Digital Twins
Research Gaps & Future Directions

Institute for Mathematical and Statistical Innovation
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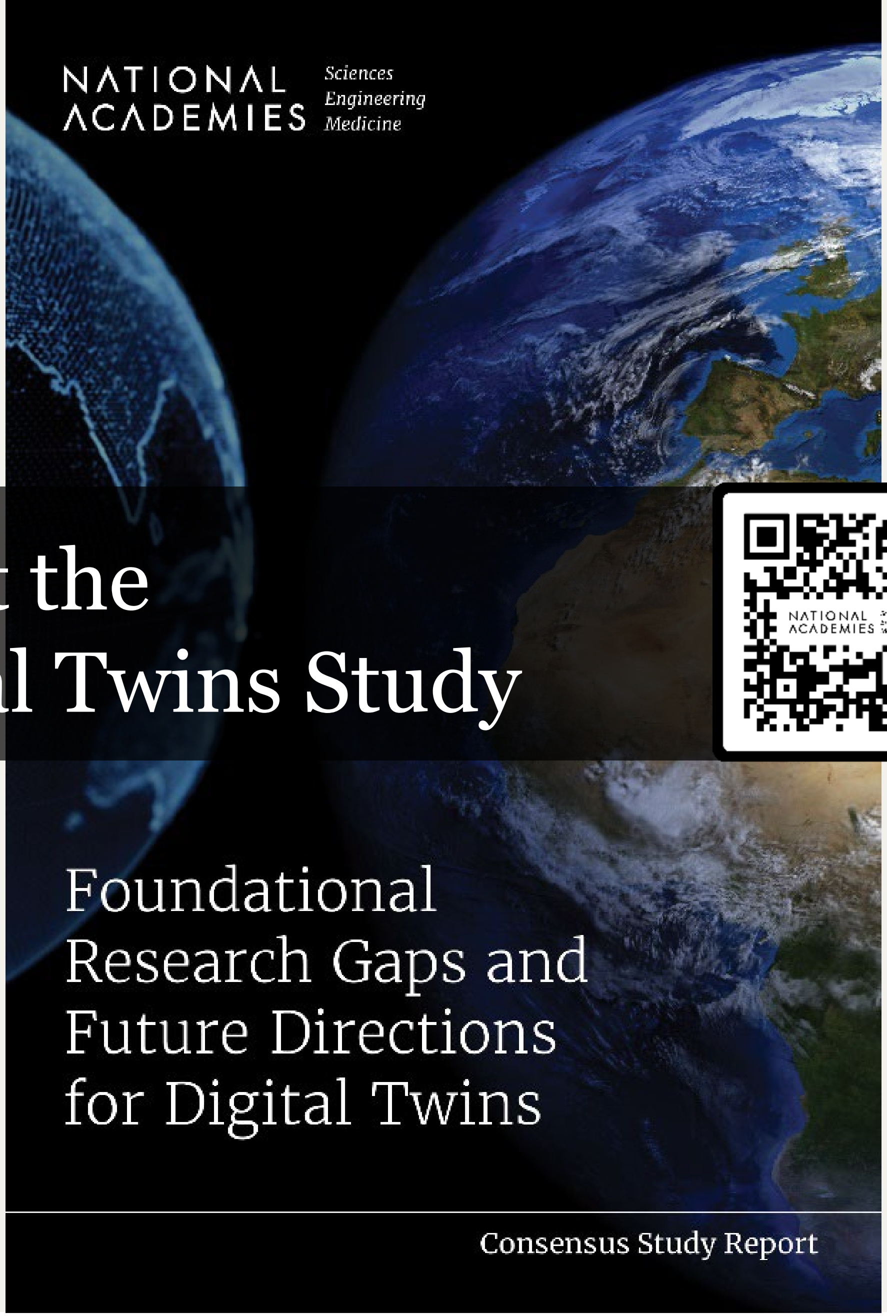
FOR COMPUTATIONAL ENGINEERING & SCIENCES

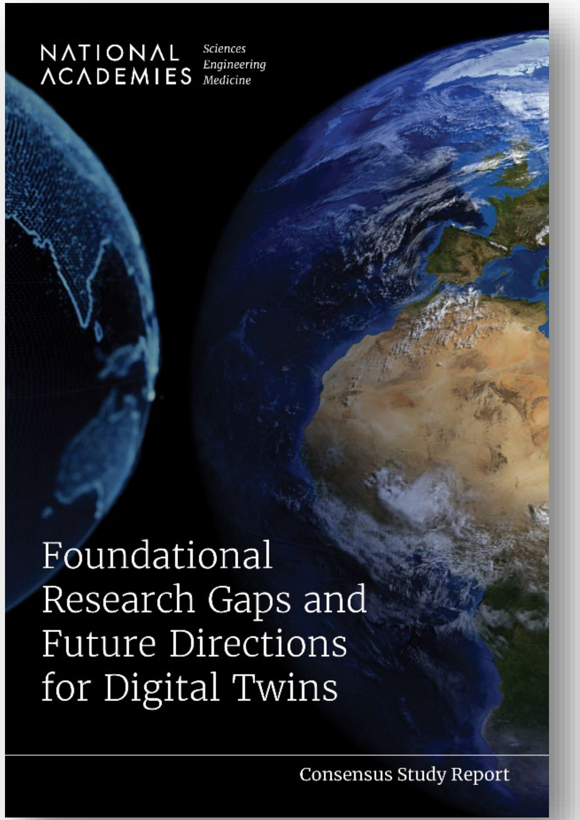
About the Digital Twins Study



Advancing mathematical, statistical, and computational foundations

- How are digital twins defined across different communities?
- Foundational research needs and systemic gaps
- Promising practices across domains and sectors
- Opportunities for translation of best practices across domains
- Use cases for awareness and building confidence
- Key opportunities in research, development, and application

A digital twin is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems), is dynamically updated with data from its physical twin, has a predictive capability, and informs decisions that realize value. The bidirectional interaction between the virtual and the physical is central to the digital twin.



National Academies Study on Foundational Research Gaps and Future Opportunities for Digital Twins (2024)

Outline

1 **PREDICTIVE MODELING CHALLENGES**
for complex systems

2 **DIGITAL TWINS**
an opportunity for transformation beyond forward simulation

3 **DIGITAL TWIN MODELING & SIMULATION**
the critical role of reduced-order modeling

4 **BUILDING TRUST IN DIGITAL TWINS**
verification, validation & uncertainty quantification

5 **DIGITAL TWINS FOR COMPLEX SYSTEMS**
complexity, scalability & sustainability

The predictive modeling challenges for complex systems

Complex phenomena
nonlinear, multiscale, multiphysics, dynamic

Cyber-physical interactions
software, hardware, sensors, automation

Complex lifecycle
multiple stages, multiple stakeholders

Evolving system state
degradation, damage, maintenance, upgrades

Limited data
observations are noisy, indirect & expensive/intrusive to acquire

Decades of high-impact advances based on modeling & simulation for complex systems

Forward Simulations
Advancing scientific discovery & engineering innovation

Forward simulation has been the backbone of engineering analysis for many decades

Decades of high-impact advances based on modeling & simulation for complex systems

Forward Simulations
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Optimization & Inverse Problems
Advancing estimation, design & control

Uncertainty Quantification
Design under uncertainty, risk assessment, …

Machine Learning & AI
Learning from data, accelerating workflows, …

Use of computing for complex systems spans well <u>beyond forward simulation</u>.

Decades of high-impact advances based on modeling & simulation for complex systems

Forward Simulations
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Optimization & Inverse Problems
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Design under uncertainty, risk assessment, …

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Learning from data, accelerating workflows, …

Use of computing for complex systems spans well beyond forward simulation.

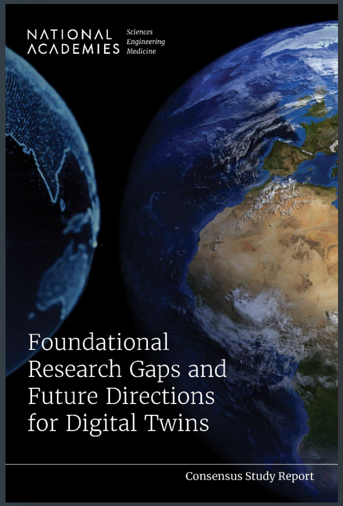
But: (1) UQ, ML & AI still in their infancy;
(2) not yet seen full impact across the entire lifecycle.

2 DIGITAL TWINS

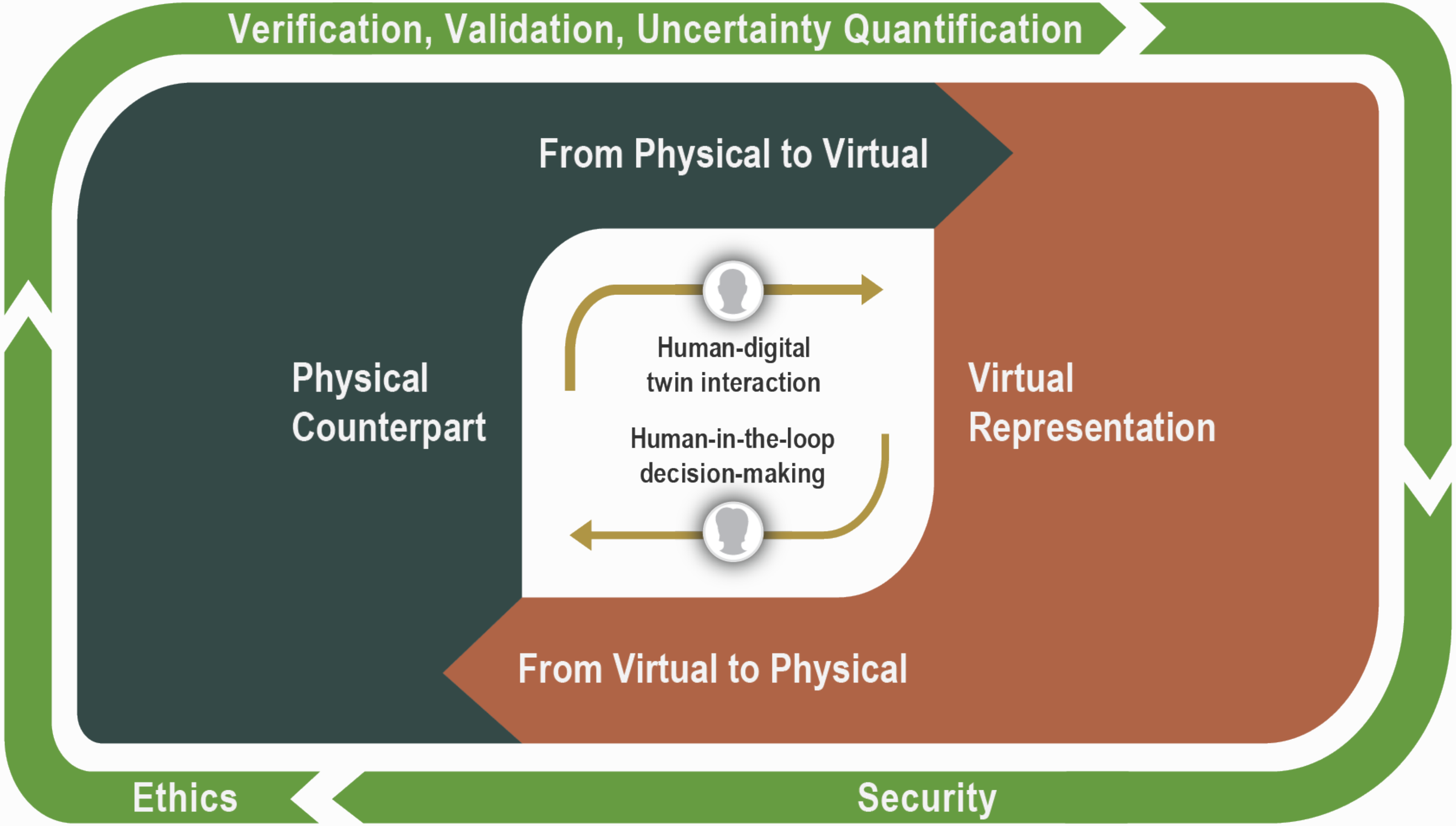
an opportunity for transformation beyond forward simulation

"A **digital twin** is a set of virtual information constructs that mimics the structure, context, and behavior of a natural, engineered, or social system (or system-of-systems), is **dynamically updated** with data from its physical twin, has a **predictive capability**, and informs **decisions** that realize value. **The bidirectional interaction between the virtual and the physical is central to the digital twin.**"

- National Academies Study on Foundational Research Gaps and Future Opportunities for Digital Twins, 2024



A Digital Twin provides a new mathematical paradigm for integrating data, models & decisions



A Digital Twin is more than just simulation and modeling

NATIONAL ACADEMIES Sciences Engineering Medicine

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Digital Twins represent a key opportunity for model and simulation transformation over the next decade

NATIONAL ACADEMIES Sciences Engineering Medicine

National Academies Study on Foundational Research Gaps and Future Opportunities for Digital Twins (2024)

FOCUSED RESEARCH NEEDS

SYSTEMIC, TRANSLATIONAL & PROGRAMMATIC

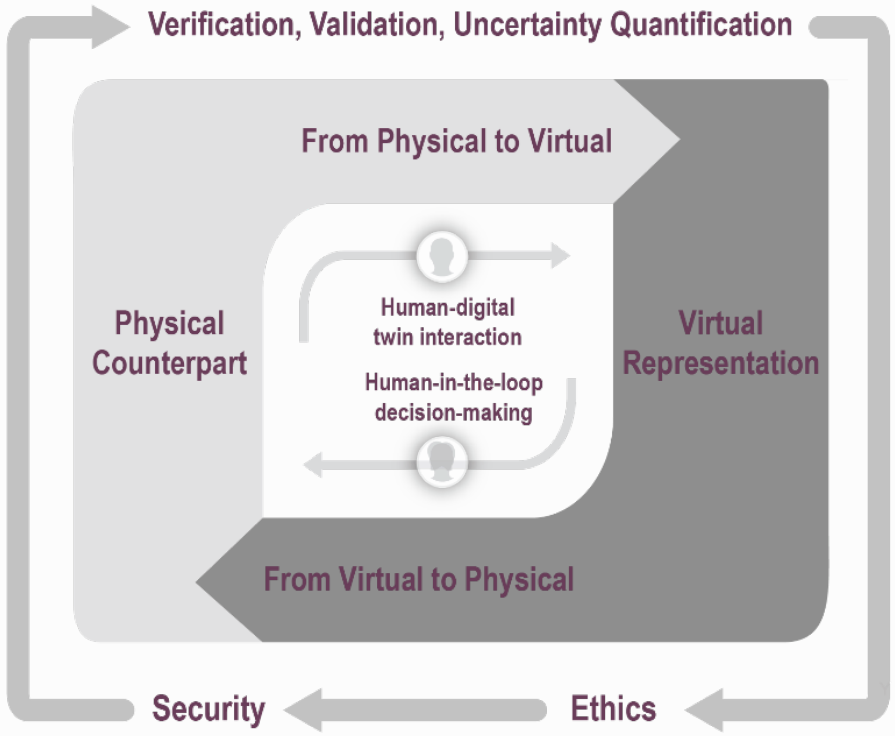
Virtual Representation
multiscale modeling, machine learning & hybrid modeling, surrogates, coupling, system integration, validation, …

Physical Counterpart
data acquisition, imputation, integration, interoperability, …

Physical-to-Virtual
scalable data assimilation, Bayesian inversion, UQ, …

Virtual-to-Physical
scalable optimization under uncertainty, quantifying risk, optimal experimental design, human-in-the-loop decision making, …

Human–digital twin interactions
user-centered digital twin design, ethics, privacy, communicating UQ, …



