Brookhaven National Laboratory

U.S. DEPARTMENT of ENERGY

Computing and Data Challenges for the Virtual Human Twin

Meifeng Lin

Chair, Computational Science Department

Director, Digital Twins Institute

mlin@bnl.gov

Virtual Human Global Summit II

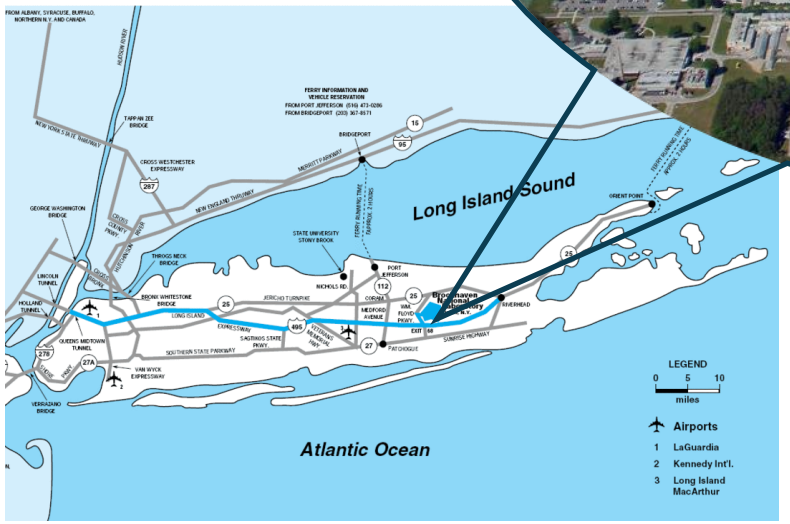
Barcelona & New York City, October 23-24, 2025

@BrookhavenLab

Brookhaven National Laboratory

- Located at Long Island, New York
- ~60 miles east to NYC (~1.5 hr train ride)
- Funded by US Department of Energy
- A multi-purpose lab:
  - Nuclear and High Energy Physics
  - Energy and Photon Sciences
  - Environment, Biology, Nuclear Science and Nonproliferation
  - Discovery Technologies
  - **Computing and Data Sciences**

- ~3000 employees
- ~4000 guests every year
- Founded in 1947



Brookhaven National Laboratory

Computing and Data Sciences

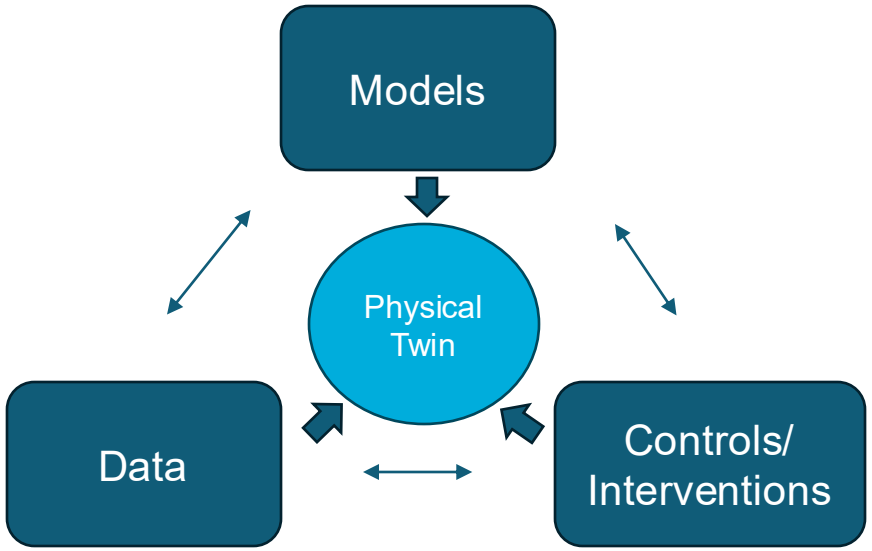
- Established in 2024
- Evolved from former Computational Science Initiative
- 3 Divisions:
  - Computational Research (AI, Applied Math, Computational Science)
  - Systems, Architectures and Computing Technologies
  - Scientific Computing and Data Facility

