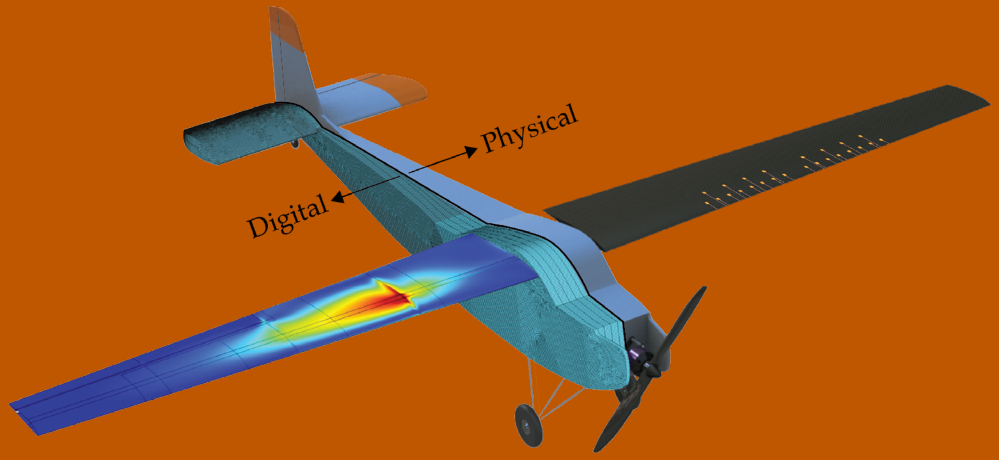
Enabling Predictive Digital Twins at Scale

Professor Karen E. Willcox
Multicore World
Wellington, New Zealand | February 13, 2023



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TEXAS
The University of Texas at Austin

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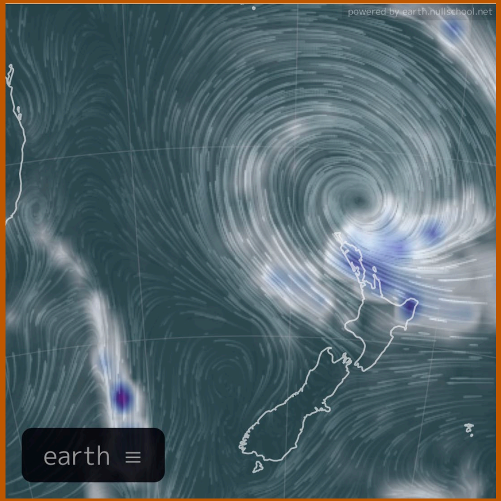

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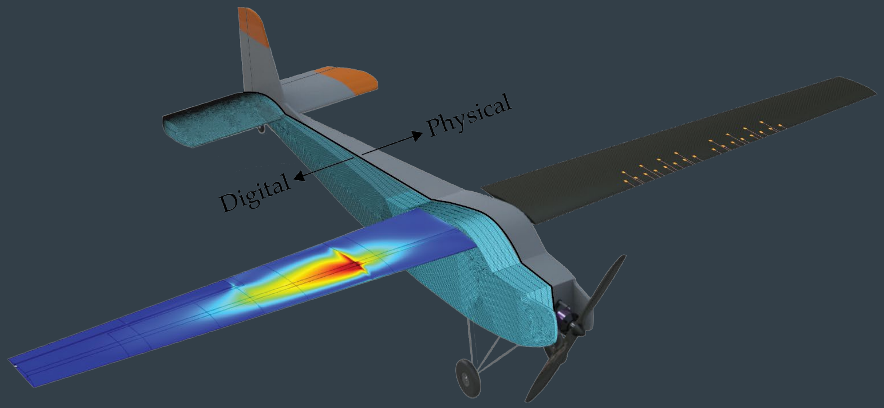
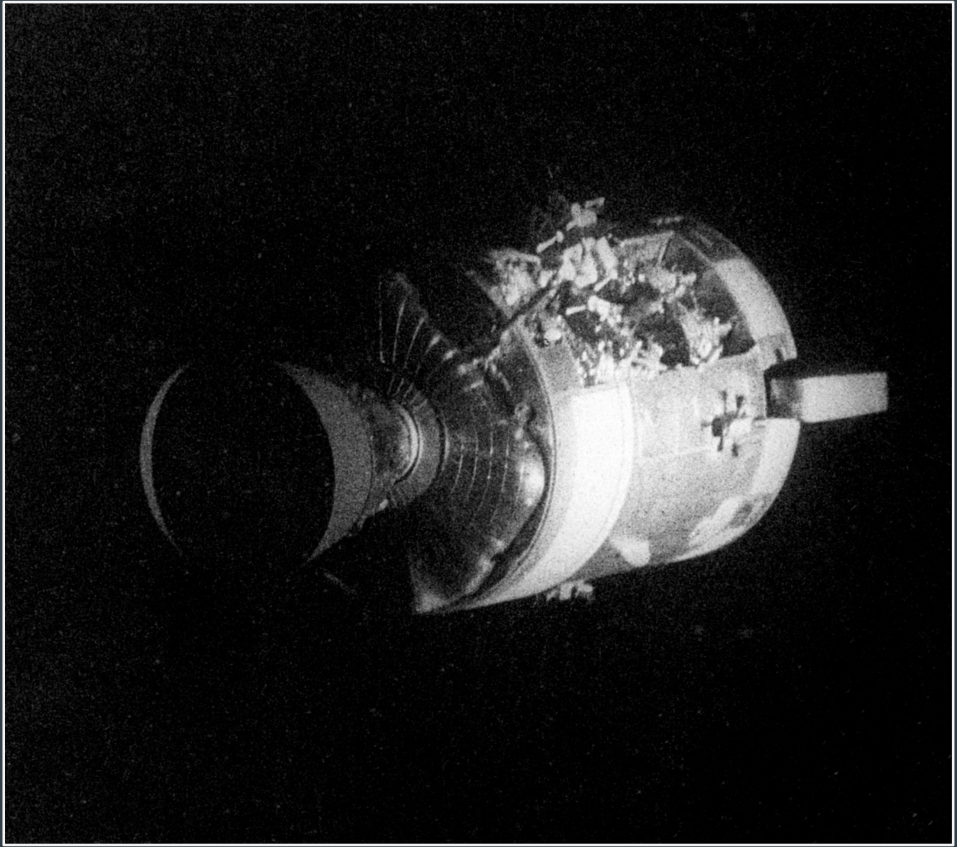
TEXAS
The University of Texas at Austin

"A Digital Twin is a set of **virtual information constructs** that **mimics the structure, context, and behavior of an individual/unique physical asset**, is **dynamically updated** with data from its physical twin **throughout its lifecycle**, and **informs decisions that realize value**"