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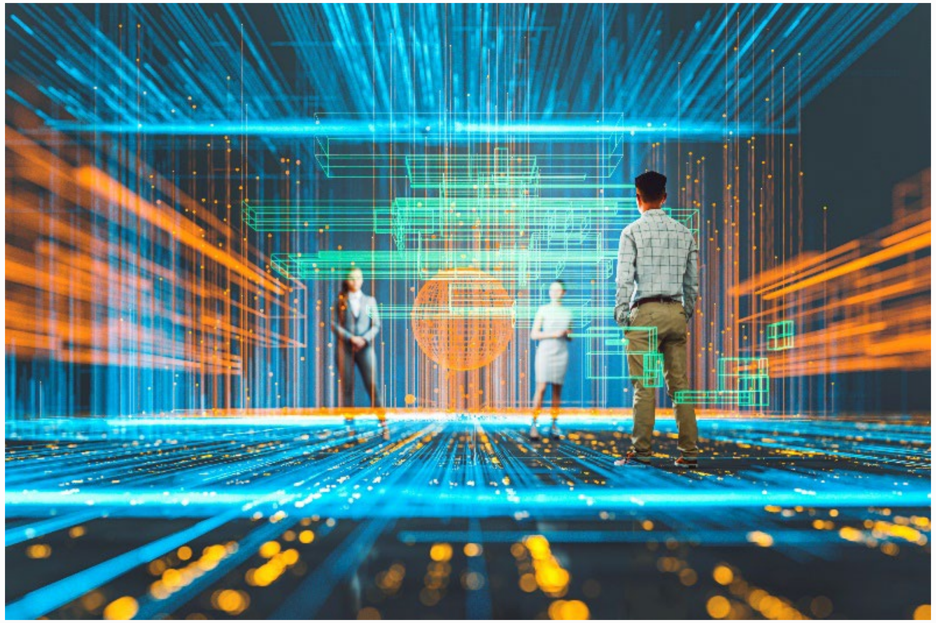
FOCUSED RESEARCH NEEDS

SYSTEMIC, TRANSLATIONAL & PROGRAMMATIC



Digital twin sustainability

Translational & collaborative research

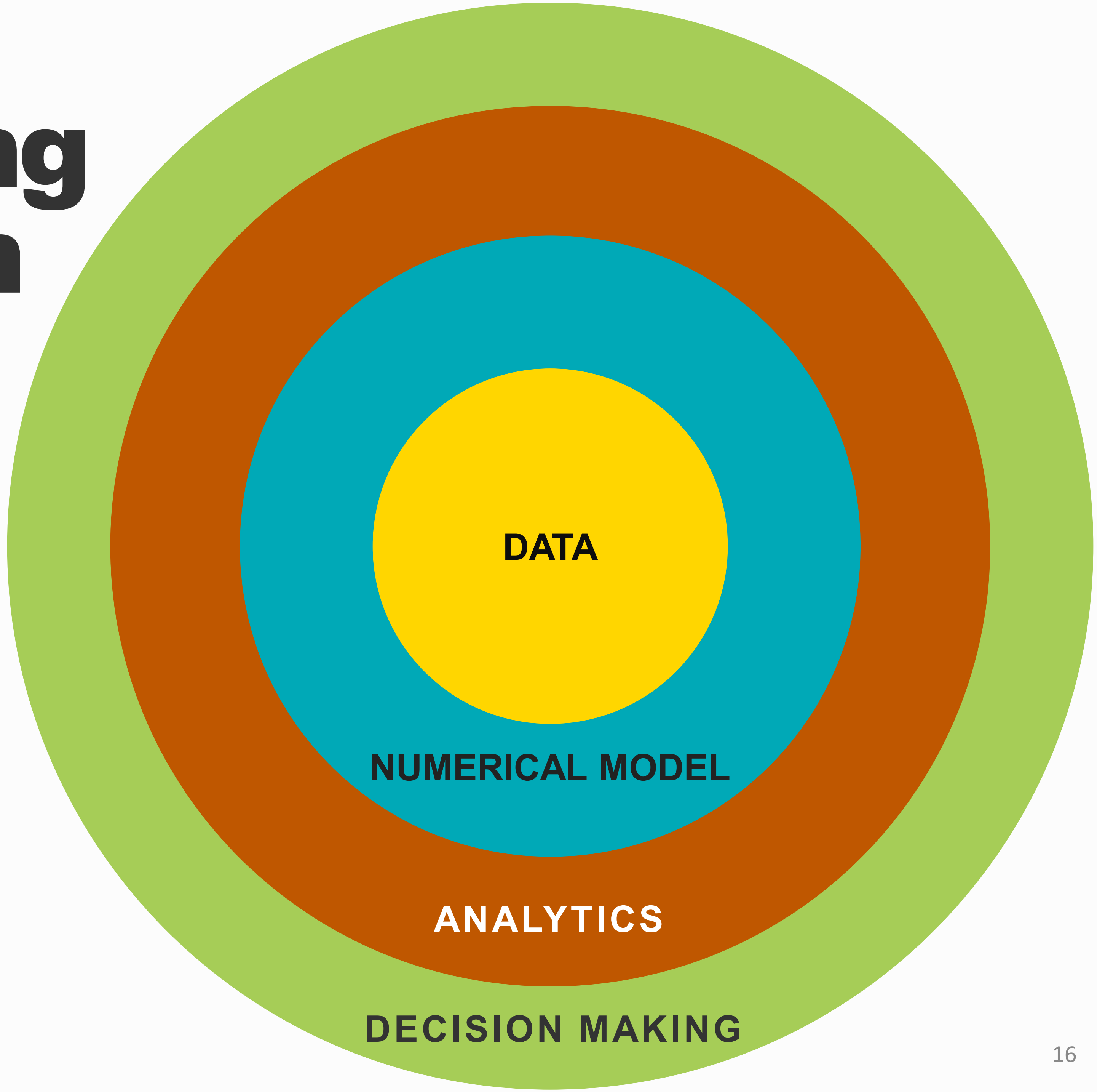
Fostering model & data collaborations

Preparing an interdisciplinary workforce

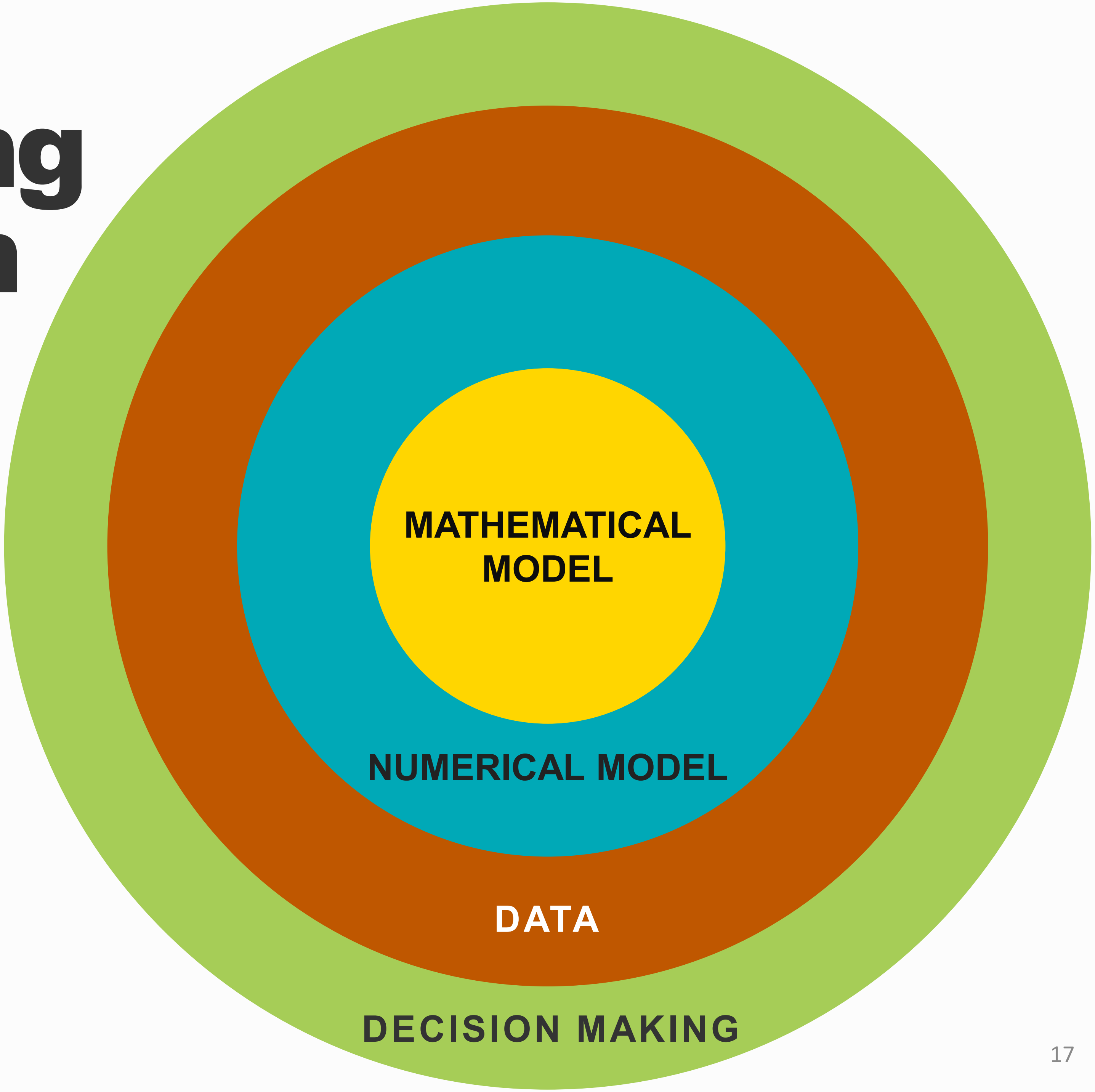
3 DIGITAL TWIN MODELING & SIMULATION

the critical role of reduced-order modeling

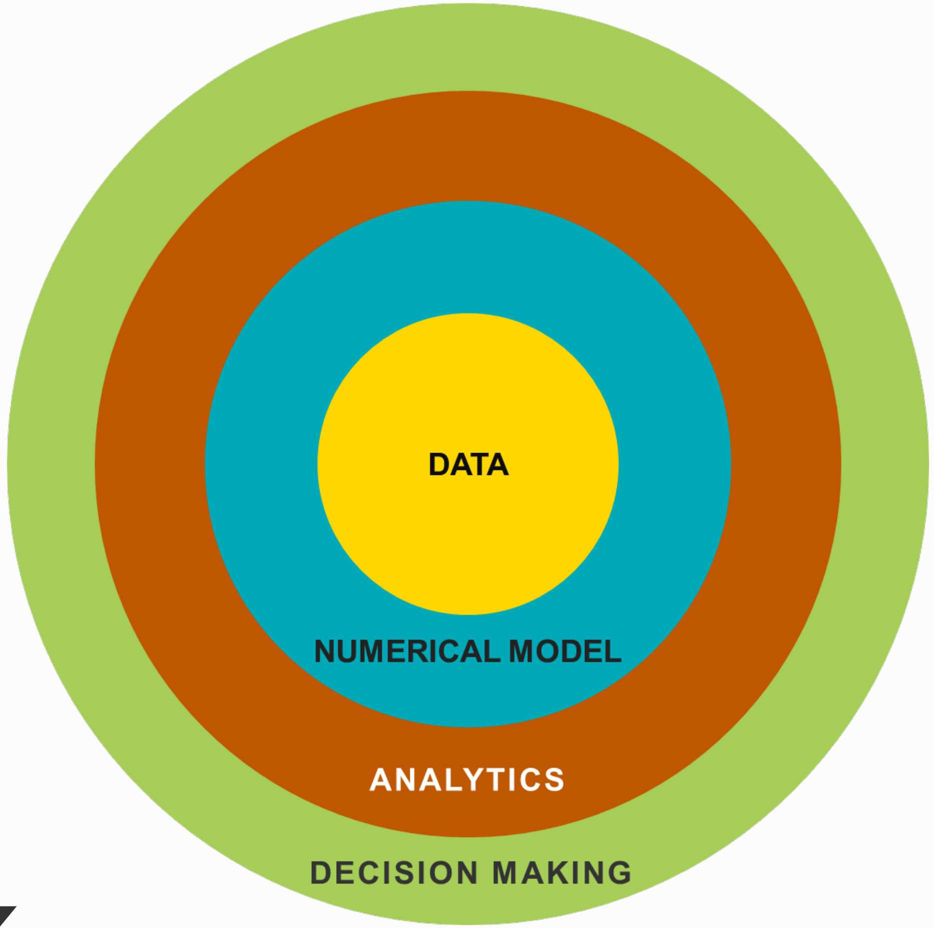
Conceptualizing a Digital Twin

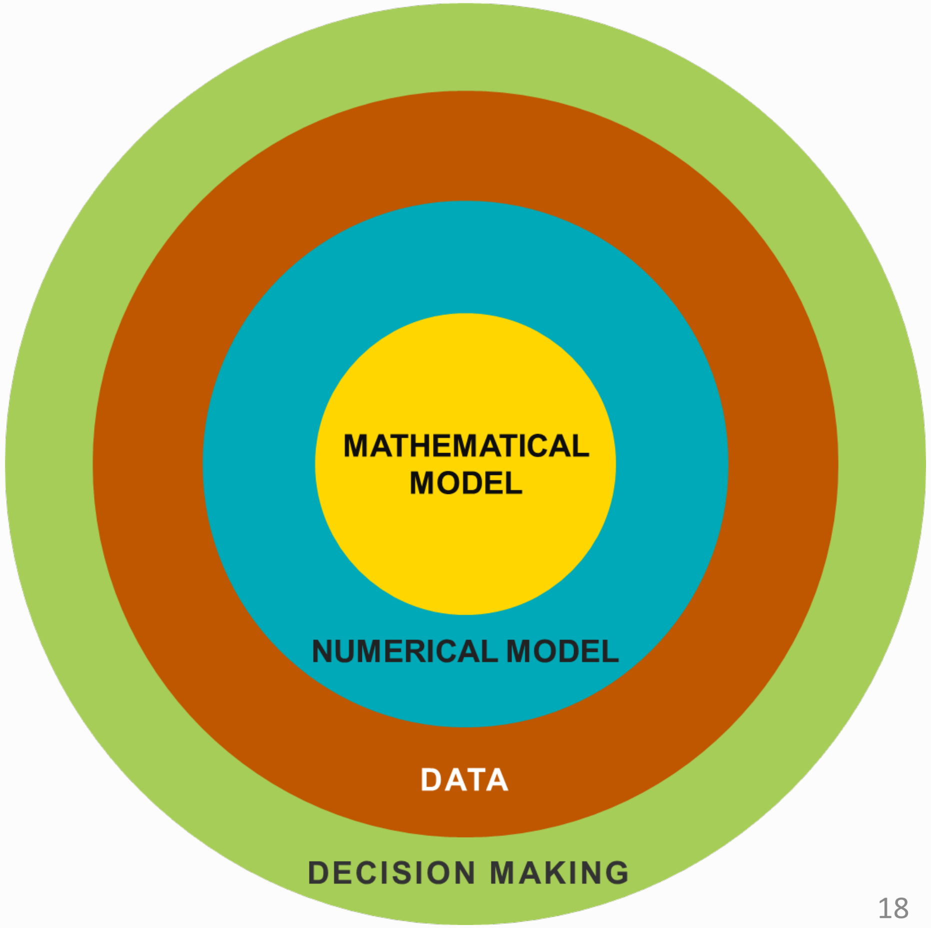


Conceptualizing a Digital Twin



Conceptualizing a Digital Twin



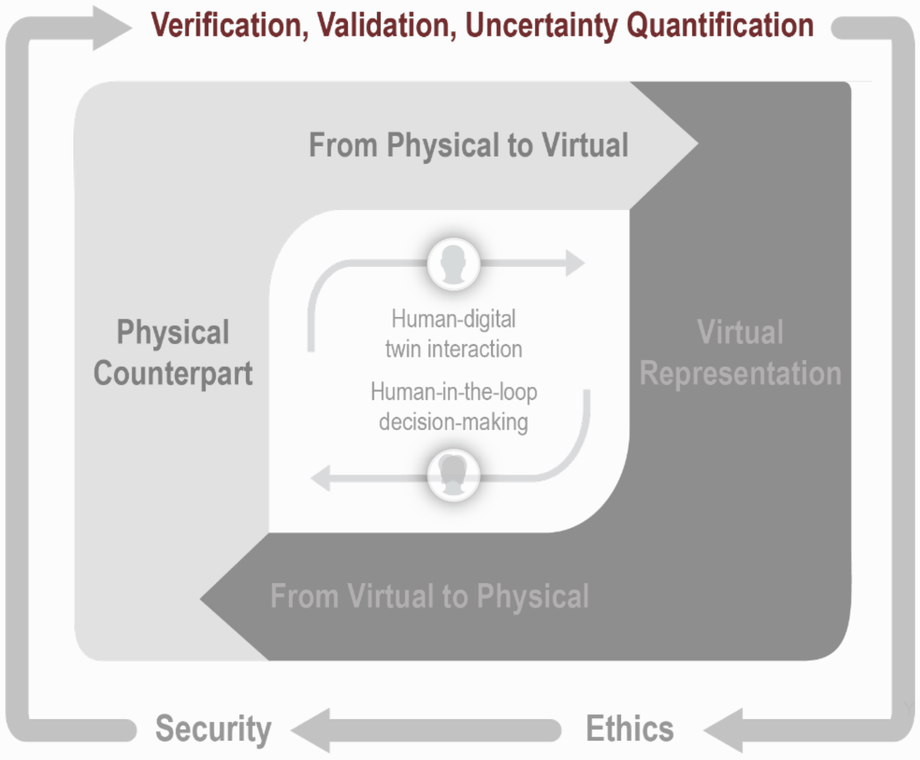


A Digital Twin should be Fit for Purpose

Balancing required fidelity for prediction, available resources, and acceptable costs

