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Request for Information on the National Digital Twins R&D Strategic Plan

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NASA, Earth Science Technology Office (ESTO), Advanced Information Systems Technology (AIST) Program

Response to "Networking and Information Technology Research and Development Request for Information on Digital Twins Research and Development"

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Who We Are

This response to the NITRD RFI for Digital Twins is from NASA's Advanced Information Systems Technology (AIST) program. As part of NASA Earth Science Technology Office, the Advanced Information Systems Technology (AIST) Program identifies, develops, and supports the adoption of software and information systems, as well as novel computer science technologies expected to be needed by NASA's Earth Science Division in the 5-10-year timeframe. Projects under this Program start at a Technology Readiness Level (TRL, [1]) from 1 to 3 and usually advance one or two TRLs before completion. AIST information systems and software technologies contribute to the entire data lifecycle, as represented in Figure 1, from the acquisition of new measurements and the design of new observing systems to onboard intelligent data understanding and decision making and all the way to data analytics and extraction of the "science data intelligence" needed to create actionable information. Within that framework, AIST focuses on three thrusts:

(1) The first one, *Novel Observing Strategies (NOS)*, enables new observation measurements and new observing systems design and operations through intelligent, timely, dynamic, and coordinated distributed sensing. This contributes to the first part of the data lifecycle.

(2) The second thrust, *Analytic Collaborative Frameworks (ACF)*, enables agile science investigations that fully utilize the large range of diverse observations using advanced analytic tools, visualizations, and computing environments. This addresses the second part of the data lifecycle.

(3) The third thrust, *Earth System Digital Twins (ESDT)*, enables the development of integrated Earth Science frameworks that mirror the Earth with state-of-the-art models (Earth system models and others), timely and relevant observations, and analytic tools. These information systems can be used for supporting near- and long-term science and policy decisions. Here "science decisions" include planning for the acquisition of new measurements, development of new models or science analysis,

integration of Earth observations in novel ways as well as various applications to inform choices, support decisions, and guide actions, e.g., related to climate change or for societal benefit. ESDT frameworks will build upon NOS and ACF technologies to integrate a continuous stream of observations, interconnected models, data analytics, data assimilation, simulations, advanced visualizations and the ability to conduct "what-if" scenarios, for example to assess the impact of human activity on natural phenomena. Therefore, technologies associated with ESDT contribute to the entire data lifecycle, as shown in Figure 1.

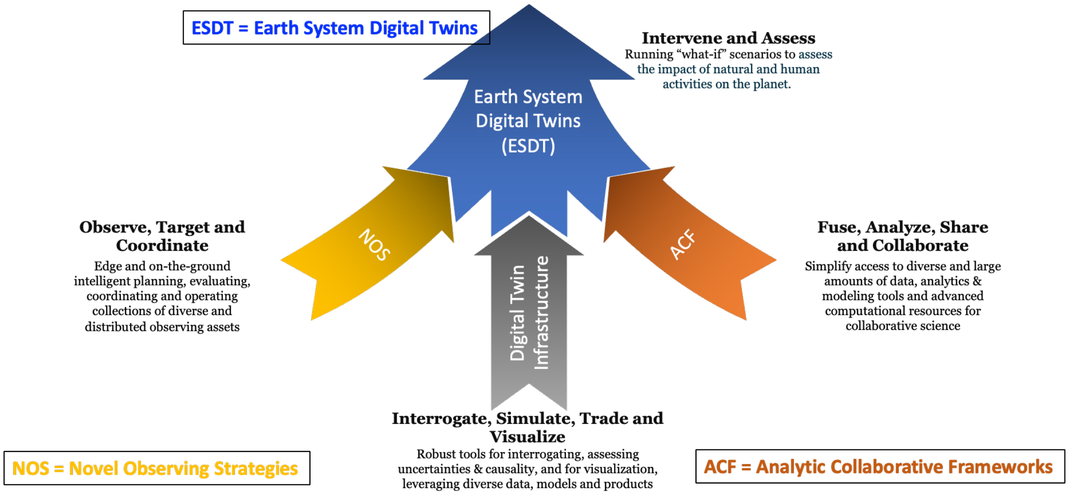

Figure 1 – ***The AIST Program Spans the Entire Earth Science Data Lifecycle***

This response document addresses several topics of interest stated in the RFI: **Artificial Intelligence, Data, Ecosystem, Long Term, Standards, and VVUQ.**

What is a Digital Twin?