- AIAA Institute Position Paper, 2020





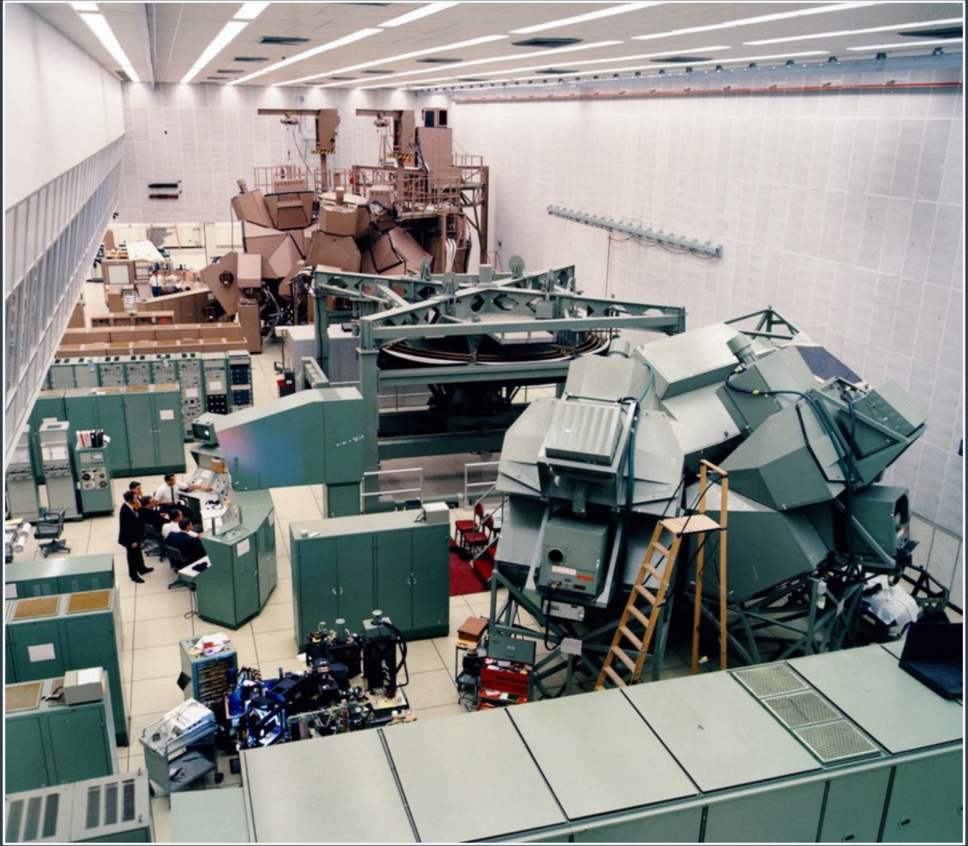


Figure credit: NASA

Digital twins have the potential to revolutionize **decision-making across science, technology & society**

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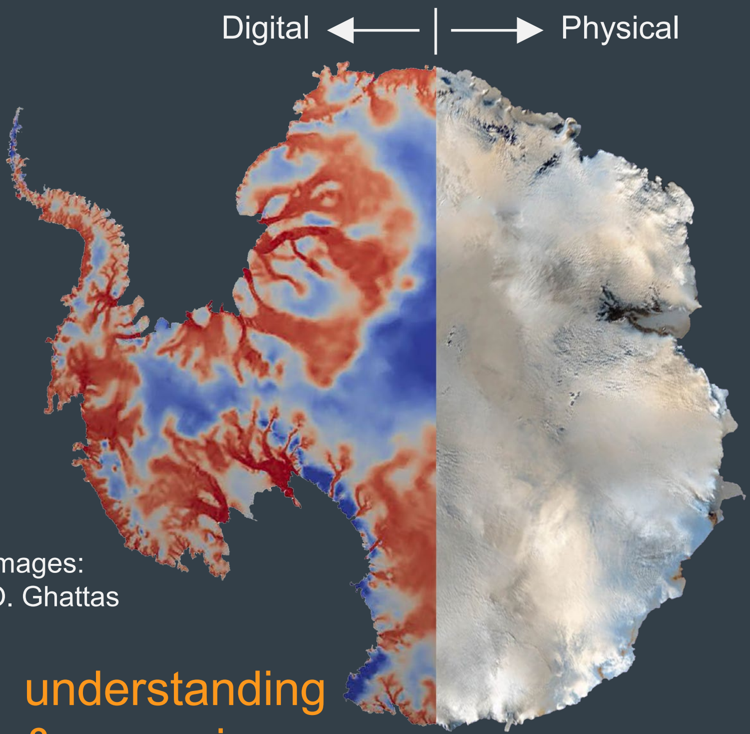
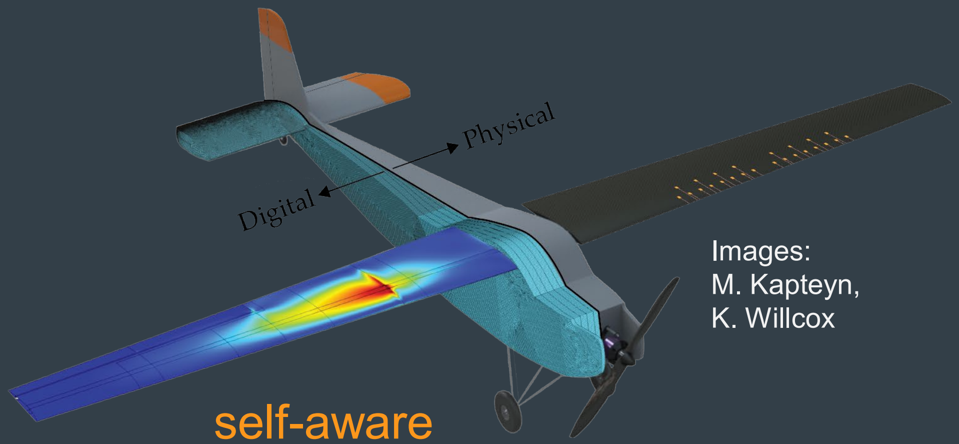