- Different digital twin purposes drive different fitness requirements related to modeling fidelity, data availability, visualization, time-to-solution, etc.

- For many potential use cases, achieving fitness-for-purpose is currently intractable



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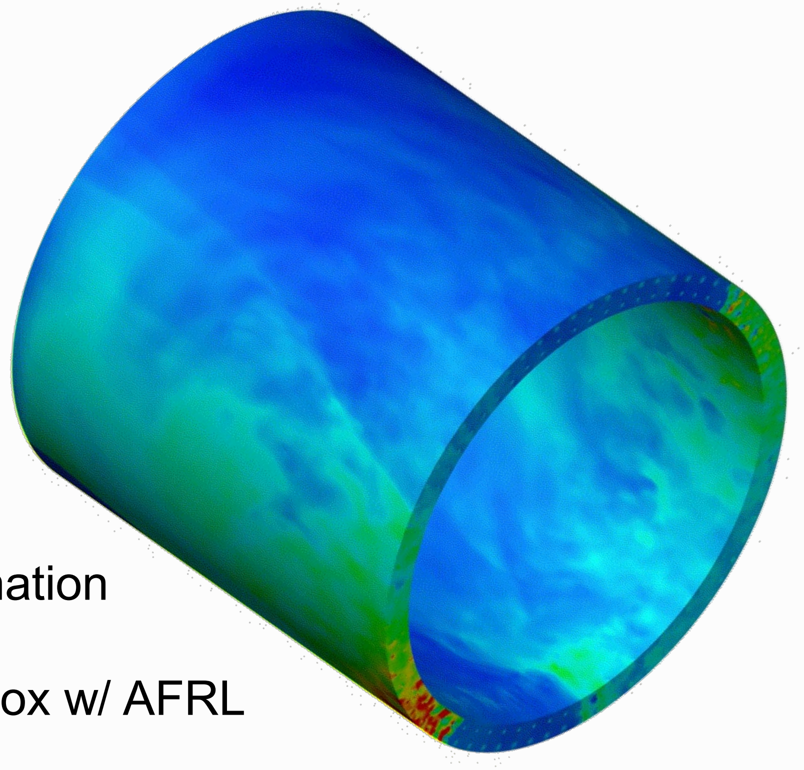
Physics-based models are essential to achieve predictive capabilities



Rotating detonation rocket engine
Farcas & Willcox w/ AFRL

Large eddy simulation (LES) of reactive Navier-Stokes equations with 136M spatial dof and $\Delta t = 10^{-9}$

but they can be COMPUTATIONALLY PROHIBITIVE for design, control, UQ, or digital twins

ML surrogates vs. model reduction

Machine learning

"…statistical algorithms that can learn from data and generalize to unseen data and thus perform tasks without explicit instructions." [Wikipedia]

Reduced-order modeling

"Model order reduction (MOR) is a technique for reducing the computational complexity of mathematical models in numerical simulations." [Wikipedia]

Model reduction methods have grown from Computational Science, with focus on *reducing* high-dimensional models that arise from physics-based modeling, whereas machine learning has grown from Computer Science, with focus on *learning* models from black-box data streams.

[Swischuk et al., *Computers & Fluids*, 2019]

We aim to blend the predictive power of physics-based methods & the speed of ML

Define the **structure of the reduced model**

$$\dot{\hat{\mathbf{x}}} = \widehat{\mathbf{A}}\hat{\mathbf{x}} + \widehat{\mathbf{B}}\mathbf{u} + \widehat{\mathbf{H}}(\hat{\mathbf{x}} \otimes \hat{\mathbf{x}})$$

Non-intrusive learning by inferring reduced operators from simulation data [Peherstorfer & W., 2016]

OpInf

We aim to blend the predictive power of physics-based methods & the speed of ML

Our Operator Inference approach blends reduced-order modeling & machine learning

ÔpInf

physics-based models
typically PDEs or ODEs

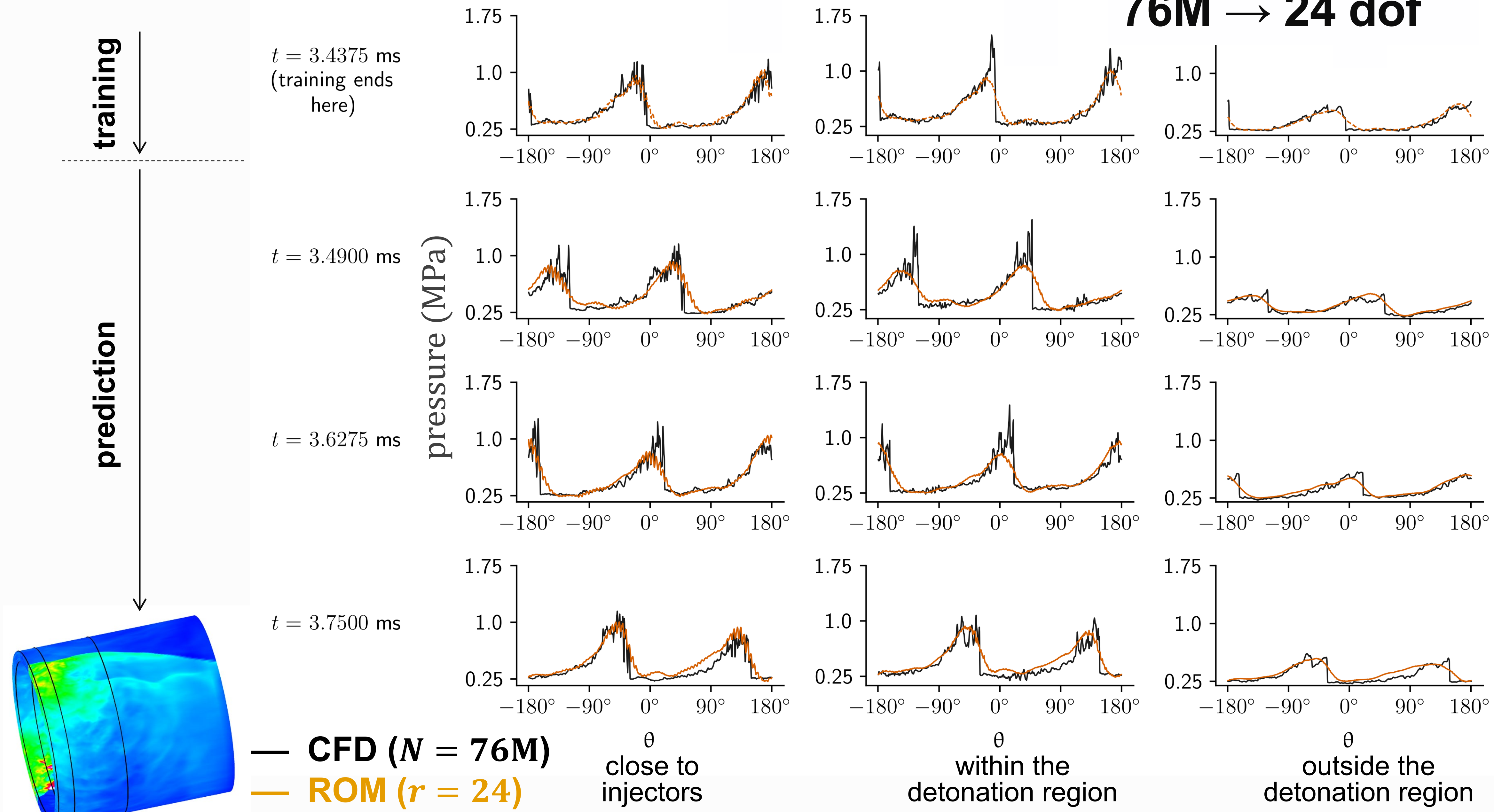
+

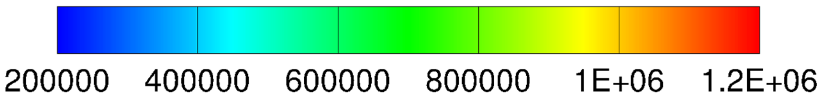
classical mathematical
lens of **projection**

defines the form of a structure-preserving low-dimensional model
which we then learn directly from limited training data

Reduced-order models are solved in <1sec, bringing **physics predictive power** off the designer's supercomputer and **into the operational world.**

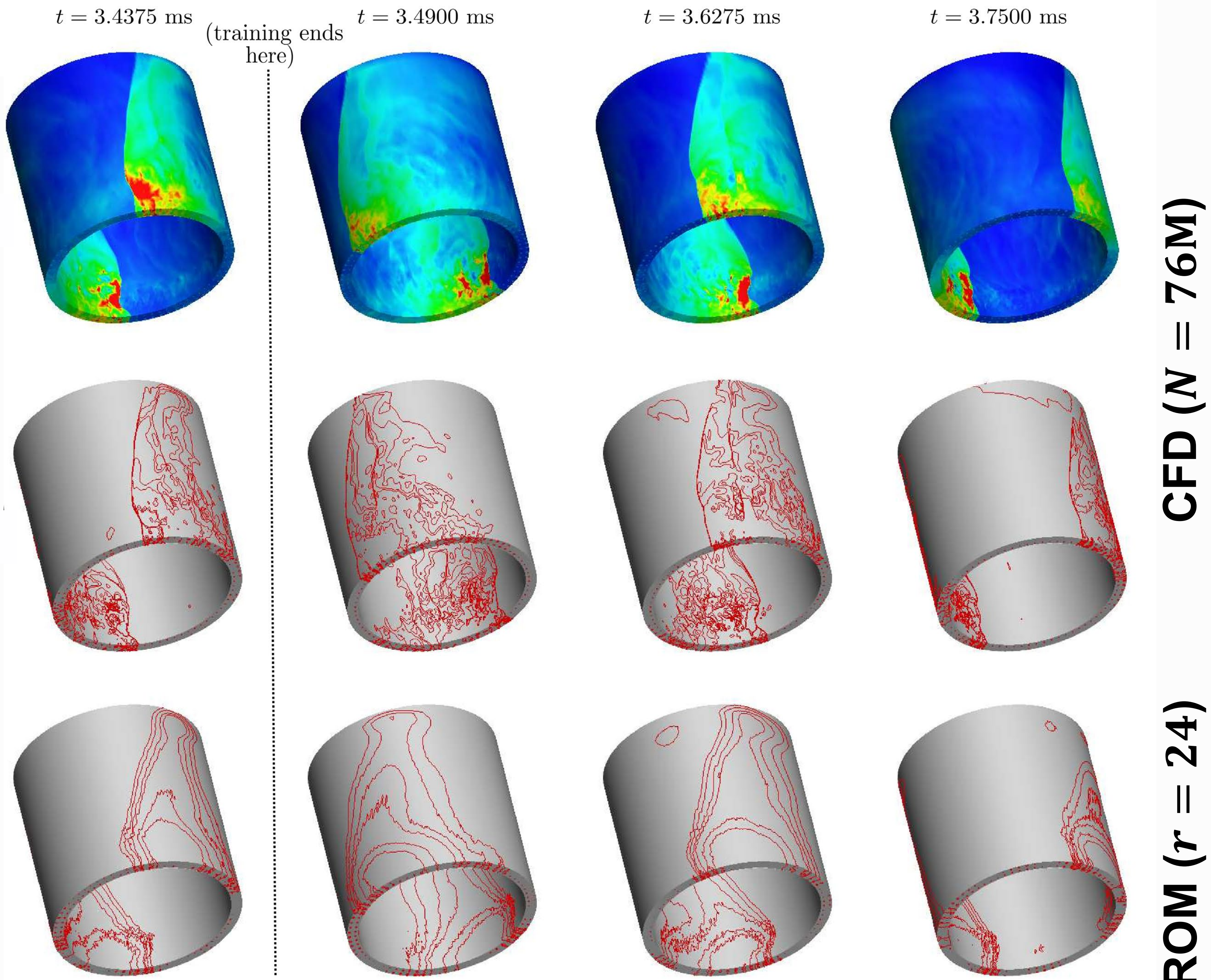
Rotating detonation rocket engine simulation: weeks → milliseconds
76M → 24 dof





RDRE pressure contours:

Reduced model captures coarse behavior but does not resolve all the fine-scale dynamics



Distributed Operator Inference
Farcas, Gundevia, Munipalli & Willcox
Computer Physics Communications, 2025.

