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

Argonne National Laboratory

RFI Response: Digital Twins Research and Development

Input from Argonne National Laboratory

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Contributors:
Scott Collis, Environmental Science Division
Zhiling Lan, Advanced Leadership Computing Facility
Jeffrey Larson, Mathematics and Computer Science Division
Sven Leyffer, Mathematics and Computer Science Division
Todd Munson, Mathematics and Computer Science Division
Tarak Nandi, Data Science and Learning Division
Tom Peterka, Mathematics and Computer Science Division
Krishnan Raghavan, Mathematics and Computer Science Division
Hemant Sharma, X-ray Science Division
Richard Vilim, Nuclear Science and Engineering Division
Haoyu Wang, Nuclear Science and Engineering Division
Orcun Yildiz, Mathematics and Computer Science Division

Background

Argonne National Laboratory is a multi-purpose Department of Energy (DOE) Laboratory. Argonne is home to five U.S. DOE Office of Science national user facilities, including the Aurora exascale supercomputer and the upgraded Advanced Photon Source, and one DOE Office of Nuclear Energy national user facility. These facilities support nearly 8,000 users annually. Argonne is actively developing and employing digital twins across the laboratory complex, often in a multi-disciplinary environment.

This response summarizes some of Argonne's capabilities and visions for the future of digital twins in science and engineering in seven areas.

1 Artificial Intelligence (AI)

Artificial intelligence (AI) is revolutionizing scientific discovery and engineering innovations throughout Argonne. Here, we highlight how two sample applications combine digital twins and AI, namely nuclear engineering and biomedicine.

Artificial Intelligence (AI) for Nuclear Engineering. AI is revolutionizing nuclear engineering research through the development of digital twins, offering unprecedented advancements in diagnostics, monitoring, and simulation. At Argonne National Laboratory, several digital twin research and development projects are carried out by leveraging AI, and these innovations collectively drive forward the research in nuclear engineering, fostering safer, more efficient, and cost-effective solutions. On-going research projects and future research opportunities and are in (a) Equipment Health Monitoring for Control of At-Power Operation, which focuses on enhancing the diagnostic capabilities of nuclear power systems by integrating AI during the development of digital twins for diagnostics purposes; (b) Real-Time Operating Performance Optimization, which leverages AI-based digital twins to optimize the operational performance of commercial nuclear plants by predicting moisture carryover (MCO) in boiling water reactors (BWRs) due to insufficient liquid phase removal from steam exiting the primary vessel; and (c) Simulation-informed and data-driven Field reconstruction techniques for Monitoring for Control of At-Power Operation, which utilizes AI to develop a digital twin for real-time online monitoring of nuclear reactors and provide a continuous and intelligent oversight of process variables that cannot be experimentally measured during at-power operation, thus addressing the limitations of current data-driven algorithms which often lack diagnostic specificity.

AI and Digital Twins in Biomedicine. Recently, there has been an increased focus at Argonne on AI for biomedicine, and one such ongoing collaborative project is in the area of mathematical oncology aimed at developing digital twins for personalized radiation therapy (RT) strategies. Conventional RT for cancers usually utilizes a single set of imaging acquired prior to the start of treatment and selects a treatment plan that has been shown to work well on an "average patient" However, cancer is a complex, evolving system that exhibits significant inter-patient variations that depend on various factors, including the underlying genomic instability and tumor microenvironment. Physics-informed neural networks (PINNs) are being developed by integrating mechanistic modeling with MRI data to model the spatio-temporal response of tumors to RT, to create therapy plans based on individual tumor biology. Such a PINN model, trained over a broad range of relevant parameters (e.g., diffusion coefficients, tumor proliferation rates, RT dose) and regularized/guided using available MRI data, can be used to carry out near-instantaneous predictions for the tumor trajectory based on parameters corresponding to any new patient, thus streamlining RT planning and precluding the need for a huge number of parameter-specific computer simulations.

2 Data

Research opportunities are in (a) heterogeneous data integration, (b) real-time data transport, and (c) data orchestration workflows. Heterogeneous data integration involves management of multimodal data for physical experiments, numerical simulations, and AI surrogate models. Real-time data transport involves efficient bidirectional data movement between the physical and virtual twins and the analysis of raw data to produce useful high-level knowledge. The orchestration of heterogeneous data in the digital twin ecosystem needs to be automated with workflows capable of managing disparate scales in time and space. Workflows need to designed with intelligence to determine optimal data models, accuracies, and routes.