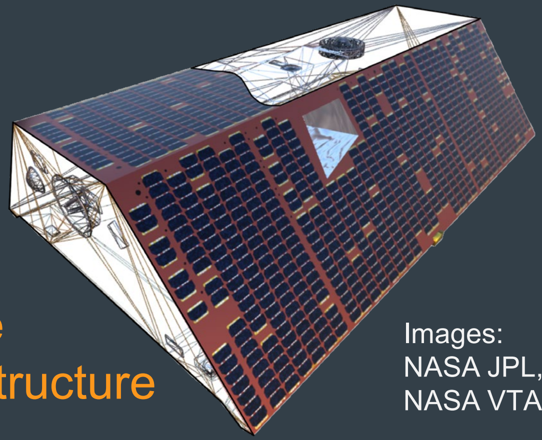
Images:
O. Ghattas

understanding
& managing
climate change



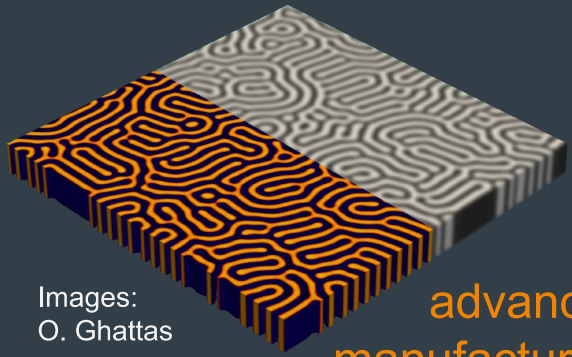
Images:
M. Kapteyn,
K. Willcox

self-aware
aerospace
vehicles



space
infrastructure

Images:
NASA JPL,
NASA VTAD



Images:
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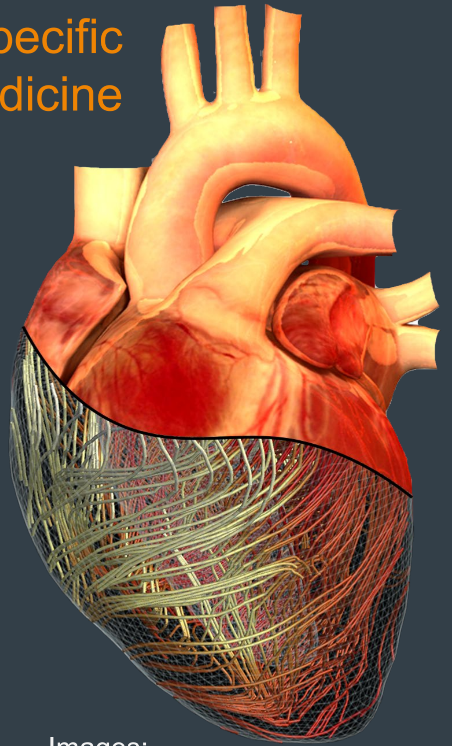
advanced
manufacturing

patient-specific
medicine



Images:
G. Foss, H. Liu,
M. Sacks

The predictive modeling challenges for complex systems

Complex physical phenomena
multiscale, multiphysics

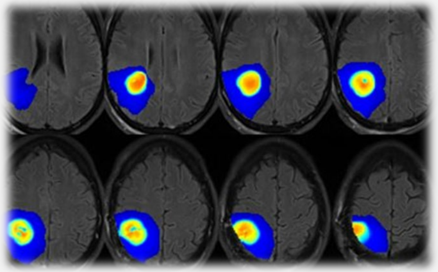
Cyber-physical interactions
software, hardware, sensors, automation

Complex lifecycle
multiple stages, multiple stakeholders

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

Evolving asset state
degradation, damage, maintenance, upgrades

BIG DATA alone is not enough.



DIGITAL TWINS must incorporate the **predictive power**, **interpretability**, and **domain knowledge** of physics-based models.

DOMAIN KNOWLEDGE

PREDICTIVE PHYSICS-BASED MODELING & SIMULATION

UNCERTAINTY QUANTIFICATION

OPTIMIZATION & CONTROL

HIGH-PERFORMANCE COMPUTING

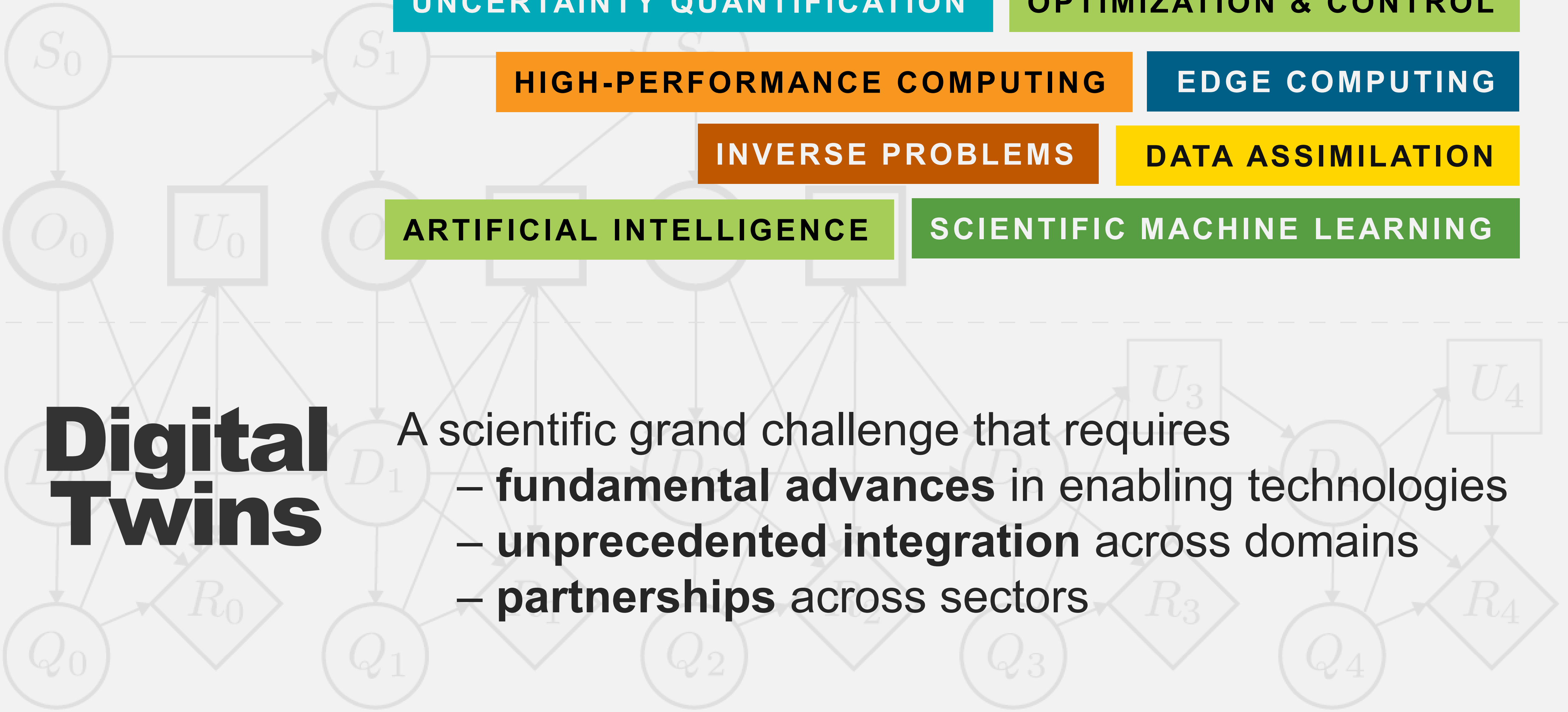
EDGE COMPUTING

INVERSE PROBLEMS

DATA ASSIMILATION

ARTIFICIAL INTELLIGENCE

SCIENTIFIC MACHINE LEARNING



Digital Twins

A scientific grand challenge that requires

– **fundamental advances** in enabling technologies

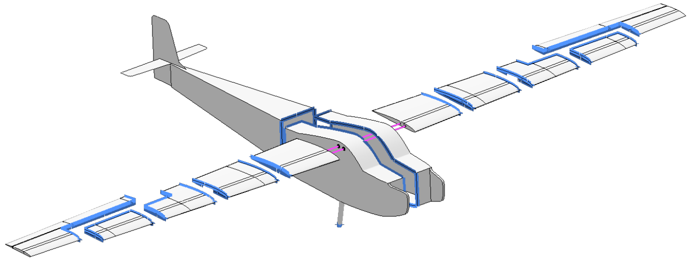
– **unprecedented integration** across domains

