Predictive Digital Twins

From physics-based modeling to scientific machine learning

Professor Karen E. Willcox
CIS Digital Twin Days | November 15, 2021

ODEN INSTITUTE
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Aerospace Engineering and Engineering Mechanics
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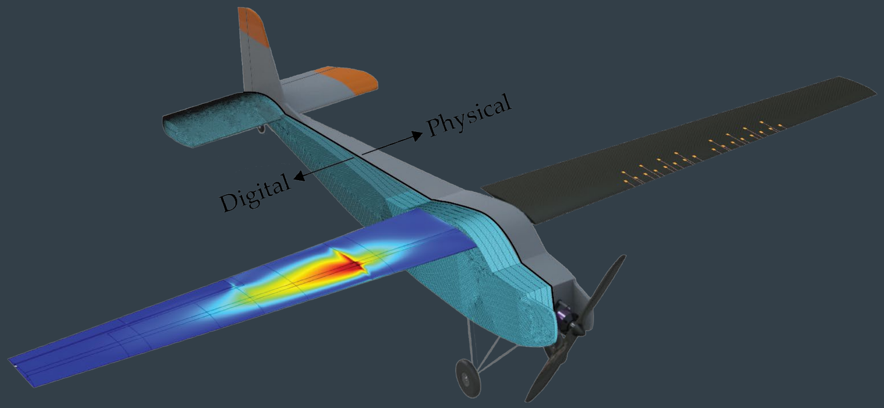
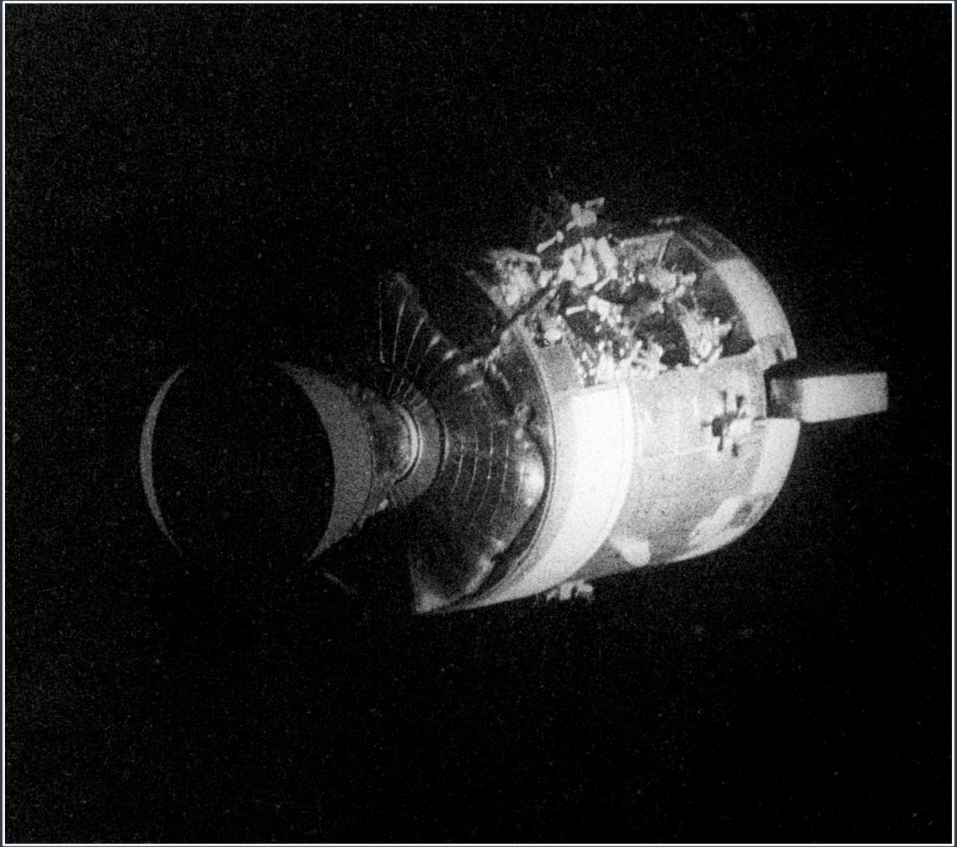
US Air Force **Dynamic Data Driven Application Systems** Program (E. Blasch)
US Department of Energy **Applied Mathematics** Program (W. Spotz)
SUTD-MIT **International Design Centre**

Disclosure: Willcox has a family member who is co-founder of Jessara.

"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





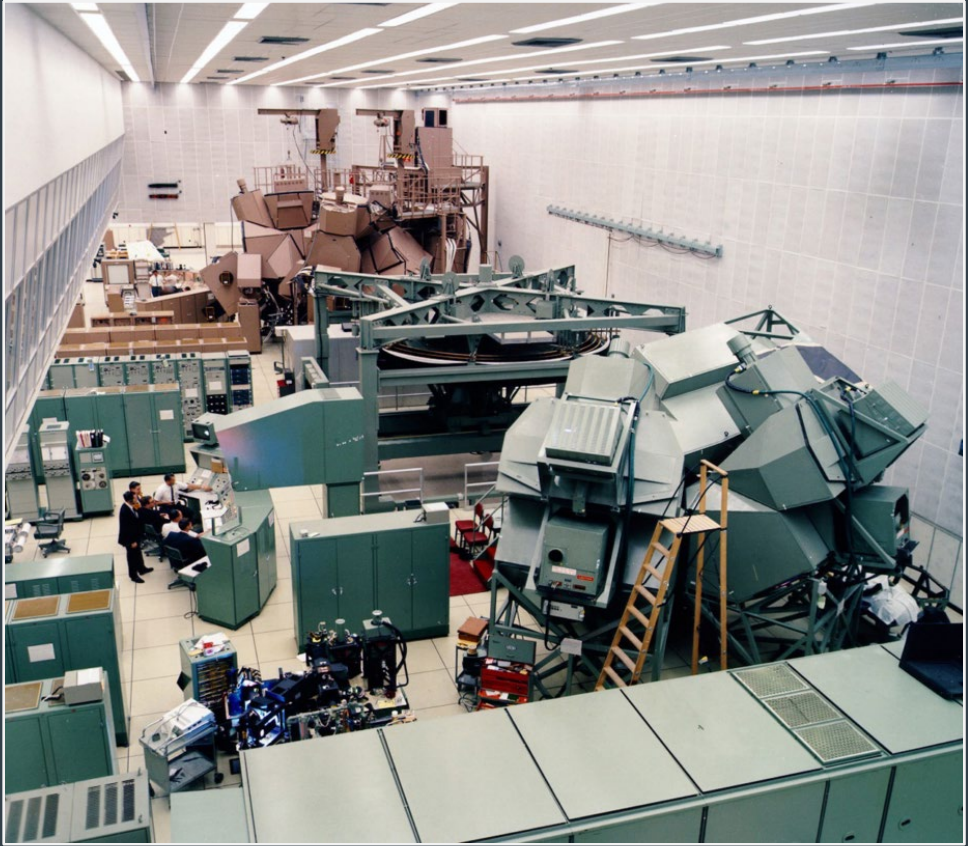
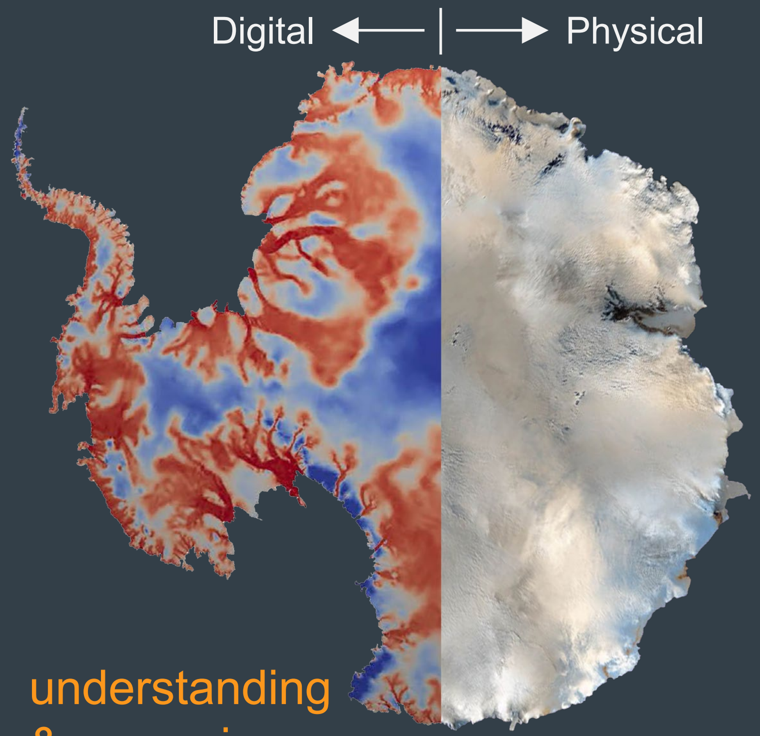


