

Advanced Information Systems Technology (AIST) Earth Systems Digital Twin (ESDT) Workshop Report

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Workshop Co-Organized with Earth Science Information Partners (ESIP) Report Edited by ESDT Workshop Participants

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Executive Summary

In October 2022, NASA Earth Science Technology Office (ESTO) **Advanced Information Systems Technology (AIST)** Program in collaboration with the **Earth Science Information Partners (ESIP)** conducted a workshop that brought together both Earth Science and Information Systems Technology communities to explore the use and benefits of Digital Twins for Earth Science and to identify which software and information systems technologies will support these Earth System Digital Twins (ESDT) and/or Digital Twin-like capabilities. This workshop represents one of the first steps in developing ESDT reference use cases and corresponding technology needs to guide the development of ESDT technologies that will be needed by NASA Earth Science within the next three to ten years.

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 advanced computing and visualization capabilities.

With a long history in engineering (e.g., aerospace, infrastructure and automotive), Digital Twins have recently attracted a lot of interest for health and economic as well as for environmental and Earth applications. Contrary to the engineering domain, digital replicas of the human body or of the Earth cannot be as exact, but they represent the best approximation possible as long as they have high degrees of accuracy and are fed by timely observations continuously updating these replicas. In the Earth domain, the interest in digital twins stems from the convergence of several developments:

- Well-documented data covering the entire Earth have now been collected continuously for more than 50 years, not only from space but also from airplanes, balloons, and insitu sensors. With the addition of commercial remote sensing providers and many more Internet-of-Things sensors, these incredible amounts of data already collected will soon be augmented by even larger amounts of diverse data and therefore will become more and more difficult to access, understand, and utilize.
- At the same time, because of climate change and its impacts the information produced by all of this data is becoming of interest to many new non-traditional users for analyzing and predicting various phenomena. As a consequence, the information derived from all of the data described above will need to be accessed and analyzed by multiple and diverse users for various uses and applications.
- Because of advances in computational and visualization capabilities and the parallel unprecedented development of artificial intelligence (AI) technologies, especially

machine learning (ML), extracting relevant information from these large amounts of data and running complex models faster has become possible.

As a result, it is becoming necessary and possible to build intuitive and interactive frameworks that will enable users with various skill levels and/or organizational hierarchy levels to easily access large amounts of targeted information along with the relevant tools and models (Earth system and human activity models) to support them in analyzing and visualizing this information, to help them understand interactions among models, to visualize the potential outcomes of various impacts, and to support decision or policy making.

The full power of digital twins is that, through an integrated representation and standardized tools and software technologies, the same digital replica can address the needs of multiple users at various resolutions (spatial and temporal) and for various applications (science, economic, policy, etc.). For scientific experts in Earth Science Models (ESMs), ESDT capabilities can be built around ESMs to leverage more advanced machine learning tools, build emulators and surrogate models, and provide the capability to consider many different scenarios and various boundary conditions in a timely manner. For science and applications users, especially when looking at Earth systems evolving more rapidly, ESDTs provide a dynamic representation with up-to-date and timely data and can therefore generate more accurate forecasts and what-if simulations from varying initial and impact conditions. For decision makers, digital twins' what-if capabilities provide a comprehensive interactive environment for understanding and monitoring current conditions and their evolution. Finally, the general public could use Earth System Digital Twins to inform daily activities and understand our changing planet.

In this context, the purpose of this workshop was to determine how to build impactful Earth System Digital Twins. With all these interests at stake, the challenges of building optimal digital twins are many and complex. The first challenge is to determine if a Digital Twin should be global or local, and multi-domain or thematic. For example, some domains such as Climate or Weather will require a global Digital Twin or Digital Twin capabilities while science areas such as Biodiversity might be more local. We can also envision that multiple thematic ESDTs, e.g., Air Quality, Wildfires, Hydrology could be federated or provide input to other ESDTs, either on a regional level or to a more global ESDT. Overall, we can imagine a future "web" of Digital Twins co-existing in a hierarchy or in a network, and capable of being connected or federated depending on the needs. This last point brings up the very important challenge of interoperability, including standards and protocols that will need to be built into these systems from the beginning. Interoperability will need to be defined not only at the syntactic level but more importantly at the semantic level. Each individual digital twin would have full flexibility in internal construction but would need standards-based interfaces (input and output) or hooks to make it compatible with others. Another challenge when building digital twins will be to decide how to organize each digital replica. Based on the application targeted by the DT under implementation, various amounts and types of raw data, Analysis Ready Data (ARD) and information will need to be incorporated. Depending on the required latencies and needs of the users, various solutions can be considered, including Data Cubes, Data Lakes, pointers, or computing information on demand. We envision that each ESDT will choose a solution adapted to its specific objectives. Another important challenge is the type(s) of visualization that will be used, as well as the level of interactivity and refresh rate that will be required. Again, this will depend on the objectives of the ESDT, but also on the various users' needs. In most cases, several types of visualizations and human interfaces will need to be offered depending on the projected users of that system.

In parallel to the challenges highlighted above, there are also many tools and technologies that will need to be developed or improved for all types of digital twins. Among those are improved machine learning technologies, for example providing explainability, but also ML techniques for causality and providing a better integration of physics models. Additionally, reliable uncertainty quantification methods will be needed for all ESDT components, from validating data fusion and assimilation to assessing the accuracy of ML models and weighing the values of decisions supported by those systems.

Based on those considerations, the workshop goals were to:

- Identify driving Earth-science use cases that will benefit from unique ESDT capabilities.
- Identify emerging **technologies** that will enable such ESDT systems within the next five to ten years.
- Identify **early pilot opportunities** that will provide lessons learned and directions for future technology developments.
- Understand **opportunities and technologies for federating ESDTs** and creating more capable systems.

With about 70 in-person and on-line participants, this hybrid workshop featured keynote speakers and panelists from a wide range of organizations who provided perspectives on Earth System Digital Twins from many diverse viewpoints. Workshop participants identified five Earth Science use cases for Digital Twins. These pose science and application questions that would benefit from digital twin capabilities to provide an integrated picture of Earth systems that answer, "what now?", "what next?" and "what-if?" questions. Those use cases address the following domains:

- Wildfires
- Ocean Carbon
- Water Cycle
- Central Africa Carbon Corridors
- Atmospheric Boundary Layer

The Workshop was also followed by additional studies which identified a use case addressing a future Coastal Zone Digital Twin.

Similarly to artificial intelligence, which is now revolutionizing many aspects of our daily lives, Earth system digital twin technologies have the potential to revolutionize the way Earth Science research will be conducted in the future, and how results and knowledge from this research will provide information to support decision making and yield impactful societal benefits.

1. Introduction

The Digital Twin concept was defined in 2002 [Gri17] and was first developed for industry for Product Lifecycle Management purposes. Its goal was to create a digital information system that would be a "twin" of the physical system through its entire lifecycle, utilizing both the initial construct of that system as well as all the continuous information available from sensors embedded within the physical system. Over time the concept has been applied to other domains such as infrastructure development and cars, and more recently to the human body and to the Earth System [Bau21]. In Earth Science, the concept of Digital Twins enables the development of integrated Earth Science frameworks that mirror the Earth with various models (Earth System Models and others), timely and relevant observations, and analytic tools. By integrating a continuous stream of observations, interconnected models, data analytics, data assimilation, simulations, advanced visualizations and the ability to conduct "what-if" scenarios, 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. In particular, these systems will be able to support the assessment of human activity impact on natural phenomena, and conversely the impact of climate change on human populations.

In its 2021 solicitation, the Advanced Information Systems Technology (AIST) Program introduced Earth System Digital Twins (ESDT) as a new thrust, with the goal of developing novel software and information system technologies that will facilitate future development of digital twins for the Earth Science domain. The objective of the workshop that was conducted in collaboration with ESIP in October 2022 was to bring together science and technology communities to explore the use and benefits of EDST and their enabling technologies. This workshop marks one of the first steps in developing ESDT reference use cases and corresponding technology needs to guide the development of ESDT technologies that will be needed by NASA Earth Science within the next three to ten years.

1.1 Workshop Goals

The workshop goals were to:

- Identify driving **Earth science use cases** that will benefit from unique ESDT capabilities.
- Identify emerging **technologies** that will enable such ESDT systems within the next three to ten years.
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- Understand **opportunities and technologies for federating ESDTs** and creating more capable systems.

With those goals in mind, the workshop was organized as a combination of plenary talks and panel discussions, followed by lightning talks describing current technology efforts and leading to several breakout sessions focusing on defining science use cases, identifying required technologies and gaps, and investigating ESDT systems vision and federation. The detailed agenda is shown below.

Wednesday, October 26, 2022				
9:30	10:00	Gathering		
10:00	10:30	Welcome Plenary	Jacqueline Le Moigne, AIST Susan Shingledecker, ESIP	
10:30	11:30	Panel: Digital Twins for NASA Earth Science		
11:30	Noon	Interactive discussion		
NOON	1pm	LUNCH		
1:00	1:30	Earth System Digital Twins and the European Destination Earth initiative	Peter Bauer, ECMWF	
1:30	2:30	Panel: Federating Earth System Digital Twins		
2:30	3:00	BREAK		
3:00	3:30	Global Digital Twin of the Earth System Environment in NOAA - for Monitoring and Prediction	Sid Boukabara, NOAA	
3:30	4:30	Panel: Technologies for Earth System Digital Twins		
4:30	5:00	Wrap up discussion		

1.2 Workshop Agenda

Thursday, October 27, 2022

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8:00	8:30	Gathering and Welcome
8:45	9:40	Lightning talks I
9:40	10:00	Science reference scenarios overview
10:00	10:30	BREAK
10:30	Noon	Breakout Session A: Science Use Cases
NOON	1pm	LUNCH
1:00	1:30	Session A brief-outs
1:30	3:00	Lightning talks II
3:00	3:30	BREAK
3:30	5:00	Breakout Session B: Technologies and gaps
5:00	5:30	Brief out
5:30		ADJOURN

Friday, October 28, 2022

8:00	8:30	Welcome/plan for the day
8:30	10:00	Session C: ESDT Systems Vision and Federation
10:00	10:30	BREAK
10:30	Noon	Brief outs
12:00	12:15	Wrap up
12:15		LUNCH / Adjourn

The first day was run in a hybrid fashion, focusing on plenary presentations and panel discussions, and was attended by about 40 participants in-person and 45 on-line. Days two and three featured in-person breakout discussions on science use cases, technologies, and digital twin architectures, with an average of about 35 attendees each day.

1.3 Keynote Speakers and Panelists

The workshop featured keynote speakers and panelists from NASA and other U.S. Government Agencies, as well as academia and international organizations, to provide diverse perspectives on Earth System Digital Twins from science, technology and programmatic standpoints. Below is a list of all keynote speakers and panelists.

Jacqueline Le Moigne, NASA ESTO AIST	Nadine Alameh, Open Geospatial Consortium (OGC)
Peter Bauer, ECMWF	Simon Baillarin, French Space Agency (CNES)
Sid Boukabara, NOAA	John Stock, U.S. Geological Survey (USGS)
David Considine, NASA Earth Science Division (ESD)	Daniel Crichton, NASA JPL
Richard Eckman, NASA ESD	Michael Little, NASA GSFC
Jared Entin, NASA ESD	Nikunj Oza, NASA ARC
Garik Gutman, NASA ESD	Amitabh Varshney, University of Maryland
Tsengdar Lee, NASA ESD	Olivier De Weck, MA Institute of Technology (MIT)
Woody Turner, NASA ESD	

Panelists and speakers addressed questions such as: What is a Digital Twin? What is an Earth System Digital Twin? What are their use and applications for Earth Science? Although slightly different definitions were proposed, they all share the same core elements. The definition used during the workshop is shown in Figure 1; other definitions are described in the next section.

1.4 Earth System Digital Twin Definition Used for the Workshop

For NASA's Advanced Information Systems Technology Program, an *Earth System Digital Twin* is defined as composed of three components:

- 1. A *Digital Replica*, i.e., an integrated picture of the past and current states of Earth systems, based on up-to-date, diverse and continuous observations as well as on historical records
- 2. *Forecasting Capabilities*, providing an integrated picture of how Earth systems will evolve in the future from the current state
- 3. *Impact Assessment* capabilities, providing an integrated picture of how Earth systems could evolve under different hypothetical what-if scenarios, and how they could be impacted by other Earth systems as well as by human systems and activity.

This is the definition that was utilized during the workshop.

Digital Replica

An integrated picture of the past and current states of Earth systems.

Forecasting . An integrated picture of how Earth systems will evolve in the

future from the current state.

Impact Assessment ."

An integrated picture of how Earth systems could evolve under different hypothetical what-if scenarios.

- Continuous observations of interacting Earth systems and human systems
- From many disparate sources
- Driving inter-connected models
- At many physical and temporal scales
- With fast, powerful and integrated prediction, analysis and visualization capabilities
- Using Machine Learning, causality and uncertainty quantification
- Running at scale in order to improve our science understanding of those systems, their interactions and their applications

Figure 1. AIST Definition of ESDT for the Workshop

As was described previously, developing such a vision will require technologies related to integrating continuous observations from various disparate sources; developing frameworks that builds on inter-connected models; improving the speed and accuracy of integrated prediction, analysis and visualization capabilities (e.g., by using machine learning); and utilizing causality and uncertainty quantification to improve our understanding of the evolution of Earth Science systems as a function of their interactions with other Earth and human systems. Additionally, interoperability standards to federate multiple Digital Twins, as well as computational resources and visualization capabilities required by those systems will also need to be investigated.

2. Keynote Presentations

2.1 Destination Earth (DestinE) – Peter Bauer

Peter Bauer, ECMWF, Director of Destination Earth, gave a keynote entitled "Earth System Digital Twins and the European Destination Earth initiative." Destination Earth (DestinE) is a flagship initiative of the European commission to develop a highly accurate digital model of the Earth on a global scale. This model will monitor, simulate and predict the interactions between natural phenomena and human activities.

In this talk and in "A Digital Twin of Earth for the Green Transition" [Bauer, 2021a], a digital twin is defined as a digital replica of a living or non-living physical entity, and a digital twin of Earth is an information system that exposes users to a digital replication of the state and temporal evolution of the Earth system constrained by available observations and the laws of physics.