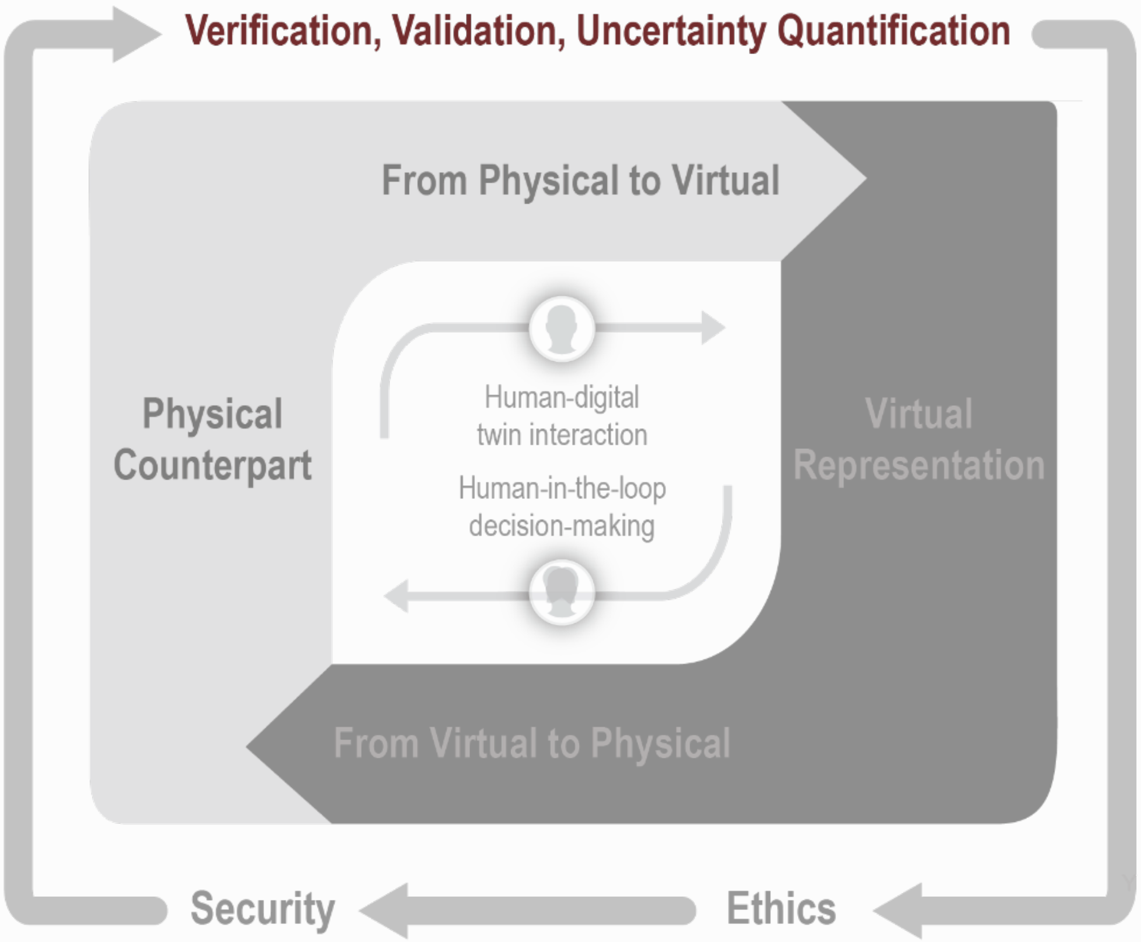
Reduced-order models are critical enablers for predictive digital twins

- There have been many advances in methods for parametric ROMs and nonlinear ROMs – these play an important role
- But ROM ability to handle complexity and wide range of operating conditions falls short for many digital twin applications
- Huge interest in medical digital twins, but relatively little ROM work for medical applications
- Cost of generating training data remains a barrier for many digital twin applications $\rightarrow$ this is a significant research need

4 DIGITAL TWIN VERIFICATION, VALIDATION & UNCERTAINTY QUANTIFICATION

Verification, Validation & Uncertainty Quantification (VVUQ)

Methods for continual VVUQ and monitoring of digital twins are required to establish trust.



Verification. Does a computer program correctly solve the equations of the mathematical model?

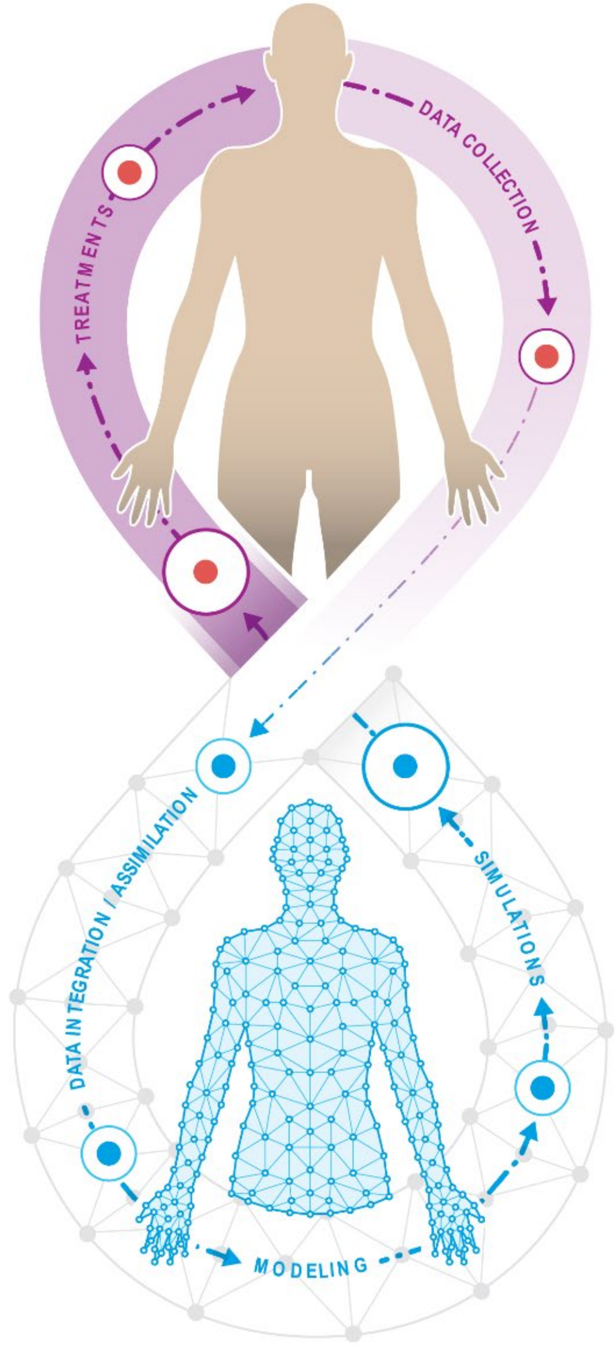
Validation. To what degree is a model an accurate representation of the real world, from the perspective of the intended model uses?

Uncertainty Quantification. What are uncertainties in model calculations of quantities of interest?

RECOMMENDATION 2

VVUQ is Critical to the Success of Digital Twins

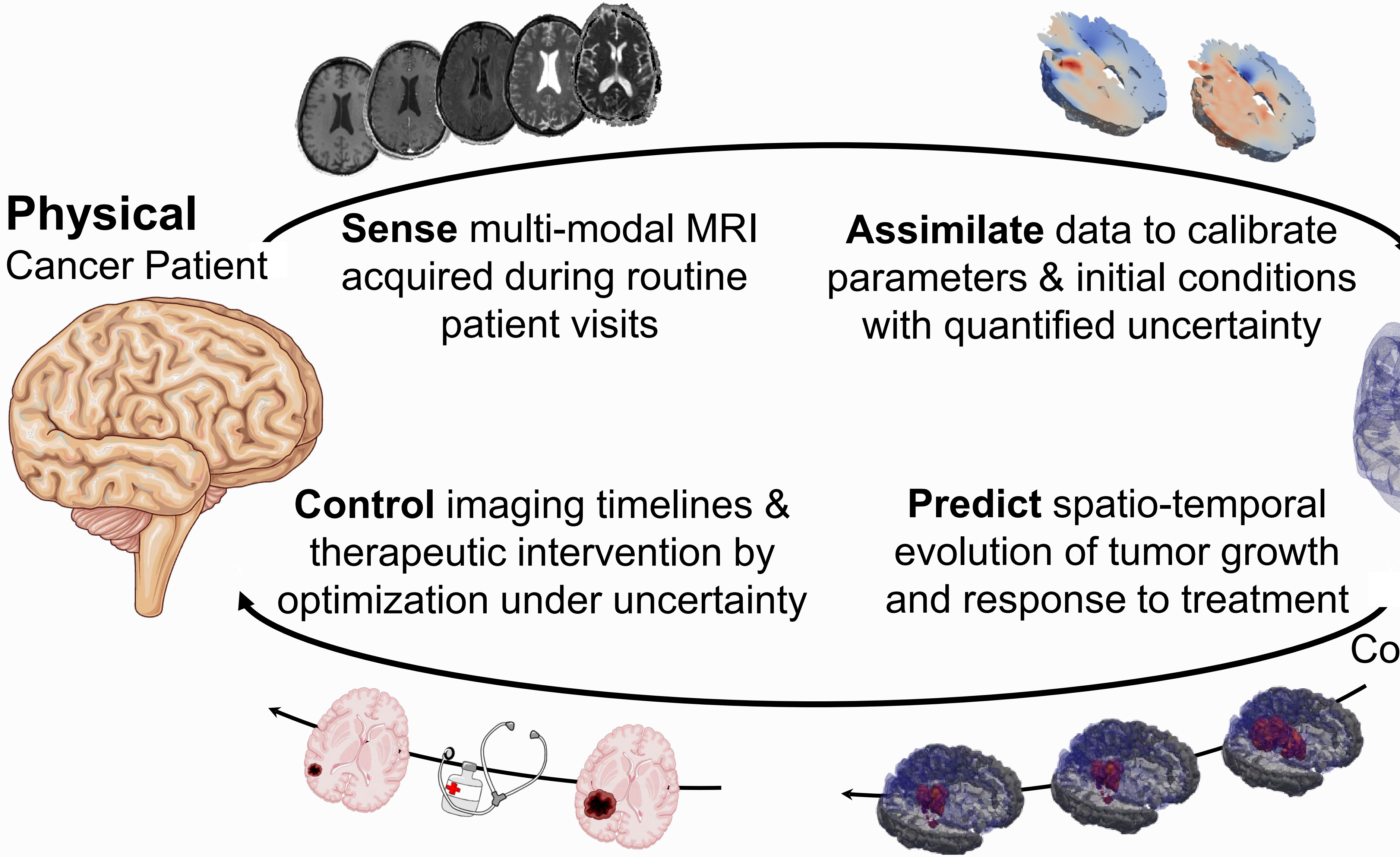
- VVUQ must be deeply embedded in the design, creation, and deployment of digital twins
- Need new methods for continual VVUQ that adapt to changes in models, data, and decision contexts
- AI, machine learning, and empirical models pose particular VVUQ challenges
- In future digital twin research and development, VVUQ should play a core role, and tight integration should be emphasized

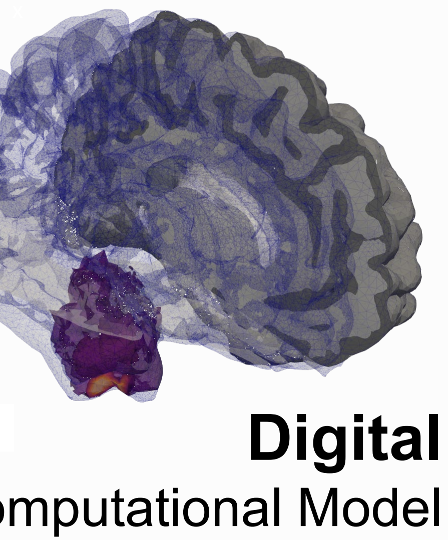


DIGITAL-TWIN-ENABLED CANCER TREATMENT

Anirban Chaudhuri
(Research Scientist)

Graham Pash
(PhD student)



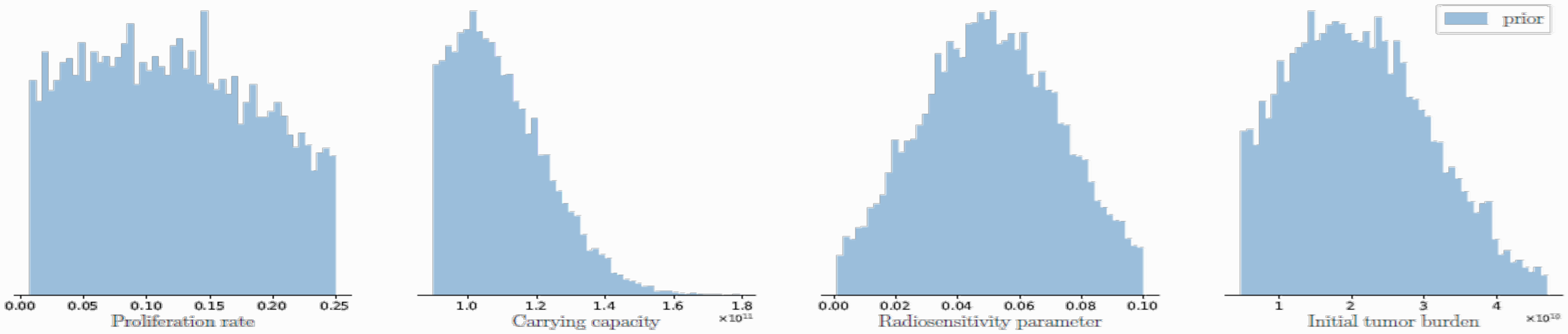


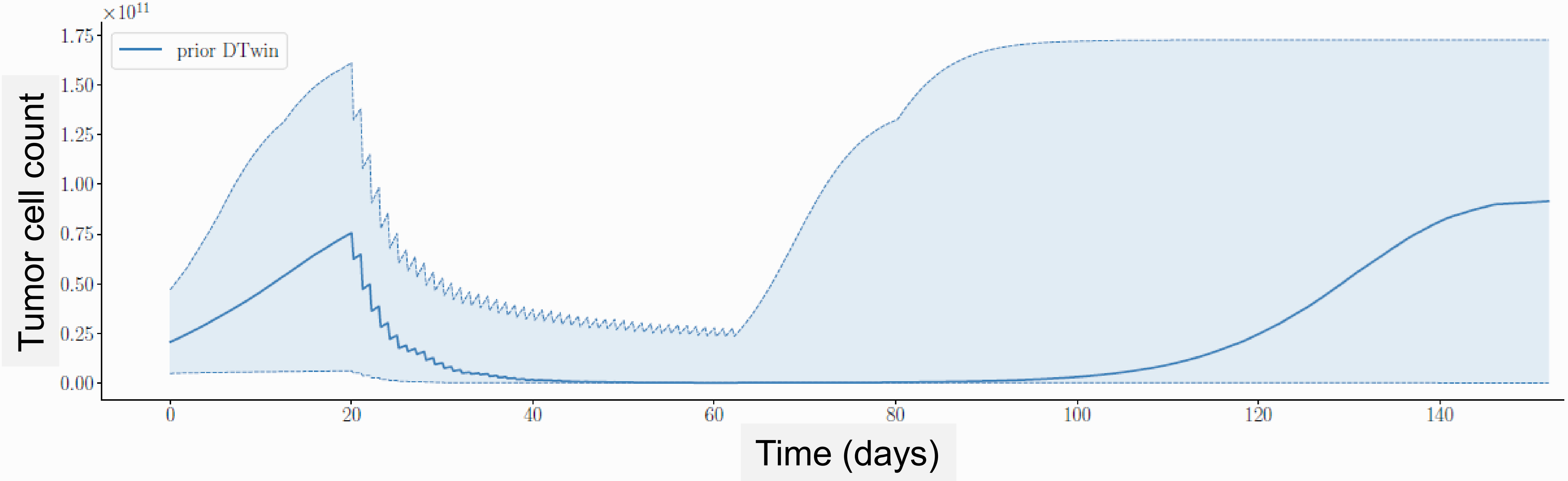
Patient Prior

Patient parameters:

Proliferation Rate
Carrying Capacity
Radiosensitivity parameter
Initial Tumor Burden

Proliferation Rate | Carrying Capacity | Radiosensitivity parameter | Initial Tumor Burden