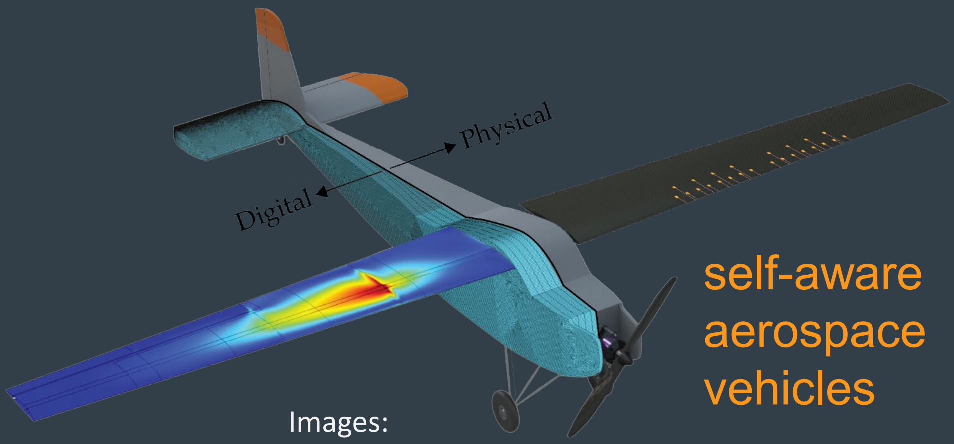
Figure credit: NASA

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



understanding & managing climate change

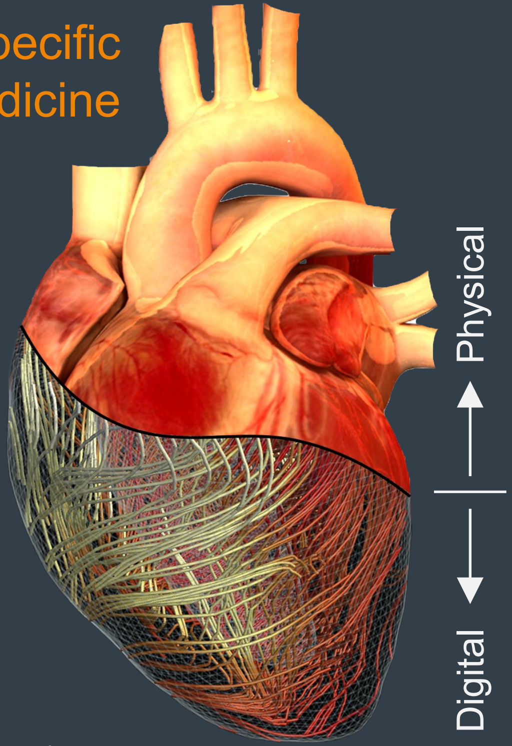
Images:
O. Ghattas



self-aware aerospace vehicles

Images:
M. Kapteyn,
K. Willcox

patient-specific medicine

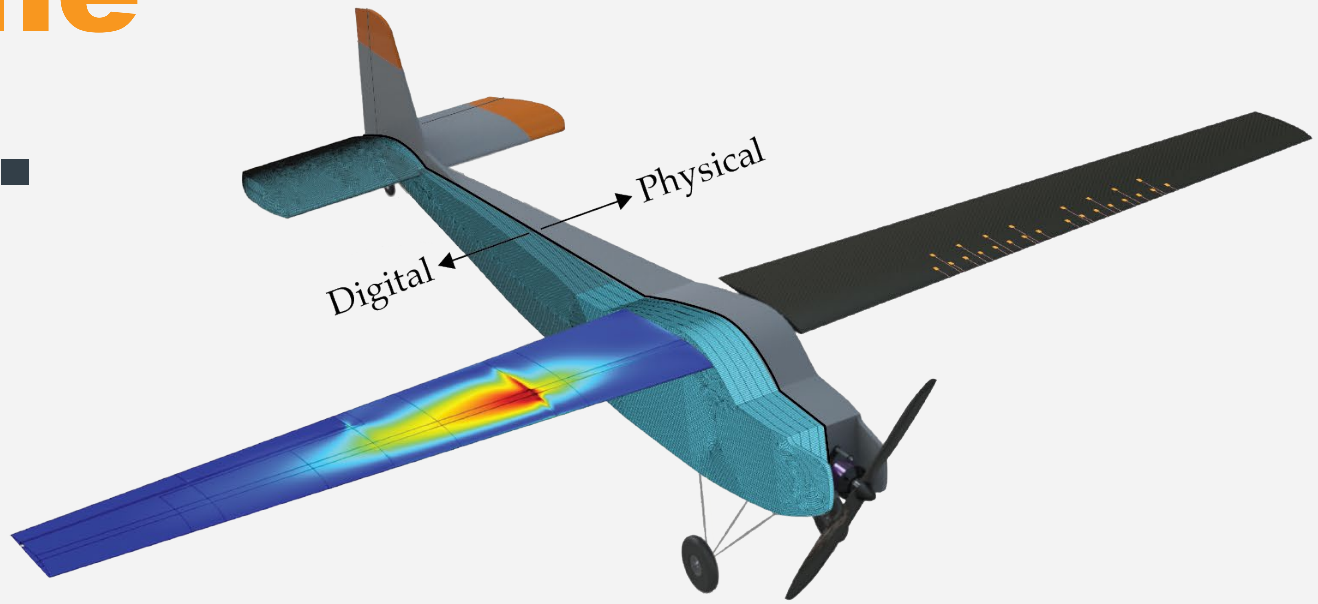


Images:
G. Foss, H. Liu,
M. Sacks

To move from the one-off expert-driven digital twin implementation to **accessible robust digital twin implementations at scale** requires many things, including computing and data infrastructure, software, standards, partnerships, …

To move from the one-off expert-driven digital twin implementation to **accessible robust digital twin implementations at scale** requires rigorous and scalable mathematical foundations.

BIG DATA alone is not enough.



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

Mathematical & computational foundations for Digital Twins

1 **Physics-based Modeling**

A predictive window on the future

2 **Reduced-order Modeling**

Blending physics-based modeling & machine learning to accelerate predictive computations

3 **Probabilistic Graphical Model**

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

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What is a physics-based model?

A representation of the **governing laws of nature** that innately embeds the concepts of **time, space, and causality**

In solving the governing equations of the system, we constrain the **predictions** to lie on the **solution manifold** defined by the laws of nature

Example: equations of linear elasticity

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} + \frac{\partial \sigma}{\partial y} + F$$

equation of motion (Newton's 2nd law)

$$\varepsilon = \frac{1}{2}\left[\nabla u + (\nabla u)^{\mathsf{T}}\right]$$

strain-displacement equations

$$\sigma = C : \varepsilon$$

constitutive equations

+ boundary conditions
+ initial conditions

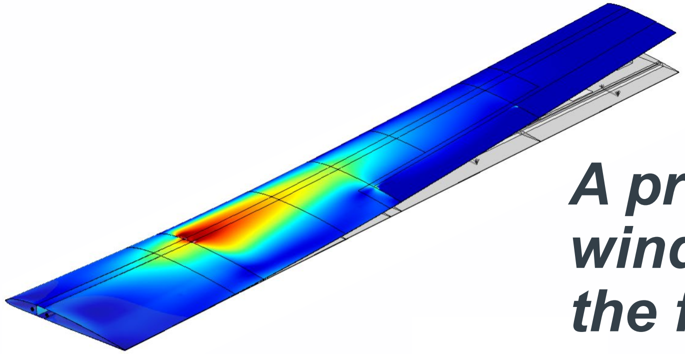
a mathematical model of how solid objects deform, relating stress σ, strain ε, displacement u, and loading F

The unreasonable effectiveness of physics-based models [Wigner, 1960]

Solving a physics-based model:

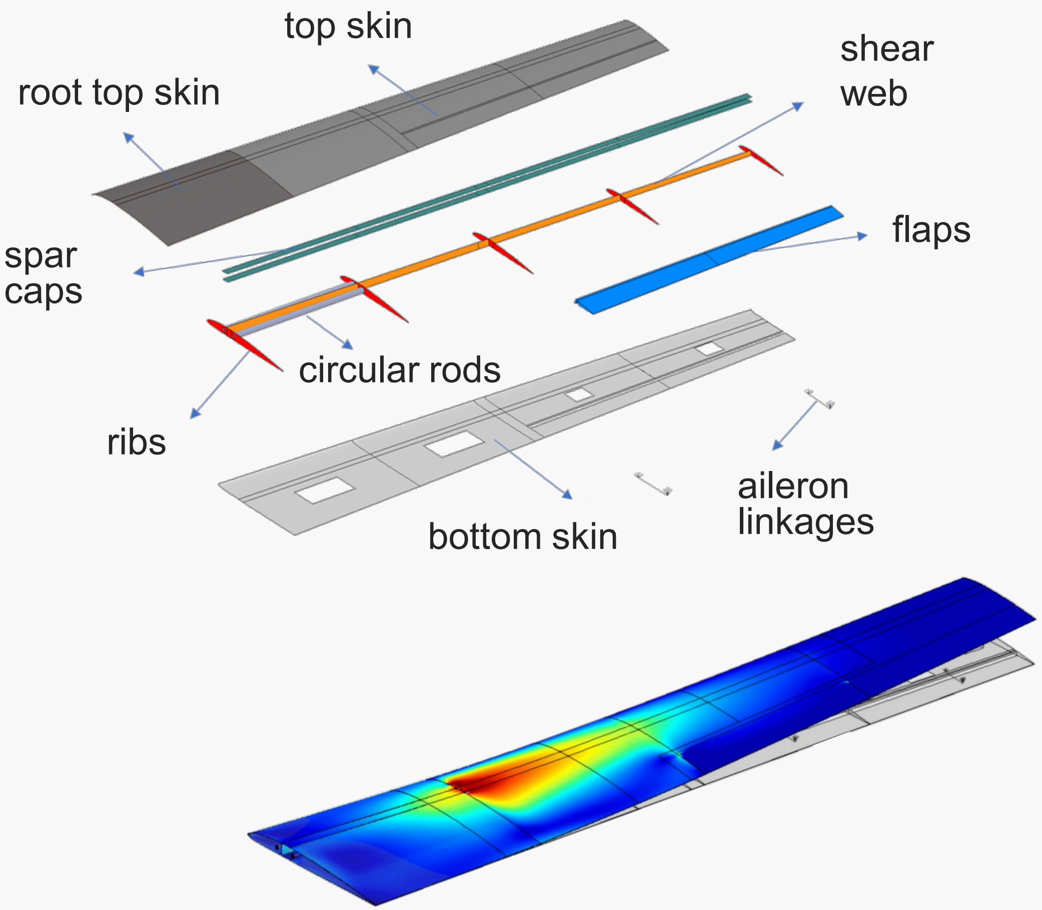
Given initial conditions, boundary conditions, loading conditions, and system parameters

Compute solution trajectories $\sigma(x, y, t), \varepsilon(x, y, t), \mathrm{u}(x, y, t), \ldots$

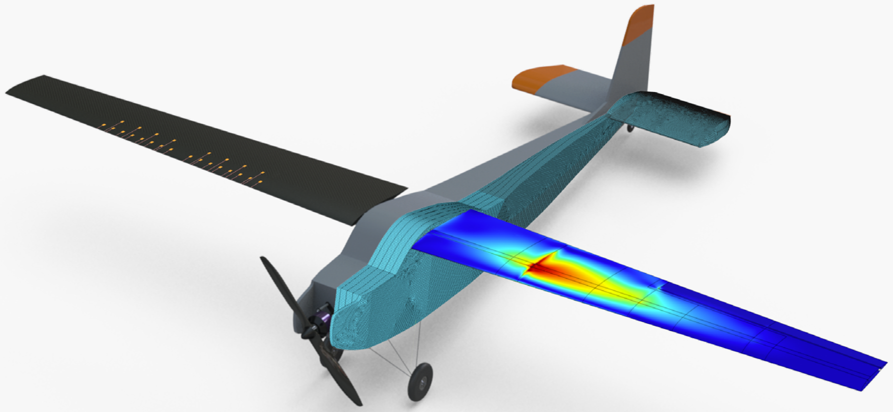


A predictive window on the future

PHYSICS-BASED MODELS are **POWERFUL** and bring **PREDICTIVE CAPABILITIES**



but they can be **COMPUTATIONALLY EXPENSIVE**



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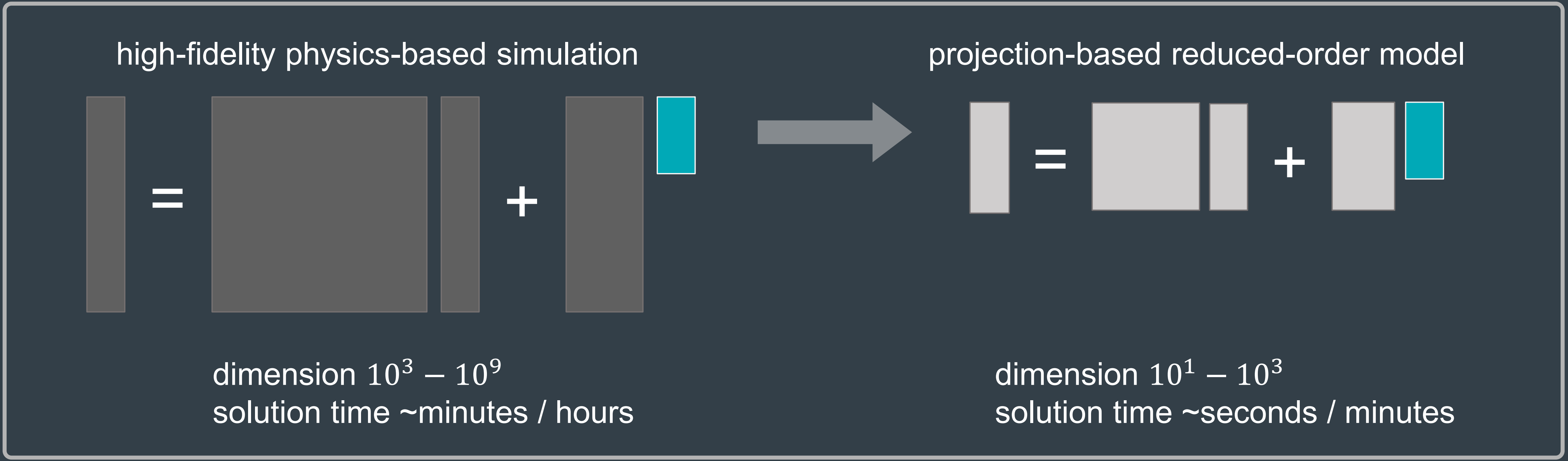
Reduced-order models are critical enablers for Predictive Digital Twins