The digital twins created in DestinE will give expert and non-expert users tailored access to high-quality information, services, models, scenarios, forecasts and visualizations. This includes models of the climate, weather forecasting, hurricane evolution and more. Digital twins rely on the integration of continuous observation, modeling, and high-performance simulation, resulting in highly accurate predictions of future developments. [DestinE, 2021]



Figure 2. Destination Earth (DestinE) Earth Digital Twin

2.2 NOAA Digital Twins – Sid Boukabara

Sid Boukabara, from the NOAA Office of Systems Architecture and Advance Planning (OSAAP), presented a vision for a NOAA Global Digital Twin of the Earth Environment for Monitoring and Prediction [NOA22]. He highlighted that this Digital Twin system is envisioned to have three components as described in figure 1.

- (1) Component 1: An observations-based, grid-flexible, multi-component, high spatialtemporal resolution DT capturing all available observations and feeding a variety of direct observation users. This component could be viewed as the fusion of all observations from multiple sources including space-based and ground-based sensors, to represent all Earth system components (atmosphere, ocean, land, hydrology, space weather). This first component could also contain short-term forecasts in its inputs to allow gap-filling and to permit data assimilation in order to feed NWP systems.
- (2) Component 2: An Earth System model digital twin, which would be multi-scale, coupled, with a flexible/high spatial-temporal resolution and flexible grid capability. The purpose of this component is to project the Earth system state into future timescales,

from short-term to long-term scales. The input for this component is the output of Component 1.

(3) Component 3: This component is an assessment aomponent. This is the component that allows the execution of impact assessment experiments. This will be useful to answer questions regarding 'what if' scenarios, which are extremely useful for a range of applications. The scope and nature of the questions to be answered in this component depend directly on the capabilities of Component 2. In theory, if Component 2 applies to short term and long term (climate) time scales, then Component 3 will allow researchers to answer questions such as "what will the extreme weather events frequency or the climate trends be, based on different scenarios of greenhouse gases restrictions?" It could also address observing systems architecture questions like "How well will we be able to monitor (and short- or medium- term predict) the Earth system, with a variety of space architectures (with multitude of sensors including sounding, imaging, Infrared, Microwave, etc)?"



Figure 3. NOAA Vision for Earth System Digital Twin.

It was noted in Sid Boukabara talk, that a project is underway to demonstrate Component 1 of the Digital Twin vision highlighted above. The 2 years project is called 'Earth Observations Digital Twin EO_DT' and will be executed in parallel by 3 different vendors.

3. Panel Discussion

3.1 Panel: Digital Twins for NASA Earth Science

Earth System Digital Twins provide unique capabilities for understanding the evolution of interacting Earth systems. Panelists discussed science needs and applications for ESDTs from the NASA Earth science perspective.

Moderator

Emily Sylak-Glassman, Manager NASA Applied Sciences Program

Panelists

Rich Eckman	Atmospheric Composition
Tsendgar Lee	Weather and Atmospheric Dynamics
David Considine	Climate Variability & Change
Jared Entin	Global Water and Energy Cycle
Woody Turner	Carbon Cycle and Ecosystems (CCE) – Biodiversity
Garik Gutman	Carbon Cycle and Ecosystems (CCE) – Land Cover Land Use Change

Panelists addressed questions about science needs and applications, needed capabilities, and opportunities to make progress without major increases in funding. Below are the overall questions that guided the discussions and a summary of the discussions:

- 1. **General:** What do you see as the high impact capabilities of ESDTs for your area of work?
- 2. **Public excitement:** There's been a lot of excitement in the public about the promise of digital twins, perhaps beyond what we've seen with other modeling capabilities. How should NASA leverage this excitement?
- 3. What-ifs: ESDTs allow experts and non-experts to "experiment" with models interactively. One of the ESDT capabilities is running "what-if" scenarios:
 - a. What kind of "what-if" scenarios would you, personally, like to run?
 - b. How do you see that "what-if" capability contributing to science questions and applications?
- 4. **Spatial scales:** Some concepts for the use of ESDTs involve bringing together information about the built environment and infrastructure with local or even global environmental data. This may mean bridging radically different spatial scales. Do you have suggestions for how we can think about doing so in a way that provides actionable information?
- 5. **Temporal scales:** What are some examples of science problems or applications that cut across temporal scales, from weather to climate? How might we design ESDTs to accommodate these different scales?
- 6. Fitness for purpose: One challenge we've seen many times in communicating Earth science is that different data products and models are optimized for different regions, scales, conditions, etc. As we think about an ESDT with a wide range of users, with a wide range of research and application goals, how should we think about ensuring that users are using the most appropriate data and models for their purpose?
- 7. **Visualization:** A key part of ESDTs is visualization of the Earth system. Which type of visualizations would be particularly useful for science insights or applications?

- 8. **ESO Era:** NASA is moving toward an Earth System Observatory, where multiple missions will observe related Earth systems. What are some examples of Science problems and applications that cut across Earth systems? How could ESDTs address those or provide new insights?
- 9. **Uncertainty:** Where do you see Uncertainty Quantification (UQ) being particularly important for digital twins? Do digital twins raise any new UQ concerns?
- 10. **Assimilation:** Accurate replication assumes that the current state is modeled while continually assimilating new data. What would it take to also assimilate observations to replicate the current state and conduct forecasts?

What are the potential needs and applications?

Atmospheric Composition:

- Urban Air Quality is an opportunity for ESDT in the Atmospheric Composition domain. (Recommendations from Topping *et al.*, 2021 doi: 10.3389/frsc.2021.786563)
- Need/Benefit: Provide digital tools to inform decision-making process of relevant bodies, leading to policies that enhance the health of the population and improve environmental outcomes (both urban and wildfire relevance).
- Digital Replica: Ingests near to real-time data from range of disparate sources from across city, providing an end-to-end decision system capturing local dependencies (both environmental and transportation increasingly decarbonized related).
- Current models of urban AQ are computationally expensive and cannot be easily coupled to activity models across urban domain.
- Metadata standards unifying low-cost public sensors with government measurements and the communications challenges of near real time (NRT) ingestion.
- Source and process identification / Edge computing: provide NRT information to users on source types, combining with ancillary data from traffic flows and meteorological data.

Weather and Atmospheric Dynamics:

- Digital Replica: Surrogate models utilized in data assimilation efforts greatly reduce time to solution.
- Forecasting: DT contribute to the ensemble forecasts enable larger ensembles.
- Impact Assessment: Digital Twins will be used in OSSE efforts for future instruments and observing systems design and trade studies. DT will also be used in scenario analysis for climate change resilience and mitigation.

Climate Variability & Change:

• Higher resolution in the "digital replica" of the Earth's climate system will enable – to the extent that the intrinsic variability of the Earth system allows it – investigation of climate impacts at local and regional scales.

- Short-term climate forecasting requires improved initialization using observations and data assimilation methods (ESDT benefits). Long-term forecasting requires realistic digital replicas that are continuously improved with new observations. ESDT efforts should improve forecasting over all timescales relevant to Climate Variability & Change.
- The most unpredictable component of the Earth system is human behavior. For years, we have used multiple scenarios to bound the possible human responses that affect climate change. Having improved scenario/ensemble capabilities would allow more rigorous bounding of these possibilities.
- "What if" scenarios could be filtered to look at differences between worlds where tipping points occur and worlds where they do not.

Global Water and Energy Cycle:

- Ice sheets are melting and ocean temperatures are changing, and there is growing
 interest in understanding systems such as snow and hydrology in relation to variables
 such as weather, temperatures, and ocean data, and in integrating better science
 systems interaction, tracking the cooling of the Earth as ice melts, understanding and
 tracking sea level rise, etc.
- There is need for technology and science to work together, and using Digital Twins to conduct what-if scenarios is essential.
- With SWOT we are entering an era in which we can do much better assessments of surface water, river conditions, etc., and with better assessments we will be able to get better predictions.
- The main question is to be able to make longer range projections and give communities better advice on how to plan for multiple decades in the future.

Carbon Cycle and Ecosystems (CCE) – Biodiversity – Catalyst: A Biodiversity Conservation Accelerator incorporating Digital Twins:

- Our planet is in the midst of its 6th mass extinction event, driven by human impacts on Earth System processes, as biodiversity loss continues to accelerate.
- An integrated information system such as a Digital Twin would inform actions to protect biodiversity at landscape-to-regional scales and reverse ecological damage.
- The goal is to develop a regional Earth System Observatory to catalyze biodiversity conservation at large scales, -that would integrate the best spaceborne, airborne and insitu Earth observing data, analytics and models to inform conservation action.
- A new initiative for a Biodiversity Conservation Accelerator, called Catalyst, is being developed, also starting in California as a first use case.
- From its start in California, Catalyst will spread to include the Western U.S., followed by future regional expansions in the U.S. and beyond.

Carbon Cycle and Ecosystems (CCE) – Land Cover Land Use Change:

• A Digital Replica of Global Land Cover Change, powered by Data Assimilation and Fusion, and which incorporates continuous and targeted multi-source, multi-resolution

observations, will provide an accurate near-real time representation of changes in Land Cover over the globe and will support a wide range of decision support.

- Forecasting capabilities, including Seasonal to Annual Agricultural Land Use, and Annual to Decadal yearly projections of Land-Use Change driven by Climate Change and Socio-Economic Changes, will be facilitated by advanced computational capabilities, machine learning and Surrogate Modeling.
- Impact Assessment capabilities will include 1) Seasonal to Annual forecasted agricultural land use on supply chains, 2) extreme weather events on Land Use, and 3) Modeling hypothetical spatially explicit future states of global land use and land cover at landscape scale; they will also include associated societal impacts, with a 20-year horizon, based on recent and near-term land-use trajectories and projections of climate, demographics, economic scenarios and resource constraints, using elements of the above Digital Replica and Forecasting.

What major capabilities will be required?

- Development of a true climate ESDT say, a fully interactive representation of the Earth system at 1 km resolution resolving clouds and convection with ability to run many "what if" scenarios. It will require exascale computational capabilities (about 1000x what is now available to NASA).
- A computational platform that combines compute capabilities with data storage and access as well as analytical tools.
- Novel acceleration techniques ML emulators, ML parameterizations, effective use of graphical processing unit (GPU) computation.
- New multi-spectral (visible to thermal and microwave) Very High-Resolution sensor technologies and synchronized constellation data acquisition to meet global science data needs.
- New algorithmic approaches and data processing technologies that will enable efficient global large volume, multisource data fusion and product generation.
- New models for forecasting seasonal-to-annual agriculture, forest, wetland, and urban changes.
- Hyper-local forecasting using historical, near-real-time or real-time data combined with ancillary data (ML/AI). Much more cost-effective than traditional chemical-transport models.
- Replacement of traditional numerical methods with hybrid process-level ML Air Quality models.
- Visualization challenges: Augmented Reality services for enhanced delivery to affected populations (again considering communication challenges and opportunities, e.g., 5G)
- Ability to run "play-back" simulations to assess "what if" scenarios and responses using historical data streams of environmental and transportation data at hyper-local scales.

What can NASA do without major increases in funding?

- The AIST Program's competitively funded ESDT projects (current and future) represent a steady and reasonable approach, realistic under current and planned NASA resources and consistent with competed science.
- The development of the NASA Earth Information System (EIS, [EIS23]), which has seen several pilot projects funded, is a modest and realistic step to provide input to ESDT replica and forecasting components and facilitating an "open science" approach.
- NASA Center for Climate Simulation (NCCS) "Adapt" system is exploring ESDT-enabling configurations.

3.2 Panel: Federating Earth System Digital Twins

Federated Earth System Digital Twins work together to provide greater access to data, models, and capabilities. Panelists discussed emerging Earth System Digital Twins, and opportunities and approaches for federation.

Moderator

Sid Boukabara, Office of Systems Architecture and Advance Planning, NOAA

Panelists

Nadine Alameh	CEO, Open Geospatial Consortium (OGC)
Simon Baillarin	Head of Data Campus Department, CNES
John Stock	Director, National Innovation Center, USGS
Mike Seablom	Senior Strategist, ESTO, NASA
Elena Steponaitis	Program Executive, Chief Science Data Office, NASA

Which DTs could be working together and what kinds of impact would that provide?

- FloodDAM digital twin (flood detection, alerts, and rapid mapping)
- Urban Digital Twins of Coastal Zones
- Wildland Fire management
- Land use planning
- A Great Lakes Digital twin.

Where do you see opportunities to pursue interoperability efforts? What recommendations or propositions might you make to the other institutions in this panel to achieve interoperability? What are the key steps we need to take together towards a shared vision? What is that vision?

- 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.
- \circ $\;$ 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").
- Creation of software and information layers that interoperate by exchanging welldefined geophysical variables and services, rather than by tight coupling of software, models, and information.

What are the big technical obstacles to federation? Are there interfaces, standards, or frameworks that could mitigate them? What are some of the big organizational or bureaucratic obstacles to federation? Are there things we could be doing to lower those barriers?

- Legal and organizational barriers to sharing specific data, software or models (e.g., proprietary, restricted) are probably the biggest obstacles to federation.
- Almost all digital twins will have multiple data sources. The forecasting or mapping capability is likely to be developed by the agencies/organizations willing to support operations and maintenance (O&M) of technology improvement.

Common types of interoperability include syntactic (data format), semantic (meaning of the data or metadata), and organizational (alignment of organizational processes, etc.). Where do you see challenges in one or more of those? Are there capabilities or technologies that would address those challenges?

- Global Earth system understanding is very complex.
- A multiscale approach (global / regional / local) for multiples use cases would be required. Federation will be needed here.
- There needs to be a federation of all assets, data, models and competencies.

• For semantic interoperability, one solution would be to use OGC Definition Server to facilitate common understanding and enable dynamic linking.

3.3 Panel: Technologies for Earth System Digital Twins

Moderator:

Ben Smith, AIST Associate and NASA/JPL

Panelists

Amitabh Varshney	Dean of the College of Computer, Mathematical and Natural Sciences, University
	of Maryland at College Park (UMD)
Mike Little	High-End Computing, NASA
Oli De Weck	Apollo Professor of Astronautics and Engineering, MIT
Nikunj Oza	Lead, Data Sciences Group, NASA Ames
Dan Crichton	Lead, Center for Data Science and Technology, NASA JPL

Panelists discussed technologies and challenges for implementing Earth System Digital Twins. Each panelist provided their perspectives on relevant technologies and potential technology gaps.