3 Ecosystem

Digital Twins and the Environment. The use of digital twins in the MOdel Driven EXperiment (MODEX) lifecycle includes active interchange between the digital twin and field observations. Feedback from the observations are used to both improve the digital twin and to assimilate and nudge the state of the digital twin. Edge computing will enable geomorphic computing where digital twins can be run in a resource limited environments that could inclde CPU/GPU limitations, bandwidth limitations or, for off the electrical grid applications, PV limitations.

Digital Twins for Scientific Discovery in X-ray Science. Linking X-ray experiments at synchrotron sources, such as the Advanced Photon Source (APS), with AI-enabled Digital twins is essential to fully realizing the scientific potential of next-generation infrastructure (such as the APS-Upgrade). The potential of AI, high performance, and edge computing (HP-EC) to unlock process secrets by capturing rare events critical to designing and manufacturing advanced materials is truly exciting. Developments such as the high energy X-ray diffraction microscopy digital twin, a part of the Microstructure Identification using Diffraction Analysis Software package (MIDAS-DT, https://github.com/marinerhemant/MIDAS), which operates in real-time, empower scientists to conceptualize, visualize, and drive their experiments. Combining full experiment simulations with material modeling running on remote HPC resources, MIDAS-DT instantly predicts regions of interest in materials. Scientists can use this information to automate experiments adaptively, using multimodal and multiresolution techniques to gain unprecedented insights into material behavior during processes such as deformation and fatigue.

4 Long Term

The two-way coupling between the physical object and its digital twin raises a number of important foundational questions about the stability, accuracy, fidelity, convergence, and correctness of the digital twin. These questions are complex and are connected to uncertainty quantification and validation and verification of digital twins, but are more fundamental in nature, requiring long-term research investments in methodologies, coupling approaches, solution methods, uncertainty quantification, and convergence. For example, the use of a digital twin to control both the data acquisition and manufacturing process in additive manufacturing could in principle be achieved today by simply bolting together data assimilation, simulation, control. However, this simplistic coupling would fail to address the questions about convergence, fidelity, and uncertainty raised above that ultimately determine whether a digital twin can become a truly predictive tool that can be safely used in complex processes. Below, we comment on two fundamental challenges in this area in more detail, namely fidelity and how to develop optimization technology for digital twins that can be used in optimal control or data assimilation.

Fidelity of Digital Twins. With the revolution of AI-driven digital twins, the need to maintain the fidelity of AI models as the underlying data distribution evolves has become crucial. However, naively updating the model with new data can lead to "catastrophic forgetting," a phenomenon where new data erases prior information stored in the AI model. The paradigm of continual learning seeks to address this issue. There are numerous research opportunities within this context. A fundamental opportunity arises from the heterogeneity in data distribution. For instance, variations in the fidelity of underlying simulations require different AI methods to effectively assimilate such high and low fidelity information into the digital twin. Similarly, the spatio-temporal nature of the data introduces significant complexity, impacting the digital twin in ways that remain opaque. The computational demands of such a structure, coupled with the significant energy requirements, present a research challenge where energy-aware methodologies must be developed. This challenge needs to be analyzed and studied both mathematically and empirically.

Research opportunities include: (a) maintaining the fidelity and time efficiency of digital twins through hybrid modeling approaches that leverage high-fidelity and fast surrogate formulations; and (b) ensuring the computational power required to run complex digital twins in real-time by integrating energy-efficient workload management systems like PBS and Slurm. One example of hybrid modeling is to integrate high-fidelity parallel discrete event simulations (PDES) with statistical or ML based surrogate models to accelerate large-scale simulations (Kronos, https://www.anl.gov/mcs/kronos-hybrid-discrete-event-simulations).