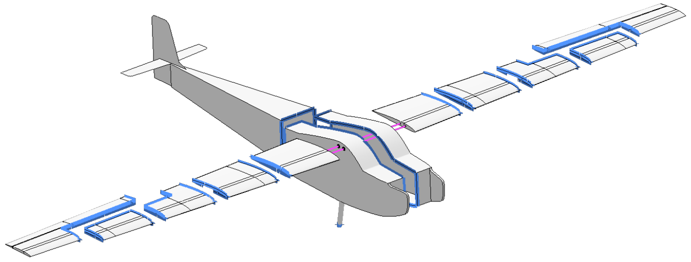
1 **Train**: Solve governing eq. to generate training data (<u>snapshots</u>)

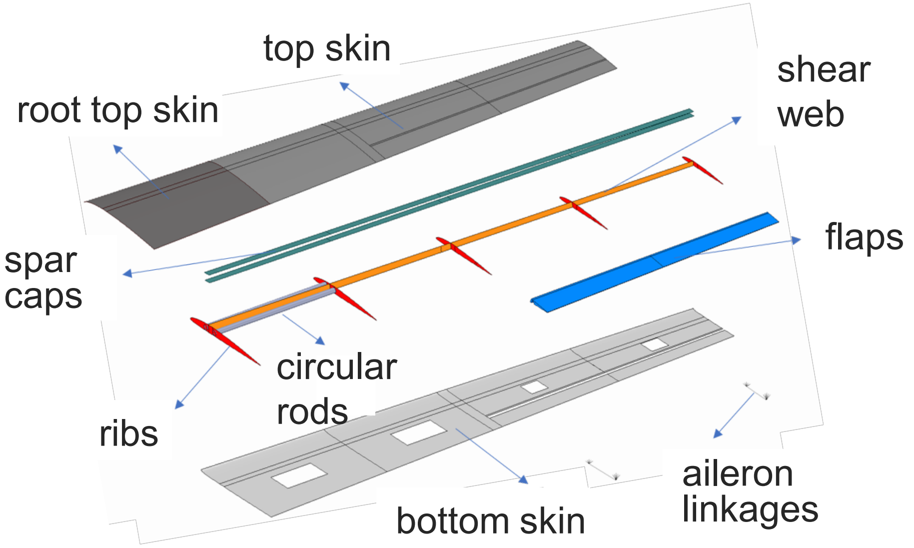
2 **Identify structure**: Compute a <u>low-dimensional basis</u>

3 **Reduce**: <u>Project</u> PDE model onto the low-dimensional subspace

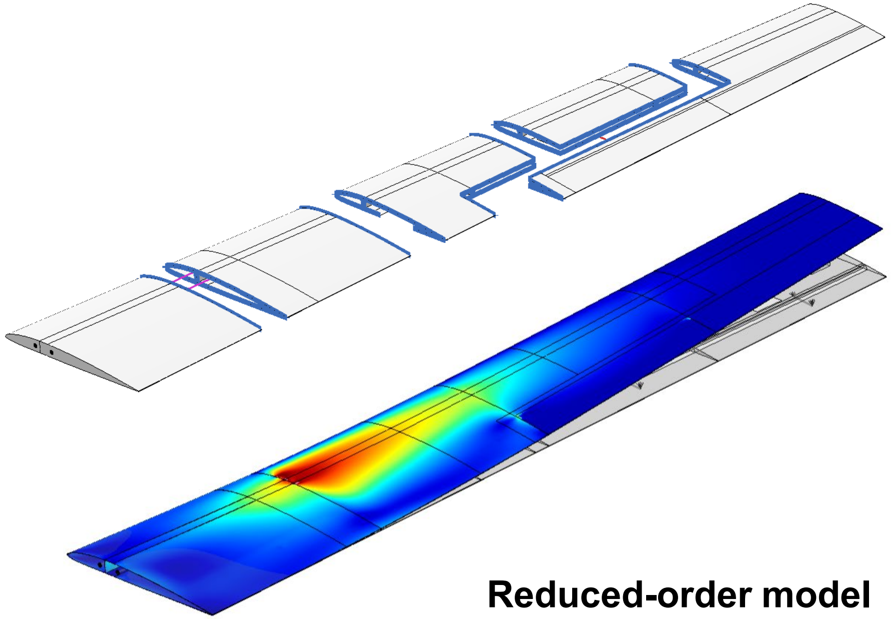
Reduced-order modeling leads to low-cost physics-based models that enable predictive digital twins

[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)

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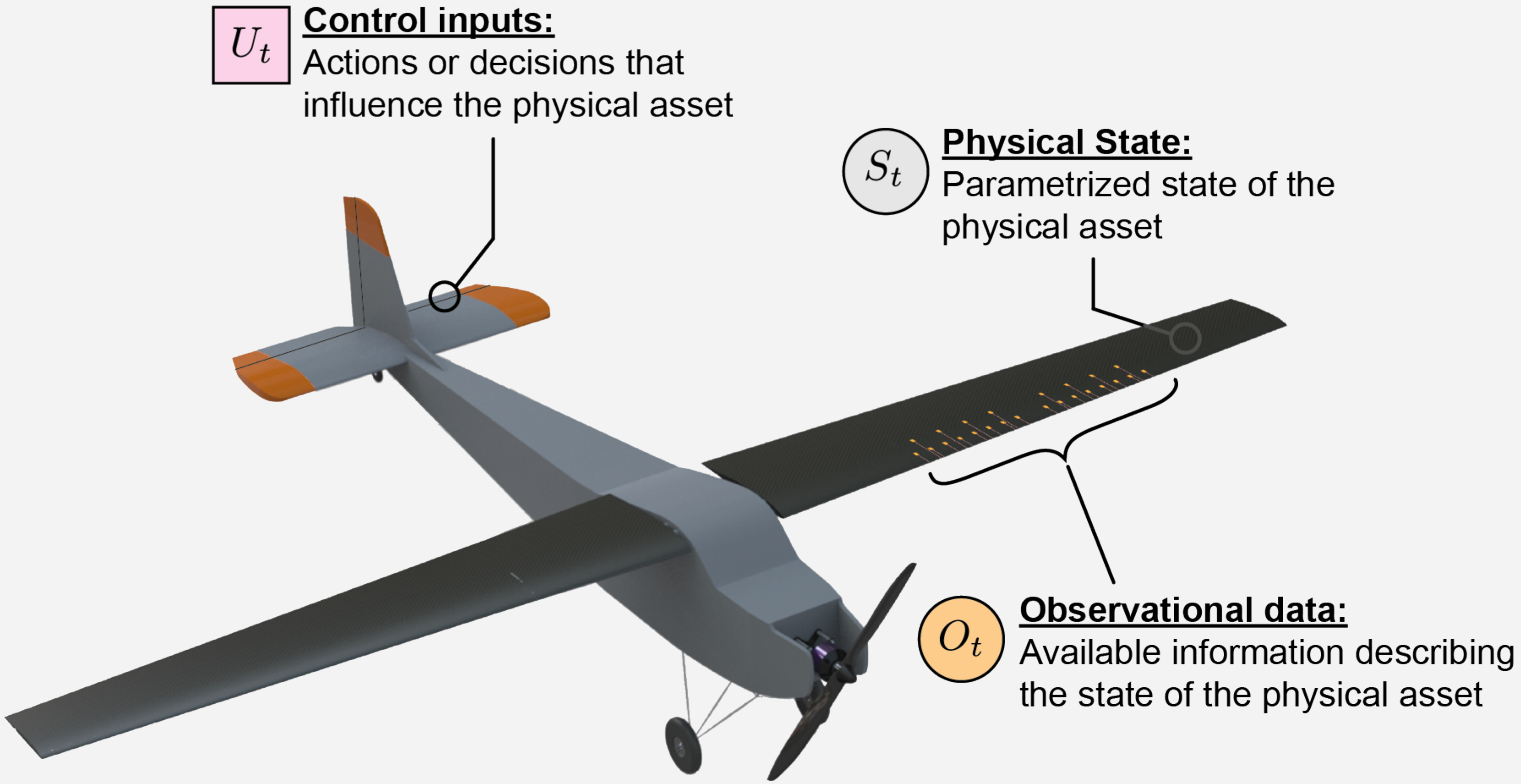
MATHEMATICAL ABSTRACTION