Machine Learning

Machine learning can play a significant role in ESDTs for analysis, data fusion, and surrogate modeling. Machine learning can provide powerful tools for analyzing ESDT data and products. Training ML models on disparate data sets can provide one form of data fusion. They can also perform inference, filling in gaps between observations or estimating higher resolution products. Compared to physics-based models, machine learning surrogate models can run faster, which is important for increasing the scale or improving interactivity. They are developed through training, rather than first principles, so it may be easier to create them.

One of the open challenges for machine learning with respect to Earth System Digital Twins is multi-resolution models. Running an entire Earth system at full resolution all the time is likely impractical. If a model can run at different temporal or spatial resolutions, one could trade resolution for computational power depending on specific needs. The remaining questions are:

- What processes (phenomena, spatial regions, etc.) can we run in parallel?
- What processes can we run only under certain conditions?
- What types of ML and other models should be used and in what situations?
- Which ones are the most accurate for forecasting vs. what-if scenarios?

High Performance Computing

Many of the models and capabilities of Earth System Digital Twins will be computationally intensive. Existing weather and climate models typically require specialized computing

environments. High-Performance and Exascale Computing will play an important role in meeting those demands.

Some of the EDST functional tools and capabilities that would be enabled by high-end computing include:

- Data Driven Models (assimilation)
- Physics Based Models
- Machine Learning Models
- Validated Near-Real-Time Models
- Running what-if exercises
- Analysis and Visualization
- Hypothesis testing (i.e., GAN)
- Continuous Validation

Some of the computing assets currently available include High-Performance Computing facilities, such as those run by NASA, NOAA, and DOE. Other assets should also be considered. These include specialized processor systems such as graphics processors (GPU), tensor flow processors (TFPU) and similar AI processors, data processing units, and FPGAs. Cloud computing will be important for running large, distributed processes at scale and managing large data volumes. Integrated Edge computing could move some processing to sensors and instruments to reduce demand on central computing. High-performance communications could also play a role for managing large data velocities.

There are several architectural models that can be considered for providing high-end computing needed for ESDT 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, and Software-Defined Systems and Networks.

Immersive Visualization

Visualization will be a critical part of understanding and interpreting the wealth of data provided by Earth System Digital Twins. Immersive visualization, such as augmented reality (AR) and extended reality (XR), is a potentially disruptive paradigm for ESDT that would allow users to explore complex data in intuitive ways to obtain insights. Immersive visualization can overcome limitations of 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 from a 2D display.

Technology gaps include:

• Human factors for improving ergonomics and productivity.

- High-level software APIs for streaming ESDT 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 largescale, multi-modal streaming datasets .
- Advances in visualization, AI/ML, human factors, and ESDT general domain expertise.
- Development of a workforce that intuitively understands and leverages the power of Extended Reality (XR).

Data Science and Interactive Data Analysis

One of the important uses of an Earth System Digital Twin will be analysis of data, models, and projections to better understand processes and their trends and impacts. Al 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
- Reduction in uncertainties (i.e., uncertainty quantification or UQ)
- Multi-disciplinary science applications of AI/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 ESDT could request supplemental observations that would reduce its forecast uncertainty, for example, or request high-resolution images in areas where events like floods or fires are forecasted so they will be available in the digital replica.

Multi-Sensor Data Fusion and Vicarious Calibration

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.

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 smallsats and cubesats within an ESDT observing framework.

Some of the technology gaps and challenges in this area include:

- Calibration for (mid-)IR
- Multi-angular concurrent observations for anisotropic albedo estimation
- Heterogeneous data fusion
- Traceability of multi-source error contributions throughout ESDTs
- Deploying a global network of land- and sea-based sensors and calibration targets

4. Lightning Talks: ESDT Systems and Technologies

A series of "lightning talks" by attendees presented current development efforts towards ESDT prototype systems and component technologies.

4.1 ESDT Systems and Prototypes

The first series of lightning talks presented ESDT systems and prototypes in development, spanning several Earth systems.

1	Rajat Bindlish	Digital Twin Infrastructure Model for Agricultural Applications
2	Allison Gray	A prototype Digital Twin of Air-Sea Interactions
3	Thomas Allen	Pixels for Public Health: Digital Twin for Coastal Resilience of Vulnerable Populations in Hampton Roads, Virginia
4	Milton Halem	Towards a NU-WRF based Mega Wildfire Digital Twin: Smoke Transport Impact Scenarios on Air Quality, Cardiopulmonary Disease and Regional Deforestation
5	Brandon Smith	TERRAHydro: Terrestrial Environmental Rapid-Replicating Assimilation Hydrometeorology
6	Laura Rogers	Earth Information Center (EIC)
7	Alexey Shiklomanov	Earth Information System (EIS)
8	Thomas Huang	CalCIS: California Climate Information System

4.1.1 Digital Twin Infrastructure Model for Agricultural Applications

This project is developing a Digital Twin Agricultural prototype framework focused on the Continental United States. This effort will establish a digital twin framework that enables remote sensing data products and land surface model products to be directly coupled with or assimilated into the crop growth model. It will implement Bayesian Neural Network (BNN) model to predict final county level crop yield and develop tools to conduct 'what if' investigations to provide agricultural guidance.

4.1.2 A prototype Digital Twin of Air-Sea Interactions

This is a prototype towards an interpretable Digital Twin for Air-Sea interactions that will advance near-real-time estimation of air-sea fluxes and their uncertainties. The core capabilities include real-time, multi-scale data fusion; a hybrid physics-informed AI model; a framework for post-hoc analysis, including feature importance and uncertainty quantification; and a visual interface for model diagnosis and "what-if" investigations.

4.1.3 Pixels for Public Health: Digital Twin for Coastal Resilience

This digital replica will link multi-source, high-velocity data to predict coastal flooding and human impacts: Earth observations, hydrodynamic models, and real-time sensor networks.

4.1.4 Towards a NU-WRF based Mega Wildfire Digital Twin

Recent persistent droughts and extreme heatwave events over the Western states of the US and Canada are creating highly favorable conditions for mega wildfires. Smoke from these Western wildfires significantly affects air quality, leading to adverse human health effects. The goal of this effort is to develop a Regional Wildfire Digital Twin (WDT) with a sub-km resolution that will run mega-wildfire smoke impact scenarios at various spatial scales and arbitrary locations over N. America. The WDT will provide a valuable planning tool to implement parameter impact scenarios by season, location, intensity, and atmospheric state. The twin will augment and couple several wildfire and atmospheric models. It will augment the NASA Unified WRF (NUWRF) model with an interactive locality fueled SFIRE parameterization that are coupled to GOCART, CHEM and HRRR4 physics models.

4.1.5 TERRAHydro

TerraHydro is developing a Terrestrial Earth System Digital Twin (TESDT) designed from the ground-up to couple state-of-the-art machine learning hydrology models with capabilities for uncertainty quantification and data assimilation. The machine learning models that will be included are at least as accurate as traditional process-based models and run significantly faster. The reduced computational complexity will enable the TerraHydro digital twin to perform classically expensive tasks such as ensemble and probabilistic forecasting, sensitivity analyses, and counterfactual "what if" experiments that will provide critical hydrometeorological information to aid in decision and policy making.

4.1.6 Earth Information Center

The Earth Information Center (EIC; [EIC23]) will allow the public to see how the Earth is changing and guide decision makers to mitigate, adapt, and respond to climate change. With resources at NASA centers from coast to coast and in close coordination with other government agencies, industry partners, and community groups and members, the Earth Information Center will deliver critical data directly into the hands of people in ways and forms that they can immediately use. EIC will provide a whole Earth view down to local information to visualize our changing planet – from temperatures in our cities to sea level rise, greenhouse gas emissions to agricultural productivity.

4.1.7 Earth Information System

The Earth Information System (EIS; [EIS23]) is a platform for understanding and answering critical questions about Earth's complex System of Systems. Using NASA's 20+ years of Earth observation data and novel modeling capabilities, it aims to support near-term and long-range analysis and decision making in support of preparation, mitigation, and resilience in the face of climate change. EIS integrates NASA's Earth science observations and modeling capabilities to produce new actionable science. EIS currently comprises four multi-disciplinary thematic areas: Fire, Freshwater, Sea Level Rise, and Greenhouse Gases. EIS will address complex Earth Science Decadal Survey (ESDS) questions using state-of-the-science models and observations from NASA and partners; deliver timely and accurate actionable information through early and consistent stakeholder engagement and co-development; demonstrate innovative and integrative science and applications enabled through ESDS unified cloud infrastructure and collaborative environment; and improve transparency and accessibility of data and methods in support of NASA's Transition to Open Science.

4.1.8 CalCIS: California Climate Information System

CalCIS is a new partnership between NASA and the State of California to leverage remote sensing to understand and manage California's natural resources in the face of a changing climate, delivered through a cloud-based information system. CalCIS will be created by NASA/JPL in collaboration with state agencies, university scientists and commercial organizations to provide a centralized data management hub that will house climate data from satellite and airborne remote sensing efforts, and climate field data for the state.

4.2 ESDT Technologies and Frameworks

The second series of lightning talks presented ESDT technologies and frameworks that are in development. Presenters indicated how the technologies contributed to advancing one or more of the ESDT components: digital replica, forecasting, and impact assessment.

1	Jon Hobbs	Scalable probabilistic emulation for Earth-system models
2	Kuo Kwo-Sen	Reproducible Containers for Advancing Process-oriented Collaborative Analytics
3	Chis Keller	Development of a next-generation ensemble prediction system for atmospheric composition
4	Jouni Susiluoto	Kernel Flows
5	Thomas Huang	IDEAS (Integrated Digital Earth Analysis System): An ESDT Framework
6	Arlindo da Silva	An Analytic Collaborative Framework for the Earth System Observatory
7	Arlindo da Silva	A Framework for Global Storm Resolving OSSEs
8	Thomas Grubb	VALIXR (Visualization And Lagrangian dynamics Immersive eXTended Reality Tool) for Scientific Discovery

Presenters indicated where technologies were positioned on a notional map, shown in Figure 4 below, illustrating how major technology areas relate to each other and to the three ESDT components. Note that some technologies contribute to several ESDT components.



Figure 4. ESDT Component Technology Areas (notional map)

The table below summarizes the technology positions on this map and the technologies investigated by each project listed above.

Technology Area (per "Atom" diagram)	Digital Replica	Fore- casting	Impact Assmt.	1	2	3	4	5	6	7	8
Seamless Access to Open Data	х		х					x	х	x	
Continuous & Targeted Diverse Observations	x		x			x					
Data Assimilation & Fusion	х	х	х			x	х	х	х	х	
Multi-Domain/ Interconnected Modeling	х	x	x			x		x			
Advanced Computational Capabilities	х	х	х								
Forecasting models		х	х		х	x		х			
Surrogate Modeling		х	х			x	х				
Advanced Visualization			х					х			x
Investigative Capabilities, incl. Uncertainty Quantification & Causality			х	x	x		x	x	x	x	x
Assisted Decision Making			х	х		х		х	х	х	

Table 1: ESDT Component Technologies in development as presented in Lightning Talks

4.2.1 Scalable probabilistic emulation for Earth-system models

Uncertainty quantification (UQ) is an important capability for Earth System Digital Twins. This effort is developing an automated capability for UQ based on a probabilistic emulator that learns the non-Gaussian distribution of spatial-temporal fields from Earth-system models nature runs. This will allow users to discover and examine nonlinear dependence structures, interpolate between observed covariate values, and run extensive what-if scenarios.

4.2.2 Reproducible Containers for Process-oriented Collaborative Analytics

Reproducibility is an important but challenging goal of open science. This effort is developing software containers for science data processing pipelines that facilitate reproducibility. These containers will be data-savvy, maintaining ties of automatic containerization, provenance tracking, and repeatability guarantees — all of which are necessary for reproducibility but missing from traditional container technologies.

4.2.3 Development of a next-generation ensemble prediction system for atmospheric composition

This effort is developing a next-generation modeling framework for the real-time simulation of reactive gases and aerosols in the atmosphere. The core innovations are the deployment of computationally efficient parameterizations of atmospheric chemistry and transport and the development of generative models based on machine learning to predict model uncertainties. Combined, these will enable improved and novel applications related to atmospheric composition, including probabilistic air quality forecasts at increased horizontal resolution, advanced use of satellite observations using ensemble-based data assimilation techniques, and scenario simulations for real-time event analysis.

4.2.4 Kernel Flows

Kernel Flows are an approach for developing machine learning emulators for high-dimensional problems such as climate models and radiative transfer. Fast machine learning emulators can make it tractable for digital twins to perform computationally complex tasks like what-if projections and ensemble forecasts for uncertainty quantification. This project is developing a versatile emulation tool based on Kernel Flows that will provide fast, accurate emulation with little tuning; scale up to very large training sets; and provide uncertainties associated with outputs gaussian process regression.

4.2.5 IDEAS: An ESDT Framework

The Integrated Digital Earth Analysis System (IDEAS) project is a software architecture for Earth System Digital Twins that can coordinate services, models and observations (data) from multiple sources to analyze interacting Earth systems. It harmonizes observations and model outputs to analyze and explore the current state of the Earth system; coordinates models and observations to perform predictions and what-if projections of interacting Earth systems; and federates with other ESDTs to allow more comprehensive analyses leveraging their data sets, models, and analytics.

4.2.6 An Analytic Collaborative Framework for the Earth System Observatory

This project is developing a cloud-based software framework that will be able to integrate data from Earth System Observatory missions to provide a holistic view of the Earth. The core elements of the framework are cloud-optimized data sets and an algorithm workbench. The framework will be demonstrated on use cases from the upcoming AOS and SBG missions.

4.2.7 A Framework for Global Storm Resolving OSSEs

Storage limitations drive traditional OSSEs to produce output at relatively low temporal resolutions that are inadequate to resolve processes of interest, such as storm convection. This new framework will overcome those limitations with two innovations. First, it will extend the parallel I/O capabilities in the GEOS model to achieve high temporal resolutions limited only by the model timestep. Second, it will use a two-phase checkpoint approach to performing nature runs that can tailor sampling resolution between checkpoints to optimize the output data volume.

4.2.8 VALIXR

Earth System Digital Twins will need to provide visualizations of complex Earth science phenomena to aid scientific understanding and discovery. This effort will develop a scientific exploration and analysis mixed augmented and virtual reality tool, with integrated Lagrangian dynamics, to help scientists identify, track, and understand Earth Science phenomena such as convective clouds, hurricanes, and wildfire smoke plumes. These move with the 3-D flow field in a Lagrangian reference frame, and it is often difficult and unnatural to understand these phenomena with data visualized on Eulerian grids.