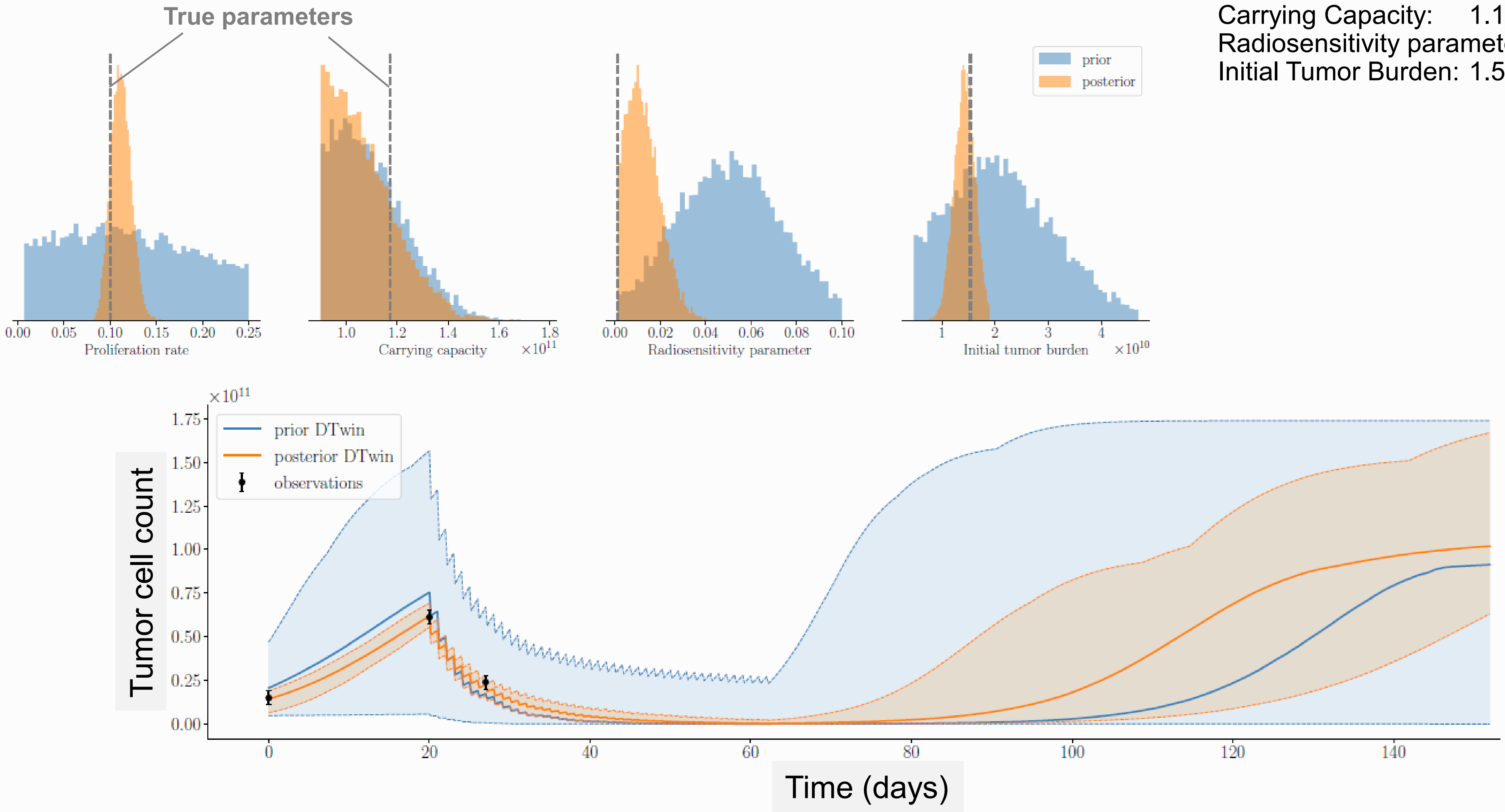




Patient 1: Calibration via Inverse UQ

Patient 1 true parameters:

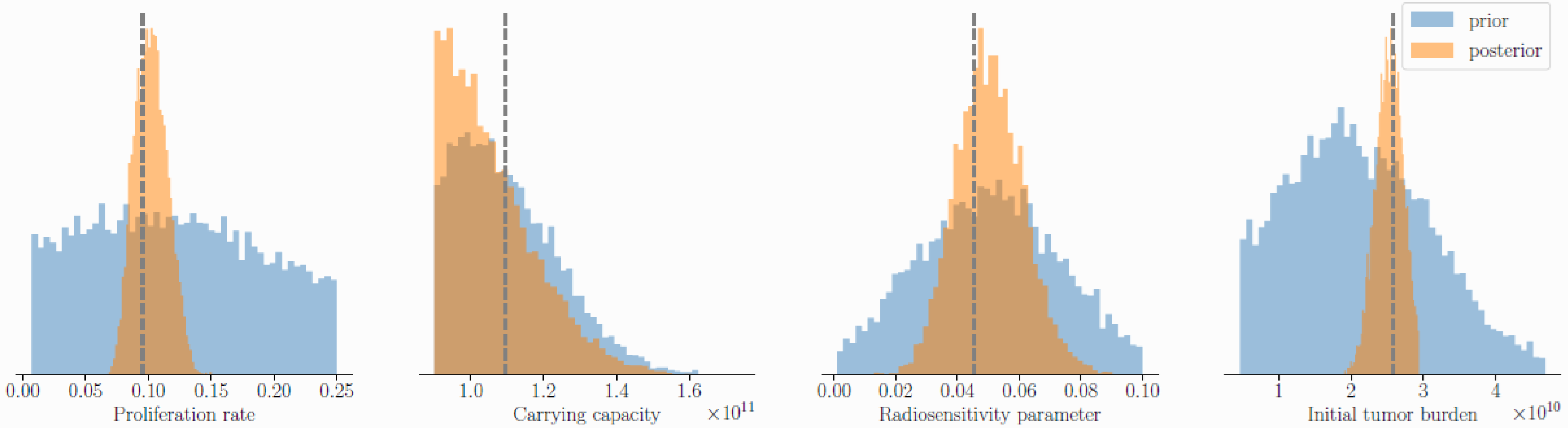
Proliferation Rate: 1.14e-01
Carrying Capacity: 1.17e+11
Radiosensitivity parameter: 1.05e-03
Initial Tumor Burden: 1.54e+10

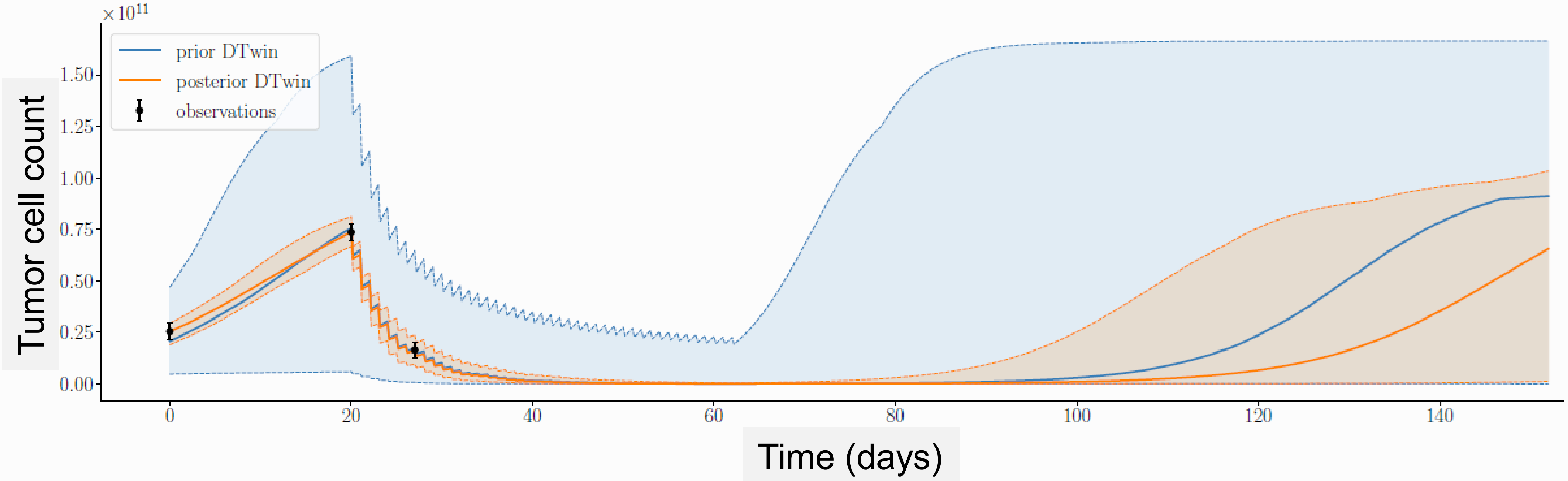


Patient 2: Calibration via Inverse UQ

Patient 2 true parameters:

Proliferation Rate: 1.09e-01
Carrying Capacity: 1.09e+11
Radiosensitivity parameter: 4.58e-02
Initial Tumor Burden: 2.60e+10

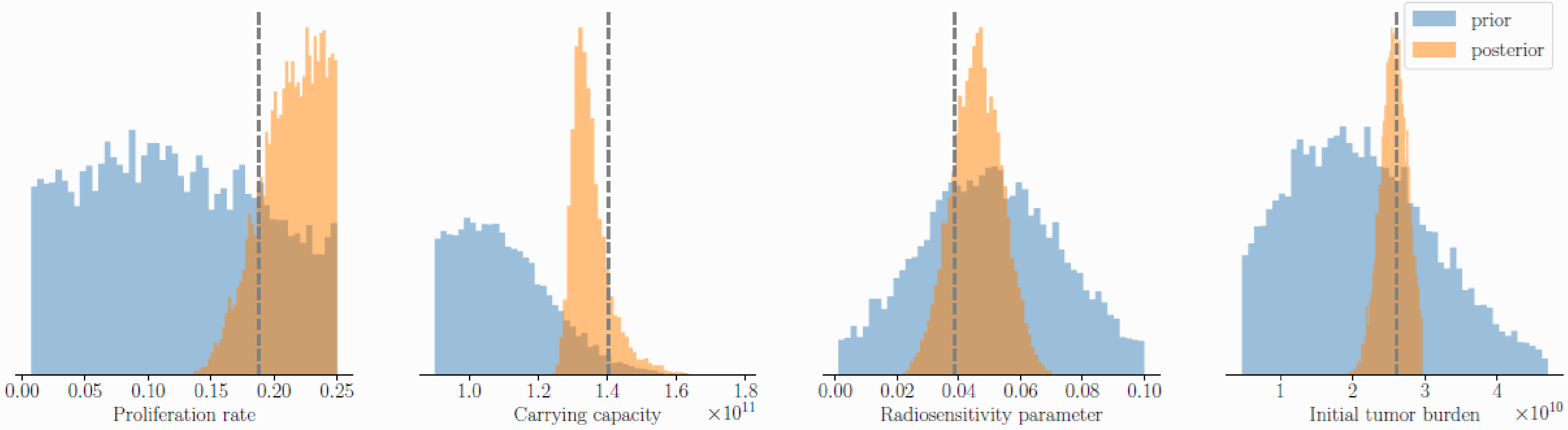


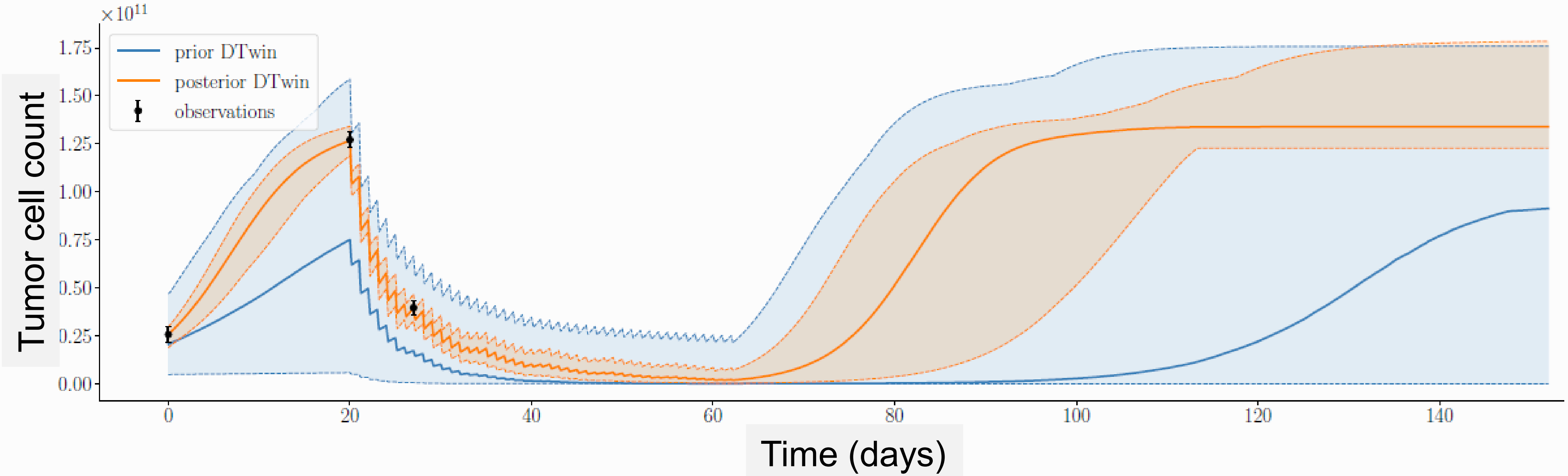


Patient 3: Calibration via Inverse UQ

Patient 3 true parameters:

Proliferation Rate: 2.25e-01
Carrying Capacity: 1.40e+11
Radiosensitivity parameter: 3.90e-02
Initial Tumor Burden: 2.62e+10



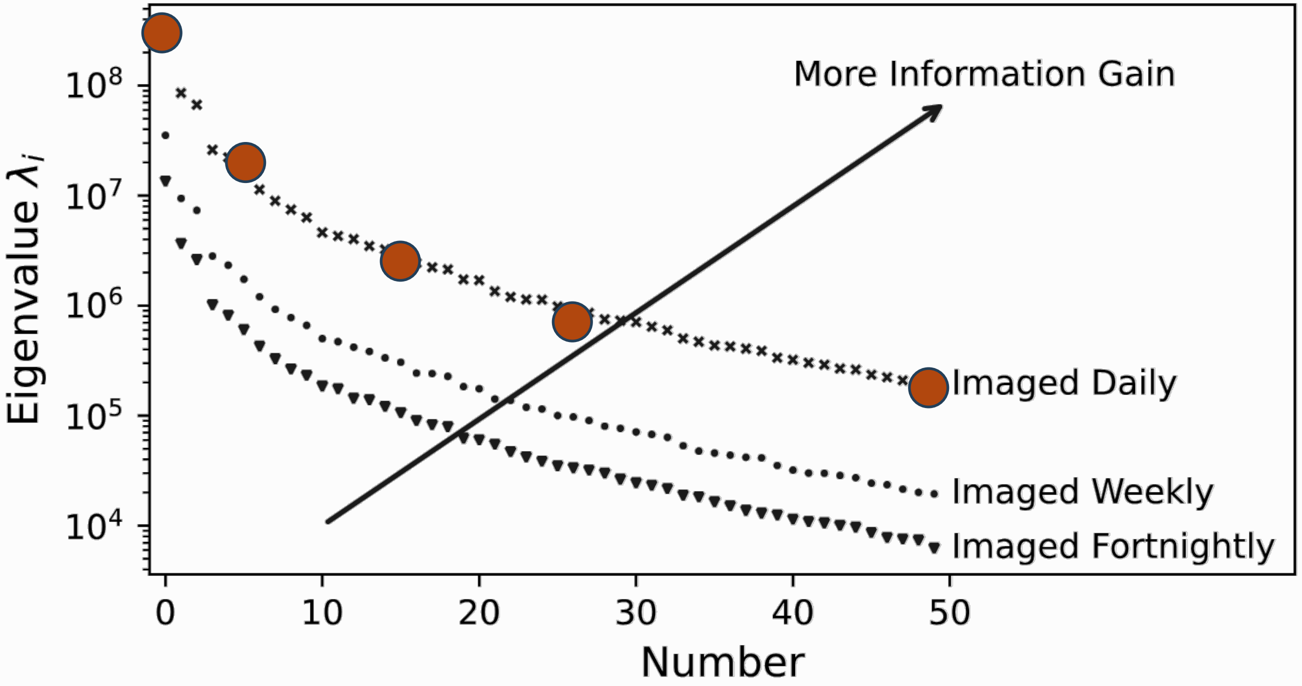


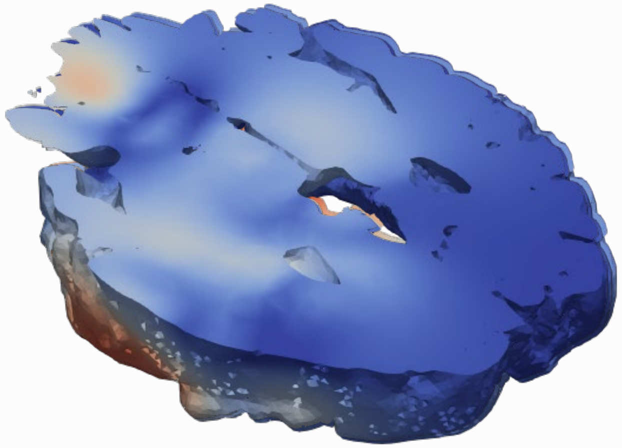
More than just trust: UQ provides valuable decision guidance