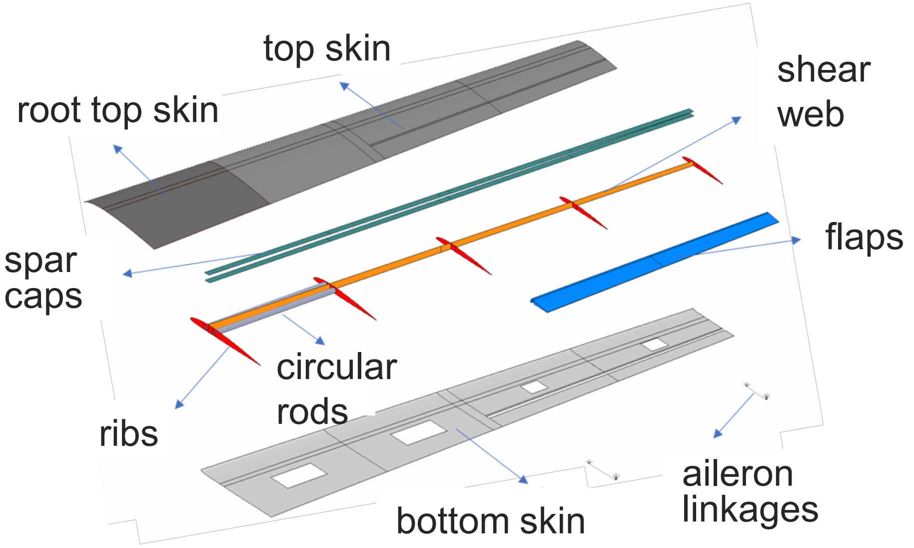
– **partnerships** across sectors

A few brief highlights of our recent and ongoing work in Predictive Digital Twins

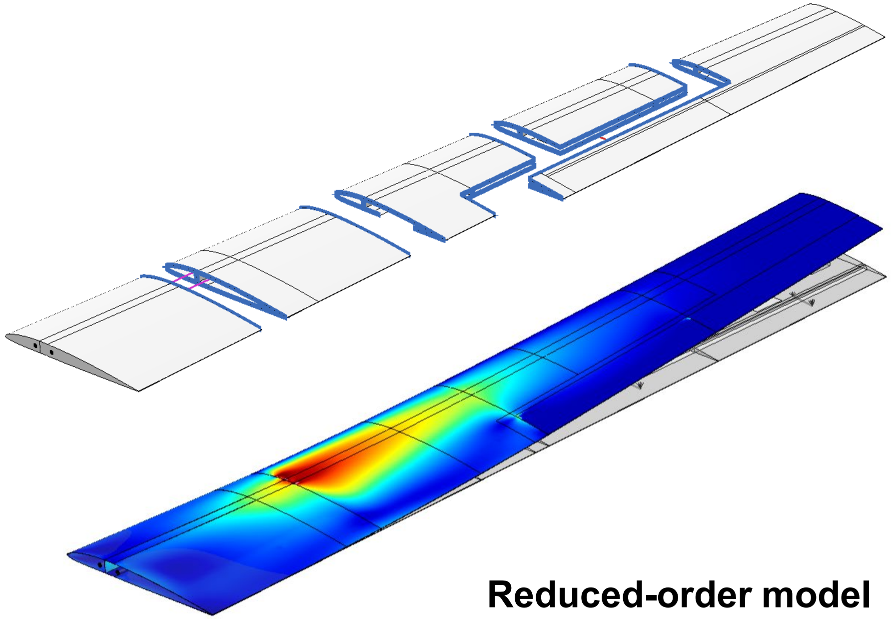
Reduced-order modeling leads to low-cost physics-based models that enable predictive digital twins

[Kapteyn et al. *IJNME* 2020]





Finite element model
multiple material types (carbon fiber, carbon rod, plywood, foam) & multiple element types (solid, shell, beam); ~55 seconds per structural analysis



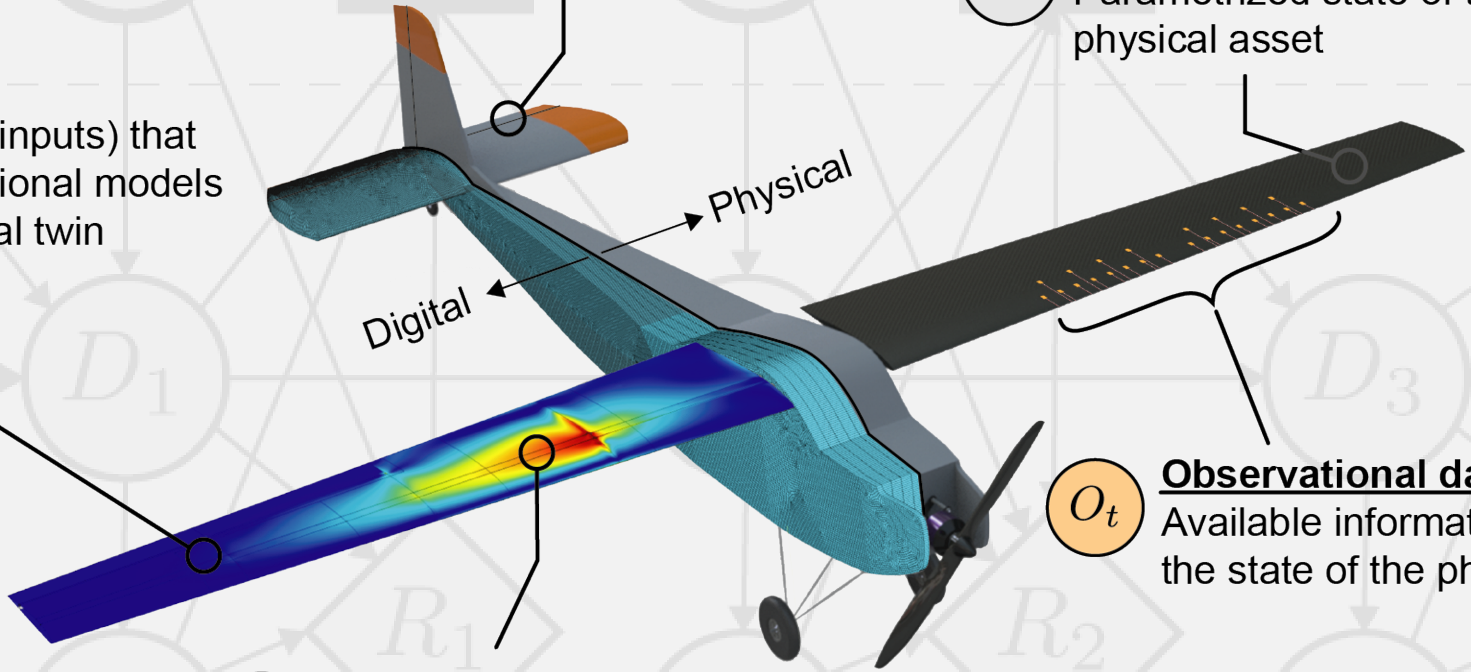
Reduced-order model
static condensation reduced basis element (SCRBE) method; ~0.03 seconds per structural analysis (1000x speedup)