5. Breakout Discussions

On days two and three, participants formed into smaller working groups to discuss key topics in a series of breakout sessions investigating:

- Science use cases
- Gap technologies
- Early prototyping opportunities and approaches for federation

Each breakout session was guided by a set of discussion topic considerations. At the conclusion of each session, the groups reconvened in a plenary session to brief their outcomes and discuss them further with the other participants.

5.1 Science Use Cases

This first breakout session refined several science-driven use cases for Earth System Digital Twins. In advance of the workshop, five use cases were developed at a high-level with a few stakeholders as a starting point; these draft use cases were then further developed by participants in the breakout sessions.

Each use case envisions a digital twin for a particular Earth science focus area. It explores how the three ESDT components — digital replica, forecasting, and impact assessment and projection — could address science and applications needs and the value proposition of a potential future digital twin in that domain.

	ESDT Domain	Abstract
A1	Wildfires	A digital twin of Earth systems involved in wildfires to represent and understand the
		origins and evolution of wildfires and their impacts on ecosystem, infrastructure, and
		related human systems.
A2	Ocean Carbon	An Earth system digital twin of: ocean, land, atmospheric Earth systems to understand
		ocean carbon processes such as carbon export and ocean-atmosphere processes and
		coupling; land-ocean continuum and interactions with human systems (e.g., urbanization,
		land use change), to understand coastal ecological changes and impacts to ecosystem
		services; ocean, land, and atmospheric system to understand feedback processes, such as
		storm intensification and sea level rise, and their impact on coastal communities and the
		blue economy; assessing feasibility and impacts of the various Carbon Dioxide Removal
		(CDR) approaches as a strategy to remove and sequester atmospheric carbon.
A3	Water Cycle	A local or regional digital twin to understand all the complexities of the Water Cycle, how
		It is affected by various Earth Systems at multiple temporal and spatial scales, and how it
		is impacted by decision making and numan influence. It would provide capabilities such
		as zooming out in time and space; neiping understand water availability and origin for
		agriculture; now events such as noods and droughts affects of weather and elimpte verificities on
		he mitigated under various scenarios
A.4	Control Africo	An Earth System digital twin of "Carbon Corridors" (i.e., connected regions of protected
~4	Carbon	forests/vegetation that store carbon and maintain habitat connectivity for hiodiversity) in
	Corridors	Central Africa. Its goal will be to: understand the current conditions: assess their ability to
	contaots	store carbon and promote biodiversity: forecast future conditions: conduct what-if
		scenarios to assess the impact of policy decisions and potential climate conditions
A5	Atmospheric	An Earth system digital twin of: the atmospheric boundary layer to provide a digital
	Boundary Laver	replica of the lowest portions of the atmosphere and of their processes and interactions
		with other systems – land, ocean, and ice surfaces – and how these interactions control
		exchanges with materials such as trace gases, aerosols; coupled atmospheric systems to
		understand the underlying processes and their relationship to climate and air quality, and
		the role of these interactions on the global weather and climate system; atmospheric
		systems related to greenhouse gasses (GHG), sources of pollution, and their transport in
		the atmosphere to understand air quality and human health impacts at multiple scales
		from hyper-local to long-term global climate projections. Proper characterization of the
		Planetary Boundary Layer (PBL) is also critically important for modeling nighttime
		minimum temperatures for agricultural applications, and for prediction of wildland fire
		risk.

Table 2: ESDT Science Use Cases

The use cases were selected to cover major Earth science domains that involve interactions among Earth systems as well as with human activity. They are intended to be representative of the potential challenges that will need to be solved when developing future ESDTs. There are certainly many more ESDT use cases. These five selected use cases also informed subsequent breakout discussion sessions on technologies and federations.

The discussion considerations for these first breakouts on science use cases were the following:

- What is the vision for an Earth System Digital Twin in this science area?
- What ESDT capabilities are needed for this scenario?
- What science questions and needs would be addressed by those capabilities?
- What is the value proposition?

These use cases represent preliminary scenarios that were produced during the workshop brainstorming discussions. Over time, we envision ESDT use cases to be refined and developed in a more systematic fashion and fully corresponding to NASA Earth science interests, for example, as they relate to the Earth Action initiative [StG23].

5.1.1 A1: Wildfires

Scope	A digital twin of Earth systems involved in wildfires to assess risk (pre-fire),				
	guide response (active fire), and understand cascading post-fire impacts				
	(post-fire).				
Key capabilities	Pre-fire Active Fire Post-fire				
Digital Replica	Digital replication of current	Digital replication of the fire	Digital replication of post-		
(what now)	conditions to assess fire	evolution.	fire systems to understand		
	risk. What are the fuel		post-fire burn extent and		
	loads, where is it dry; wind		severity.		
	conditions; where are those				
	near infrastructure?				
Forecasting	Model-derived predictions	Digital replication of fire	Understand how interacting		
(what next)	of near- and long-term	crews, air assets,	system processes change		
	ignition risks and	infrastructure, evacuation,	after a fire.		
	uncertainties.	etc.			
Impact	Assess risk under alternate	Model-derived real-time	Forecast cascading impacts,		
Assessment	future conditions (e.g., wet	prediction of fire and smoke	such as flooding due to		
(what-if)	or dry winter).	plume evolution and spread	burn scars, impacts to air		
		to guide response. and water quality, and			
	impacts to human health.				
Earth Systems	Fuel load, soil moisture, ecosy	vstem/biodiversity, climatology,	, winds, smoke transport,		
	river systems.				
Human Systems	Infrastructure, crew disposition, air assets, evacuation routes.				
Resources now	SMAP, MODIS, in situ sensors, AIRS, MAIA, NIFC systems.				
Resources	TBD Missions/Sensors/Data.				
future					

A wildfire digital twin would contribute to the management of wildfires and to our scientific understanding of their causes, processes, and impacts. Wildfires are typically divided into three phases: pre-fire, active fire, and post fire. The pre-fire phase focuses on activities prior to a potential fire such as risk assessment and mitigation; active fire is the response to an active wildfire; and post-fire is managing and understanding the recovery. A Wildfire Earth System Digital Twin could address all three phases.

CAPABILITIES

A Wildfire Earth System Digital Twin would provide what-now, what-next, and what-if information about the multiple Earth systems that contribute to a wildfire. These include information about the forest, fuel loads, and soil moisture; propagation of the fire; winds and atmosphere; smoke; and ecosystems and biodiversity. In addition to Earth systems, the digital twin would also need to include information about human systems, such as firefighting assets, roads, and buildings and infrastructure.

Pre-fire: During the pre-fire phase, a Wildfire ESDT would provide information about the state of the forest in order to understand risks and mitigations. What-now capabilities would include measurements of the current conditions, from remote sensing, airborne, and in situ sources, augmented with nowcasting and models to fill in gaps. What-next capabilities would include forecasts and risk assessments. What is the forecasted fire risk, and where are the areas of greatest concern? What-if capabilities would provide longer-term risk projections and support mitigation efforts. How would fire risk change if certain mitigation efforts were implemented? What does the risk look like under different assumptions about future climate conditions, such as worsening drought or beetle infestation? Where are smoke plumes likely to go, what communities would be affected, and how will that impact health and air quality?

Active-fire: In this phase, a wildfire is actively burning. A Wildfire Digital Twin would support incident response teams' management efforts. What-now capabilities would provide the most up-to-date information on the current state of the fire. This would include measurements from remote sensing, airborne, in-situ sensors and ground crews. Some of these sources have latencies of several hours or more. Nowcast models would provide estimates of current conditions with appropriate uncertainty estimates. The state of the fire would be augmented with state and location of fire crews and airborne assets. Information about buildings, roads, and other infrastructure would also be valuable for understanding risks and planning evacuation efforts.

The what-next capabilities would provide near-term forecasts of fire spread, smoke plumes, and fire weather in support of response efforts. Accuracy and low latency forecasts are important given the operational cadence.

What-if capabilities would provide projections for different response scenarios and conditions. What are the likely outcomes if we make a fire break here or an air drop there? What will happen if the winds change? The breakout discussion focused further on what-if projections and impact assessments, and identified the following gap capabilities:

- Wildfire susceptibility models at 1-2 weeks out using fuel load and forecast of live fuel moisture
- Near real-time Ember-cast models using wildfire thermal and wind data
- Machine learning models to forecast live fuel moisture using soil moisture at surface and depth

Post-fire: After a fire, the digital twin would support recovery efforts and understanding the scope of the impact. What-now capabilities would provide information about the current state of the forest and affected ecosystems. What-if would provide recovery projections under different assumptions and under different recovery strategies. What-if projections would also provide new risk projections, such as flooding in burn scars.

MODELS AND DATA SOURCES

The breakout group identified several models that could contribute to a wildfire digital twin. These include fuel load, soil moisture, ecosystem/biodiversity, climatology, winds, and smoke transport.

Two particularly high-impact models are:

- Fuel loads to understand wildfire susceptibility
- Plume dynamics for situational awareness and forecasting

Other potential models and data sources discussed included:

- Lower-latency fuel load measurements from synthetic aperture radar (SAR)
- Communications
- Plume forecasts and bulk characteristics
- Near real time fire weather (wind & moisture)-embercast derivatives
- Human behavior

Forecast Models would be needed for:

- Fuel load (ladder fuels, fuel type, etc.). These would be climate/ecosystem map driven.
- Fuel moisture-soil moisture as leading indicator
- Rainfall intensity-Topo, windspeed and IWV driven
- Wildfire plume content using source and wildfire thermal data
- Wildfire spread processes, such as wind-driven embercast models
- Runoff areas: geologic and geomorphic constraints

OTHER CONSIDERATIONS

The breakout group identified a few additional considerations for the development of Wildfire Digital Twins:

- Technologies are needed to reduce latency.
- There is a training data gap for wildfires; training data sets would be valuable.

- Human-centered design should be considered in development to facilitate operational use.
- It is beneficial to use existing data and capabilities wherever possible.
- Having partners with regional capabilities is important for effective use of a digital twin for wildfire management and ensuring it has the right capabilities.

5.1.2 A2: Ocean Carbon

The ocean carbon cycle plays a vital role in Earth's carbon cycle. The ocean interacts with atmospheric and land systems to exchange carbon and is a key component of climate processes. An Earth System digital twin for Ocean Carbon would encompass ocean, land, and atmospheric systems that participate in those ocean carbon processes to better understand science questions and applications such as:

- Ocean carbon processes, e.g. carbon export, ocean-atmosphere processes, and oceanatmosphere coupling.
- Land-ocean continuum and interactions with human systems, such as urbanization and land use change, to understand coastal ecological changes and impacts to ecosystem services.
- Ocean, land, and atmospheric system to understand feedback processes, such as storm intensification and sea level rise, and their impact on coastal communities and the blue economy.

Scope	A digital twin of ocean, land, and atmospheric Earth systems to understand the role of ocean carbon processes such as carbon export and ocean-atmosphere-land interactions.		
Capabilities			
Digital Replica (what now)	 Digital replica of nutrient run off following precipitation and resulting coastal algal activity. Digital replica of carbon exchange from ocean-atmosphere coupling. Digital replica of the effects of anthropogenic pressure on oceans (rivers, increasing 		
	atmospheric CO2, increasing temperature, etc.).		
Forecasting	 Where and when are we likely to get algal blooms? 		
(what next)	 Can we improve severe storm and extreme event projections? 		
Impact Assessment (what-if)	 How will carbon exchange from ocean-atmosphere coupling impact sea level rise under different assumptions about key climate variables? How would sea level rise impact coastal communities under different assumptions? Assess feasibility and impacts of various Carbon Dioxide Removal approaches. 		
Earth Systems	Ocean, land, and atmospheric processes contributing to ocean carbon		
Human Systems	Agriculture, infrastructure, tourism, health, and safety		
Resources now	Ocean currents, SST, ocean color; ECCO; floats, gliders, and other in situ sensors (e.g., ARGO); land surface models; river flow models; ocean physical and biogeochemical models, atmospheric carbon data (OCO-2, TGO, MAIA, GOSAT)		
Resources future	Expanded measurements of carbon processes: sea surface temperature, ocean color, and currents; ocean circulation and biogeochemical models; atmospheric gasses such as carbon dioxide, methane, and water vapor; ocean sensor buoys, and gliders.		

• Assessing the feasibility and impacts of the various **Carbon Dioxide Removal (CDR)** approaches as a strategy to remove and sequester atmospheric carbon.

CAPABILITIES

A **Digital Replica** would provide the current state of ocean carbon. It would integrate ocean remote sensing data that contribute to ocean carbon processes, such as currents, sea surface temperature, ocean color plus related land and atmospheric data such as winds, river outflows, and atmospheric gasses such as carbon dioxide, methane, and water vapor. Observations would drive models to provide a more complete picture of the current state. A replica would address science questions such as ocean carbon exchange in ocean-atmosphere coupling. It would also support ocean carbon applications, such as coastal algal activity.

The **Forecasting** capability would project how coupled ocean carbon systems would evolve over time. There are several existing models for both individual and coupled ocean systems that could contribute to this capability. Applications range from forecasting when and where we are likely to get algal blooms, to storm and extreme event projections as well as investigate the various Carbon Dioxide Removal (CDR) approaches.

The **Impact Assessment** capability of this digital twin would project how ocean carbon systems could unfold in different hypothetical future scenarios and analysis of their impact. These would include scenarios such as how carbon exchange from ocean-atmosphere coupling would impact sea level rise under different assumptions about key climate variables; or how ocean carbon sinks and sources would evolve under different assumptions. The digital twin could also assess the impact of those projections. For example, how would harmful algal blooms change under different scenarios, and what impact would that have on fisheries and aquaculture? Or how would sea level rise impact coastal communities. Assessing economic and community impacts could be accomplished either by incorporating that information within the digital twin or by federating with another digital twin with that focus.

MODELS AND DATA SOURCES

There are many data sources and models that could contribute to an Ocean Carbon digital twin. Ships, buoys, gliders, drones and global sensing could all contribute to improved measurement, leading to better models and understanding of the carbon processes. Current and future data sources and models include sea surface temperature, ocean color, and currents; ocean circulation and biogeochemical models; atmospheric gasses such as carbon dioxide, methane, and water vapor; ocean sensor buoys, and gliders; reanalysis products and earth system models.