Analysis of the Bayesian inverse problem Hessian provides insight into the value of imaging data

- Eigenvalues tell *how* well-informed
- Eigenvectors show *where* is well-informed

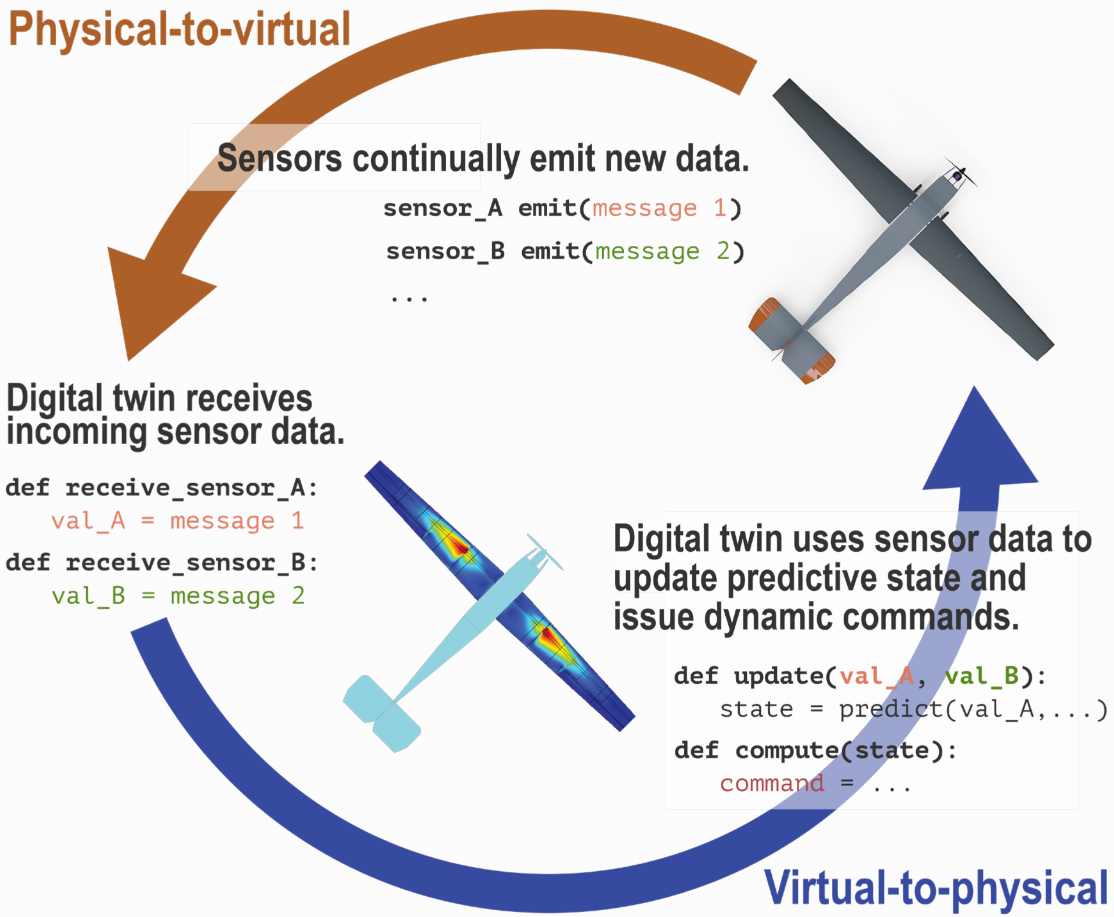
$$\mathbf{H}_{\mathrm{MAP}}^{\mathrm{data}}\mathbf{v}_j = \lambda_j \mathbf{\Gamma}_{\mathrm{pr}}^{-1}\mathbf{v}_j$$

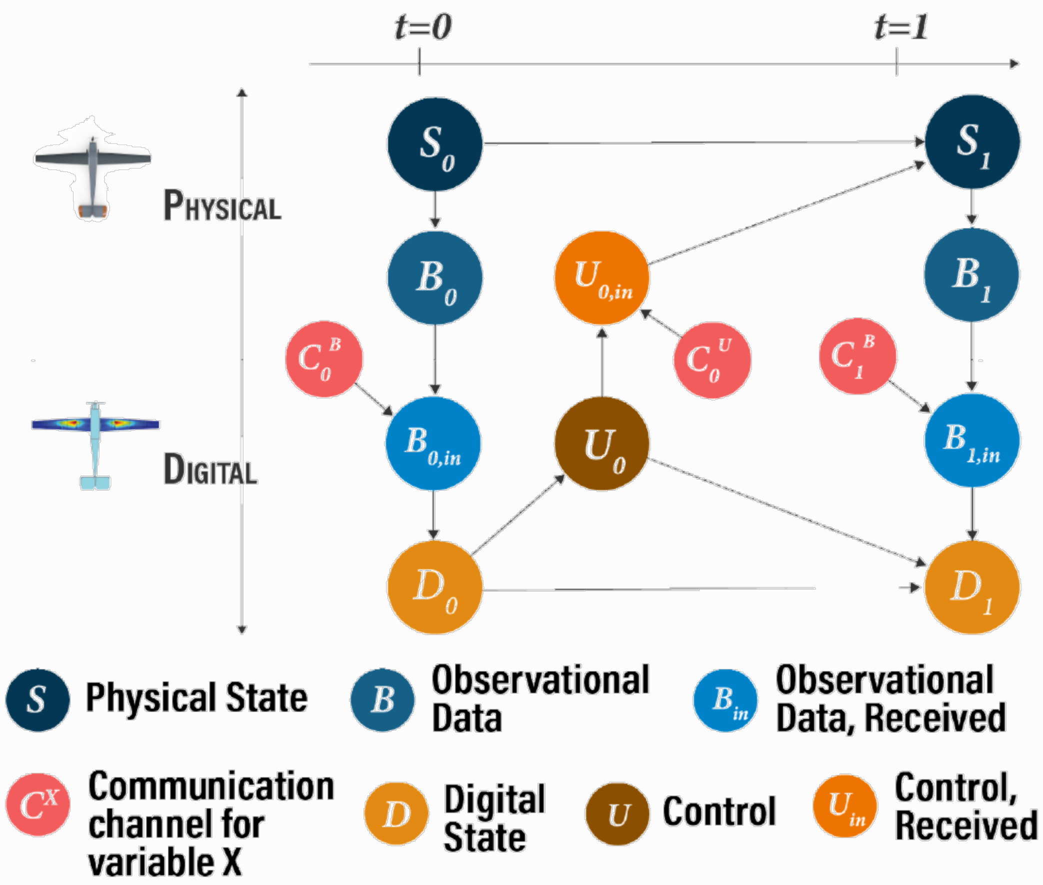




Research need: scalable methods for digital twin verification & security

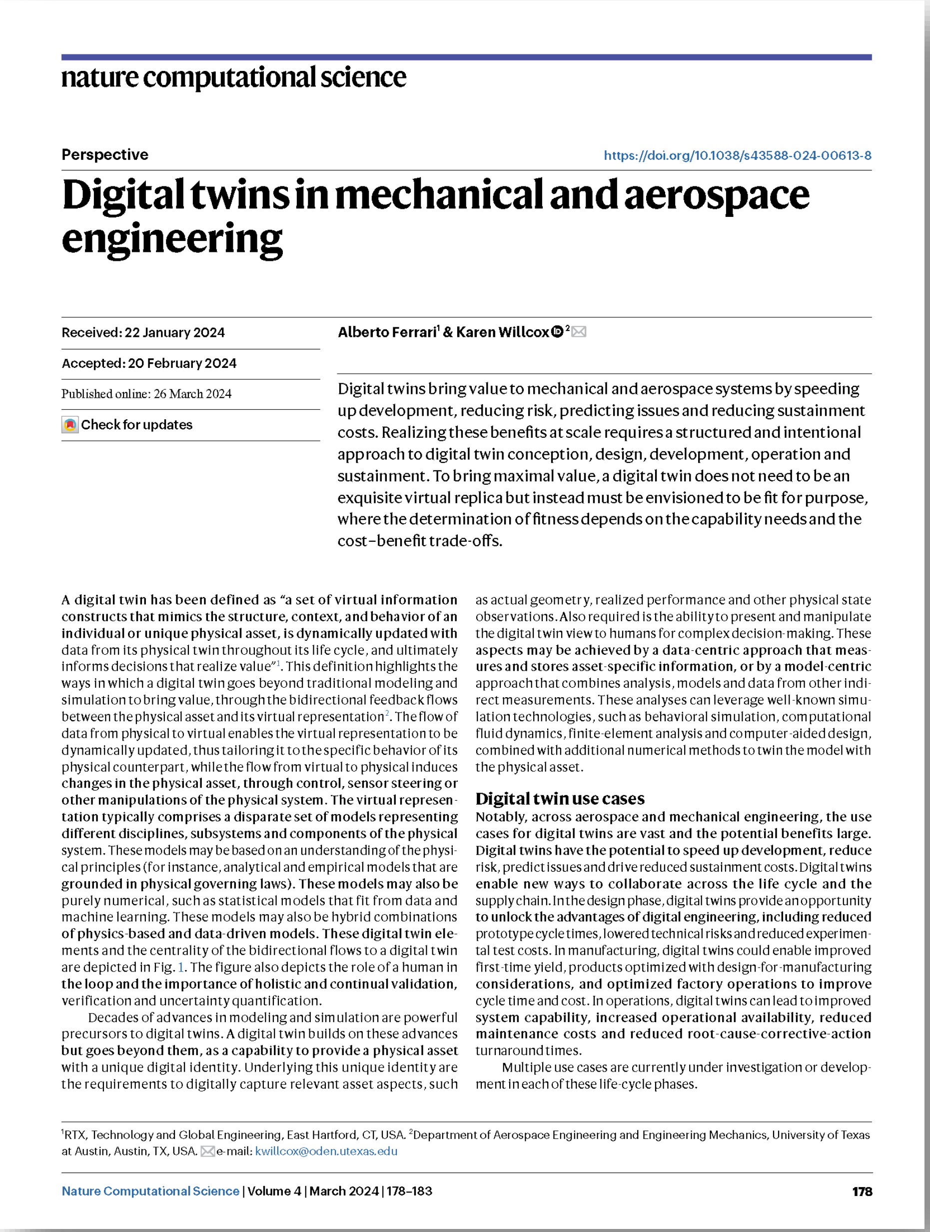
Luwen Huang
(PhD student)





Huang, Topcu, Varshney & W. Submitted *J. Computational Physics*.

5 DIGITAL TWIN SUSTAINABILITY, COMPLEXITY & SCALABILITY



nature computational science

Perspective

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Digital twins in mechanical and aerospace engineering

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Check for updates

Alberto Ferrari[1] & Karen Willcox[2]

Digital twins bring value to mechanical and aerospace systems by speeding up development, reducing risk, predicting issues and reducing sustainment costs. Realizing these benefits at scale requires a structured and intentional approach to digital twin conception, design, development, operation and sustainment. To bring maximal value, a digital twin does not need to be an exquisite virtual replica but instead must be envisioned to be fit for purpose, where the determination of fitness depends on the capability needs and the cost–benefit trade-offs.

A digital twin has been defined as "a set of virtual information constructs that mimics the structure, context, and behavior of an individual or unique physical asset, is dynamically updated with data from its physical twin throughout its life cycle, and ultimately informs decisions that realize value"[1]. This definition highlights the ways in which a digital twin goes beyond traditional modeling and simulation to bring value, through the bidirectional feedback flows between the physical asset and its virtual representation[2]. The flow of data from physical to virtual enables the virtual representation to be dynamically updated, thus tailoring it to the specific behavior of its physical counterpart, while the flow from virtual to physical induces changes in the physical asset, through control, sensor steering or other manipulations of the physical system. The virtual representation typically comprises a disparate set of models representing different disciplines, subsystems and components of the physical system. These models may be based on an understanding of the physical principles (for instance, analytical and empirical models that are grounded in physical governing laws). These models may also be purely numerical, such as statistical models that fit from data and machine learning. These models may also be hybrid combinations of physics-based and data-driven models. These digital twin elements and the centrality of the bidirectional flows to a digital twin are depicted in Fig. 1. The figure also depicts the role of a human in the loop and the importance of holistic and continual validation, verification and uncertainty quantification.

Decades of advances in modeling and simulation are powerful precursors to digital twins. A digital twin builds on these advances but goes beyond them, as a capability to provide a physical asset with a unique digital identity. Underlying this unique identity are the requirements to digitally capture relevant asset aspects, such as actual geometry, realized performance and other physical state observations. Also required is the ability to present and manipulate the digital twin view to humans for complex decision-making. These aspects may be achieved by a data-centric approach that measures and stores asset-specific information, or by a model-centric approach that combines analysis, models and data from other indirect measurements. These analyses can leverage well-known simulation technologies, such as behavioral simulation, computational fluid dynamics, finite-element analysis and computer-aided design, combined with additional numerical methods to twin the model with the physical asset.

Digital twin use cases

Notably, across aerospace and mechanical engineering, the use cases for digital twins are vast and the potential benefits large. Digital twins have the potential to speed up development, reduce risk, predict issues and drive reduced sustainment costs. Digital twins enable new ways to collaborate across the life cycle and the supply chain. In the design phase, digital twins provide an opportunity to unlock the advantages of digital engineering, including reduced prototype cycle times, lowered technical risks and reduced experimental test costs. In manufacturing, digital twins could enable improved first-time yield, products optimized with design-for-manufacturing considerations, and optimized factory operations to improve cycle time and cost. In operations, digital twins can lead to improved system capability, increased operational availability, reduced maintenance costs and reduced root-cause-corrective-action turnaround times.

Multiple use cases are currently under investigation or development in each of these life-cycle phases.