of an asset-twin system



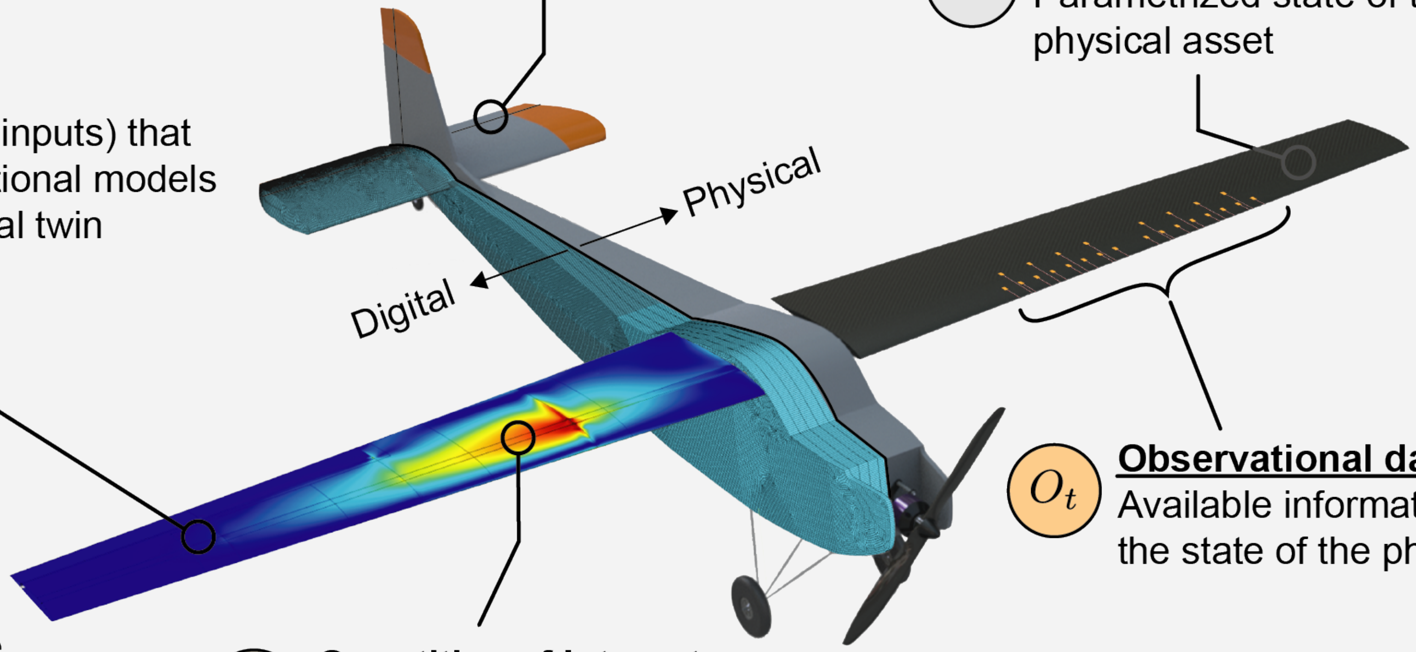
MATHEMATICAL ABSTRACTION

of an asset-twin system

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



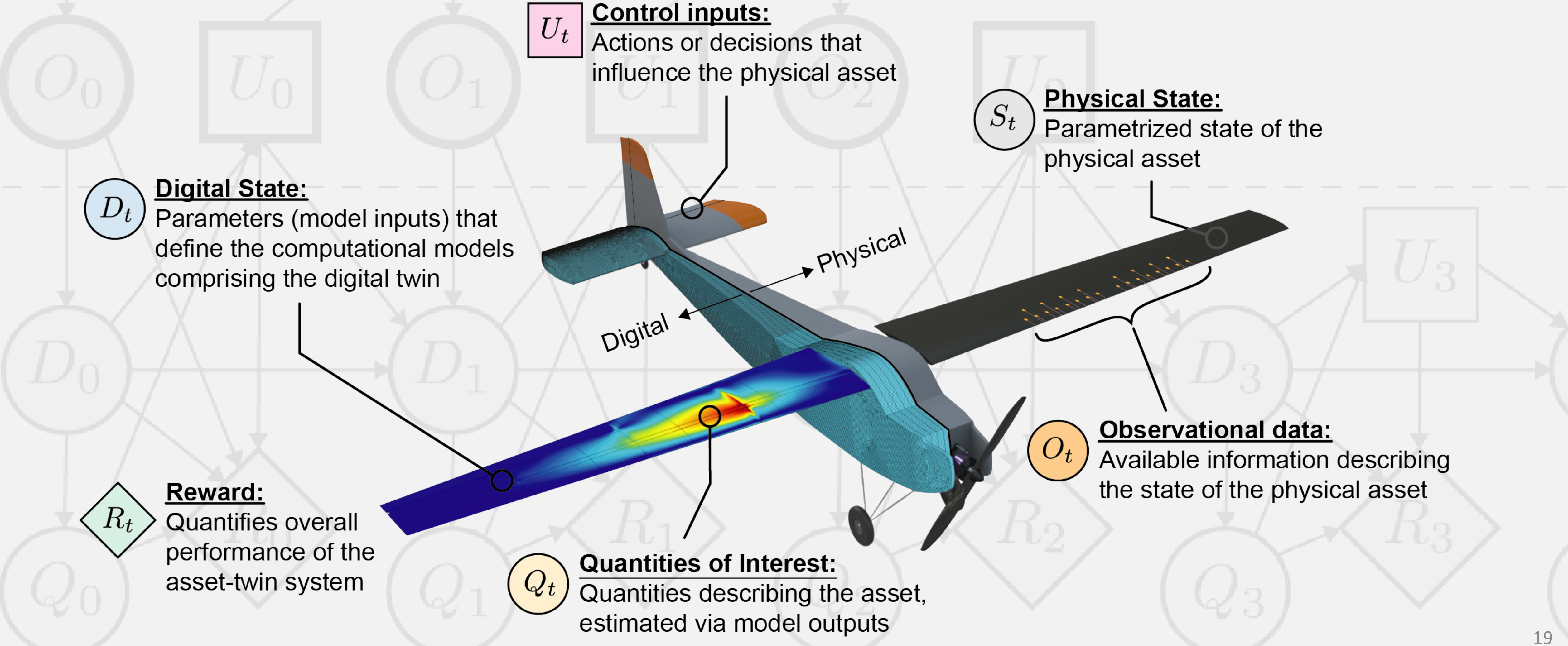
O_t **Observational data:**
Available information describing the state of the physical asset

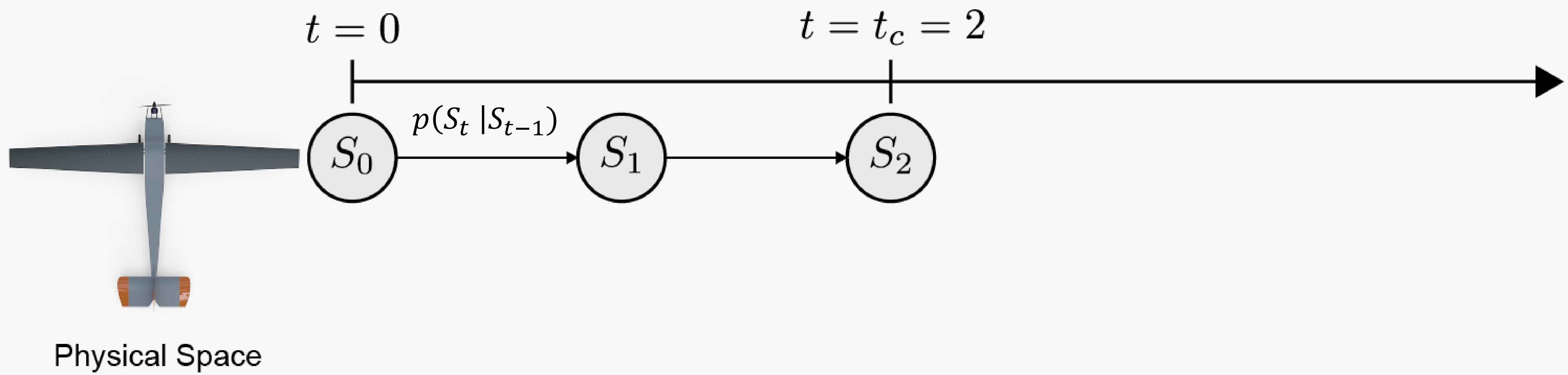
R_t **Reward:**
Quantifies overall performance of the asset-twin system

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

Image adapted from Kapteyn et al., *Nature Comp. Sci.*, Vol. 1, No. 5, 2021.

PREDICTIVE DIGITAL TWINS

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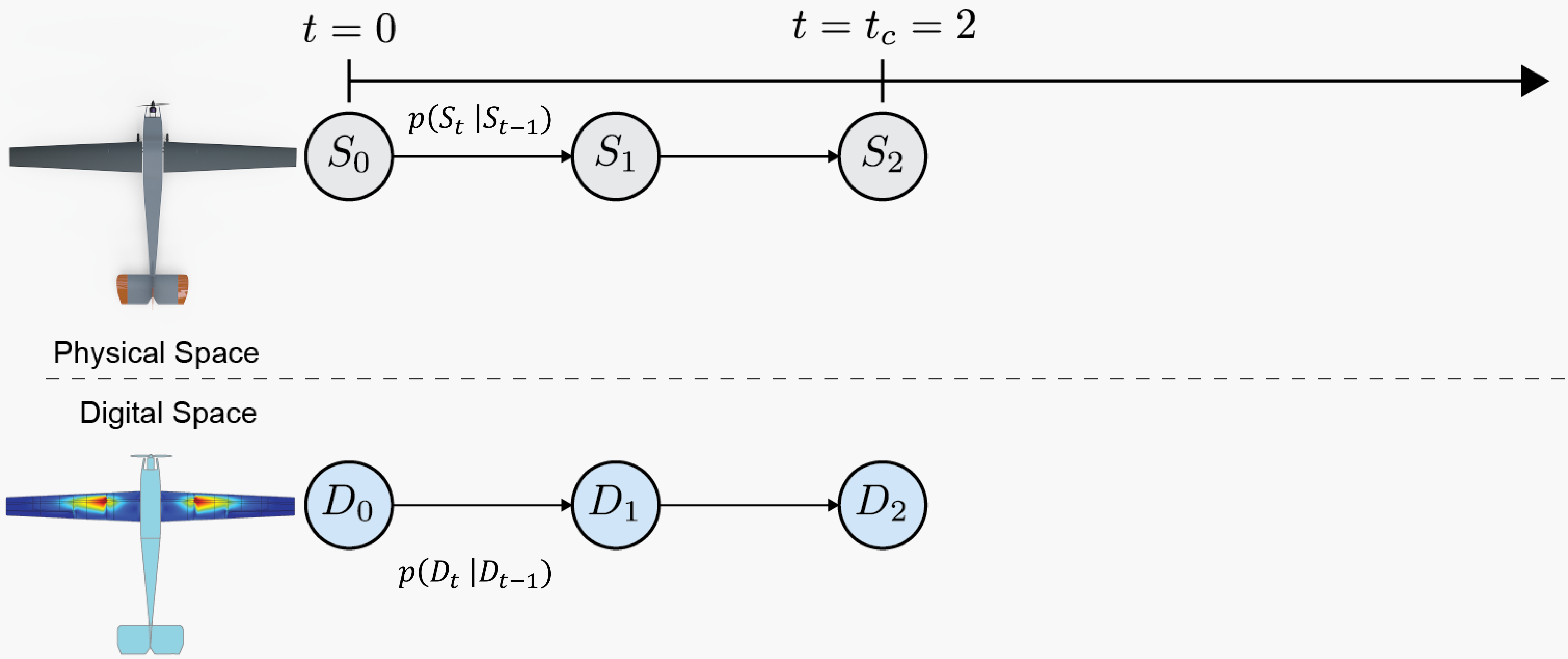
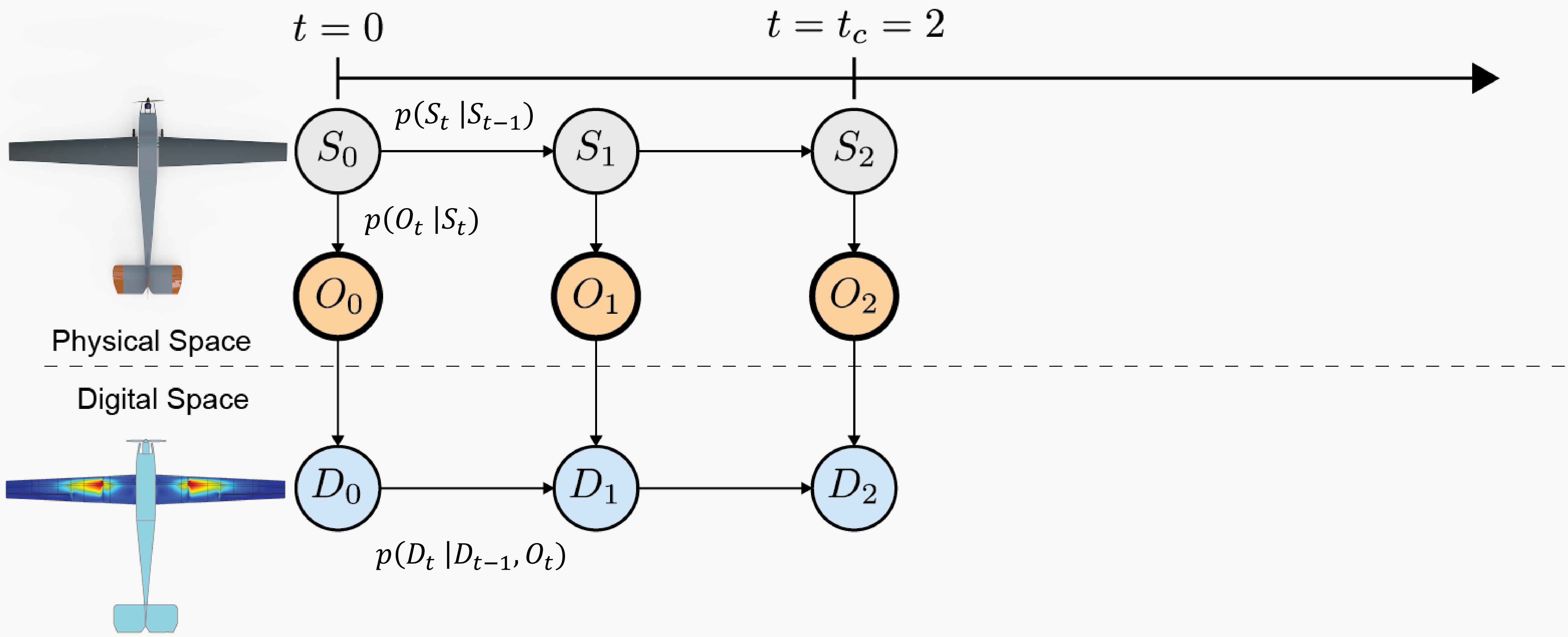
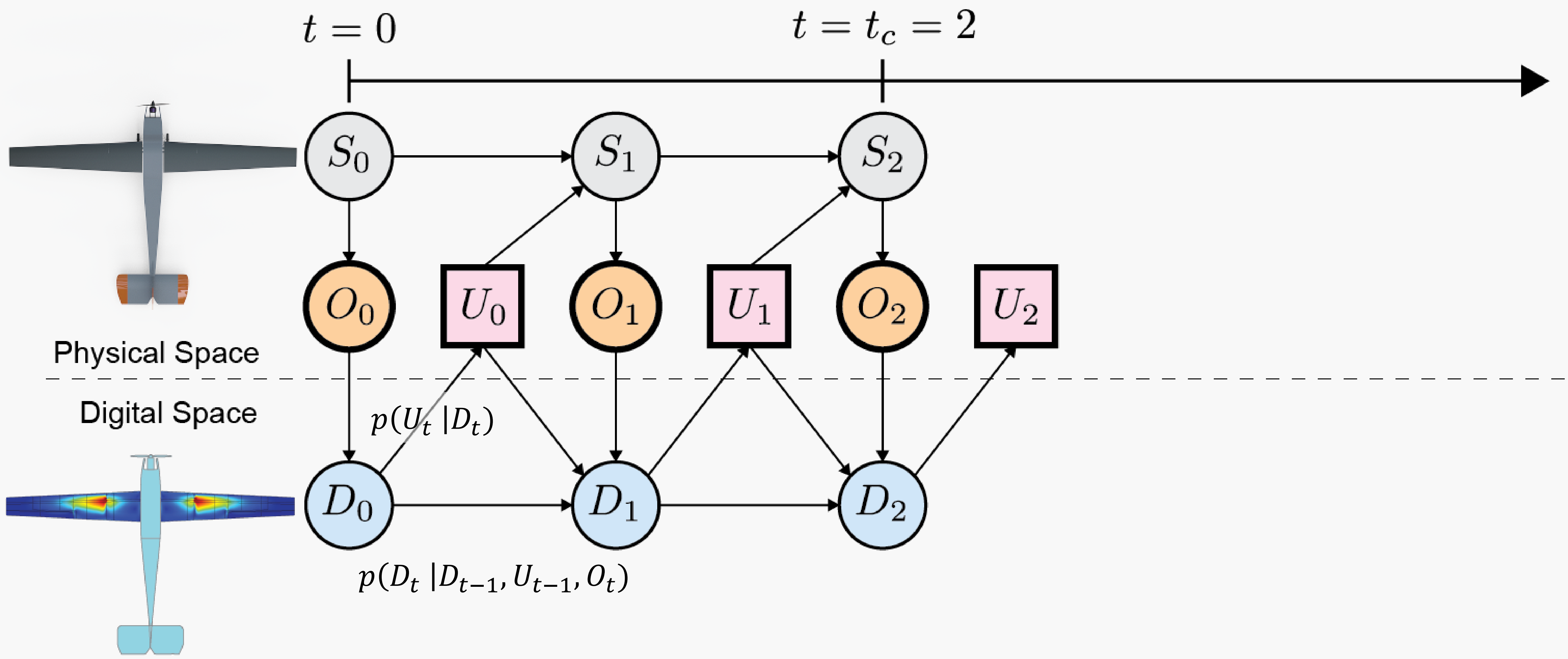
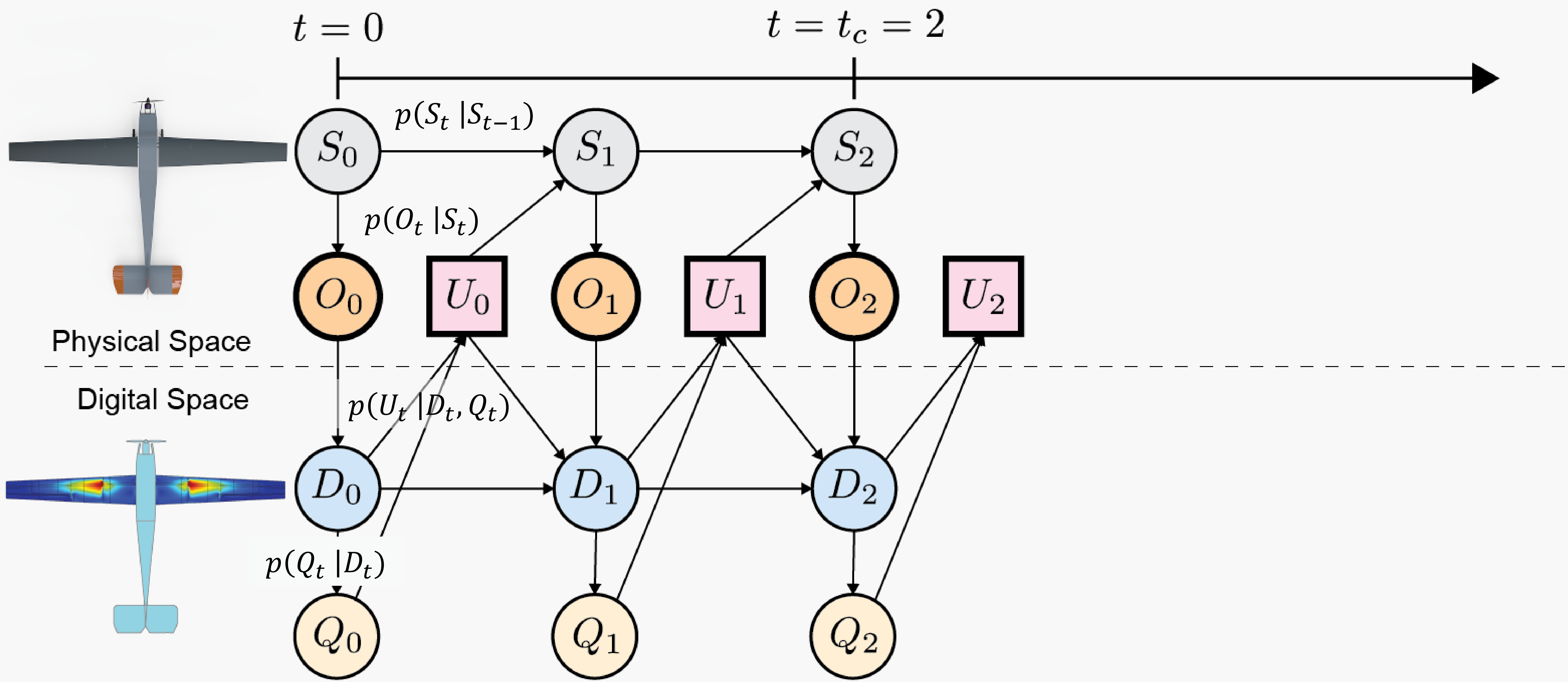
$t = t_c = 2$
$p(S_t \mid S_{t-1})$
S_0
S_1
S_2
Physical Space