OTHER CONSIDERATIONS

The carbon cycle is a complex interaction among ocean, land and ocean systems that operates at various spatial and temporal scales. To really answer the fundamental questions, such as how climate change will affect ocean carbon uptake and its long-term impacts, we should consider a global carbon digital twin. One could then "zoom in" to specific concerns, such as algal bloom effects in coastal zones; or the global carbon digital twin could federate with more specialized twins. In a federated approach, the global carbon twin could provide coarser boundary conditions that the specialized twin could refine to regional scales.

A global carbon digital twin would be an ambitious undertaking. Some of the challenges include:

- Coupling of ocean, land, and atmospheric models
- Global models that do well at open ocean don't necessarily work well at coastal scales
- Atmosphere-ocean interactions are better resolved than land-ocean
- High uncertainties in some boundary processes, such as river input to ocean (land toocean)

5.1.3 A3: Water Cycle

The ultimate goal of a Water Cycle digital twin is to understand all the complexities of the Water Cycle, how it is affected by various Earth systems at multiple temporal and spatial scales, and how it is impacted by decision making and human influence. It would provide capabilities such as zooming out in time and space; helping understand water availability and origin for agriculture; how events such as floods and droughts affects life, property and infrastructure; and more generally how the effects of weather and climate variability can be mitigated under various scenarios.

Scope	A digital twin to understand all the complexities of the Water Cycle, its relation to weather and climate, and the impact from human influence as well and its impact onto human systems.
Capabilities	
Digital Replica (what now)	 What is the current state of hydrologic systems: rivers, reservoirs, snow pack, etc. Observe current state of hydrologic systems to understand how they are interacting (rivers, snow pack, reservoirs, etc.). Understand current state of hydrologic systems following floods and droughts, including data from human systems (e.g., rivers, snow pack, aquifers, precipitation, soil moisture and their interactions with cities, agriculture, etc.).
Forecasting (what next)	 Under probable evolution of current conditions, what will be the future state of the water cycle in 5, 10, 20 years, considering multiple systems (snow pack, precipitation, river networks subsurface, land surface models, etc.)?
Impact Assessment (what-if)	 How might hydrology systems evolve under different climate or policy assumptions, and how would that impact human activities? Improve our understanding of the processes driving interacting hydrologic systems by conducting what-if projections under different assumptions.
Earth Systems	Evapotranspiration, river systems, snowpack, subsurface aquifers, meteorology/climatology, surface water (reservoirs/lakes), and land use/land cover.
Human Systems	Reservoirs, dams, agriculture, infrastructure.
Resources now	NISAR, SMAP, GPM, VIIRS, Landsat, SBG, PACE, GRACE/FO/MC, CYGNSS/SoOP, Sentinels, river gauge sensor network, GCMs/Reanalyses (i.e., MERRA-2), LIS.
Resources future	ТВО

CAPABILITIES

A Water Cycle Earth System Digital Twin would provide what-now, what-next, and what-if information about the multiple Earth systems that contribute to the water cycle, understanding its relationship to weather and climate, and information on how the water cycle contributes back to the multiple Earth systems that contribute to it.

The breakout group quickly realized that the water cycle is quite broad and therefore limited the scope of its discussion to the terrestrial water cycle. The discussion spanned from regional to global scales. Regional twins would be valuable for studying water cycle processes specific to different environments (e.g., polar, tropical, urban). Global Water Cycle Digital Twins would provide insight into the interactions among hydrologic processes at the global scale. Twins at all scales could be federated.

Digital Replica: The water cycle consists of many components, such as rivers, reservoirs, and snowpack. All of these are significantly impacted by various local conditions. For example, rivers near Earth's poles are driven by glaciers to a significant extent, but this is not true for tropical rivers. For this reason, the group discussed developing a Digital Twin architecture with object types, such as rivers, that can be instantiated with their characteristics, such as their locations, neighboring object types, and others. We need significantly more data and systematic study of the various elements of the water cycle and the elements that impact them. This will need to be performed separately depending on the environmental characteristics. For example, polar regions will need to be studied separately from the tropics, and areas close to urban centers will need to be studied separately from rural areas and forests. Separate digital twins could be developed for these various environments and then we could explore tying these twins together. These various digital twins may serve to "fill in" missing data and information to help assess the true states of the water cycle following floods and droughts, and other environmental occurrences. There are also national security concerns with regards to the water cycle, such as one nation extracting underground water from a neighboring nation. Digital twins may help to inform these concerns and enable better decision making.

Forecasting: The key benefits of forecasting are to different users, such as farmers, who can decide what crops to plant given expected precipitation. Forecasts can also provide key information for assessing risks, which is important for all users. For example, better informed assessment of the risk of flooding is important for homes, businesses, and their insurers.

Impact Assessment (what-if): The ability of digital twins to allow what-if assessments is quite important for the water cycle, essentially allowing forecasts of alternate futures. The breakout group discussed potential policy decisions on land use, and adding and removing dams, as examples of alternative futures that could be explored.

MODELS AND DATA SOURCES

There are many models and data sources that could be part of a Water Cycle Digital Twin. Some of these are listed in the use case summary table above as an example. A specific

implementation would need to select models and data sources based on the needs of the system, and may use all, some, or none of these. These models would need to be integrated to constitute an accurate digital replica and provide the ability to do forecasting and impact assessment along the lines discussed above. The breakout group also discussed the need for uncertainty quantification. This is especially critical for filling in missing data for the current state of the water cycle and forecasting and impact assessment. The value of different data sources can also be assessed in terms of the reduction in uncertainty that they yield in the digital twin.

The breakout group identified many relevant users of a water cycle digital twin, all of which may provide relevant data and models: water utilities, agriculture, hydropower, shipping industry, Army Corps of Engineers (for dam maintenance), NOAA, USGS, EPA, and national security. Their perspectives on how they would use such a digital twin are critical to developing a useful system.

OTHER CONSIDERATIONS

There are many additional gaps that the breakout group identified beyond user perspectives. Water issues are mostly local; however, if local digital twins were developed, they would need to be interoperable with other similar digital twins and federated to inform a global perspective. Standards for how the various digital twins could be tied together will facilitate rapid, independent developments of the component digital twins. Other considerations include: the importance of identifying and representing natural and anthropogenic factors in the water cycle, especially for forecasting and impact assessment; and the need for comprehensive data at different resolutions to develop an accurate digital twin and to allow the resulting digital twin to assess the true value of each data source and the different resolutions.

5.1.4 A4: Central Africa Carbon Corridor

Carbon and biodiversity corridors are connected regions of protected forests and vegetation. They store carbon and maintain habitat connectivity for biodiversity. This use case envisions an Earth System Digital Twin for carbon and biodiversity corridors in Central Africa that would enable users to:

- Understand the current conditions
- Assess the ability of carbon and biodiversity corridors to store carbon and promote biodiversity
- Forecast future conditions
- Conduct what-if scenarios to assess the impact of policy decisions and potential climate conditions (e.g., helping inform the Democratic Republic of the Congo (DRC) about the best lands to lease for oil/gas exploration while minimizing negative impacts on carbon sequestration and maintaining the DRC's unique biological heritage)

One concrete and timely application is supporting land-use decisions. In the summer of 2022, the Democratic Republic of the Congo announced auctions of oil and gas blocks. These blocks

intersect peat lands and high carbon stock corridors, which are major carbon sinks and also connect wildlife habitats. Decision makers would like to understand how proposed land-use strategies would impact carbon stores and biodiversity composition and abundance, as well as the agricultural and economic impacts. A digital twin could provide a more detailed and comprehensive picture of the short-term and long-term impacts to better inform such decisions. One example of goals for this ESDT is to inform DRC decisions on which lands to lease for oil and gas while conserving the most important areas for maintaining carbon sinks and biodiversity conservation, as well as habitat connectivity.

Scope	A digital twin of Carbon and Biodiversity Corridors in Central Africa.			
Capabilities				
Digital Replica (what now)	 Digital replica of carbon/biodiversity corridors to understand the current conditions. Estimate carbon storage, biodiversity composition and abundance, and the potential for wildlife dispersal and migration. Effects/interactions with agriculture, infrastructure, and other land uses. 			
Forecasting (what next)	 Forecasts of carbon storage, biodiversity conservation, and habitat connectivity. Interconnected system of systems forecasts (e.g., hydrology, vegetation, atmosphere, carbon exchange, biodiversity, and land use/land cover (LCLUC) together). 			
Impact Assessment (what-if)	 How would carbon storage capacity and/or biodiversity composition/abundance and/or habitat connectivity change under different land use scenarios? Where would adding protected area coverage help? Which areas would have the most/least impact on the above? How would different scenarios of change impact agriculture? How would carbon storage/biodiversity loss evolve under alternate future climate assumptions? How would habitat corridor intactness respond to different wildfire scenarios? 			
Earth Systems	Forests, hydrology, atmosphere (CO2 exchange), biodiversity, fires.			
Human Systems	Agriculture, infrastructure, other land uses, trade in bushmeat.			
Resources now	Landsat, MODIS, SMAP, Terra, Aqua, GEDI, NISAR, commercial high-resolution imagery, biodiversity assessments, in-situ sensors (AQ, telemetry tags, etc.).			
Resources future	Activity from nighttime lights, in-situ acoustic sensors, bushmeat reports, roads, economic reports.			

CAPABILITIES

The digital twin would need to encompass at least three core concerns:

- The amount of above-ground and below-ground carbon
- Biodiversity composition and abundance
- The connectivity between habitats in space and time and this connectivity's relationship to biodiversity.

The twin would allow the user to answer questions about the interrelationship among these domains, as described in the following sections. The core question, informing land use, falls under impact assessment.

Digital Replica: The digital replica would reflect the current state of existing carbon and biodiversity corridors, including above and below ground carbon, biodiversity composition and abundance, and habitat connectivity. Some of the core science applications and questions that could be addressed by the digital replica capability include:

- How are habitats connected and how does this impact biodiversity?
- How is the forest growing? How does it interact with fire? Is the understory recovering?
- Monitor carbon dynamics and biodiversity composition and abundance. Are they changing, and how are they related to human activities?

Forecasting: The digital twin's forecasting capability would show how carbon and biodiversity corridors are likely to change in the near future. Current biodiversity models are limited. One science use of a digital twin is to improve those models through better understanding of the underlying system processes and interactions between them. The ability to compare forecasts with observations (the digital replica) would facilitate model improvements and thereby improve future forecasts and modeling:

- Forecast near-term changes to biodiversity and carbon stores.
- Understand interactions to improve models and process understanding. For example, elephants push down trees which reduces forest cover in the near-term, but they disperse seeds of large, high wood density species, spurring growth for a net gain in carbon and biodiversity.

Impact assessment (what if). This digital twin capability speaks most directly to the goal of informing land-use decisions:

- How will developing specific plots of land impact carbon storage and biodiversity composition and abundance in the short term and in the long term?
- Which areas will have the least impact?
- How will changes to carbon storage and biodiversity impact economic concerns such as agriculture and trade?

DATA SOURCES AND MODELS

An Earth System Digital Twin of carbon and biodiversity corridors would require data about land cover and land use; forest structure; carbon in the land and air; species distribution and abundance; and human activity. It will also need models for biodiversity and carbon processes, as well as habitat connectivity.

Existing Data Sources: Existing data sources that could contribute to this digital twin include satellite remote sensing, including assets like Landsat, MODIS, SMAP, Terra, Aqua, GEDI, NISAR, high-resolution commercial imagery; in situ sensors such as air quality and animal tracking tags; and analysis products such as biodiversity assessments.

These could be augmented with potential future data sources, especially those for understanding how carbon and biodiversity corridor systems interact with human activity. Integrating such data into the digital twin will be important for improving our understanding of carbon and biodiversity corridor dynamics.

- Nighttime light sources visible in satellite imagery could indicate human social and economic activities, including burns to convert lands to agriculture and other uses. There are some limited static data sets available now, but a continuously integrated data set could be a valuable indicator of human activities.
- Roads
- Human trade data (e.g. bushmeat consumption)
- In situ biodiversity measurements such as expanded tagging, acoustic sensors, and trail cameras

Models: There are a few commonly used biodiversity models that could be part of the digital twin. The Madingley model [Har14, Mad23] takes a process-based approach to estimating abundance and biomass distributions of animal functional groups and can be applied from pixel to global scales. An alternate approach would be agent-based models [AnG21], which are finer grained but do not scale as well due to computational complexity. Neither of these fully integrate models of human activity. A digital twin would need to be able to model biodiversity at multiple spatial scales; provide finer grained detail about interactions; and consider human activity.

OTHER CONSIDERATIONS

Value Proposition

Current models are inadequate to answer the kind of questions we would like to ask of a digital twin. Current tools can perform static point analyses, but they cannot do detailed projections of how exploiting an acre of land will impact biodiversity in that area 10 years from now. Current data sources are stove-piped. Having them all available and integrated within a single digital twin would greatly facilitate science analysis.

A Proposed Development Strategy

Current biodiversity models are inadequate to support some of the envisioned forecasting and impact assessment capabilities. The breakout group proposed a two-phased development strategy for a carbon and biodiversity corridor digital twin that could close this gap.

In Phase 1, several digital twins could be piloted to address the three core domains: (1) Aboveground / below-ground carbon, (2) Biodiversity composition and abundance, and (3) Measurements of the habitat connectivity focusing on the connectivity between "patches" of carbon and biodiversity. The pilots would be validated against satellite remote sensing and insitu observations, accounting for uncertainty, to assess the quality of the digital replicas and their forecasting capabilities. In Phase 2, a more comprehensive digital twin could be constructed that would build on top of the lessons and systems from the pilot phase. This twin would also be validated, as above. It could also be used to answer questions such as what needs to be modeled in order to answer impact and forecast questions. It may be possible to simplify the pilot approaches. This phase would also address issues of coupling and interoperability among various models.