The National Academies report "Foundational Research Gaps and Future Directions for Digital Twins (2023)" defines digital twins as follows:

> *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.*

A key omission from this definition is within the predictive capability. The digital twin should not only allow for prediction given the current and past states and actions and planned future actions, but also given **alternative** current and past states and actions and various future actions – What-if scenarios. The AIST program conducted a workshop on Earth System Digital Twins (ESDT) October 26-28, 2022 in Washington, D.C., USA. The workshop report [2] defines ESDTs, but the definition can be easily generalized to digital twins:

> *An Earth System Digital Twin or ESDT is a dynamic and interactive information system that first provides a digital replica of the past and current states of the Earth or Earth system as accurately and timely as possible; second, allows for computing forecasts of future states under nominal assumptions and based on the current replica; and third, offers the capability to investigate many hypothetical scenarios under varying impact assumptions. In other words, an ESDT provides the integrated "What-Now, What-Next, and What-If" pictures of the Earth or Earth system, by continuously ingesting newly observed data and by leveraging multiple interconnected models, machine learning as well as advanced computing and visualization capabilities.*

In particular, our definition of Earth System Digital Twin **distinguishes *what-next* from *what-if***. The what-if capability enables predictions of the outcomes of different decisions to enable exploration of new ideas and their benefits and drawbacks (e.g., how much the average temperature in a city decreases as a function of the density of trees planted). This what-if capability is likely helpful in many other domains as well, such as engineered systems, where changes in maintenance strategies (time between maintenance, conditions under which maintenance is performed, specific tasks conducted during maintenance) can be explored for short-term and long-term impact.

Core components of digital twins

1. Sources of Data

The Novel Observing Strategies (NOS) AIST thrust described above illustrates the need for not only different sensors and platforms as sources of raw data, but also the need for coordinated, distributed, timely sensing. The data lifecycle in figure 1 is a true cycle---in many cases, data collected in the past is run through data analytics and visualization to produce not only useful insights, but suggestions for additional data to be collected in the future. Such a sensing system is necessary for digital twins, as they must be able to assimilate the latest data and request additional data in some cases to help improve the twin's accuracy. The types of data needed will vary across domains. However, in general, the data required may relate to the system for which the digital twin is produced, the environment in which the system operates, and the actions of people who interact with the system, and possibly others.

Earth System Digital Twins will fuse data from multiple sensors to build a digital replica and to drive forecasts and what-if scenarios. Calibration (geometric and radiometric) has a big impact on data fusion quality and uncertainty. Well-calibrated instruments have a higher effective data value due to smaller errors propagating through the data processing, fusion, and analysis chain. Vicarious calibration against a network of reference sites can provide frequent, accurate calibration.

2. Domain Knowledge

The knowledge of domain experts who know the system for which the digital twin is being produced is important and should be codified for use within the digital twin. In some cases, the knowledge is in the form of physics-based mathematical models (e.g., global climate models), while in other cases, the knowledge may be a set of rules. In some cases, the experts themselves may serve as direct sources of knowledge during the operation of the digital twin. For example, there are human in the loop (HITL) simulations of the National Air Space (NAS) in which human air traffic controllers issue instructions to simulated aircraft.

3. Data-Driven Models

Data-Driven Models are models developed to fit past data. Machine Learning is a discipline within Artificial Intelligence that develops such methods. There is much press currently around generative models, which are a class of Machine Learning models that learn to model the process that generated the data or could have generated the data. Machine Learning models are a critical component of digital twins. These would be used in cases where the domain knowledge is limited (e.g., physics-based models are inaccurate) or the mathematical models are too slow to run in a real-time simulation. Machine Learning models that quickly provide approximations to physics-based models are often referred to as surrogate models. In many cases, both physics-based models and data-driven models may be used, with each one being used where most appropriate, for example, trading off accuracy and speed, or different models being more accurate in different situations (e.g., physics-based models may not work well in off-nominal situations), or output of physics-based models being used to train data-driven models. Data may be an important part of this tradeoff between accuracy and speed. For example, in Earth Science, data of different spatial and temporal resolutions is available, where lower resolution data enables rapid calculations but yields lower accuracy while higher resolution data enables greater accuracy but requires greater running time. Machine Learning models that provide predictions plus measures of confidence (e.g., an error bar), such as Gaussian Processes, can be particularly helpful, as they can quickly provide an answer which may be deemed good enough if the error bar is small, or which can prompt running a physics-based model if the error bar is too high. Overall, one may obtain comparable accuracy to running a physics-based model every time, but at much lower computational cost.