Digital-Twin-Aware Optimization Tools. Optimization plays a fundamental role in digital twins as a tool for optimal control and optimal data acquisition, for example. The development of digital-twin-aware numerical optimization tools is a long-term need, driven by the increasing complexity and scale of digital twins across scientific domains. These optimization tools must be able to handle such dynamic, evolving, data-driven models. Research in methods is needed to ensure that the optimization solutions remain robust and efficient as the underlying digital-twin changes. Addressing this need will require creating novel, sophisticated optimization algorithms that can integrate real-time data and adapt to new environmental conditions, while maintaining previous critical domain knowledge.

5 Sustainability

The design and development of systems and architectures for digital twin sustainability are pivotal for advancing the sector's safety, efficiency, and longevity. By leveraging cutting-edge digital twin technology, researchers can create dynamic, real-time simulations of nuclear systems, providing comprehensive insights into their operations. These digital replicas facilitate predictive maintenance, optimize performance, and enhance decision-making processes. At Argonne National Laboratory, several digital twin research and development projects focus the integration of robust, scalable architectures that ensure the long-term sustainability and adaptability of digital twins, enabling continuous improvement and resilience in nuclear power systems. This approach not only addresses current operational challenges but also sets the foundation for future advancements in nuclear engineering. On-going research projects and future research opportunities and are in (a) Control Strategies Informed by Prediction of Equipment Condition, which focuses on developing control systems that enable semi-autonomous operation, addressing the challenge of ensuring continued safe operation despite component performance degradation, which conventional control systems may struggle to manage; (b) Control for Meeting Equipment Constraints in Integrated Energy Systems, which focuses on the sustainable deployment of digital twins for controlling multiple production assets, addressing the challenge of achieving economically optimal electricity dispatch in integrated energy systems; (c) Control of Advanced Reactors Using Reinforcement Learning, which focuses on the sustainable deployment of digital twins through the development of reinforcement learning-based control algorithms thus addressing the need for self-learning control systems to expand the range of upsetting events that can be managed by the plant control system, and reducing the reliance on protection systems; and (d) Asset management approach through Integrated Online Monitoring and Diagnostics, which aims to enhance the economic competitiveness of advanced reactors by integrating intelligent online monitoring with asset management decision-making methods, thus optimizing the operation and maintenance cost and plant performance through the sustainable deployment of digital twins.

6 Trustworthy

The trustworthiness of digital twins is paramount for their effective implementation and acceptance in nuclear power systems. Digital twins, as virtual replicas of physical systems, offer transformative potential in optimizing operations, enhancing safety, and predicting maintenance needs. At Argonne National Laboratory, multiple research projects focus on enhancing the trustworthiness of digital twins, involving rigorous validation and verification processes by integrating data from physical sensors or high-fidelity simulations, and adherence to regulatory standards. By incorporating advanced algorithms, real-time data analytics, and comprehensive simulations, researchers can build digital twins that accurately reflect the complexities in nuclear systems. Establishing trust in these digital replicas not only bolsters operational efficiency but also strengthens safety protocols and decision-making processes, paving the way for their widespread adoption in the nuclear industry. On-going research projects and future research opportunities and are in (a) Stability and Control in Boiling Water Reactor Feedwater Systems, which focuses on employing a physics-based digital twin specifically developed for the feedwater heater string to enhance the understanding of the underlying phenomena contributing to cycling behavior, and then design an operational control system to address the prevalent issue of oscillatory behavior in the feedwater heater levels of boiling water reactors (BWRs); (b) Dispatch of Electricity for Nuclear Plants with Energy Storage, which focuses on the control of energy storage systems coupled with nuclear plants to match electrical power output with instantaneous fluctuations in net demand; and (c) Control and monitoring for semi-autonomous operation, which focuses on enhancing the economic competitiveness of advanced reactors by optimizing costs and plant performance through the trustworthy deployment of digital twins.

7 Workforce

The inherent complexity of digital twins raises the barrier-for-entry into this critical technology and therefore requires a sustained investment into workforce development. The next-generation of scientists must be competent domain scientists in addition to having fundamental knowledge in AI, numerical simulation, uncertainty quantification, etc. Argonne National Laboratory provides internship opportunities for undergraduate and graduate students that should be expanded to provide training and workforce development opportunities in the area of digital twins. We must extend these opportunities to R2 universities and MSI institutions that may not be sufficiently well-resourced to provide courses and experience with digital twins, in order to democratize access to digital twin technology and development opportunities.