5.1.5 A5: Atmospheric Boundary Layer

The atmospheric boundary layer (ABL), or planetary boundary layer (PBL), is the lowest layer of the Earth's atmosphere. It interacts with processes at the Earth's surface and plays an important role in weather, air quality, and climate. A digital twin of the atmospheric boundary layer would encompass the lowest portions of the atmosphere and their interactions with the Earth's surface to better understand science questions and applications such as:

- How interactions between the atmospheric boundary layer and Earth surfaces control exchanges with materials, such as **trace gases and aerosols**
- Understand the underlying processes of **coupled atmospheric systems** and their relationship to climate and air quality, and the role of these interactions on the global weather and climate system
- Atmospheric systems related to greenhouse gasses (GHG), sources of pollution, and their transport in the atmosphere from hyper-local to long-term global climate projections
- Proper characterization of the PBL , which is also critically important for modeling nighttime minimum temperatures for agricultural applications and for prediction of wildland fire risk

Scope	A Digital Twin of the Atmospheric Boundary Layer
Capabilities	
Digital Replica (what now)	 Digital replica of current lower atmospheric systems and processes including planetary boundary layer (PBL) processes that impact surface exchange of greenhouse gases and air pollutants. Of particular interest is capturing the interactions of PBL dynamics with human activities (e.g., urban and agricultural systems) and terrestrial and marine ecosystems.
Forecasting (what next)	 Forecast evolution of these PBL processes in various environments, and for different climate scenarios Forecast air quality and carbon cycle Transport of wildfire smoke
Impact Assessment (what-if)	 Long term climate projections and relationship to GHG under different assumptions about key variables and trends. How would air quality evolve under different assumptions about human activity or policies, and what would the impact be on human health?
Earth Systems	Terrestrial ecosystems (forests, grasslands, etc.), Marine ecosystems (coastal), precipitation, atmospheric chemistry, land/sea interactions
Human Systems	Cities, infrastructure, transportation, agriculture emissions
Resources now	MODIS, AIRS, CrIS, VIIRS, CALIPSO, TROPOMI, TEMPO, GEMS, MAIA, OCO-2/3, GOSAT, MethaneSat, GHGSat, GOES-R, in situ AQ sensors
Resources future	CO2-M, GOSAT-GW, SBG, AOS, Geo-XO, /Sensors/Data

CAPABILITIES

A **Digital Replica** would encompass the lower atmosphere systems and their interactions with planetary surface systems, such as land, sea, and ice. It would integrate models and observations to provide insight into science questions and applications such as understanding surface exchange of greenhouse gasses and air pollutants; and for understanding the composition of carbon in the atmosphere and the impact of boundary layer processes on the carbon cycle. Of particular interest is the capturing of interactions of PBL dynamics with human activities (e.g. urban and agricultural systems) and terrestrial and marine ecosystems. These applications would also require information about ecosystems and human systems, either as part of the digital twin or in federation with other digital twins.

The **Forecasting** capability would project how atmospheric boundary layer systems would evolve over time. Applications include air quality predictions and transport of wildfire smoke.

The **Impact Assessment** capability of this digital twin would project how atmospheric boundary layer processes could unfold under hypothetical future scenarios and assess their potential impacts. Applications include climate projections under different assumptions and analyzing their relationship to greenhouse gas; and atmospheric transport of pollutants and GHG under various scenarios and their impacts on human health.

MODELS AND DATA SOURCES

There are a wealth of data sources and models that could contribute to an Atmospheric Boundary Layer Digital Twin. These include remote sensing of atmospheric conditions and composition, such as MODIS, AIRS, TROPOMI, and OCO; in situ sensors for air quality and meteorology; and a rich set of models for atmospheric transportation, composition, and chemistry. An ABL digital twin could include interactions with land cover / land use change (LCLUC).

An ABL digital twin would benefit from additional data sources. An ABL digital twin that encompasses surface air quality — such as fires, Volatile Organic Compounds (VOCs), Ozone (O3), Methane (CH4), and Nitrous Oxide (N2O) — would need measurements from surface air quality networks, PBL precipitation, and temperature. 3-D surface structure data could improve deposition estimates. Emissions from land are important to ABL processes, but critical measurements near the ground are lacking. Additional in situ or remote sensing measurements would improve a digital replica of those processes.

At the neighborhood scale, an ABL digital twin could integrate fine scale emission data from sources such as traffic, wildfires, and human activities to understand air quality, ozone, and landcover change.

OTHER CONSIDERATIONS

The breakout group identified several considerations for digital twins of the atmospheric boundary layer.

- Planetary Boundary models are important for understanding carbon in the atmospheric quality. The ability to see processes at multiple scales, including finer grids, would be useful for understanding those processes.
- Weather models do not simulate the atmospheric boundary layer, which differs between regions. A digital replica of the ABL could improve weather models, perhaps through federation.
- Machine learning models could be useful for forecasting. They can complement physicsbased models or be trained from measurements and principles where there are no existing models.
- The neighborhood scale is important for many air quality applications. Physics models are different for different neighborhoods. There are models for wildfire plume modeling for several US cities that work well when fire location and characteristics are known at fine scale. Measurements at that scale could be used to train physics-based machine learning models to address additional cities and processes. Smaller scale models could also provide insight into the resolutions at which current larger scale models break down. For example, chemistry and plume models differ for distributed cases, and atmospheric chemistry needs to be modeled at the appropriate scale.
- It should be possible for digital twins to characterize uncertainty and extend to public health. Visualization of those science scenarios will need high resolution emissions and deposition for neighborhood level air quality. Techniques are needed to better characterize and quantify uncertainties, especially for ML models.

5.2 Technologies

The technology breakout sessions were organized around ESDT capabilities. Each group focused on a different ESDT capability: digital replica, forecasting, and impact assessments. The main objectives were to identify technologies needed for those capabilities, including those that could be available in the near-term and those with longer development timeframes.

The breakout groups considered the following discussion guidance:

- What are the main ESDT capabilities needed in this area? Consider the needs from the science scenario breakouts as a starting point.
- What are the key technologies needed for those capabilities?
- What DT capabilities could be achieved in the near-term? What are the key technologies?
- What ESDT capabilities are farther term and would need more significant technology advances?
- Are there any "tall tent pole" technical challenges that need particular attention?

	ESDT Capability	Moderator	Scribe
B1	Digital Replica A (Science) Evolution of Earth systems from historic to now.	Mike Little	Louis Nguyen
B2	Digital Replica B (Applications) Evolution of Earth systems from historic to now.	John Stock	Jon Ranson
B 3	Forecasting What will Earth systems do next starting from current state	Sujay Kumar	Nikunj Oza
B4	Impact Assessments and Projections What would happen over the long-term under different scenarios or assumptions. How will that impact natural and human systems?	Laura Rogers	Dedelolia Olungwe

5.2.1 B1: Digital Replica (Science)

Breakout groups B1 and B2 both considered technologies needed for *digital replica* capabilities of a digital twin. Science and application users have different needs and therefore somewhat different requirements for a digital replica. Group B1, described in this section, focused on technologies to support digital replica needs for science users. Group B2 focused on applications users and is discussed in the next section (5.2.2).

5.2.1.1 Science User Needs for a Digital Replica

The group discussed needs that science users would have for a digital replica and then explored the technologies that would address those needs.

Near-real-time science data processing is needed to enable updates to the digital replica so that it is as contemporaneous to reality as possible. This includes the data assimilation needed to make the data smooth (e.g. removing jitter) without removing measurements of actual anomalies.

Computational Capacity: Computational capacity sufficient to create and maintain the digital replica (observations) and to project ahead nominal forecasting, including the uncertainty quantification needed to create appropriate confidence in the DT. Both research and applications users also need sufficient computational capacity to run alternative forecasts derived from varying input conditions and constraints.

Collaboration Tools: Future use of such digital twins requires collaboration tools, including easy to use access controls with varying levels of user authorization. Shared workspace available to all members of the investigation team is essential to harnessing the full power of the group.

Standards: Application of standards to the instrument output data products to enable faster data fusion and assimilation. 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.

Intuitive "Low Drag" Search and Browse of Datasets: Processing an entire dataset to extract a region or timeframe is computationally expensive and significantly time consuming during an investigation. In several discussions, scientists indicated a need for a rapid-turnaround way to narrow down to the desired space and to extract only necessary data without spooling through the entire set of files. One point of discussion was whether it is better to provide (and store) multiple versions of analysis ready datasets or to develop a translator to transform data from various authoritative sources into a format preferred by the PI for that investigation.

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

- DTs are not owned by an individual organization or community but have structured means to encourage inclusive contribution.
- Access to diverse inputs and a guide to help discover unrecognized assets.
- Permitting others to contribute to a shared DT (NASA is only one part of the community).
- Leverage developments from other agencies.
- Current concepts of intellectual property blocks openness.
- A new model to give credit for intellectual advances earlier than publication.

Confidence in the validity of the DT will be essential to its usability. Confidence in the validity is distinctly different than validation. What is required to establish credibility in the DT and confidence in using it varies widely across communities but is important to all. There seems to be two different camps at either end of the spectrum: the public and non-scientific decision makers, and the research scientists.

5.2.1.2 Technologies for a Science-focused Digital Replica

Technologies needed for Digital Twins were discussed around five technology areas:

- Information system frameworks
- High-performance computing
- Machine learning, surrogate models and data fusion
- Visualization and Virtual/Augmented Reality
- Multi-sensor data fusion and vicarious calibration

Much of the needed technology is under development by programs such as AIST. However, a few other technologies and challenges were identified that need maturation:

• Reusable and interchangeable components.

- Edge Computing
- Accelerated forecasting models
- Advanced, fast, data visualization
- Geospatial registration
- Easy to use control console

Reusable and interchangeable components: In the Science scenario breakout, scientists indicated that they would like to be able to explore alternative algorithms and tools in a pipeline, and that development of a framework permitting interchangeability is important. Swapping out different algorithms to perform similar functions can help with improving accuracy, precision, uncertainty and throughput, as well as letting the investigator to explore sensitivity of the results to the tools. A computing environment that enables this would permit a more thorough exploration of the phenomenon or process as well as improved validation of the conclusions.

Edge computing: Further development of capable computing platforms, models, algorithms, and tools for use in processing data and commands at the instrument is essential. The integration of edge computing with central facilities is important and computer security is an important consideration to ensure that data is processed accurately and that the results are returned to the central computing site without disruption. Understanding the full breadth of commercial computing development work in this area is a key component of solving this problem without developing the technology from scratch and an opportunity for collaboration with various firms and universities. This will also involve consideration of the data communications technologies needed to link the pieces together. Software defined networking is likely to be instrumental.

Accelerated forecasting models: Forecasting models must be fast to yield analyzable results in order to be useful in a DT. These results can be delivered in stages but should be consistent with the Human Factors discipline imposed. They must also provide estimates of UQ in some apparent and obvious way, also with some Human Factors Engineering (HFE) guidance.

Accelerated models are a cross-cutting need. Digital replicas need fast models for nowcasting and hindcasting to create a timely and complete picture of the current state and recent events. The Forecasting breakout (5.2.3) identified a need for accelerated forecasting models, and the Impact Assessment breakout (5.2.4) identified a similar need for accelerated climate scenario models.

Advanced, fast, data visualization: Scientific visualization with low latency is important to enabling the understanding of the physical phenomena or natural process. Scientific visualization in this context means data-driven visualizations with access to the parameters, not just a pretty graphic. Work in AR/VR is ongoing at multiple locations, notably GSFC and JPL. Visualization of the uncertainty quantification (UQ) is critical to using the DT in an effective way. Decision making on data and products that lack quantified uncertainties will lead to misuse and misinterpretation and rapid discrediting of the DT.

Geospatial registration: The subject of co-registration came up several times during the discussion, both in the context of co-registration of instrument scientific data and model output and in the context of co-registration against the GIS coordinate system. The DT, to be usable, must handle both issues. Small registration errors will render the coordination of the data ineffective for scientific uses. Scientific investigations relying on the Digital Replica are particularly demanding. This is also an element of the Uncertainty Quantification – if the region (in a topological sense) in which the individual observation is located is too large or misstated it will render the DT useless and unreliable at as virtual instrument.

Easy to use control console: There was considerable discussion of how to interact with the DT itself. Part of what's needed is rapid, multi-scale visualization, but that is only one part of the answer. To derive effective value, the user must be able to steer the focus of the forecasting and spawn what-if exercises with easy-to-use controls. Good human factors design is an important feature of this development (e.g., the importance of human factors engineering in the Macintosh initial development).

5.2.2 B2: Digital Replica (Applications)

Breakout group B2 considered technologies needed for digital replica capabilities of a digital twin focused on the needs of application users. The companion group, B1, focused on science users as described above in Section 5.2.1. To guide the discussions, three use cases were considered: Use Cases A1/Wildfires and A3/Water Cycle that were described previously as well as an additional use case not previously discussed, but of great importance, focusing on Smart Cities/Urban Planning. The Wildfires use case considers a fine scale 3-D wildfire surface model including hyperspectral-derived species types for locating ground and ladder fuels; the Water Cycle use case is based on an end-to-end hydrology model based on NASA's GSFC's Land Information System (LIS); and the Smart Cities/Urban Planning use case is based on a French study which considers fine to course scale modeling, autonomous mapping, and a user interface.

Capabilities and Challenges

The main capabilities for a Digital Replica in the Applications area are centered around a dynamic three-dimensional model. This type of model can consider problems at different scales (e.g., cities, watershed). They can handle modeling gaps such as human impacts, impervious surfaces, dams, and land cover change.

The current level of digital twin capability with available technology is achievable for a learning behavior model for water resources. Key technologies needed to support applications include model development and integration. Important features discussed included human feedbacks (e.g., wastewater and dam operators), semantic interoperability, high-resolution surface height models, and increased spectral, spatial, and temporal resolutions from satellite systems.

For all three use cases, the following general challenges were identified:

- Workflows to fuse very different kinds of data (citizen science, IoT, etc.) and weight their role in the Digital Twin outputs
- Development of architectures for data computation and visualization for multi-scale storage and output
- Ingestion of Quality Assurance/Quality Control (QA/QC) methods for untrusted data
- Improvement of semantic interoperations to ingest real-time human sourced data feeds; initiation and development of potential partnerships with industry
- Development of protocols for source data that require a legal framework to protect personal privacy

Other needed capabilities also include:

- Acceleration of forecast models by about 10X compared to current runtimes
- Overcoming common observation gaps including sub-meter GSD data, with frequent updates
- Availability of required sources of training data for machine learning
- Building trust and awareness of users in the consistency of DT with physics
- Development of human-centered design to enable and facilitate trust and interactivity of DTs by/with end-users

Technologies

Among the technologies corresponding to the challenges listed above, some of the most important are data fusion and assimilation from multiple sources, zooming in and out at various spatial scales, modeling to fill in between observations, running at scale, and data visualization.