4. Computational Systems

All of the digital twin components described earlier require computer systems. One or more systems ranging from desktop computers to traditional on-prem supercomputers, cloud-based systems, and edge computers may be used. Within these, there may be different types, such as traditional CPUs, GPUs, TPUs, and FPGAs may be used. Of course, significant data storage is also needed. Whenever multiple computer systems are used, the communications infrastructure will be critical. In some domains, such as Earth Science, the digital twin may span a vast geographic area, so the computer and communications infrastructure will span a large area. The communications reliability will be relatively low over a large geographic area, therefore, having more compute power closer to the data required is preferred. There are several architectural models that can be considered for providing high-end computing needed for digital twin tools and services. Conventional High-Performance Computing (HPC) batch processing is perhaps the most obvious, and other architectures include interactive HPC environments, Jupyter Notebook Orchestration, Dedicated Project Environments, edge computing, and Software-Defined Systems and Networks.

5. Visualization

Domain experts and others must be able to understand the insights produced by the digital twin. In some domains, traditional simple plots may be sufficient or even preferred. However, in data-intensive areas such as Earth Science, immersive visualization, such as Virtual Reality (VR), Augmented Reality (AR), and eXtended Reality (XR), is a potentially disruptive paradigm that would allow users to explore complex data in intuitive ways to obtain insights. Immersive visualization can overcome limitations of two-dimensional (2D) displays, such as constrained screen size. Immersive visualizations also provide interactions that are more natural to our senses, which can improve understanding and retention. For example, studies have shown that people are better at remembering items they experienced in an immersive visualization than a 2D display.

Technology gaps include:

- Human factors for improving ergonomics and productivity.
- High-level software Application Programming Interfaces (APIs) for streaming digital twin data for ingestion into extended reality systems.
- If needed, headsets that are lightweight with high-resolution and wide field-of-view.

And some of the major challenges include:

- Development of algorithms for analyzing, visualizing, and deriving insights from large scale, multi-modal streaming datasets.
- Advances in visualization, Artificial Intelligence (AI), ML, human factors, and digital twin general domain expertise.
- Development of a workforce that intuitively understands and leverages the power of VR, AR, and XR.

6. Data Science and Interactive Data Analysis

One of the important uses of a digital twin will be analysis of data, models, and projections to better understand processes and their trends and impacts. AI and Data Science technologies can address challenges in developing interactive data analysis and modeling capabilities, such as:

- Interactive analytics
- Automated multi-scale, multi-temporal event detection
- Integrated workflow management
- Understanding and Reduction of uncertainties, i.e., uncertainty quantification (UQ)
- Multi-disciplinary science applications of ML

Some of the relevant AI and Data Science capabilities include anomaly detection, data assimilation, ML, uncertainty quantification, and computational workflows, among others.

Data science technologies, in addition to aiding in analysis, could also be used to identify supplemental observations that would improve models or provide important data about ongoing events. Data-driven observing systems are an emerging concept in which observations are requested based on an analysis of models and other data. The digital twin could request supplemental observations that would reduce its forecast uncertainty, for example, high-resolution images in areas where events like floods or fires are forecasted.

7. Federation

For some systems, a single digital twin will be sufficient. However, for larger systems, such as the Earth, a single twin will not be practical. Multiple twins representing smaller local/regional or thematic Earth systems will be developed, likely by different groups of people with different expertise, and they will need to be connected in some ways.

Some of the challenges related to federation are the following:

- Sharing the same needs and definitions would be a catalyst for federation
- Ongoing standards and collaboration efforts that would contribute to federating Earth System Digital Twins are:
    - Findable Accessible Interoperable Reusable (FAIR)
    - OGC APIs: Maps/Tiles/Routes/Styles.
    - Processes and Environmental Data Retrieval (EDR).
    - Cloud-native geospatial standards (COG, COPC, STAC, ZARR, GeoParquet, etc.)
    - Proposal for joint OGC-ISO standard with framework and Analysis Ready Data for land, ocean, atmosphere, earth system, etc.
    - Standard for training and validating data for ML
    - Standard for assessing data quality, data fitness for use, etc.
    - OGC pilot and testbed programs for developing and evaluating standards.
- Where to start federating efforts? In addition to federation, the community could develop specific reusable building blocks.
- As a community, there could be prioritization of a common outcome with public value, e.g., forecasting water flow, or land level change, or subsurface hazards and resources;
- Agree on how to promote and federate with each other's digital twins and/or source data to enter a cycle of improvement
- Interoperability of data layers, models, services will be needed.

- Another opportunity would be to develop the capability to systematically generate local, thematic and dated Digital Twins to address specific territorial needs/usages, to support decision making (a “Digital Twin Factory” [5])
- Creation of software and information layers that interoperate by exchanging well defined geophysical variables and services, rather than by tight coupling of software, models, and information.