Core Research Areas
AI-enhanced Accelerators, Detectors, and Sensors
AI for Science
Optimal Experimental Design and Steering
Uncertainty Quantification
Safe, Secure, and Trustworthy AI
High-performance Computing
Systems, Architectures, and Computing Technologies
Quantum Computing, Networking, and Sensing
Exploring the Intersection of QIS, Applied Math, and Physics

Brookhaven National Laboratory

Digital Twin vs Virtual Human Twin

- A Digital Twin (DT) is a virtual representation of a physical object, system, or process through computer simulation and modeling, high-performance data analytics and active control.
- Assists in design, optimization, control and/or prediction of the physical counterpart.



- A **virtual human twin** is a special case of a digital twin but has additional requirements and challenges.
- Multiscale Modeling (from cellular to whole body) and Multimodal Integration (sensor data, simulations, diagnostics…)
- Individuality/Personalization
- Privacy and Ethics Concerns
- High-stakes applications, requiring stringent VVUQ

DT Data and Computing Challenges

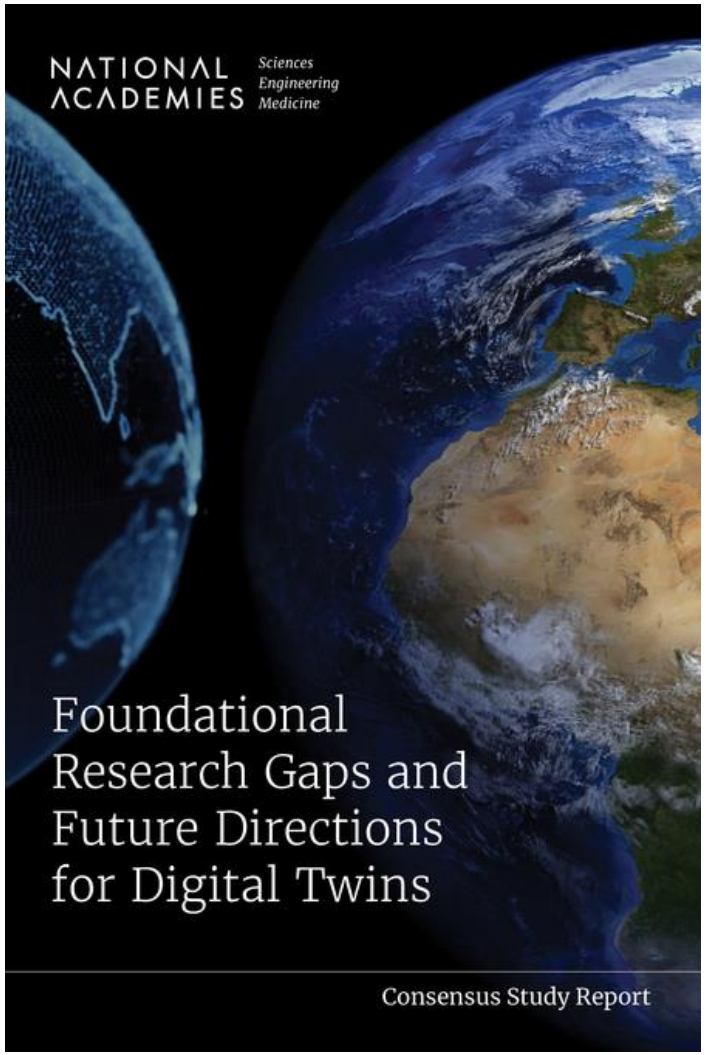
To develop functional digital twins, there are still several challenges that need to be addressed:

- **Data:** Data-related issues are of paramount importance: Data availability, access, quality, security, provenance, real-time visualization, etc.
- **Inference and Prediction:** Efficient surrogate models for fast inferencing and predictive modeling methods are still lacking.
- **Speed and Scale:** To support responsive DT applications, we need to integrate multiscale modeling capabilities with high performance computing and ML..
- **VVUQ Challenges:** Validation, verification and uncertainty quantification are all crucial in digital twins, especially for high-stake applications, such as VHT.
- **Computational Infrastructure:** DTs require the integration and interaction of many heterogeneous computational modules. But it is challenging to have a **general DT framework** that is usable by different DT applications.