More specifically, technologies identified for each of the three use cases (wildfires, water cycle, and smart cities) are listed below:

Wildfires

- Development and delivery of analysis ready data and fusing different data types
- Acceleration of models, e.g., going from 4 hours to 4 minutes
- Need for diverse training data (e.g., orbital, air, ground, IoT, citizen crowd sourcing)
- Approaches such as decision trees to process data and workflows to fuse very different kinds of data and achieve the required output layers
- Computational latency for hourly plume forecasts, more importantly for local rather than regional or continental plumes; a gap in technology exists between the generation of a plume forecast and human response; decision making support and operations and enhancement assisted by human-centered design would help fill that gap.
- QA/QC for crowd sourced data, especially in collaboration with industry
- Knowledge Graph Process Frameworks
- Development of accurate models for wildfire spread, wildfire susceptibility, and smart city response to wildfires

Water Cycle

Water resource systems have a large stakeholder base, e.g., U.S. Army Corps of Engineers (USACE), as well as many other federal agencies and private sectors. The main required technologies include:

- Multiscale modeling approach (e.g., wastewater vs. transit)
- Capturing human infrastructure changes as they relate to water resource systems, e.g., capturing operator-driven changes to a dam, or in agriculture
- Integrating additional variables such as wastewater infusion and ground water recharge
- Real-time data feeds from human sources
- Improving semantic interoperability to onboard more data streams

A learning behavior model for human water action with cultural input and a boundary layer are considered achievable capabilities. Software systems such as Autodesk and Trimble may fit the needs, among others, with not much human decision making in the loop.

Smart Cities/Urban Planning

For this use case, the key technology needs that were discussed include:

- Availability of high-resolution imagery (e.g., 10 cm)
- Structure from motion (SfM) software to provide building details
- Autonomous navigation above and on ground to provide full coverage of the city
- Updatable hyperspectral imagery for land-use mapping
- 4D modeling of the city with layers labeled with purpose and object characteristics, as well as uncertainty estimates for each characteristic

Overall, it would be useful to generalize existing smart city digital twin architectures, e.g., leveraging industry models of smart cities and add variables such as air quality. Also needed is a better understanding of the longer-term legal issues associated with the implementation of a digital twin for disaster prediction.

5.2.3 B3: Forecasting

Group B3 discussed technologies needed to support the *forecasting* capabilities of an Earth system digital twin. That is, how will the Earth systems evolve in the foreseeable future from the current state?

Key capabilities needed for forecasting include uncertainty quantification, connecting existing physics-based models, surrogate models of sufficient accuracy and that run faster than existing physics-based models, and policy models that allow what-if scenarios over different policies and allow for cost/benefit assessments. Machine learning will be needed to fill in the gaps not modeled accurately by physics-based models or their surrogates, and to connect the various models together when they do not have common variables. Reinforcement Learning can help with identifying policies that will be best in terms of cost/benefit. For the forecasts to be useful, the technologies must be able to separate the influence of initial and boundary conditions, as well as the influence of random versus systematic factors.

Accelerated models are a cross-cutting need. The Digital Replica breakout (5.2.1) identified accelerated models as a need for timely nowcasting and hindcasting, and the Impact Assessment breakout (5.2.4) identified a similar need for accelerated climate scenario models.

It was felt that, within the near term, we can assess current forecasting skill under different conditions through benchmarking of hindcasts, start using machine learning to "glue" various pairs of physics-based models, and better quantify non-stationarities given increased observational capabilities. Farther term developments include firmly describing how we will assess forecasting skill as we grow the scope of the digital twin, identifying emergent constraints from various models and their relationships, and predicting "tipping points." Another key development needed is identifying "levels" (e.g., spatio-temporal fidelities and scopes) of ESDT capability as relevant technologies are developed and assessing the true benefits of these relevant technologies.

All these developments are likely to proceed along very different trajectories and with different rates of progress depending on the Earth science area due to variations in the availability and usability of data and models. However, ultimately, we would like to tie these forecasting technologies together. Therefore, ways need to be developed to standardize forecasting technologies and their interfaces to allow for the technology developments to proceed largely independently but still work together.

5.2.4 B4: Impact Assessments and Projections

Group B4 discussed technologies needed to support the impact assessments and projection capability of a digital twin. This is the ability to project what could happen over the long-term under different scenarios or assumptions and to assess the impacts on human and natural systems.

The group concentrated on ESDT capabilities needed for impact projections in the 30-year plus timeframe. Important factors for long range impact projections are the effects of human interactions and the (limits of) predictability.

The key technologies are:

- Climate scenario emulators
- Climate model downscaling using machine learning
- Predictive Modeling

Climate scenario emulators are the most mature capabilities. They generate possible climate futures for a standard range of scenarios. They could be expanded to consider tailored scenarios out of those standard ranges, such as major regional disruptions or different ENSO possibilities.

Downscaling of General Climate Models to local scales is less mature and would need further technology advances. Speed ups on the order of 10⁵ would be needed to downscale models from approximately 600km resolution to 10s of meters to understand local impacts. Machine learning technologies are one promising approach.

Accelerated models are a cross-cutting need. The Digital Replica breakout (5.2.1) identified accelerated models as a need for timely nowcasting and hindcasting, and the Forecasting breakout (5.2.3) identified a need for accelerated forecast models.

Another area for consideration is interactive exploration. How can users provide information about human activities, and interactively explore different scenarios?

A few scenarios include:

- Users should be able to specify parameters to interactively explore scenarios and their impacts.
- Can these kinds of actions be "gamified" to allow interactive exploration? What if we plant more trees? What if convert this area into crop land?
- Consider capabilities for "layers" or user options. For example, how would actions like planting trees be expressed in the digital twin so that it can project long term impacts?

Intuitive interfaces are another cross-cutting need. The Digital Replica breakout (5.2.3) independently identified a need for an **easy-to-use control console.** There was considerable discussion of how to interact with the DT itself. Part of what's needed is rapid, multi-scale visualization, but that is only one part of the answer. To derive effective value, the user must be able to steer the focus of the forecasting (5.2.3) and spawn what-if exercises (5.2.4) with easy-to-use controls. Good human factors design is an important feature of this development.

5.2.5 Key Outcomes from Technology Session

Table 3 below summarizes key outcomes from the technology breakout sessions.

Capabilities and Needs	Technologies			
Digital Replica (Science and Applications)				
 Models, Observations, and Analysis Near-real-time science data processing Accelerated, multi-scale, and inter-connected models Accurate fusion of disparate, multi-scale instrument and other types of data Integration of human systems information Intuitive workflows for analysis and fusion Computational capacity Intuitive user interfaces Collaboration tools Easy to use control console. Low-drag (intuitive) search/browse of datasets Advanced and fast data visualization Reusable and interchangeable components. Validation, Confidence/Trust 	 Modular and open source information system frameworks Standards and interfaces for interoperability High performance computing, GPU Models optimization Edge computing Machine learning for data fusion and surrogate modeling Multi-scale modeling Accurate and fast multi-source geo-registration Advanced and fast visualization including VR/AR/MR/XR Uncertainty Quantification 			
Forecasting (what next)				
 Connecting/coupling models Accelerated forecasting models Integrating multiple spatial and temporal scales 	 Machine learning (surrogate models, model coupling, semantic mapping, multi-resolution and multi-source analysis) Reinforcement learning Uncertainty quantification 			
Impact Assessment (what if)				
 Downscaling projections to local scales (spatial and temporal) Interactive exploration of scenarios and impacts Policy models for what-if scenarios Visualization 	 Climate scenario emulators Climate modeling downscaling (e.g., ML) Predictive and causal modeling Frameworks for interactive exploration, visualization, and analysis What-if models and impact analysis 			
Cross Cutting				
 Fast and responsive computations Handling multiple spatial and temporal scales Interoperability and federation Reusable and interchangeable components Interactive visualization and exploration Validation and Trust 	 Modular and open-source information systems frameworks and architectures Standard and interfaces Data fusion High performance and cloud computing Edge computing/smart instruments and sensors Augmented/Virtual/Mixed/Extended Reality Uncertainty Quantification 			

Table 3. Technology Breakout Summary

5.3 ESDT Systems, Prototypes and Federation

	ESDT Capability	Moderator	Scribe
C1	Architectural Frameworks for ESDTs	Dan Duffy	Tom Grubb
C2	Interfaces and Standards	Marge Cole	Jon Ranson
С3	Near-term opportunities for ESDT Prototypes	Nikunj Oza	Jon Hobbs
C4	Long term opportunities for prototyping and/or federating	Laura Rogers	Toshiro Tokunaga
	ESDTs		

The ESDT Systems, Prototypes and Federation breakout session explored which types of architectural frameworks and which general interoperability interfaces and standards would be needed to build ESDTs, which prototypes could be built in the near-term and what are the long-term opportunities for prototyping and for federations of Earth System Digital Twins. Federating digital twins will be necessary to create more comprehensive systems.

5.3.1 C1 Architectural Frameworks for ESDT

The Architectural Frameworks group explored architectural considerations and components for building digital twins. Discussion topics included:

- What are the main components of an ESDT information system?
- How could models be inter-connected and interact with this information system?
- How could traditional and surrogate models co-exist/work together?
- Which kind of layered architecture could be envisioned that would facilitate the development of an ESDT (e.g., hierarchical, GIS, CADD-like)? Are there multiple solutions?
- Where would data reside and how would it be organized to be accessed easily?
- How could multiple temporal and spatial scales be considered?
- How could what-if scenarios run fast enough? Could prior scenarios be buffered or stored as intermediate products?
- What architectural capabilities already exist (or what do we already know how to do)? Which ones need to be developed/designed?

Summary and Key Takeaways

The subject of architectural frameworks for Earth System Digital Twins is a complex topic that merits further discussion and a deeper analysis. The breakout group was only able to scratch the surface despite a spirited and ranging discussion.

We are in the early stages of architecture development. It is too early to lock in a specific architecture. The community should be open to different architectures during these early days, and to experiment with alternate approaches depending on the use cases. Industry should be a part of this discussion. Partnerships should be explored for appropriate capabilities, services, and computing platforms. A conceptual "cookbook" would be beneficial for sharing

architectural approaches that worked well for various use cases and could be one product of the early exploratory phase.

Federation is an important capability for digital twins. The architecture should facilitate interoperability and provide common high-level solutions. The shape of that framework is not yet clear, but it will likely include common APIs to expose services and exchange processing pipelines.

ESDTs appear to be a system of systems, both in terms of systems contributing to an individual digital twin and in terms of federation across twins. One of the core elements is process-oriented sharing among systems: for example, sharing between models, models and data repositories, and among federated digital twins. It is not yet clear how that would be implemented. ESDT architectures could be informed by design patterns and practices that have proved successful for systems-of-systems engineering.

Two limiting requirements unique to digital twins are geospatial data coupled with real-time processing. Addressing these requirements will be one key driver for the architecture.

Considerations

This remainder of this section is organized as a set of considerations that emerged from the breakout discussion that should inform future studies.

Federation and Interoperability

- Organizations will build DTs for themselves that will not necessarily be consistent with how other organizations build things hence, the need for a framework.
- Various organizations excel at different things. A federated approach allows us to play to all strengths. Different DTs can have different capabilities and share them with each other.
- There is a need for standards. See the parallel breakout group on standards and interoperability.
- Data or data products might often be "owned," but processes are more readily shared. There are legal and organizational restrictions around what can be shared and what is proprietary. Architectural support for those requirements should be considered. The framework should be able to interact with closed or proprietary digital twins, data sets, and models.

Stakeholders and Requirements

- Need to consider the stakeholders: what drives the vision and how to meet this vision?
- Different stakeholders will need different components or different integrations across DTs and applications.

- Use cases include:
 - Decision support tools
 - o Science
 - Exploration: DTs will need to provide information sufficiently close to reality so they could lead to decisions and or new connections.
 - Applications: users will ask context specific, knowledge-based questions to an ESDT. For example, insurance companies might ask about the risk of extreme weather in specific geospatial areas over specific times.
- Computational requirements are one driver, especially for near-real-time processing and interactivity.
- Another driver is efficient management of geospatial data at multiple spatial and temporal scales from disparate sources.

Process First View

The group discussed an approach for developing an architecture that focuses on the processing perspective. What data products need to be generated and which workflows are needed to support the use cases?

- Process creator, consumer, maintainer, operator
- Process chaining
- Data cubes to pass between processes
- Lineage and provenance

Data

How available is the data needed for a complete DT?

- There are proprietary data sources that are not publicly available. How important are those to the DT? Are they amenable to uncertainty quantification?
- Highlight the value of the source data sets to identify what needs to improve over time; gaps also need to be identified.
- Citations/DOIs for data sets are important and can help.
- NASA has models and global satellite data sets that are publicly available.

Data in an Earth System DT

- Data generally needs to be geolocated.
- There is a lot of 2D data, but the DT architecture also needs to be able to handle 3D and 4D data. Those are also geolocated and/or mapped to a (sphere) geometry.
- Most models need geolocated data, but a few are agnostic.
- Unstructured data, such as financial/market data, should be considered. Additional capabilities might be needed to work with it.

Modeling and Analysis

- ML is playing some central role in the various components of any DT system. The system needs to be designed with this in mind.
- Various machine learning techniques will need to be considered; among those, one possible technology to study further is swarm learning. This is a decentralized ML technique in which each member of the swarm controls their own data, but the learning can be shared. The ability to share learning while keeping data private could be an approach to learning in the presence of proprietary or protected data. The decentralized nature of swarm learning could distribute the computing and networking load. For example, swarm nodes could run on in situ platforms at the edge. They could train on local sensor data, where it is produced, and communicate only the learned results with other swarm nodes.

Potential Industry Role

- Industry has already developed digital twin capabilities, especially in domains such as aerospace and manufacturing, and is making significant progress in those areas. There could be opportunities for collaboration and knowledge transfer to accelerate ESDTs' development.
- Earlier engagement might have a larger impact.
- Industrial capabilities, data, and services are not necessarily open-source. There is a need to understand how to leverage these capabilities and at the same time make them interact with open science requirements.
- Even though we want to be as open as possible, the framework should still contain the capability of being able to interact with closed or proprietary data and DTs. Some mechanisms might include cooperative agreements, such as Cooperative Research And Development Agreements (CRADA) and Space Act Agreements (SAA).
- DTs can utilize new observations that go beyond what has traditionally been considered. Industry could provide some of these new type of observations.
- Community assessment reports (CAR) are mostly done for applications. Users of the DT outcomes will need to be identified and invited to provide input to CAR, including industry.