$t = 0$
$t = t_c = 2$
$p(S_t \mid S_{t-1})$
S_0
S_1
S_2
Physical Space
Digital Space
D_0
D_1
D_2
$p(D_t \mid D_{t-1})$

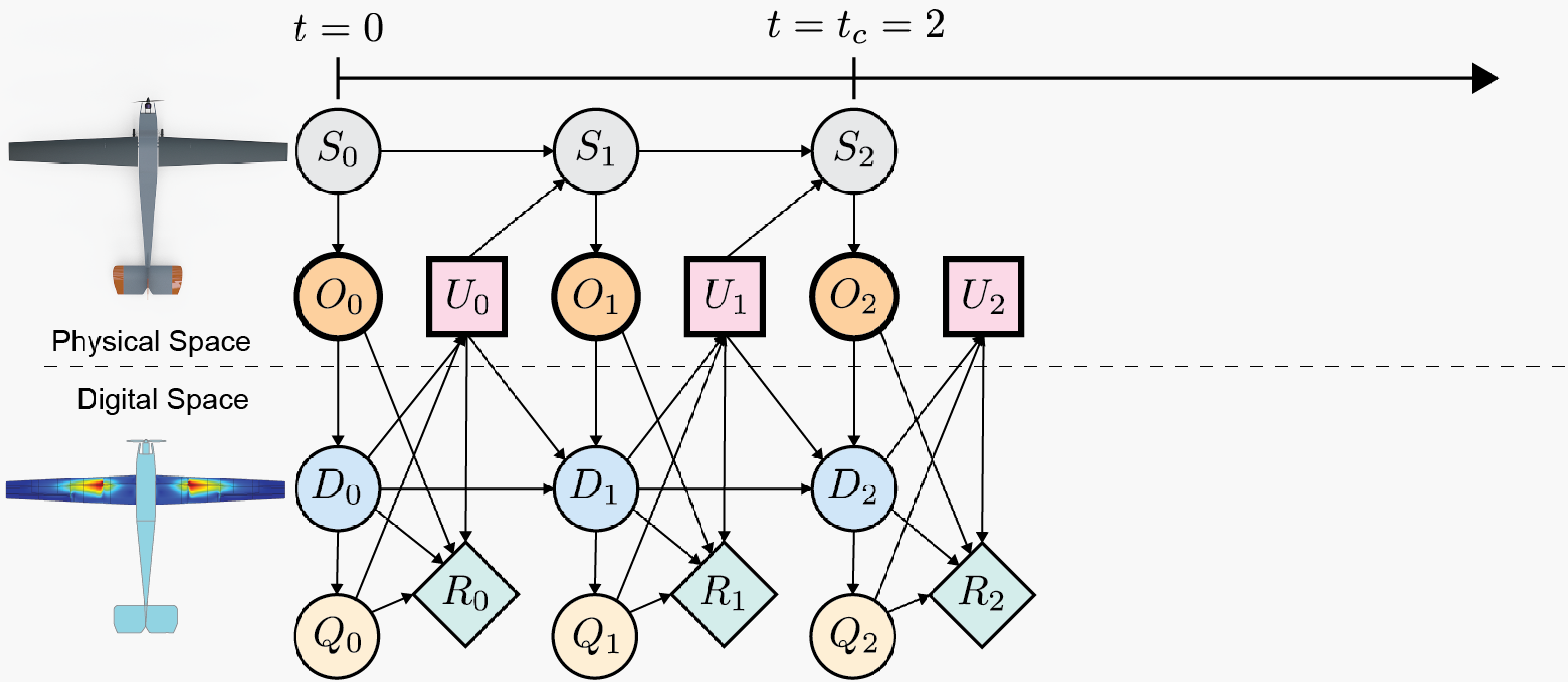


$t = 0$
$t = t_c = 2$
$p(S_t \mid S_{t-1})$
$p(O_t \mid S_t)$
$p(D_t \mid D_{t-1}, O_t)$
S_0
S_1
S_2
O_0
O_1
O_2
D_0
D_1
D_2
Physical Space
Digital Space