Our Research Focus

The challenges identified are inline with the National Academies for Science, Engineering and Medicine report in 2023 on digital twins, which shape our research focus:

- **Continuous data assimilation and model calibration**, as well as predictive or decision-making capabilities in DTs, are not necessarily mature or fully integrated with traditional simulation methods
- **Speed and Scalability** are imperative, requiring the use of new computational techniques such as AI, and novel hardware
- **Safe, Secure and Trustworthy** data handling and AI/ML applications

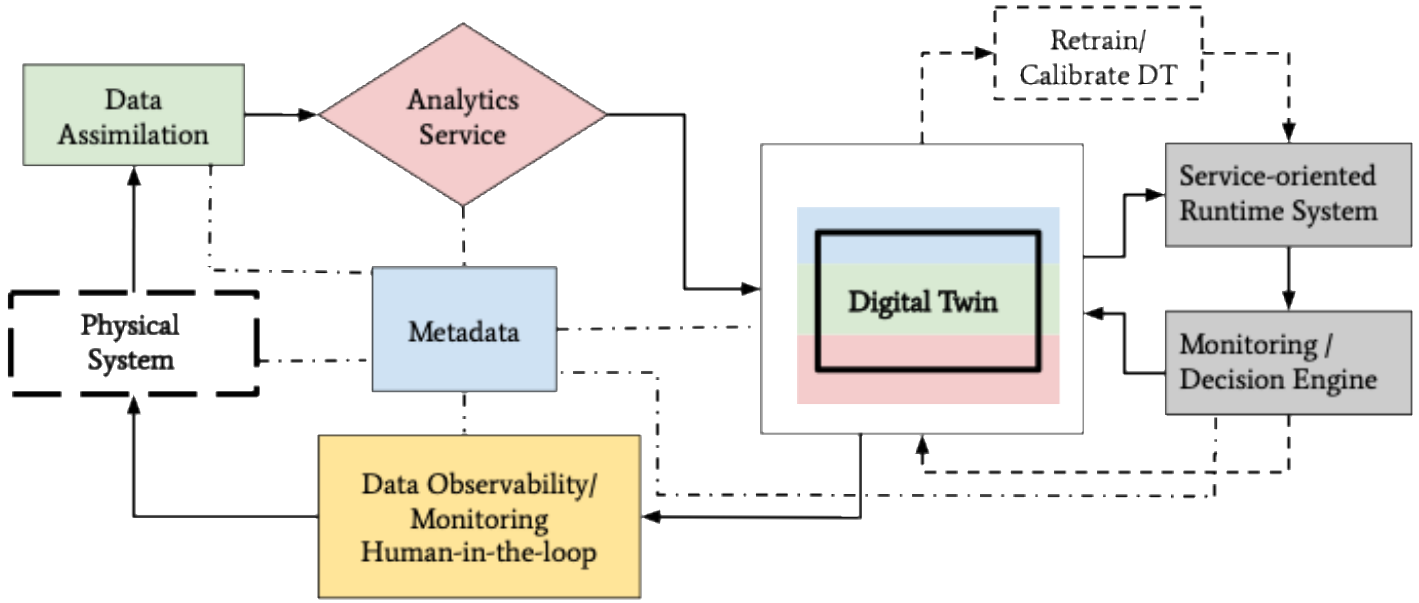


Example Project 1: UniDT

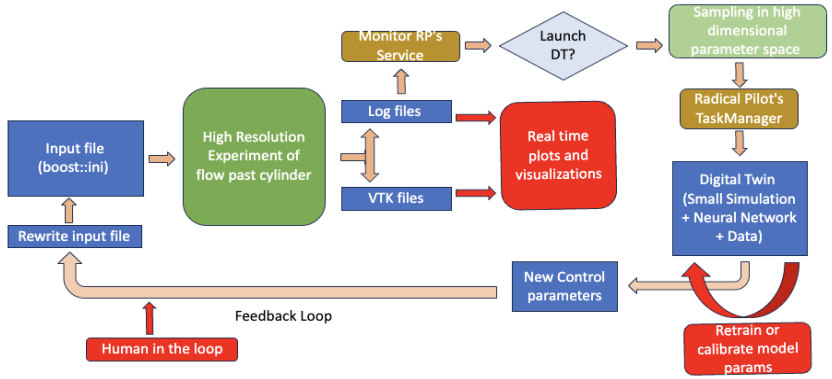
POC: Mohammad Atif, fmohammad@bnl.gov

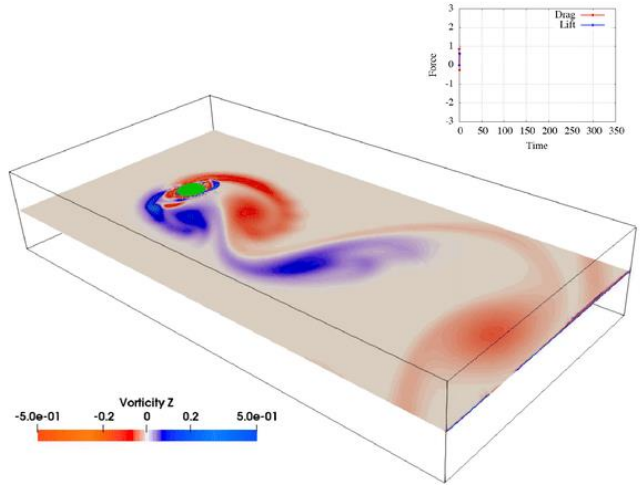
Goal:

- Create a universal digital twin (UniDT) framework for diverse DT applications
- Modular and composable; enables bidirectional feedback loop
- Prototype implementation for CFD
- Can be generalized for other applications



