric Sciences and Climate based on the report *Foundational Research Gaps and Future Directions for Digital Twins* (2023).

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