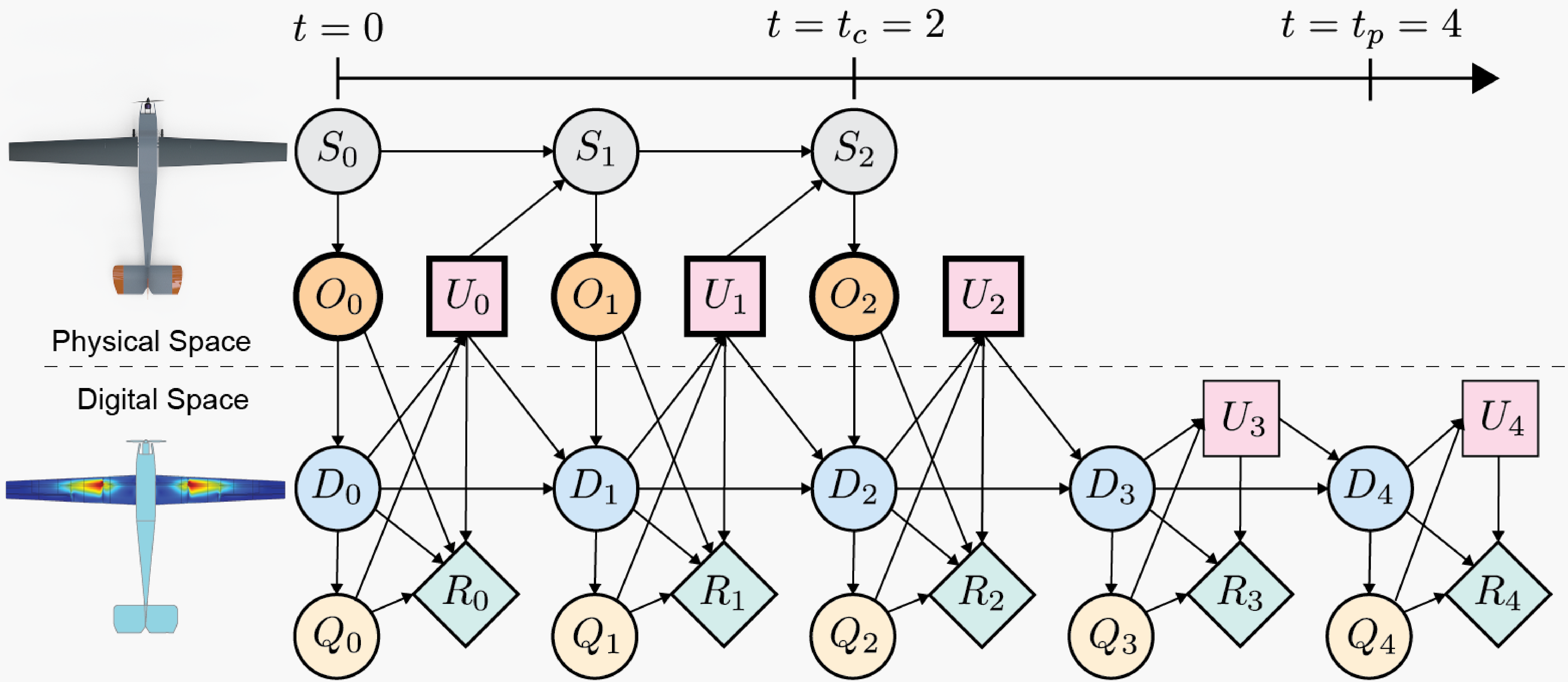

$t = 0$
$t = t_c = 2$
S_0
S_1
S_2
O_0
U_0
O_1
U_1
O_2
U_2
Physical Space
Digital Space
$p(U_t \mid D_t)$
D_0
D_1
D_2
$p(D_t \mid D_{t-1}, U_{t-1}, O_t)$



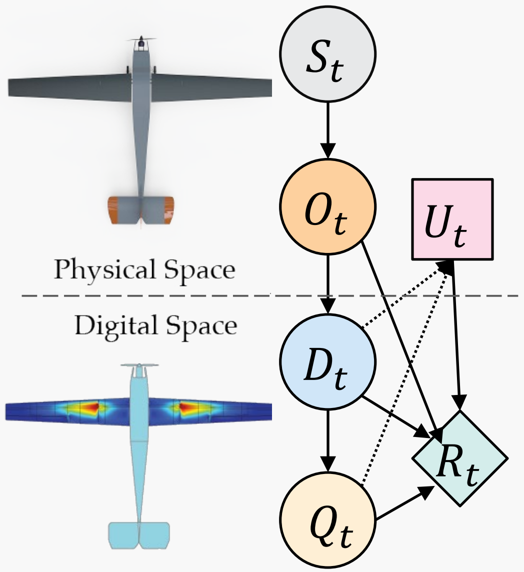
$t = 0$
$t = t_c = 2$
$p(S_t \mid S_{t-1})$
$p(O_t \mid S_t)$
$p(U_t \mid D_t, Q_t)$
$p(Q_t \mid D_t)$
S_0
S_1
S_2
O_0
U_0
O_1
U_1
O_2
U_2
Physical Space
Digital Space
D_0
D_1
D_2
Q_0
Q_1
Q_2



$$p(R_t \mid D_t, U_t, O_t, Q_t)$$



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



Conditional independence structure defined by the graph admits a factorization:

$$p\left(D_0, \ldots, D_{t_p}, Q_0, \ldots, Q_{t_p}, R_0, \ldots, R_{t_p}, U_{t_c+1}, \ldots, U_{t_p} \;\middle|\; o_0, \ldots, o_{t_c}, u_0, \ldots, u_{t_c} \right)$$

$$\propto \prod_{t=0}^{t_p} \left[\phi_t^{\text{dynamics}} \, \phi_t^{\text{QoI}} \, \phi_t^{\text{eval}} \right] \prod_{t=0}^{t_c} \phi_t^{\text{assim}} \prod_{t=t_c+1}^{t_p} \phi_t^{\text{control}}$$

quantity of interest

$\phi_t^{\text{QoI}} = p(Q_t \mid D_t)$

assimilation

$\phi_t^{\text{assim}} = p(o_t \mid D_t)$

control

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

digital state transition

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

reward function

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

Physics-based (reduced) models underpin the graphical model and bring predictive capability

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

Mathematical Formulation via Probabilistic Graphical Model

Automatic monitoring, virtual inspections, simulation-based certification

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

Forecasting, predictive maintenance, planning

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

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

Multi-objective optimization:

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

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

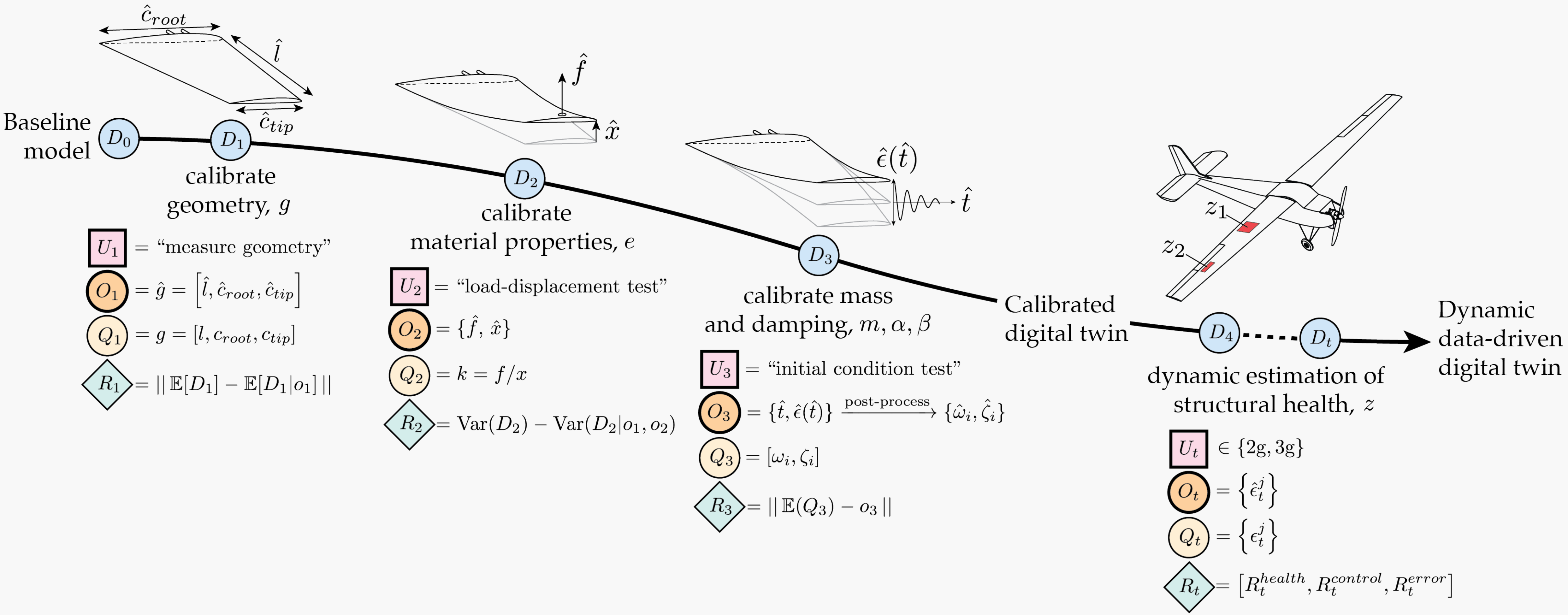
Learn from historical data, transfer insights to similar assets

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



The hardware

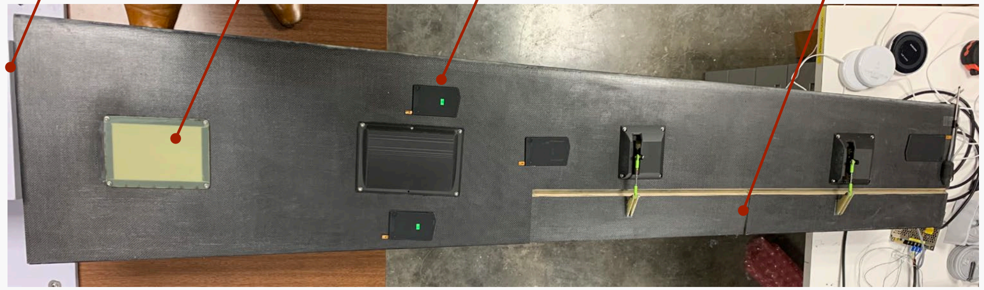
Customized 12ft Telemaster aircraft

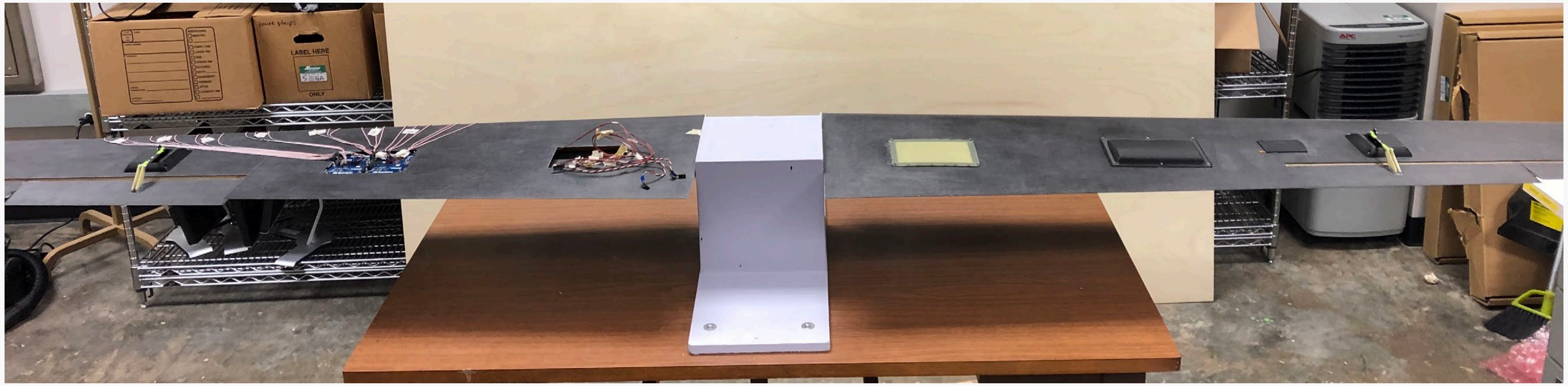
Fuselage mount

Custom sensor suite

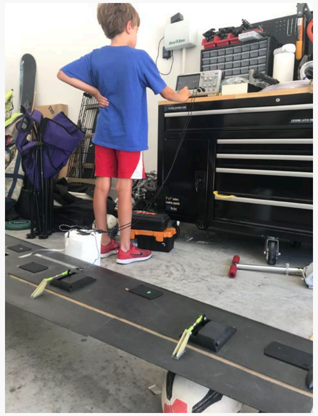
Access panel

Ailerons





Internal structure



*Willcox has a family member who is co-founder of Jessara. Purchase of the sensors for use in the research was reviewed and approved in compliance with all applicable MIT policies and procedures.