PREDICTIVE DIGITAL TWINS

U_t **Control inputs:**
Actions or decisions that influence the physical asset

S_t **Physical State:**
Parametrized state of the physical asset

D_t **Digital State:**
Parameters (model inputs) that define the computational models comprising the digital twin

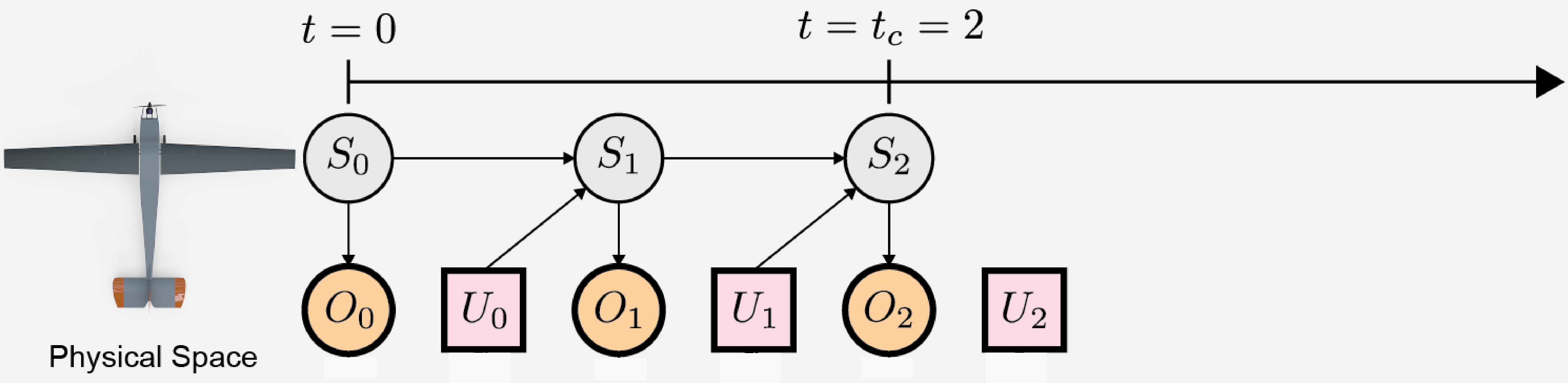


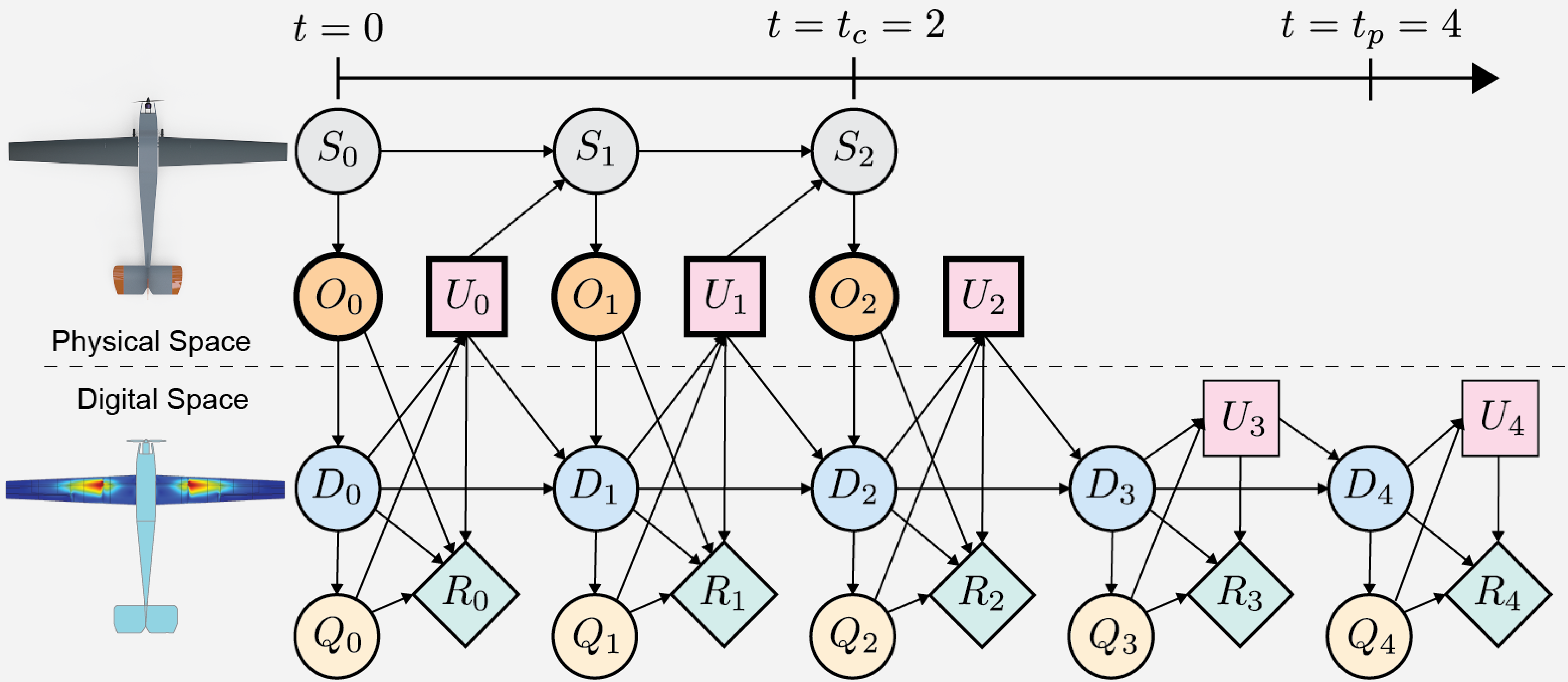
O_t **Observational data:**
Available information describing the state of the physical asset

R_t **Reward:**
Quantifies overall performance of the asset-twin system

Q_t **Quantities of Interest:**
Quantities describing the asset, estimated via model outputs