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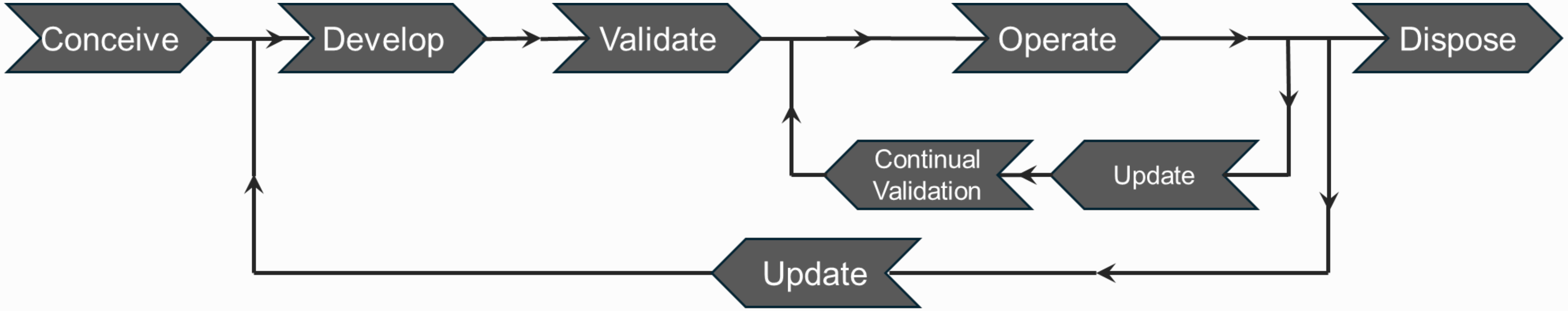
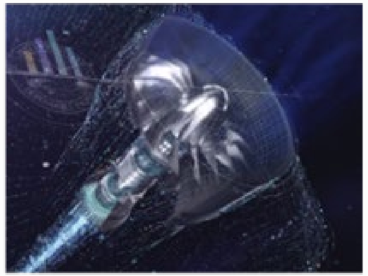
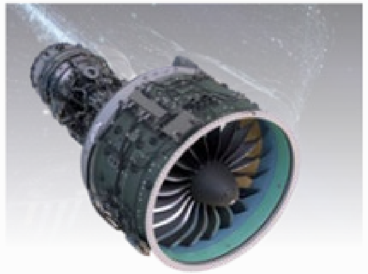
Need to view the digital twin as an asset in its own right

Ferrari & Willcox, *Nature Computational Science, May* 2024



Digital Twin Lifecycle



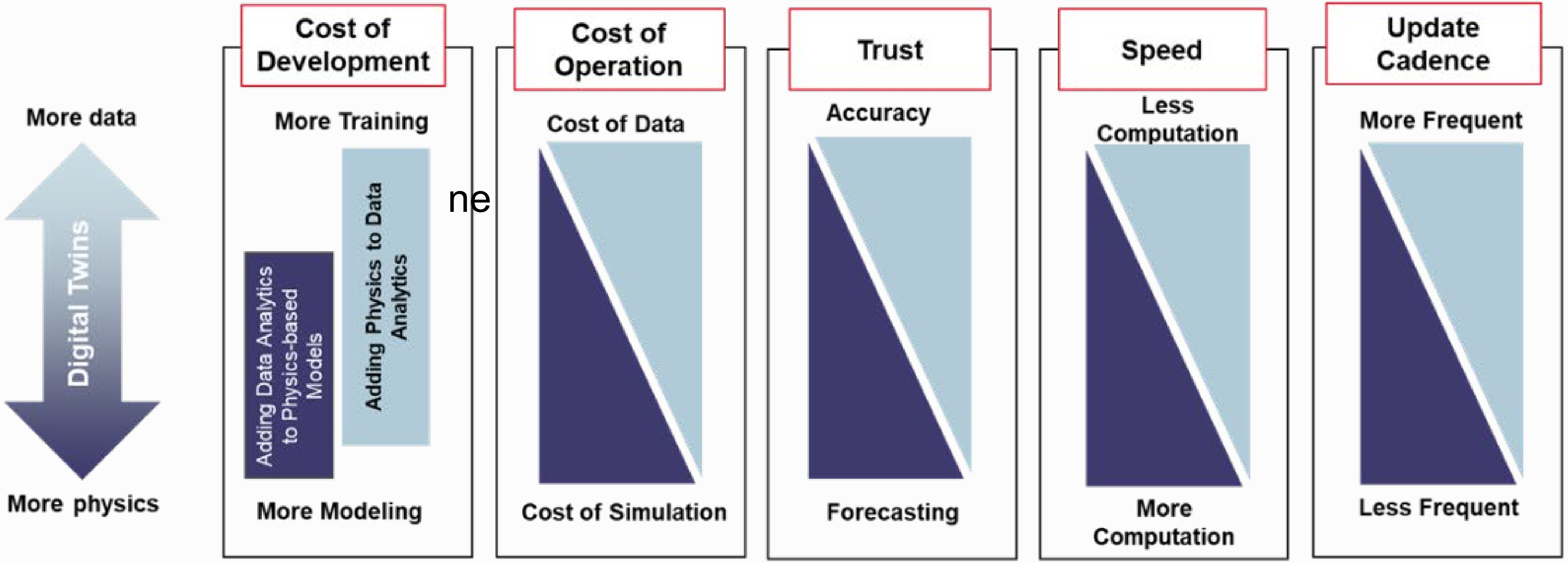


with its own lifecycle that must be conceptualized, architected, designed, built, deployed, and sustained

Need to view the digital twin as an asset in its own right

with requirements to achieve fitness-for-purpose and cost-benefit tradeoffs

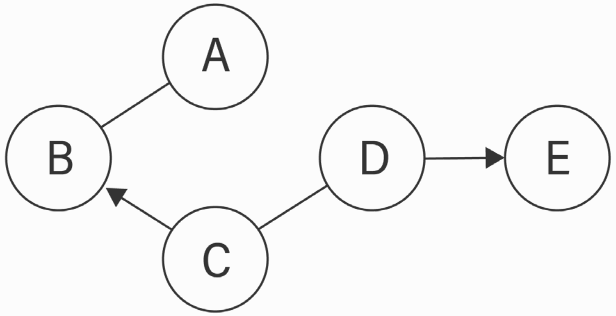
Ferrari & Willcox, *Nature Computational Science, May* 2024



but we need theoretical underpinnings & computational tools for architecting, designing & assessing digital twins

GRAPHICAL MODELS
are widely used* to represent complex systems

* but not in the PDE modeling & simulation community



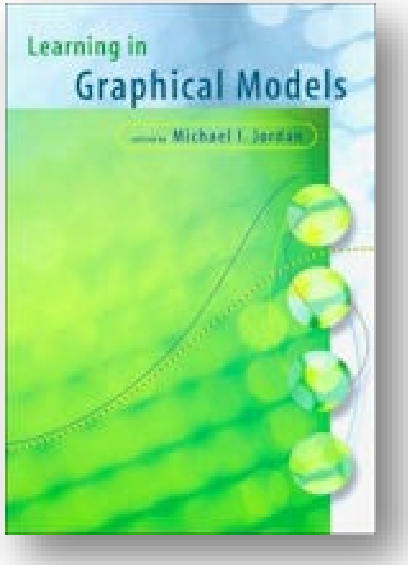
$$G = (V, E)$$

$$V = \{\mathrm{A, B, C, D, E}\}$$

$$E = \{\mathrm{A} \leftrightarrow \mathrm{B}, \mathrm{C} \rightarrow \mathrm{B}, \\ \mathrm{C} \leftrightarrow \mathrm{D}, \mathrm{D} \rightarrow \mathrm{E}\}$$

"Graphical models, a marriage between probability theory and graph theory, provide a natural tool for dealing with two problems that occur throughout applied mathematics and engineering — uncertainty and complexity."

"Fundamental to the idea of a graphical model is the notion of modularity: a complex system is built by combining simpler parts. Probability theory serves as the glue whereby the parts are combined, ensuring that the system as a whole is consistent and providing ways to interface models to data."

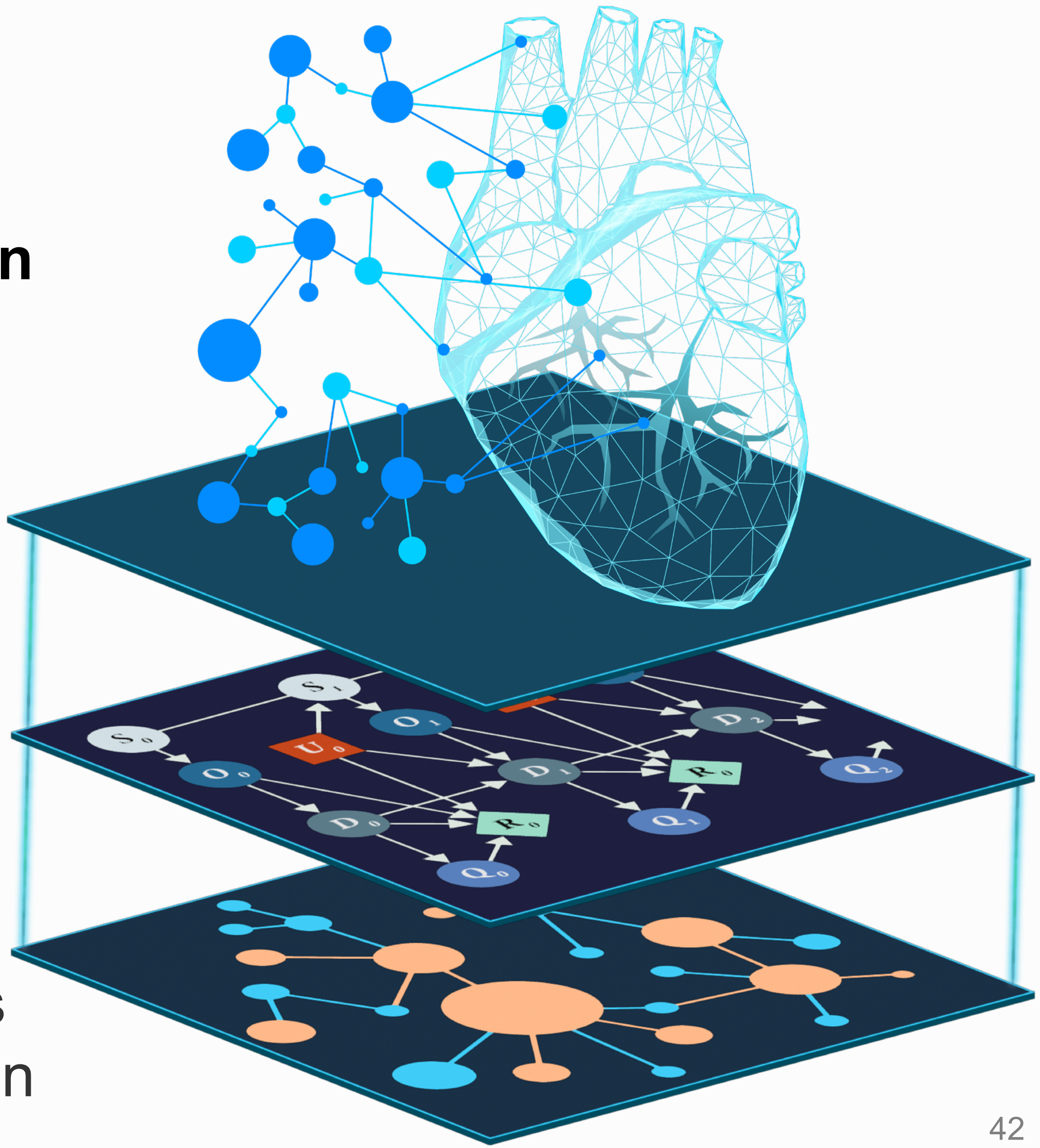


Graphical models emphasize relationships & encode uncertainty

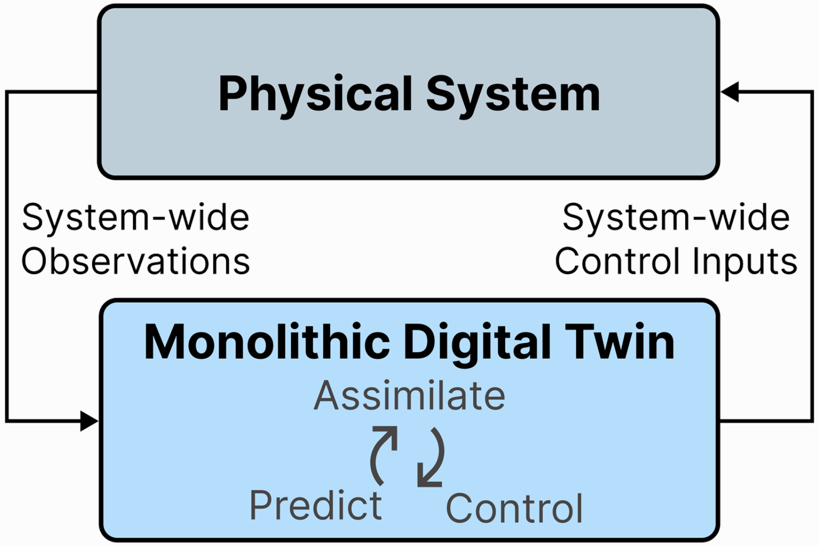
GRAPHICAL REPRESENTATION of a digital twin

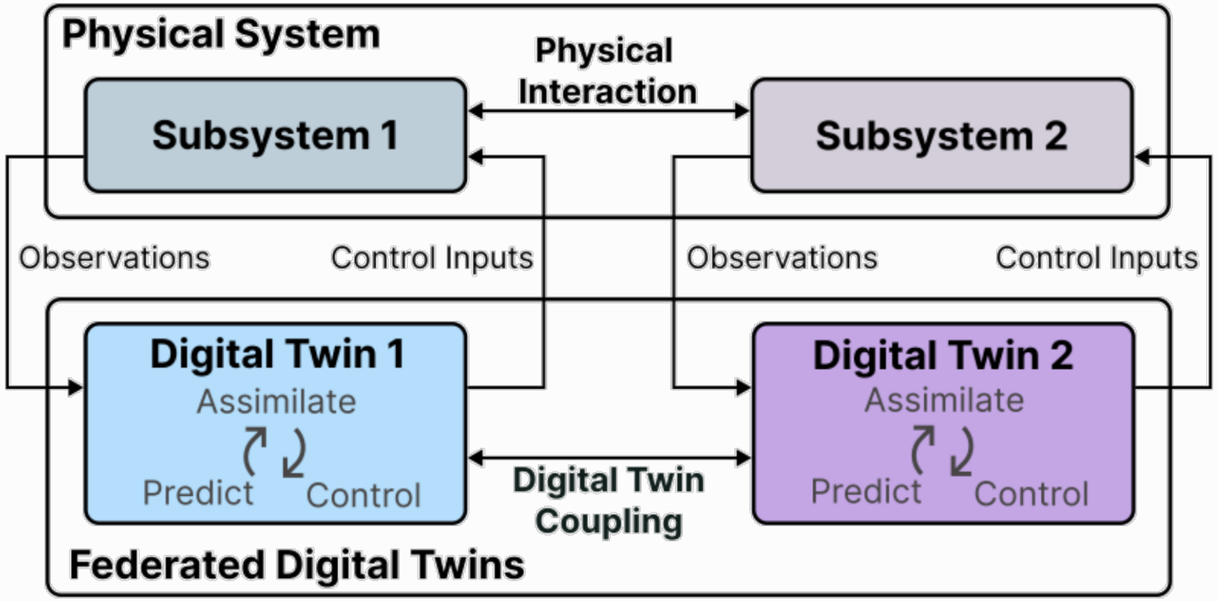
We use a **multilayered graphical formulation** to manage digital twin complexity and embed uncertainty quantification

- Foundational layer: **knowledge graph** as a mathematical structure to support semantic knowledge organization, scalable computations and bidirectional data flow
- Predictive layer: **probabilistic graphical model** encodes uncertainty and interdependence between random variables → a scalable foundation for UQ & verification



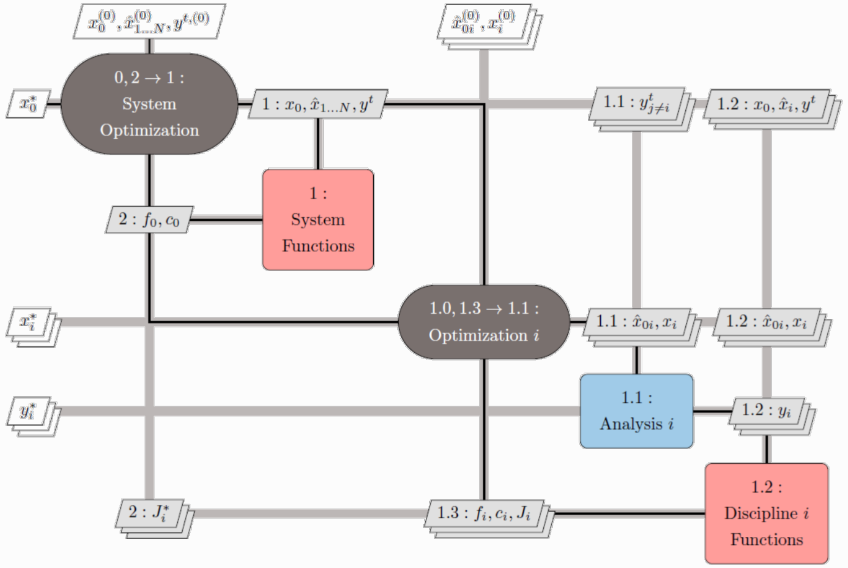
Can we move towards modular formulations for digital twins?