The structural model

Finite element model + reduced-order model

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{\partial \sigma}{\partial x} + \frac{\partial \sigma}{\partial y} + F$$

force/displacement equation of motion

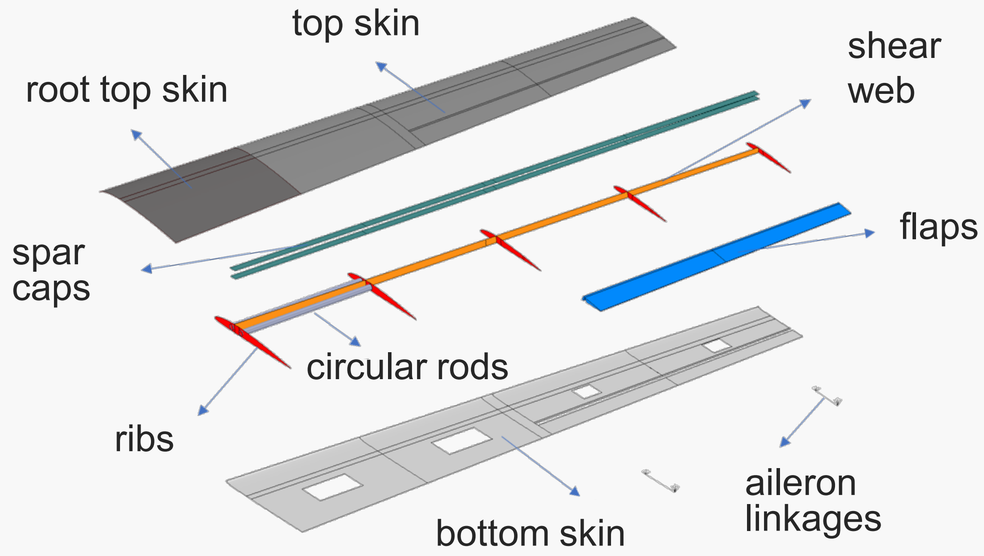
$$\varepsilon = \frac{1}{2}\left[\nabla u + (\nabla u)^{\mathsf{T}}\right]$$

strain-displacement equations

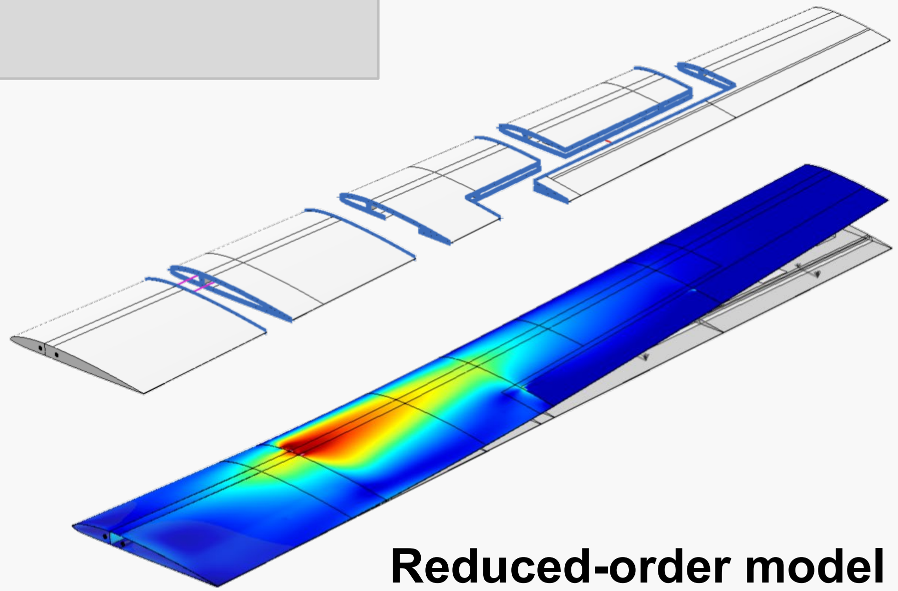
$$\sigma = C : \varepsilon$$

constitutive equations

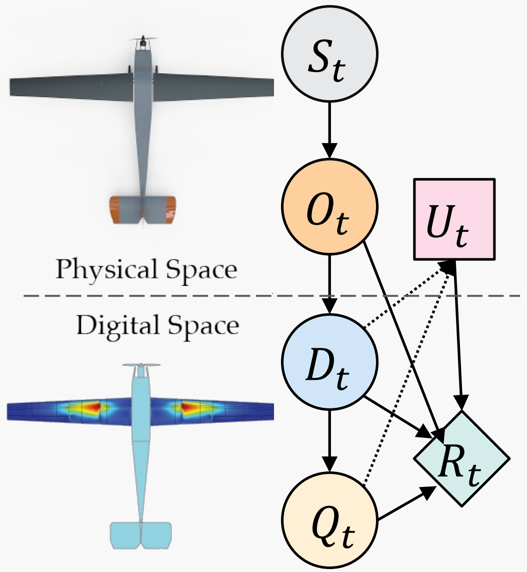
+ boundary conditions
+ initial conditions



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

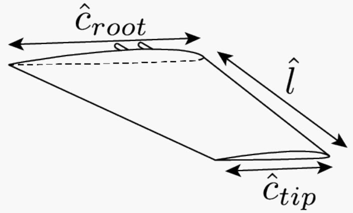


Reduced-order model
static condensation reduced basis element (SCRBE) method; ~0.03 seconds per structural analysis (1000x speedup)



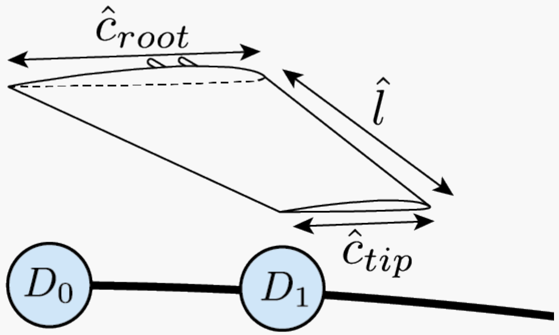
D_t Digital State

$$d := \begin{bmatrix} g \\ e \\ m \\ \alpha \\ \beta \\ z \end{bmatrix} \begin{array}{l} \} \text{ vector of geometric parameters} \\ \} \text{ Young's modulus scale factor} \\ \} \text{ vector of added point masses} \\ \left.\begin{array}{l} \\ \end{array}\right\} \text{ Rayleigh damping coefficients} \\ \} \text{ vector of structural health parameters} \end{array}$$



D_t	c_{root} [mm]	c_{tip} [mm]	l [mm]	e [-]	m_{servo} [g]	α [s^{-1}]	β [s]
Prior information	$\mathcal{N}(435.6, 1.3)$	$\mathcal{N}(261.1, 1.3)$	$\mathcal{N}(1828.8, 1.3)$	$\mathcal{N}(1.0, 0.026)$	$2m_{servo}+m_{pitot}=472$ $m_{servo}, m_{pitot} \geq 0$	0	0

Baseline model



calibrate geometry, g

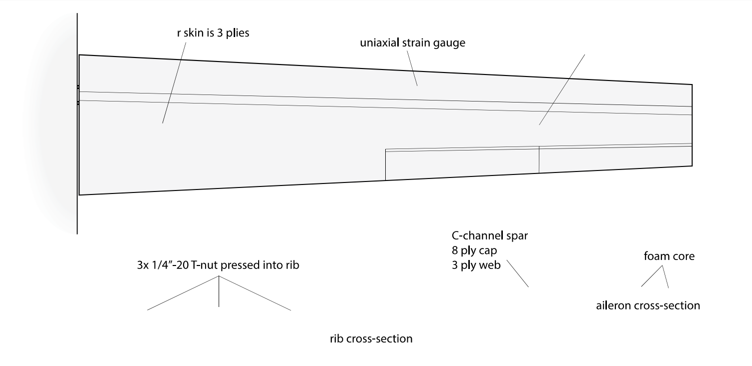
U_1 = “measure geometry”

$O_1 = \hat{g} = \left[\hat{l}, \hat{c}_{root}, \hat{c}_{tip}\right]$

$Q_1 = g = [l, c_{root}, c_{tip}]$

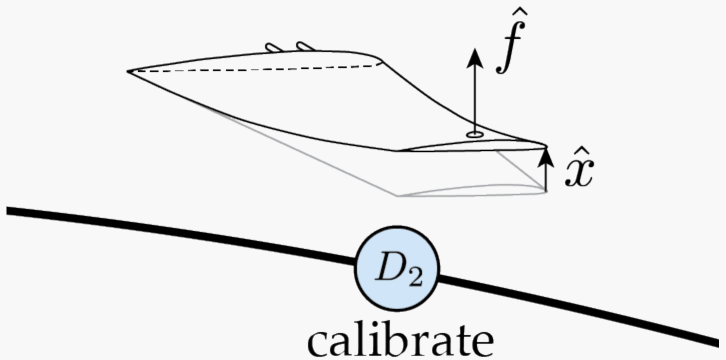
$R_1 = ||\, \mathbb{E}[D_1] - \mathbb{E}[D_1|o_1]\, ||$

Prior



Observation

D_t	c_{root} [mm]	c_{tip} [mm]	l [mm]
Prior information	$\mathcal{N}(435.6, 1.3)$	$\mathcal{N}(261.1, 1.3)$	$\mathcal{N}(1828.8, 1.3)$
Posterior estimate	433	260	1828



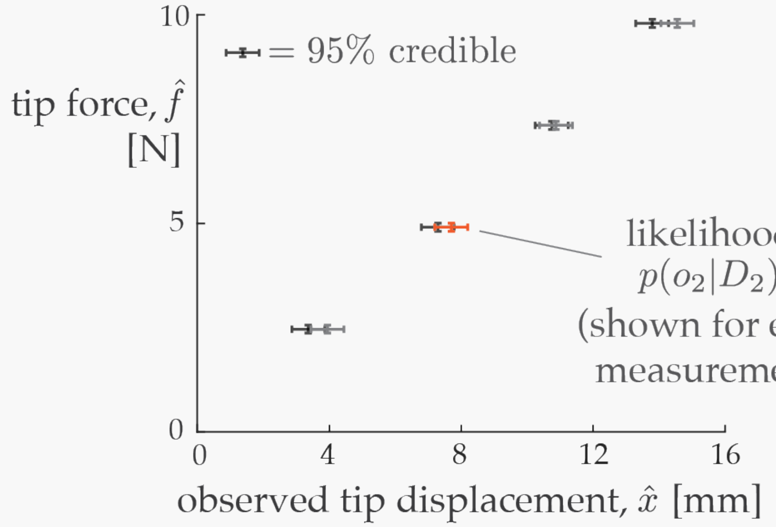
calibrate
material properties, e

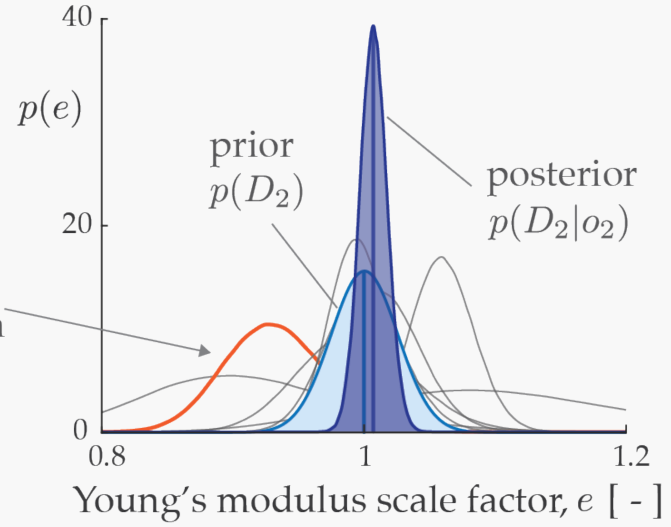
U_2 = “load-displacement test”

O_2 = $\{\hat{f},\, \hat{x}\}$

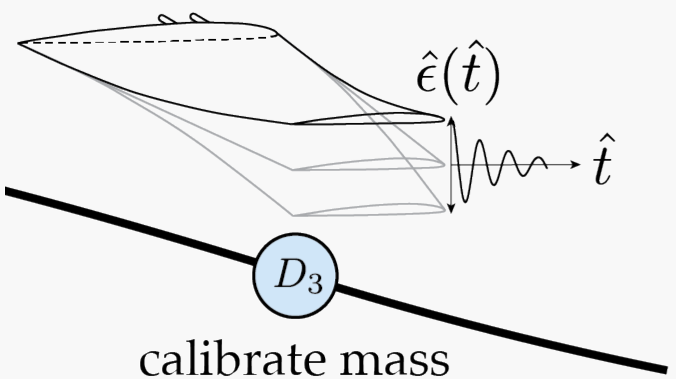
Q_2 = $k = f/x$

R_2 = $\mathrm{Var}(D_2) - \mathrm{Var}(D_2|o_1, o_2)$





D_t	c_{root} [mm]	c_{tip} [mm]	l [mm]	e [-]
Prior information	$\mathcal{N}(435.6, 1.3)$	$\mathcal{N}(261.1, 1.3)$	$\mathcal{N}(1828.8, 1.3)$	$\mathcal{N}(1.0, 0.026)$
Posterior estimate	433	260	1828	1.0073 (0.0103)