[Kapteyn, Pretorius, W. *Nature Comp. Sci.* 2021]


$t = 0$
$t = t_c = 2$
S_0
S_1
S_2
O_0
U_0
O_1
U_1
O_2
U_2
Physical Space



Graph represents joint probability distribution: $p\left(D_0,\dots,D_{t_p},Q_0,\dots,Q_{t_p},R_0,\dots,R_{t_p},U_{t_c+1},\dots,U_{t_p}\ \middle|\ o_0,\dots,o_{t_c},u_0,\dots,u_{t_c}\right)$

Representing a Digital Twin as a probabilistic graphical model gives an integrated framework for calibration, data assimilation, planning and control [Kapteyn, Pretorius, W. *Nature Comp. Sci.* 2021]

Predictive Digital Twin Use-case

Automatic monitoring, virtual inspections, simulation-based certification

Forecasting, predictive maintenance, planning

Operations: Tradeoff between
- Favorable asset state
- Digital twin accuracy
- Required control effort
- Observation acquisition cost

Learn from historical data,
transfer insights to similar assets

Mathematical Formulation via Probabilistic Graphical Model

Data assimilation: $p(D_{t_c}, Q_{t_c}, R_{t_c} \mid u_0, \ldots u_{t_c}, o_0, \ldots o_{t_c})$

Prediction: $p(D_{t_p}, Q_{t_p}, R_{t_p} \mid u_0, \ldots u_{t_c}, o_0, \ldots o_{t_c})$

Multi-objective optimization:

$$\phi_t^{\text{evaluation}} = p(R_t \mid D_t, Q_t, U_t, O_t)$$

$$\max_{U_{t_c}, \ldots, U_{t_p}} \sum_{\tau = t_c}^{t_p} \mathbb{E}[R_\tau]$$

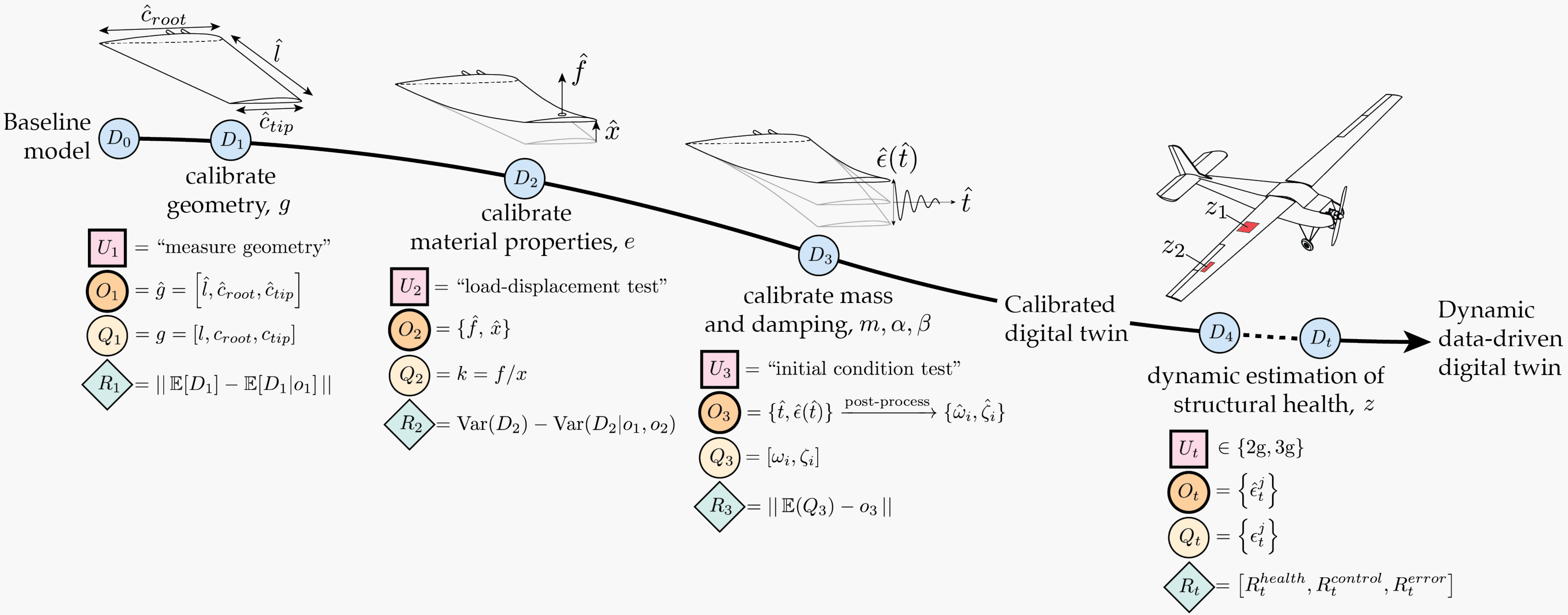
Learning:

$$\phi_t^{\text{dynamics}} = p(D_t \mid D_{t-1}, U_t)$$

$$\phi_t^{\text{assimilation}} = p(O_t \mid D_t)$$

Creating and evolving a structural digital twin

for an unmanned aerial vehicle [Kapteyn, Pretorius, W. *Nature Comp. Sci.* 2021]



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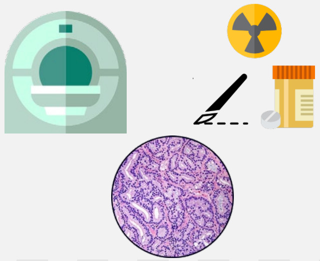
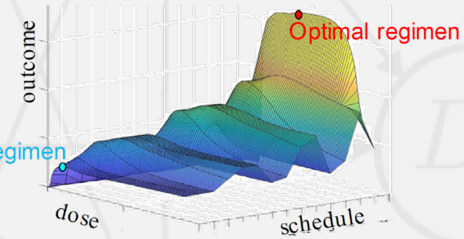
PREDICTIVE DIGITAL TWINS

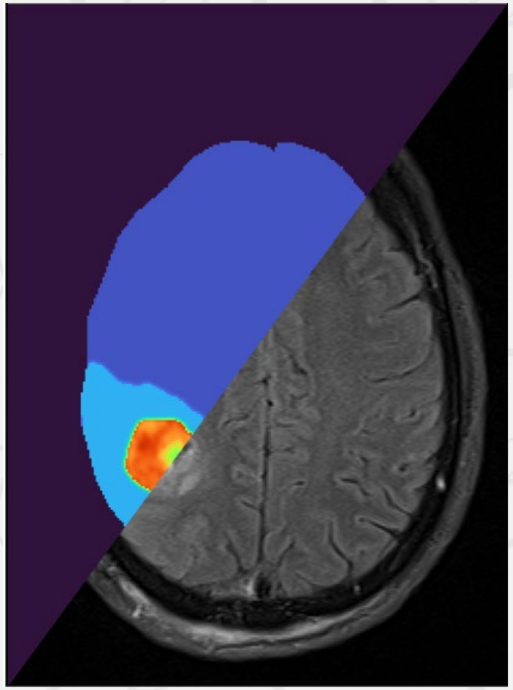
D_t Digital Twin State
Tumor dynamics, mechanics