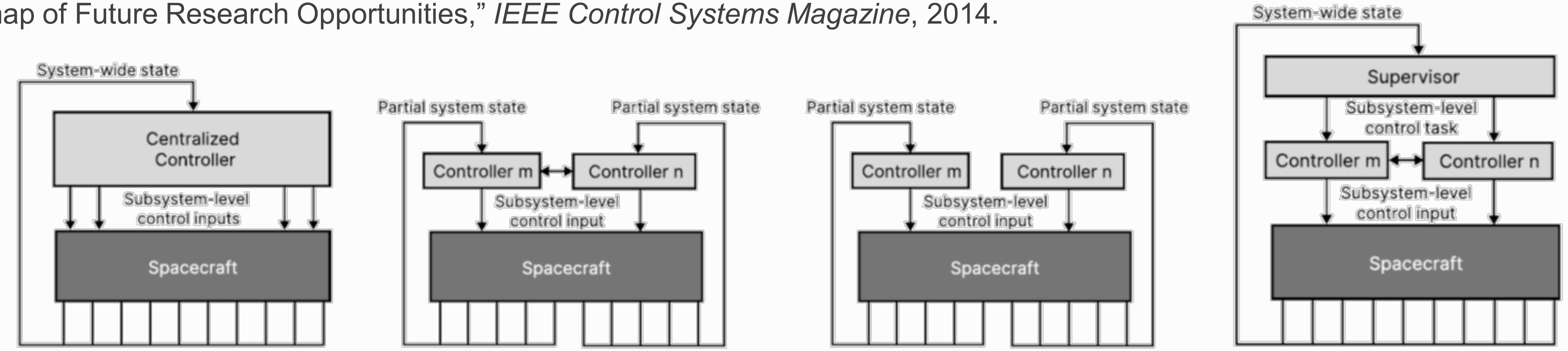
Sebastian
Henao-Garcia
(PhD student)

Distributed & decentralized formulations have been considered in control and MDO



Collaborative Optimization
Figure: Martins & Ning *Engineering Design Optimization*, 2021.

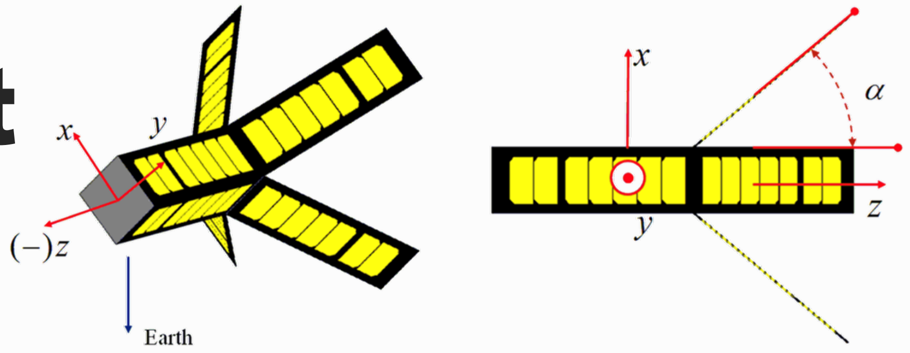
Figure: Negenborn & Maestre, "Distributed Model Predictive Control: An Overview and Roadmap of Future Research Opportunities," *IEEE Control Systems Magazine*, 2014.



(a) Centralized. (b) Distributed with communication (c) Distributed and decentralized. (d) Distributed and hierarchical.

but are fraught with mathematical challenges

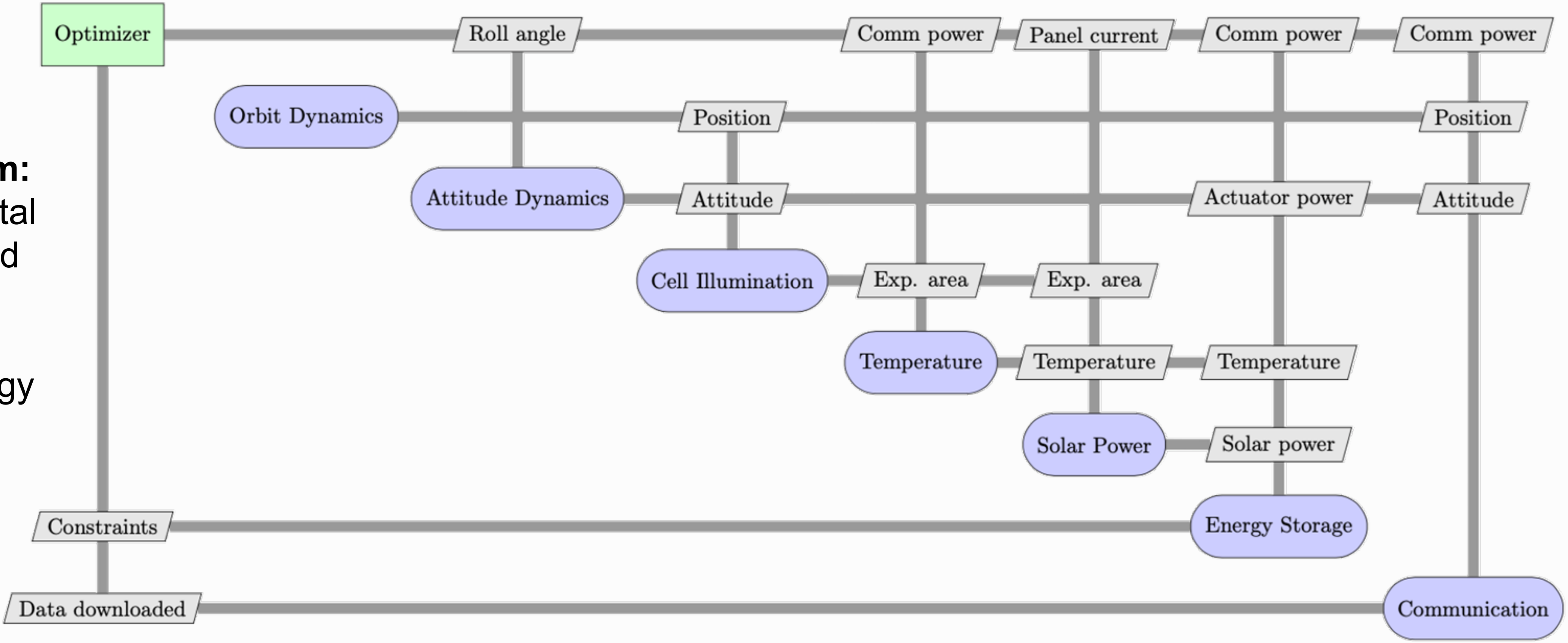
Example: CADRE CubeSat



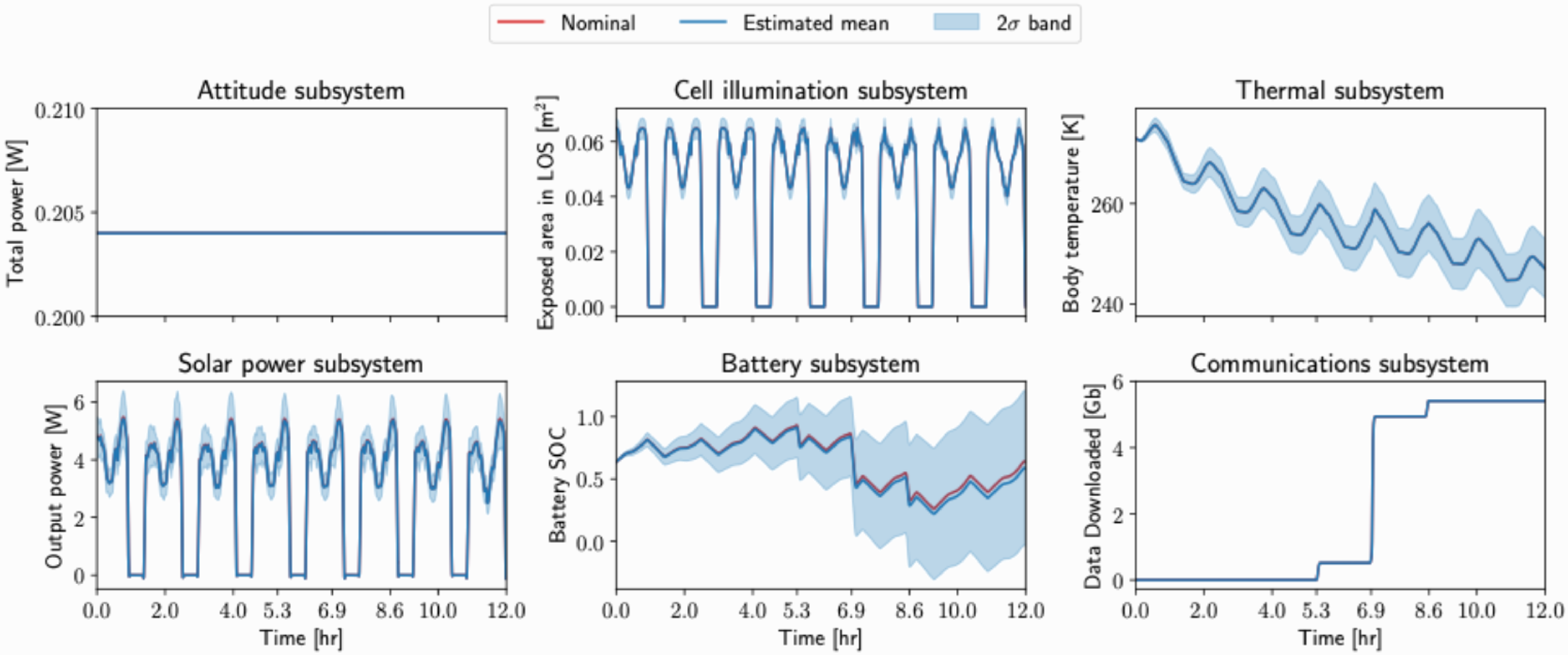
CADRE: CubeSat investigating atmospheric density response to extreme driving. Mission: continuously collect data and transmit as much data as possible to the ground stations.

Figures & problem definition: Huang, Lee, Cutler & Martins, 2014

Design problem: Maximize the total data downloaded subject to constraints on power and energy available

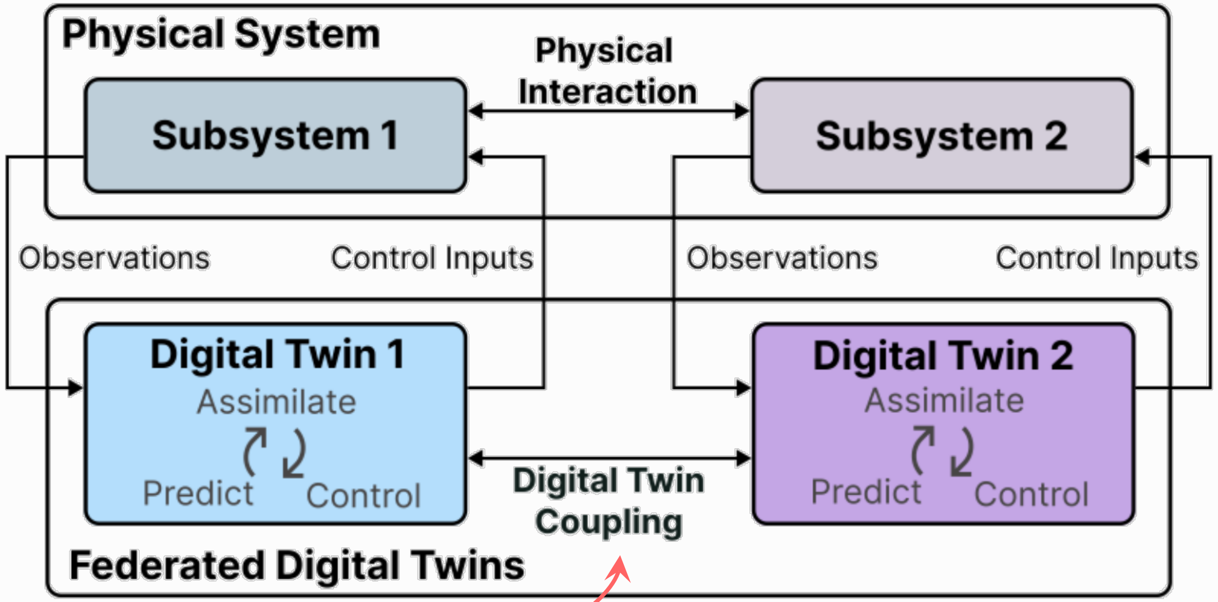


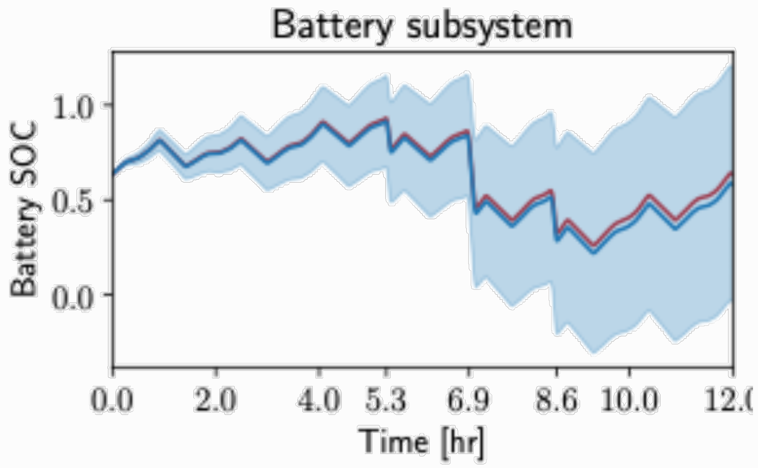
How does uncertainty in subsystem digital twin states translate into QoI uncertainty?



UQ + global sensitivity analysis defines digital twin coupling requirements

Can we achieve assimilation, prediction & control at subsystem digital twin level?
→ local computations, reduced complexity





Can we design digital twin coupling & update rates to achieve acceptable QoI uncertainty and an overall stable, trusted digital twin?

DOMAIN KNOWLEDGE

PREDICTIVE PHYSICS-BASED MODELING & SIMULATION

UNCERTAINTY QUANTIFICATION

OPTIMIZATION & CONTROL

HIGH-PERFORMANCE COMPUTING

EDGE COMPUTING

SURROGATE MODELING

INVERSE PROBLEMS

DATA ASSIMILATION

VISUALIZATION

HUMAN COMPUTER INTERACTION

ARTIFICIAL INTELLIGENCE

SCIENTIFIC MACHINE LEARNING

Digital Twins

A scientific grand challenge building on next-generation **mathematical modeling** and **computational science**