Digital Twins for Future Scientific Discoveries

Valerie Taylor and Xingfu Wu (Argonne National Laboratory) Zhiling Lan (Illinois Tech)

Imagine the ability to simulate plans or build what-if scenarios for the facilities and processes you wish to design before you actually put real-world resources behind real-world implementation. That's the promise of digital twins.

The concept of digital twins is to create computer models to virtually represent their physical counterparts. An efficient and accurate digital twin is a combination of rigorous physical models, real-time ingestion of various on-board sensor data, and predictive machine learning. With the availability of a digital twin, one may predict the behavior of the real-world counterpart so as to address potential problems before they occur. With the increase in processing power of supercomputers and the advances in artificial intelligence techniques, digital twin technology has the potential to impact science methodologies. Digital twins can become another tool to be used by scientists to advance science discovery. We argue for an aggressive exploration of the digital twin concept for DOE future scientific discoveries by leveraging ever-growing computational and data processing power of HPC systems and scientific knowledge amassed over decades.

Potential applications of digital twins:

- **Smart Labs/facilities**: Imagine that all the variables that go into the management of a lab/facility are represented via a digital twin. Digital twin helps the planners understand and improve the efficiency of energy consumption and many applications that can improve the operations.
- **Healthcare**: Digital twins along with data from IoT can play a key role in the health care to better understand and predict the impact of drug interactions, the spread of disease, or personalized drug design.
- **Environment:** Digital twins can be applied to the environment to represent the various variables that impact soil as well as plants, thereby impacting agriculture.
- **Education**: Digital twins can be applied to build AI-powered virtual teachers using ML, natural language processing and computer vision.

Another question that is raised is the combination of different digital twins, such as environment and healthcare, to have a broader view of relationships and impact. Digital twins is an exciting concept that warrants further discussion at a meeting about future scientific methodologies.