Prototype Implementation

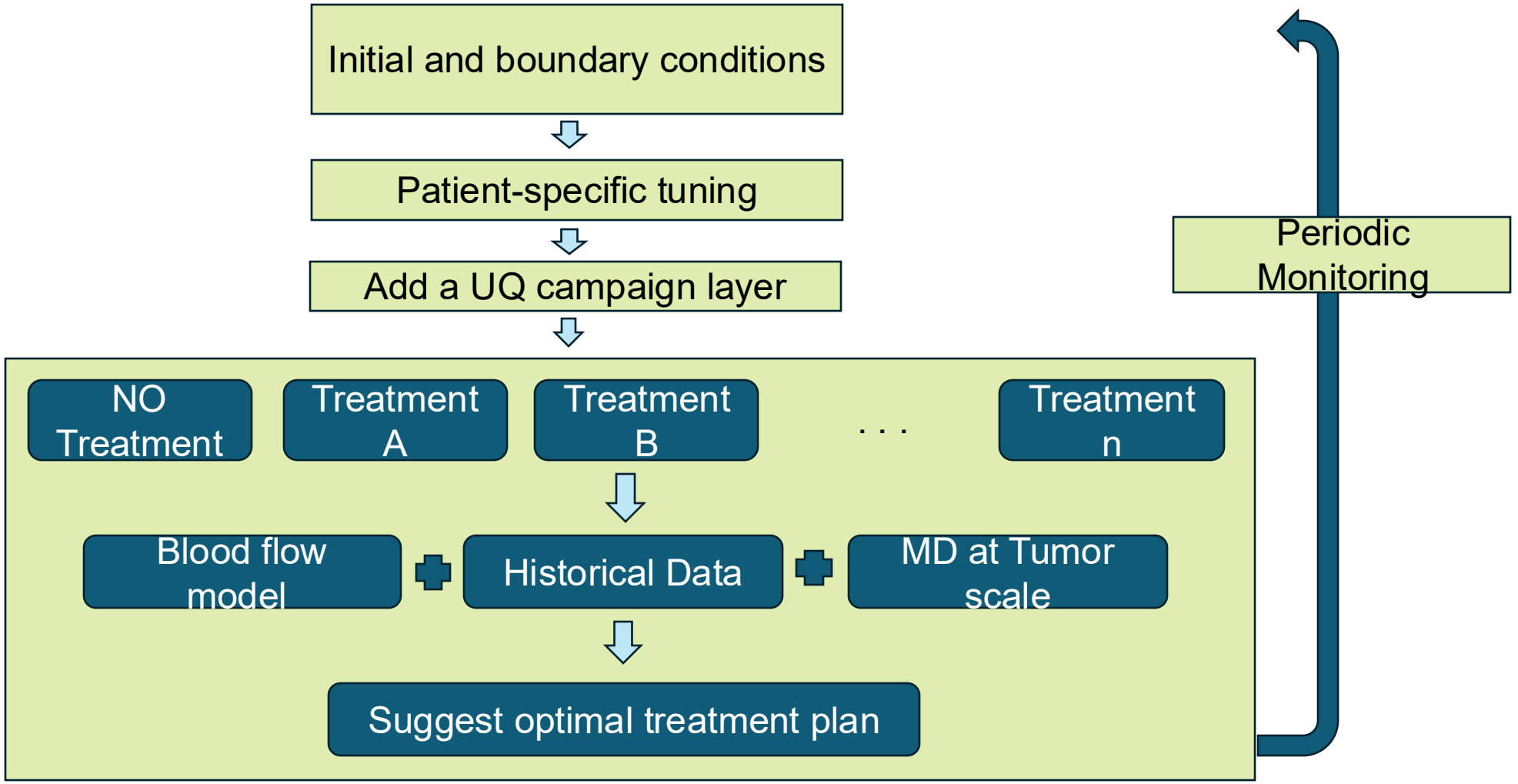




Brookhaven National Laboratory

UniDT for Cancer Research: Conceptual Workflow

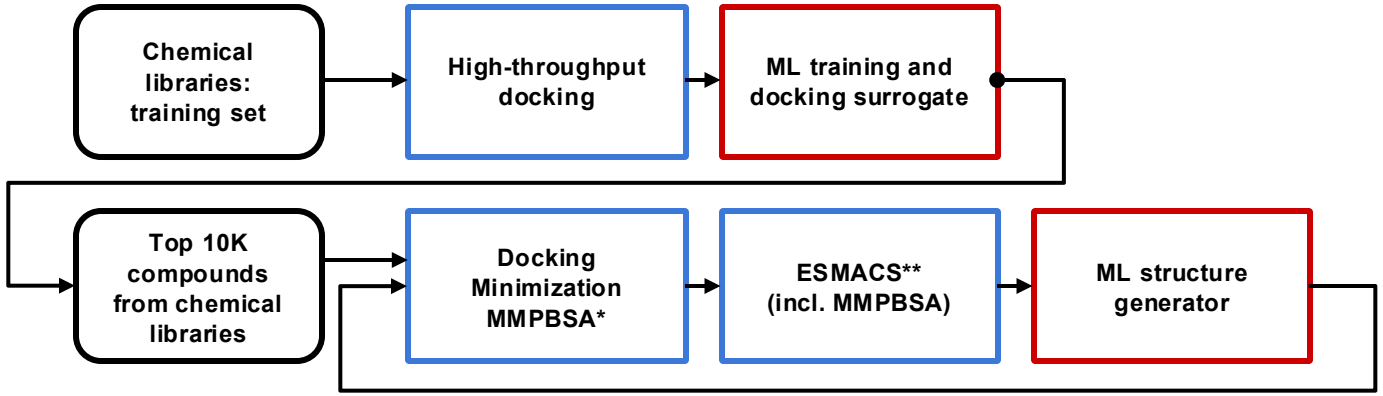
POC: Mohammad Atif, fmohammad@bnl.gov



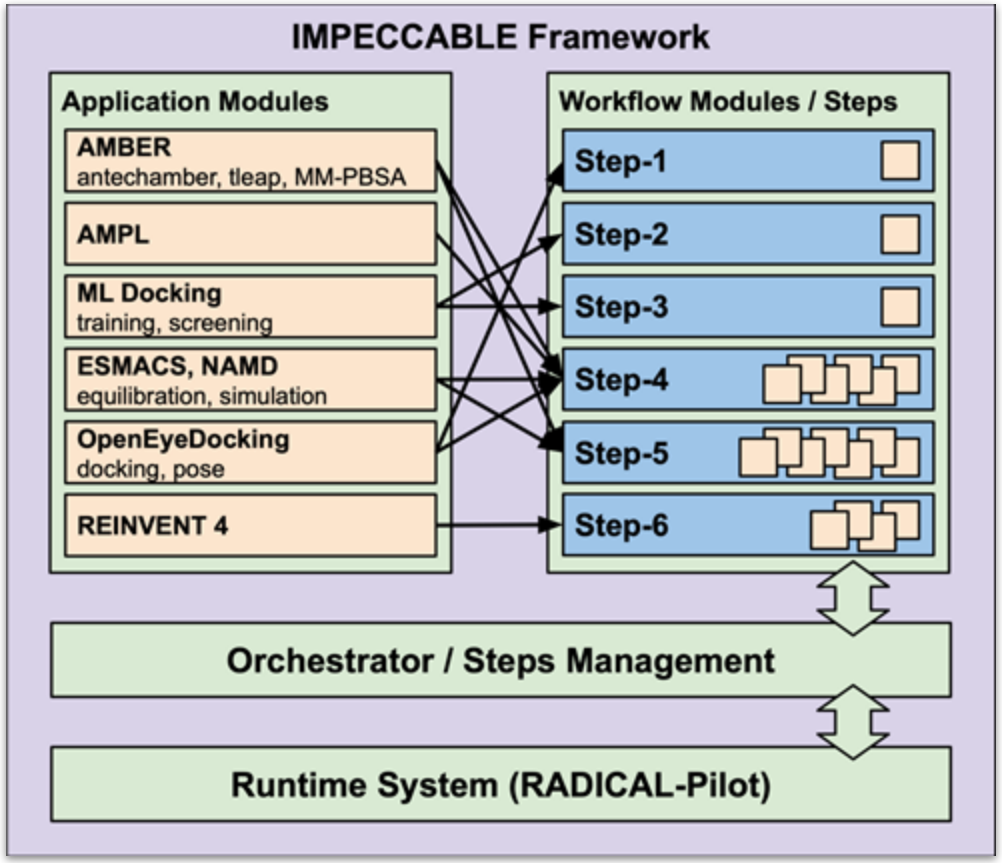
Example Project 2: Coupled ML-HPC framework

POC: Mikhail Titov, mtitov@bnl.gov

ML-HPC coupled algorithms and methods enhance effective performance of traditional HPC simulations. **IMPECCABLE** gen.2 [1] - *High-Throughput Virtual Screening* - multi-stage campaign of heterogeneous workflows, which couple ML and physics-based methods to accelerate the drug discovery process.



* *MMPBSA - molecular mechanics Poisson-Boltzmann surface area methodology;*
** *ESMACS - enhanced sampling of molecular dynamics with approximation of continuum solvent.*