U_t Control inputs
MRI studies, biopsies, treatment regimens



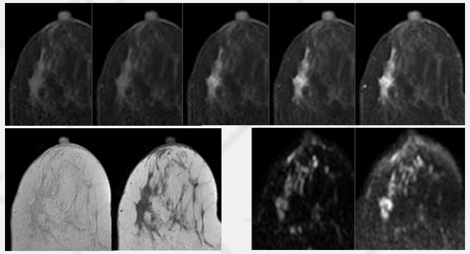
R_t Reward
Patient outcomes: treatment efficacy, toxicity

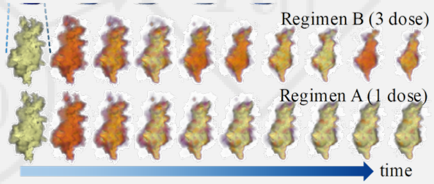




S_t Physical State
Anatomy & morphology, mechanical & physiological state

O_t Observational data
Anatomy, perfusion, permeability, cell density, metabolism

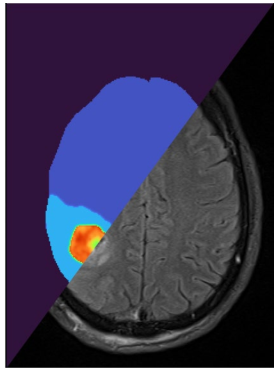


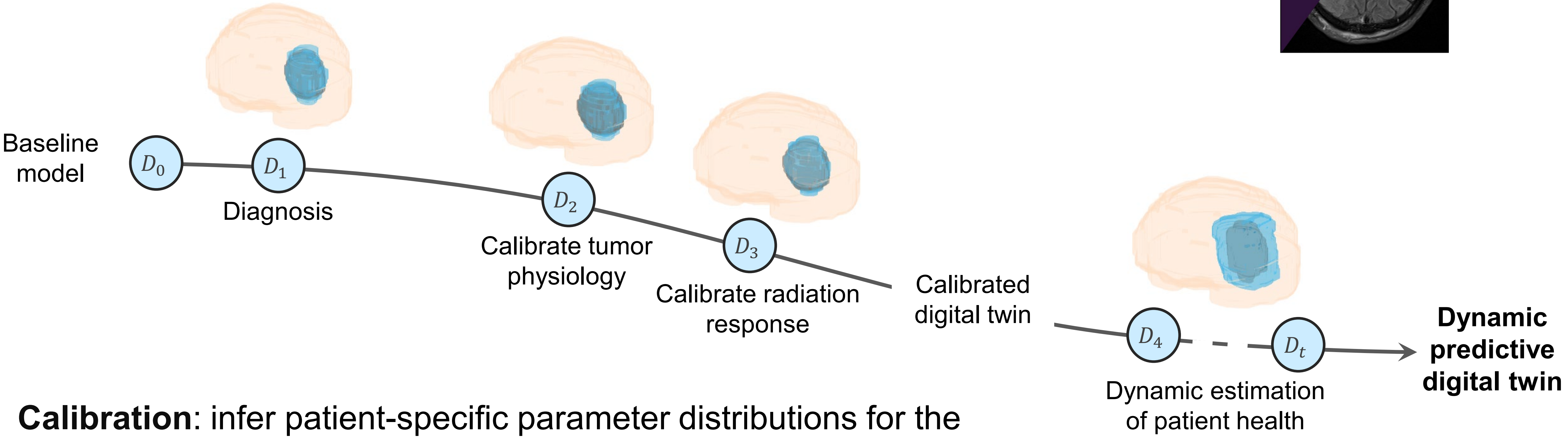


Q_t Quantities of Interest
Distribution of therapies, tumor shape, cell density

[Chaudhuri, Hormuth, Pash, Yankeelov et al.]

Creating and evolving a cancer patient digital twin





Calibration: infer patient-specific parameter distributions for the digital twin from observed data and population-based priors

Monitoring: anticipate tumor progression by forecasting the effect of radiotherapy treatment on cancer cells

Optimize therapy: use predictive digital twin to choose optimal patient-specific treatment plan under uncertainty

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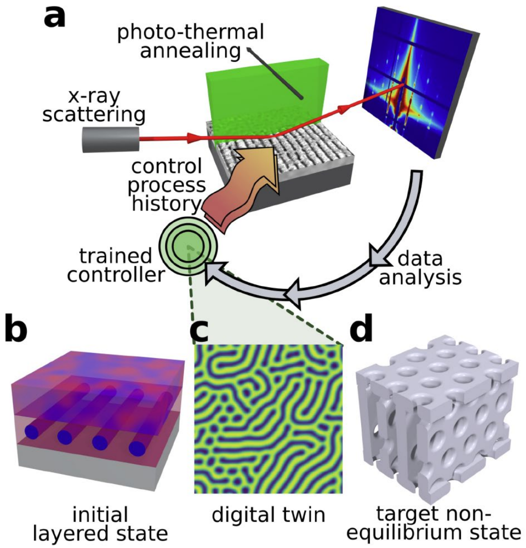
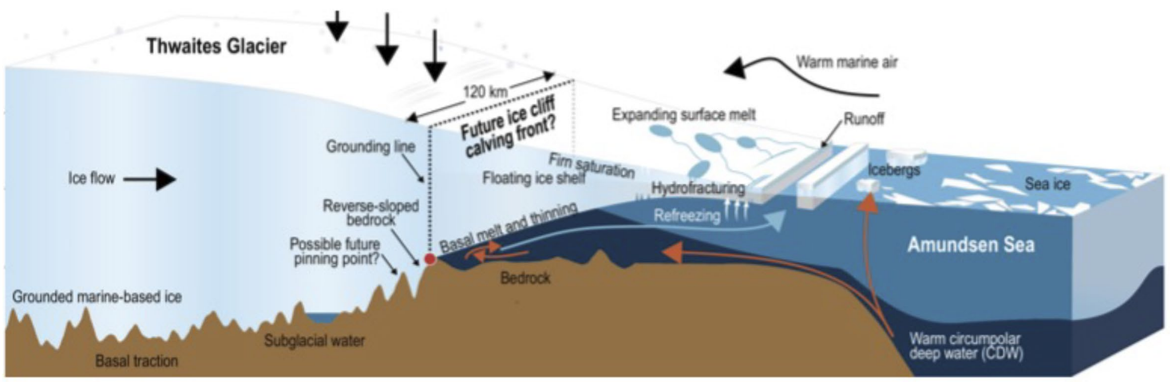
M2dt: Multifaceted Mathematics for Predictive Digital Twins

$$\int \mathcal{M}^2 \, \mathrm{dt}$$

- New Department of Energy Mathematics Multifaceted Integrated Capability Center, launched September 2022, five-year duration
- Co-directors Omar Ghattas and Karen Willcox; collaborators: MIT, Brookhaven, Argonne, Sandia
- Research Thrusts: (1) Dynamically-integrated data assimilation & decisions; (2) Reduced-order & surrogate modeling; (3) Mathematics of coupling for predictive digital twins