8. Other Technologies

Depending on the application domain, other technologies are also needed. For example, Verification, Validation, and Uncertainty Quantification (VVUQ) are important at various points throughout the digital twin to provide confidence in the results, especially if they will be used to inform decision making, and to quantify the uncertainty in the results. In Earth Science, modeling the effects of calibration and fusion errors could provide a basis for deriving traceable error bars and uncertainty distributions for digital twin state variables. Vicarious calibration could be performed “on demand” to minimize uncertainties, rather than only up front when sensors are first deployed. This might be particularly useful for fusing data from constellations of small satellites and CubeSats within an ESDT observing framework. Assessing the uncertainty in data-driven models and in running what-if scenarios will also be very important, especially in giving users metrics that will ensure confidence and trust in these digital twins.

Reinforcement Learning (RL) is a branch of Machine Learning that we have not mentioned so far. RL enables agents to learn how to behave by providing rewards (positive or negative) in response to its actions. RL can be used to learn agents that operate within the digital twin but that can be implemented in the form of real systems once there is sufficient confidence that the agent has learned how to behave. Causal models and reasoning technologies are necessary to enable the digital twins to truly model the behavior of the target system. This is especially difficult in areas like Earth Science where there are feedback loops of causes.

Foundation Models is another branch of Machine Learning that might also have a strong impact on the way Earth System Digital Replicas will be computed as well as on increasing the speed and the accuracy of forecast models. This past year has already seen tremendous progress using Foundation Models for medium-range weather forecasting, e.g. with NVIDIA FourCastNet, Google GraphCast, European Centre for Medium-Range Weather Forecasts (ECMWF) Artificial Intelligence/Integrated Forecast System (AIFS), and Microsoft Aurora.

Standards are important and necessary for the development of digital twins to enable the community to develop them and connect them. This will require standards for both software and data. The current hodge-podge of non-conforming outputs and unique formats slows their use and increases the computational requirements to translate the data products into something usable in a digital twin. This becomes more important as scientific investigations create more data products to be preserved (for transparency and reproducibility) through fusion of elements from multiple datasets.

Culture change is needed to encourage both collaboration and competition. Some specific changes include:

- Digital Twins are not owned by an individual organization or community but have structured means to encourage inclusive contribution, including modular design, plug-and-play architectures, federation, etc.
- Access to diverse inputs and a guide to help discover unrecognized assets.
- Permitting others to contribute to a shared Digital Twin
- Leverage developments from multiple agencies and organizations
- Current concepts of intellectual property block openness
- A new model to give credit for intellectual advances earlier than publication.

Confidence in the validity of the digital twin will be essential to its usability. Confidence in the validity is distinctly different than validation. What is required to establish credibility in the digital twin and confidence in using it varies widely across communities but is important to all, and digital twins will be used and will need to be trusted by a wide range of users, such as the general public, non-scientific decision makers, as well as research scientists.

Examples

Over the past 4 years, the AIST Program has funded multiple projects in the area of Earth System Digital Twins [2,6] focusing on:

- Underlying analytic capabilities needed to build Digital Replicas, such as domain-focused Analytic Collaborative Frameworks (e.g., for Air Quality or Wildfires)
- Novel infrastructure technologies such as reproducible containers and virtual reality
- Surrogate modeling and Machine Learning-based emulators
- Preliminary prototypes including the interconnection of several models, e.g., for agriculture, for wildfires, for hydrometeorology, for assessing the impact of climate change on urban environment, and for floods and their impacts on coastal populations and their health.

Two specific examples are:

a. The Integrated Digital Earth Analysis System (IDEAS), developed by several NASA Centers and in collaboration with the French Space Agency (CNES), is a Digital Twin for Water Cycle and Flood Detection and Monitoring, It interconnects several models for river discharge, for Land and Hydrology Information and for predicting worldwide energy resources as well as for flood prediction. It is being federated with the digital twin being developed in parallel at CNES, called FloodDAM-DT, with the goal of investigating, developing and promoting common interoperable standards.

b. A Coastal Zone Digital Twin (CZ-DT) is now being developed as a collaborative project between NASA, NOAA and CNES under the umbrella of the Space Climate Observatory (SCO) [7]. The overall goal is to build a multi-organization CZ-DT around relevant Earth system models and simulations related to coastal zone change (e.g., sea level rise, increasing hazardous storms, pollution, and land cover/land use dynamics) and both observed or potential impacts now and into the future. The breadth of the topic is immense and covers coastal, terrestrial and marine water quality, lagoon and estuary ecosystems, human lives and livelihood, agriculture, infrastructure and socioeconomic factors. This will address many questions of growing interest such as those related to assess: 1) the current state of coastal zones, 2) what can we expect under climate change and 3) how can we mitigate current impact and prepare for future impacts?

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