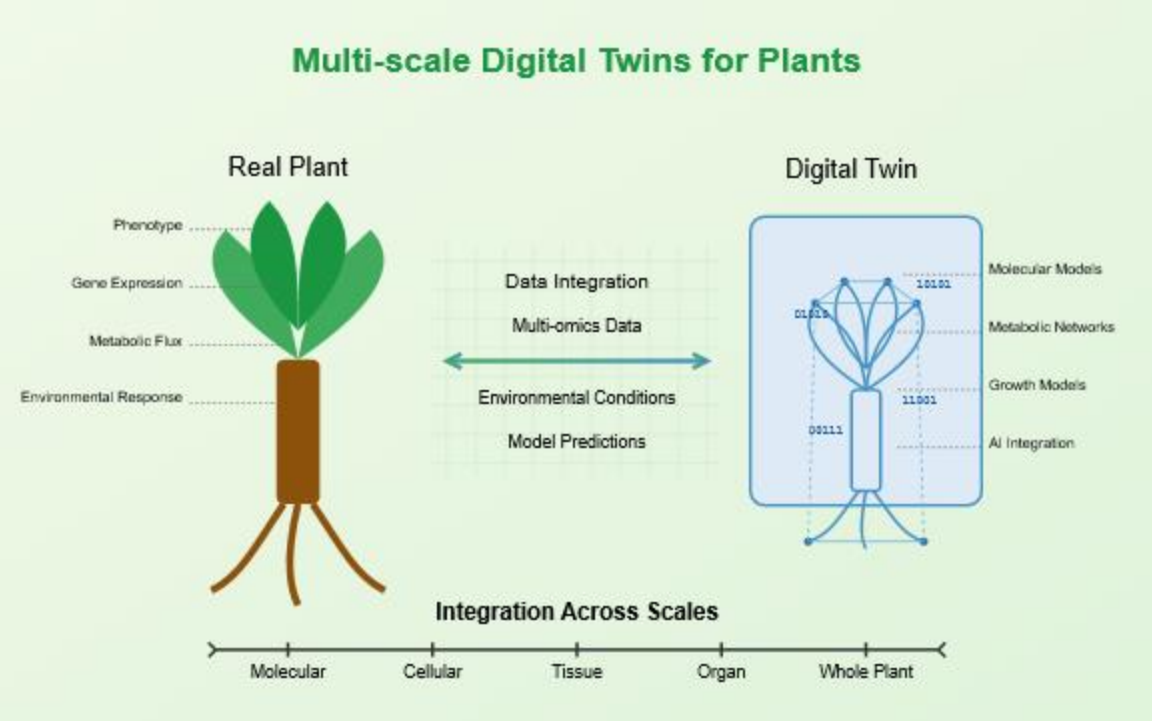


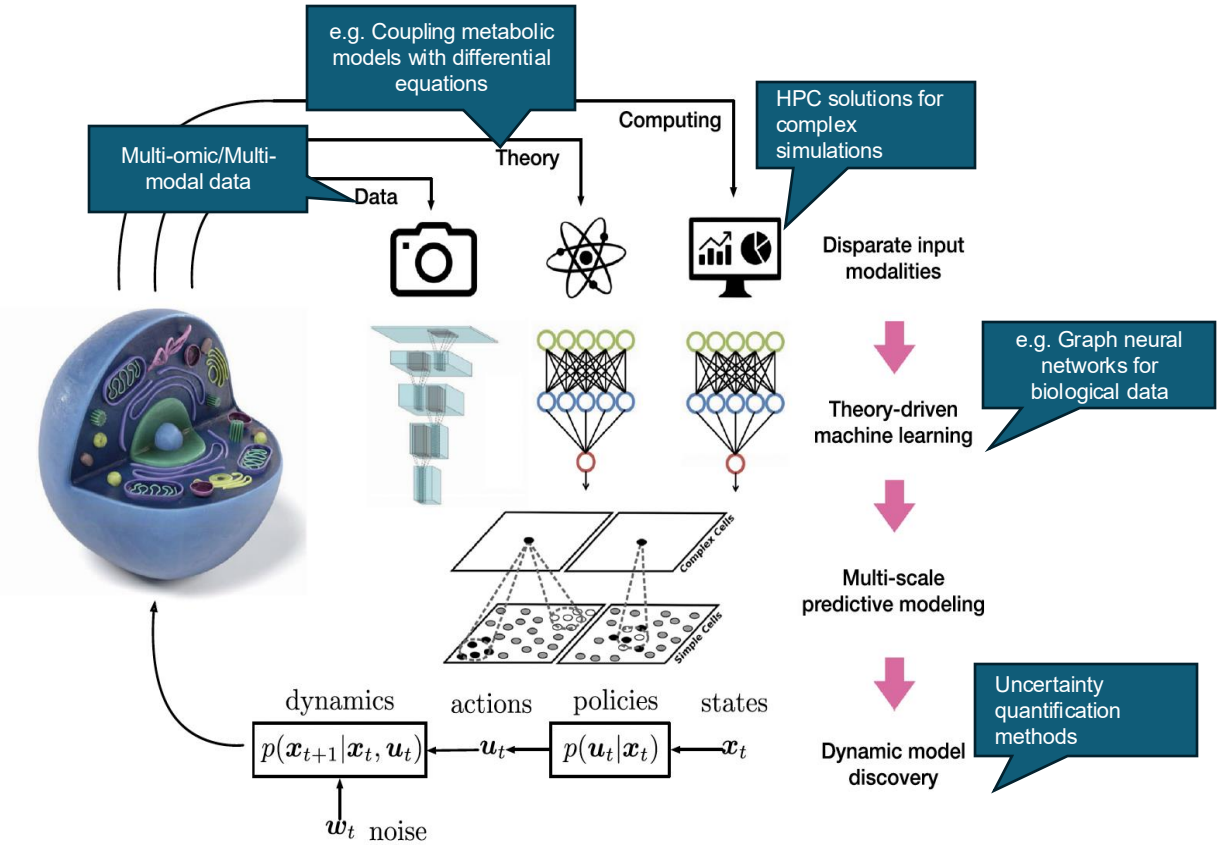
Brookhaven National Laboratory

*[1] Alsaadi, A., et al. (2021) **IMPECCABLE: Integrated Modeling PipelinE for COVID Cure by Assessing Better LEads**.*
DOI:10.1145/3472456.3473524

Example Project 3: Multi-scale Digital Twins for Plants

POC: Kriti Chopra, kchopra@bnl.gov



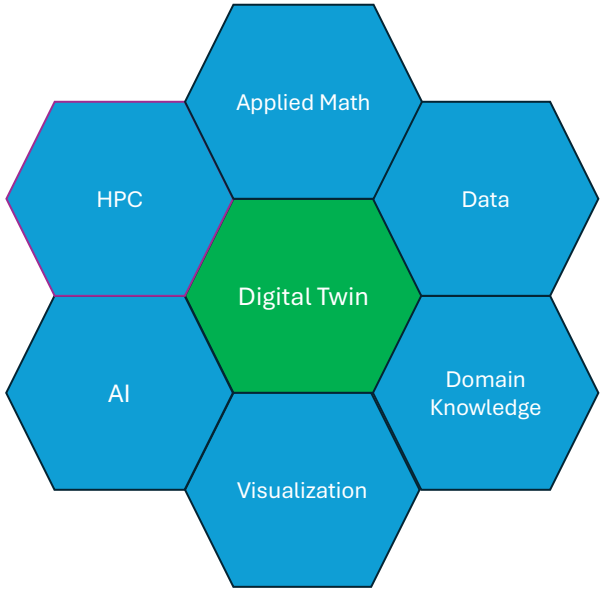


Adapted from: Alber, M., Buganza Tepole, A., Cannon, W.R. *et al.* Integrating machine learning and multiscale modeling—perspectives, challenges, and opportunities in the biological, biomedical, and behavioral sciences. *npj Digit. Med.* **2**, 115 (2019).

- **Multi-scale coupling**: Seamlessly integrate metabolic network models with mechanistic differential equation systems across molecular-to-organism scales
- **Theory-driven ML**: Develop graph neural networks and reinforcement learning architectures that learn from sparse, heterogeneous biological data with rigorous uncertainty quantification
- **Dynamic model discovery**: Create HPC-enabled algorithms that identify governing equations and causal relationships from multi-modal experimental observations
- **Can be extended for VHT!**

BNL Digital Twins Institute

- The BNL Digital Twins Institute (DTI) was established in 2024 to serve as a hub to bring together applied mathematicians, computer scientists, computational scientists and domain experts working on digital twins.
  - To address **common challenge**s in digital twins in terms of data, algorithms, software and computational infrastructure.
  - To form a **community** of digital twin researchers through better communications and coordination.
  - To respond jointly to **funding opportunities** for digital twins.
  - To accelerate digital twin research **innovations**.
- **We welcome any collaboration opportunities!**



Brookhaven National Laboratory

Summary and Outlook

- DTs have the potential to help predict the behaviors of the physical systems, including the human body.
- Fundamental research challenges remain to enable practical digital twins, such as virtual humans in clinical settings.
- Advancements in computing hardware/software and AI/ML are creating a paradigm shift for DTs.
- BNL CSD can provide computing and data infrastructure and expertise to help advance VHT and its clinical applications.

Acknowledgments

- We acknowledge the support of the funding agencies for the research presented.
  - Department of Energy
  - New York State
  - Brookhaven National Laboratory