Approaches

- One approach is to start relatively small and grow in complexity and size of the DTs. The questions are: how would components from those smaller DTS be combined later to create more complex DTs, and what architectural capabilities would facilitate that?
- A generic framework to bring specific models together will need to be established.
- How can we get all of this to fit together? Below are some of the technology concepts that were discussed and that could be useful:
 - Layers data, service, stakeholders (software concepts)

- Object-based representations
- Foundational models
- o Data, product and information discoverability
- Tensors as a building block: tensors are similar to the data cube concept, although maybe not as generic or as widely used. Interoperability will need to be investigated.
- Interfaces that wrap DTs or the information they produce, especially for DT federation purposes.
- Processes need to have identities so they can be combined, related to each other, layered, and disseminated to arbitrary end points.
- Expose digital twin capabilities and data as discoverable services with welldefined APIs and semantics to facilitate federation.
- Provide a semantic layer with discovery:
 - Find processes, data, models, services and understand what they do and how to interpret them, in an autonomous fashion (machine-to-machine) or manually by users.
 - APIs that expose interoperability so that DT frameworks can discover and use them.

Components of Digital Twin

The breakout discussion identified several possible components of a digital twin:

- Digital Replica:
 - \circ Assimilation
 - o Data management and access
 - o Data catalogue
 - o Syntactic definitions
 - Data discovery, ontology, transformations, etc.
 - Physics-based models
- Prediction/Forecasting:
 - Forecasting capabilities
- Impact Assessment:
 - Decision support tools
 - o Visualization/stakeholder focused
 - Document results/knowledge-based
 - End user portals
- Overall Information System:
 - Advertising capabilities, discoverable, semantics, interoperable federation
 - o Archival and reproducibility components
 - ML training component
 - o ML validation components
 - Data training
 - Provenance of chains of processes or components of the DTs

- Discoverability component. Processes are exposed as descriptions with contextualized keywords, using a knowledge graph to find semantic matches for use in a DT
- o Ingest, identity, context transformation, dissemination
- Nodes or processes

5.3.2 C2: Interfaces and Standards

This breakout group focused on interfaces and standards that will pave the way for interoperability and seamless interaction of ESDTs.

Which types of standards and interfaces would be needed to make ESDT a reality?

Currently, there is no single standard for Earth System Digital Twins. However, there are "building blocks" that could contribute toward such a standard. These include existing and emerging standards for remote sensing/GIS data and metadata, models, geospatial analysis, system interoperability and cloud-based workflows. There are emerging standards for digital twins in other domains such as aerospace and manufacturing that may also be relevant to ESDTs. Other considerations include translation between building blocks, end-to-end workflows, validation, and data cataloging. System-level considerations include interoperability, trust, and ease of use.

What standards/interfaces/frameworks exist now that should be considered?

There are standards from organizations such as OGC, ISO, etc. that should be considered, e.g.:

- CityGML, IndoorGML, SensorThings, 3DTiles, i3S, API-Tiles,
- STaC for federated asset catalogs
- Data representation standards such as (cloud optimized) GeoTiff and NetCDF
- The Discrete Global Grid Systems (**DGGS**) standard, which is being used successfully with datacubes

To define the best standard(s), collaborative prototyping and testing will be needed. Prototyping using existing standards, identifying what works and what does not will be needed to develop standards, workflows, and best practices where there are gaps. In particular, standards will be needed to allow drilling down through multiple scales, from global to regional to local.

General Approaches and Considerations

This breakout discussion identified possible approaches and considerations.

- A modular approach is needed for standards, product consistency, and data discovery.
- The proposed approach is to start from existing standards, to avoid starting from scratch.
- Functions between digital twins should be standardized to avoid unnecessary duplication of services.

- Standards need to be minimal. They need to provide enough guidance to create interoperability, but not be so constraining that they stifle development.
- Developing multiple standards-based protocols will need to be considered as well as using pilot and reference applications to evaluate them. Knowing the lineage of protocols would be helpful.
- Ensembles or ecosystems of interoperability standards that work together will be needed to implement digital twins. A thriving ecosystem would include standards for data formats, communication protocols, service discovery, data queries, workflows, and model-to-model interaction among other interoperability concerns.
- Starting with prototypes will help to better understand interoperability needs and evaluate alternatives, for example, to federate stable ESDTs. Other standards will also be needed to enable interoperability between models, visualization, and interactivity. Feedback and validation are important for model standards.
- Standardized user interfaces could improve users' experience and minimize the learning curve across digital twins. Comprehensive tooling and library support would make it easier to follow those standards.
- There is a government role for supporting open standards and tools. Agency programs could solicit standards.
- OGC has a testbed program for developing and evaluating standards.
- Discovery is important for finding relevant datasets, models, and analyses both within a digital twin and within a federation. Discovery is facilitated by common approaches and interfaces for advertising and using capabilities. Some possibilities are:
 - Standardized workflows for finding and retrieving data
 - Catalog searching on geophysical variables, physical properties and descriptions
 - A logical markup or metadata language model interface
 - Common data taxonomies or ontologies

5.3.3 C3: Near term opportunities for ESDT Prototypes

This breakout session was focused on discussing ESDT prototypes that could potentially be developed in the near term, in that the constituent models, data, and appropriate machine learning algorithms are in a form that the participants felt could be put together relatively easily and quickly to show the benefits of ESDTs.

The participants first discussed potential prototypes that should be explored based on the five science scenarios discussed the previous day. There are relevant capabilities developed by NASA's Global Modeling and Assimilation Office (GMAO), within which emission sources and known fires are already incorporated. The participants suggested that models for planetary boundary layer, ocean, air quality, wildfires (e.g., existing tools such as Technosylva, which is used by CalFire) and even some socio-economic models and human behavior models could be brought together in the near-term in one or more combinations. These could be used to develop improved air quality forecasts and likely other near-term or seasonal forecasts.

Several technologies that could contribute to the near-term ESDTs were discussed. One is machine learning, which can serve as a "glue" between different models and datasets. Others include uncertainty quantification (various statistical and machine learning-based methods), data assimilation, and virtual reality for model and data exploration. Refinements on all these technologies driven by the desire to improve prediction quality should be developed. Adversarial machine learning was discussed as a good way to characterize digital twins – in particular, one could define the fidelity of the twin to be such that one cannot tell the difference between real models/data and twin-generated data. Some of these technologies are being developed as part of ongoing AIST projects, so it is worth investigating the possibility of bringing some of these projects together to form digital twins.

The participants identified several communities that may be interested in the digital twin candidates that were discussed. Some examples include insurance companies and organizations involved in building and maintaining infrastructure and supply chains. Governments and others involved in health policy – and climate change – related policy would also be interested. The digital twin would need the capability of investigating counter-factuals to simulate the impacts of different policies.

5.3.4 C4: Long-term opportunities for prototyping and federating ESDTs

This breakout group discussed the opportunities for system prototypes and federations of ESDTs in the long-term. What are those opportunities? What technologies would contribute to them, and what technologies would need to be developed?

Federation System and Governance: In the long term, there could be several individual ESDTs that have been developed for focused science and application areas. ESDTs with complementary models, data sets, and analytic capabilities could be federated to create a larger, more capable system to address a broader scope. Doing that kind of federation regularly and successfully will require a community environment with effective governance that facilitates collaboration and system interoperability.

Develop a "Digital Twin Hub" to Encourage Federation: This would provide shared infrastructure that models could "plug in" to. This would make it easier for ESDTs to interoperate and would encourage federation. The hub should have a corresponding community that contributes to the hub and is part of the federation. Some lessons could be drawn from open-source community projects like Pangeo or the Earth System Modeling Framework (ESMF).

Community Evaluation: This is an important part of model development that would also apply to digital twins. A hub might host several digital twins, each with different components or services. This could also be a mechanism for community evaluation to see which components work best for which purposes.

Governance: A governance model will be needed for making decisions about which components to add, providing evaluations and standards for emerging components, and similar coordination and quality issues. This could be a centralized or a community-driven model, and various DTs could have a different governance model.

Continuity of funding: Funding must be available over the long-term to avoid fragmented efforts that start and stop. Programs with adequate funding will be needed to mature, infuse, and maintain the infrastructure and community.

Lessons from Prior Model Integration Efforts

We can draw lessons from large community development efforts in modeling and software. On the positive side, many large open-source projects have had great success. On the negative side, past problems with large modeling frameworks have included:

- Mismatch between models on embedded science assumptions
- Models that tightly interact on science
- Varying project maturities, e.g., abandonware and differences in coding quality
- Difficulty in integrating very different code bases
- Difficulty in technology refresh. Can the system accommodate them, and is it part of the planning?

Earth systems are tightly coupled, and the models reflect that fact. How that coupling is done is part of the science. This must be taken into account when federating systems and coupling models.

Many models have "legacy" issues. They often have elements that are no longer correct, either because our understanding has evolved or because of technical limitations that existed at the time they were developed. Those not-quite-right elements have become so tightly coupled with the rest of the model that it is now difficult to change them. Federations need to be aware of those issues and treat them accordingly. This is not dissimilar from legacy issues in other large software systems.

Traceability and validity of models is an important issue. Is there semantic consistency across models in a federation. Are these models all doing things the "same way," or are some of them at odds with each other?

Long-term opportunities

• ESDTs could inform the NASA decadal surveys. We could consider how observations would support analysis, forecast, and projection needs; and how a portfolio of missions

could contribute to improved understanding of multiple Earth Systems in the context of an Earth System Digital Twin.

ESDTs could also be the basis for training the next generation of scientists and providing new tools for science. How could science be conducted differently with a digital twin? It could reduce barriers to analysis and facilitate interdisciplinary and collaborative science.

5.3.5 Key Outcomes from ESDT Systems, Prototypes and Federation Session

- An ecosystem of Earth System Digital Twins tailored for different domains seems more likely than one monolithic digital twin that does everything. Federation and interoperability will be important for leveraging capabilities, data, and models.
- Pilots and prototypes will be important for identifying/adopting reusable frameworks, APIs and standards. No single organization can do it all. Standardization requires collaboration.
- Ensembles or ecosystems of interoperability standards that work together will need to be developed to implement digital twins.
- There are several standards we can use now for digital twin "building blocks," such as data formats, service discovery, and workflows. There are emerging standards for industrial and urban digital twins that might also be applicable to Earth System Digital Twins.
- It is important to consider syntactic, semantic, and organizational interoperability. All three levels are important, and each poses different challenges. Syntactic interoperability concerns the low-level interfaces and formats through which ESDTs communicate. Semantic interoperability concerns the conceptual representations; for example, whether two systems have compatible assumptions about an Earth system process. Organizational interoperability concerns the organizational environment, such as which kind of information systems are allowed to share or how their respective teams can collaborate.
- Near-term digital twin prototypes should be explored to understand needs, technologies approaches, and interoperability concerns. These could draw from the five use cases as well as other sources.
- Emerging digital twin prototypes should explore how to federate with each other. This is a "low hanging fruit" opportunity to understand federation needs and approaches, and to evaluate potential standards and interfaces.

In the long-term, a thriving ecosystem of digital twins would benefit from community governance, evaluation, and support. Like large community models, digital twins will need community engagement for development, validation, sustainment, and road mapping. Governance models can be drawn from other successful community modeling and open-source software engineering efforts. Funding agencies are an important part of that community and continuity of funding.

6. Summary Conclusions

Co-organized with the Earth Science Information Partners (ESIP), the Advanced Information Systems Technology (AIST) Earth System Digital Twins (ESDT) 2022 Workshop brought together over 70 experts from NASA, NOAA, USGS, Academia, the EU and international organizations to explore the benefits of ESDTs to Earth science, develop science use cases, identify enabling technologies, and define short-term and long-term opportunities for demonstrating ESDT capabilities.

Earth System Digital Twins bring together relevant Earth system models and simulations, other relevant human and infrastructure models, continuous and timely observations, long-time records, analytics and artificial intelligence tools, as well as advanced visualization and computational capabilities to enable more comprehensive, accurate, and in-depth understanding of Earth and human systems and their interactions. The three core components of an ESDT are a **digital replica (what now), forecasting (what next)**, and **impact assessment (what if).** Together these provide a powerful system for various levels of users to fully understand Earth system processes and their interactions and to support science and policy decisions by projecting how Earth and human systems could evolve under different scenarios and what impacts those would have on each other and human systems.

Participants identified five **Earth science use cases** that would benefit from these unique ESDT capabilities to enable science and applications that involve interactions among multiple Earth and human systems and across temporal and spatial scales. These use cases focus on:

- Wildfires
- Ocean Carbon
- Water Cycle
- Biodiversity impacts in the Central Africa Carbon Corridor
- Atmospheric Boundary Layer

These five use cases correspond or have large overlaps with some of the 13 focal areas that were identified in the Earth Action Initiative, and over time we can envision that Digital Twins could be developed for all focal areas.

ESDTs will build on a solid foundation of Earth System Models (ESM), data and information products, and large-scale science data analysis and modeling technologies. **New technology** developments will also be needed to address unique capabilities of Earth System Digital Twins including advanced data fusion and assimilation, accelerated models, machine learning, high end and edge computing, analytic frameworks, and visualization. More specifically, the workshop participants identified several technical and programmatic challenges that need to be addressed for digital twins:

- Rather than trying to develop "one digital twin to rule them all," it would be more efficient to develop digital twins for different domain areas, which could range in extent from global to local and in scope from multi-domain to narrow thematic focus.
- Digital twins should support federation to increase scope and capabilities.
- Standards and interoperability challenges need to be addressed to build digital twins efficiently and facilitate federation.
- Interoperability challenges exist at syntactic, semantic, legal and organizational levels.
- Integrating multiple data and modeling sources raises challenges in data fusion and data assimilation.
- Digital twin architectures are needed to address data representation, modeling, and analysis challenges including approaches such as data cubes, data lakes, and cloud-optimized architectures.
- Analysis technologies are needed for explainability, causality, and impact assessment.
- Improved modeling capabilities (including machine learning) are needed to enable faster run times, interaction with other models, and continuous assimilation of observations.
- Visualization and interactivity capabilities are needed for data analysis and exploration.

Various national and international organizations are developing ESDTs, ranging from research prototypes to large scale initiatives. This presents an early **opportunity for developing interoperability standards and for federation.** By sharing data products and information, models, and services, digital twins with different foci can work together to provide a more powerful capability. Prototypes and pilots are an excellent way to explore interfaces, standards, and interoperability frameworks and evaluate their utility.

Earth System Digital Twins are emerging as a powerful capability for understanding our planet and the processes that drive it. The results of this workshop took initial steps towards that goal by developing ESDT reference use cases, technology needs, and opportunities for prototyping, federation, and interoperability.

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