Driving application 1: Real-time data assimilation and optimal control of directed self-assembly of block copolymer thin films



Driving application 2: Dynamics of coupled ice shelf – ocean cavities

Looking Forward

From the Artisanal
To the Industrial

How to move from the one-off expert-driven digital twin to **accessible robust digital twin implementations at scale**?

nature computational science
PERSPECTIVE
https://doi.org/10.1038/s43588-021-00072-5
Check for updates

Scaling digital twins from the artisanal to the industrial

Steven A. Niederer[1] ✉, Michael S. Sacks[2], Mark Girolami[3,4] and Karen Willcox[2]

Mathematical modeling and simulation are moving from being powerful development and analysis tools towards having increased roles in operational monitoring, control and decision support, in which models of specific entities are continually updated in the form of a digital twin. However, current digital twins are largely the result of bespoke technical solutions that are difficult to scale. We discuss two exemplar applications that motivate challenges and opportunities for scaling digital twins, and that underscore potential barriers to wider adoption of this technology.

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, that is dynamically updated with data from its physical twin throughout its life-cycle, and that ultimately informs decisions that realize value"[1]. Although this definition targets engineering systems, a broad interpretation covers the use of digital twins in a diverse array of other application areas such as healthcare and information systems. Specifically, we interpret asset to include processes and living entities, and the life-cycle to be the period over which the digital twin is needed to support decision-making. With this broad interpretation, the definition also covers cases in which digital twins are used over fixed time periods, such as for surgery or in critical decision points for physical systems. In essence, a digital twin is an in silico model that brings together the technology to map, monitor and control real-world entities by continually receiving and integrating data from the physical twin to provide an up-to-date digital representation of the physical entity.

A schematic depiction of a digital twin is provided in Fig. 1. In practical terms, a digital twin is a model (or a collection of models) of a specific physical object—or a set of objects—that is initialized from plans, measurements, past models and/or other available information. Models can be statistical, data-driven or mechanistic (that is, physics-based), or a combination of these. The model can be used to predict observations from the physical system at future time points to validate the twin and refine the model if required. The model parameters—encoding material properties, geometry and boundary conditions—can first be initialized and then become priors that are updated as more data are acquired from the physical system. In this way, the digital twin is continuously improving and provides a dynamic digital history of the asset or entity. These core functionalities can be augmented with feedback control, networking twins and artificial intelligence (AI). Combined, these advances enable a substantial development in monitoring, control and decision support. However, to achieve this substantial development in the most societally critical application areas, the digital twin must be predictive, that is, the digital twin must be able to extrapolate and issue predictions about yet-unseen conditions and future system states, and it must do so with quantified uncertainties and acceptable levels of risk.

Digital-twin approaches and projects have been developed across a broad range of industries and disciplines[2–9]. This reflects the growing appreciation of the broader opportunities to enable asset-specific decisions, disparate data integration and optimal management across multiple disciplines through digital twins; however, many of these exemplars are limited to specific applications, using bespoke methods and technologies that are not widely applicable across other disciplines. We argue that this is limiting the wider adoption of digital-twin technologies. In this Perspective, we explore the barriers to moving digital twins from a labor intensive and highly specialized or artisanal product to a widely adopted or industrial commodity by highlighting developments in aerospace engineering and cardiology. Although aircraft and human hearts are clearly systems that serve very different functions, they share many common attributes that are relevant to the digital-twin paradigm. Both cases showcase the frontiers of digital twins, their open challenges and lessons that are applicable across the digital-twin space.

Digital twins in engineering and precision medicine

Digital twins originated in aerospace engineering, with many people pointing to the Apollo program as the first place where the idea was put in practice, where simulators on the ground mirrored the systems being put into space[10]. A notable historical example is the Apollo 13 mission, which suffered an in-flight explosion that critically damaged the spacecraft's main engine. As recounted by Ferguson[11], during the emergency, NASA mission controllers were able to use data from the damaged spacecraft to update the simulators to match the conditions of the physical twin. The dynamically updated simulators were then used to explore strategies and inform the decisions that ultimately brought the astronauts safely home. The term digital twin was coined at NASA in 2010, building on the concept outlined for product life-cycle management[12]. The past decade has brought renewed focus to the digital-twin paradigm (see, for instance, Grieves and Vickers[13]). A great deal of attention has focused on digital twins to support structural health monitoring, sustainment and predictive maintenance[14,15]. Applications are often driven by specific attributes of the digital twin. As digital twins are updated over time, this allows the structural health of an asset (for example, an unmanned aerial vehicle (UAV)[16], or a reusable spacecraft[17]) to be monitored and managed continually. As the digital twin represents a specific asset, it can provide predictive decision support on the basis of the characteristics of the specific system and its ensemble parts. This can be applied to predicting failure points

[1]School of Biomedical Engineering and Imaging Sciences, King's College London, London, UK. [2]Oden Institute for Computational Engineering and Sciences, The University of Texas at Austin, Austin, TX, USA. [3]Department of Engineering, University of Cambridge, Cambridge, UK. [4]The Alan Turing Institute, London, UK. ✉e-mail: steven.niederer@kcl.ac.uk

The finite element method had its origins >70 years ago in civil and aeronautical engineering

1 Mathematical maturity of underlying methods enable robust use by non-experts

2 Computing advances in hardware and algorithms admit routine application to realistic problems

3 Flexible software implementations make state-of-the-art methods accessible and broadly applicable

Today it is the workhorse of engineering analysis and design, and is in the hands of every engineer (and many non-engineers)

The digital twin had its origins ~2 decades ago in aeronautical engineering (concept stretches back further)

- foundational advances in the enabling methods
- computing and data infrastructure
- software
- standards
- partnerships

⋮

The world needs accessible robust digital twin implementations at scale and across domains

(SOME) RESEARCH NEEDS FOR DIGITAL TWINS

1 **Predictive modeling**

Many decisions demand a predictive window on the future

2 **Validation, verification & uncertainty quantification**

Achieving the levels of reliability and robustness needed for certified high-consequence decision-making

3 **Data, models and decisions across multiple scales**

An integrated framework for calibration, data assimilation, uncertainty quantification, planning & control

4 **Scalable algorithms for updating, prediction & control**

Incorporating physics-based modeling, data-driven learning & state-of-the-art computational science

5 **Digital twins at the system and system-of-systems levels**

Decomposition and coupling of subcomponent digital twins; multi-resolution multi-fidelity digital twins

Data-driven decisions

building the mathematical foundations and computational methods to enable design of the next generation of engineered systems

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