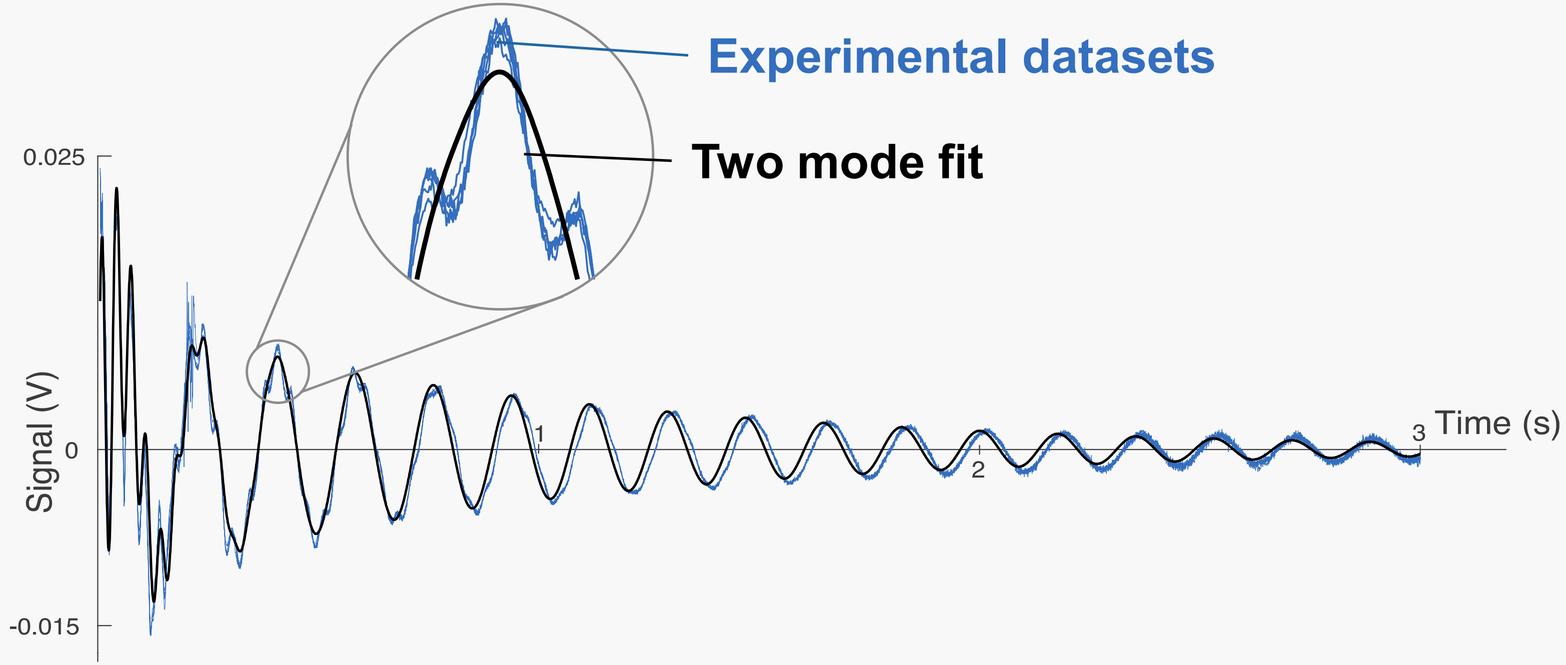
calibrate mass and damping, m, α, β

U_3 = "initial condition test"

$O_3 = \{\hat{t}, \hat{\epsilon}(\hat{t})\} \xrightarrow{\text{post-process}} \{\hat{\omega}_i, \hat{\zeta}_i\}$

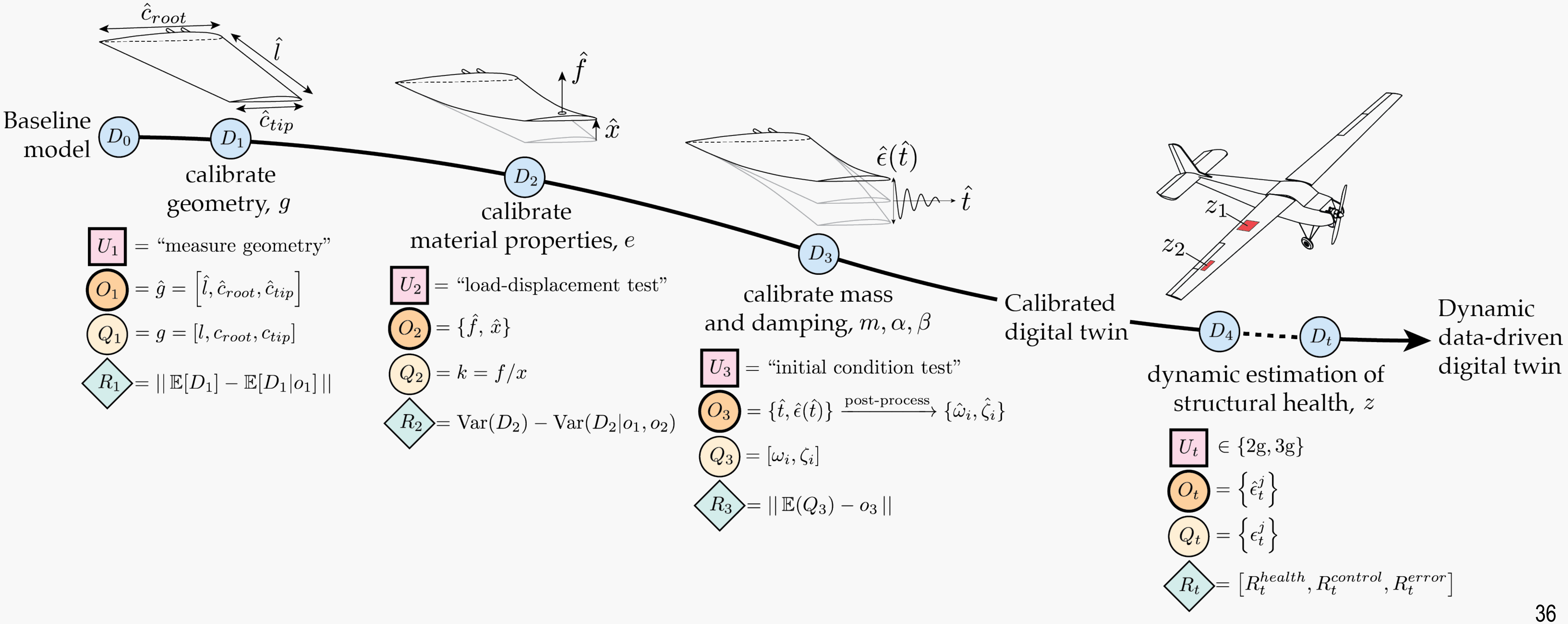
$Q_3 = [\omega_i, \zeta_i]$

$R_3 = ||\,\mathbb{E}(Q_3) - o_3\,||$

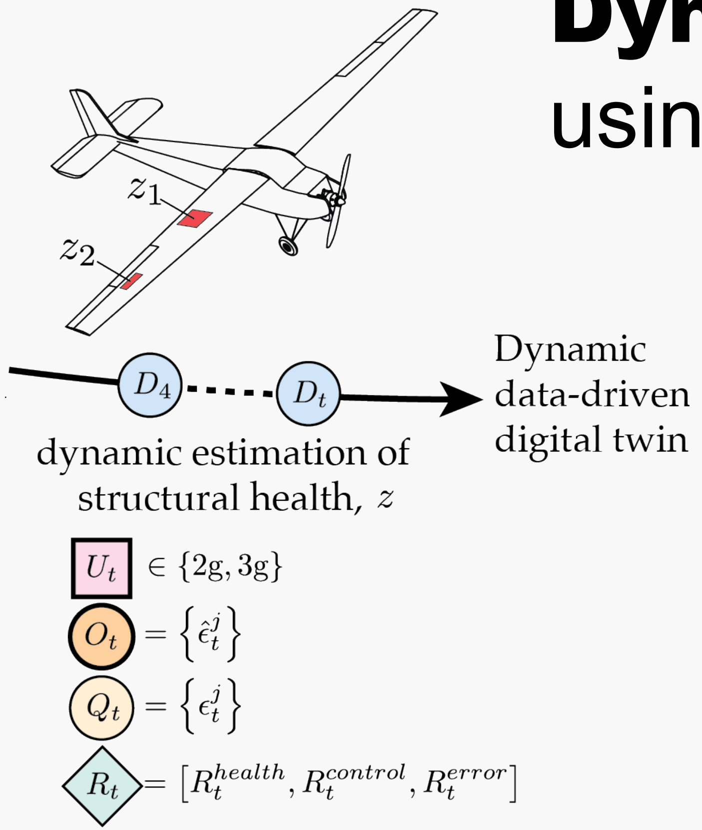


D_t	c_{root}	c_{tip}	l	e	m_{servo}	α	β
	[mm]	[mm]	[mm]	[-]	[g]	[s^{-1}]	[s]
Prior information	$\mathcal{N}(435.6, 1.3)$	$\mathcal{N}(261.1, 1.3)$	$\mathcal{N}(1828.8, 1.3)$	$\mathcal{N}(1.0, 0.026)$	$2m_{servo}+m_{pitot}=472$ $m_{servo}, m_{pitot} \geq 0$	0	0
Posterior estimate	433	260	1828	1.0073 (0.0103)	169.1 (3.9)	1.030 (0.001)	$7.66{\times}10^{-4}$ $(6.18{\times}10^{-7})$

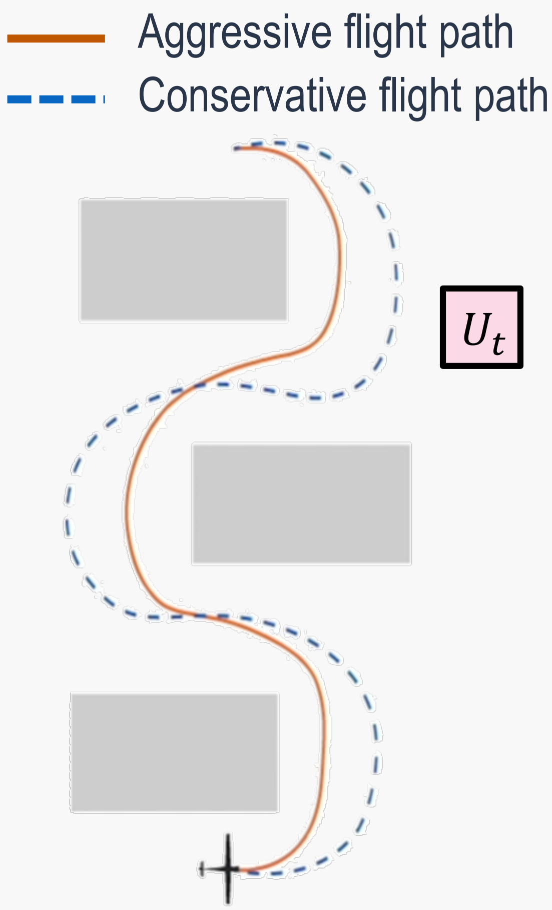
Calibrated digital twin reflects geometry, material properties, and structural properties of the physical UAV, along with estimates of our uncertainty



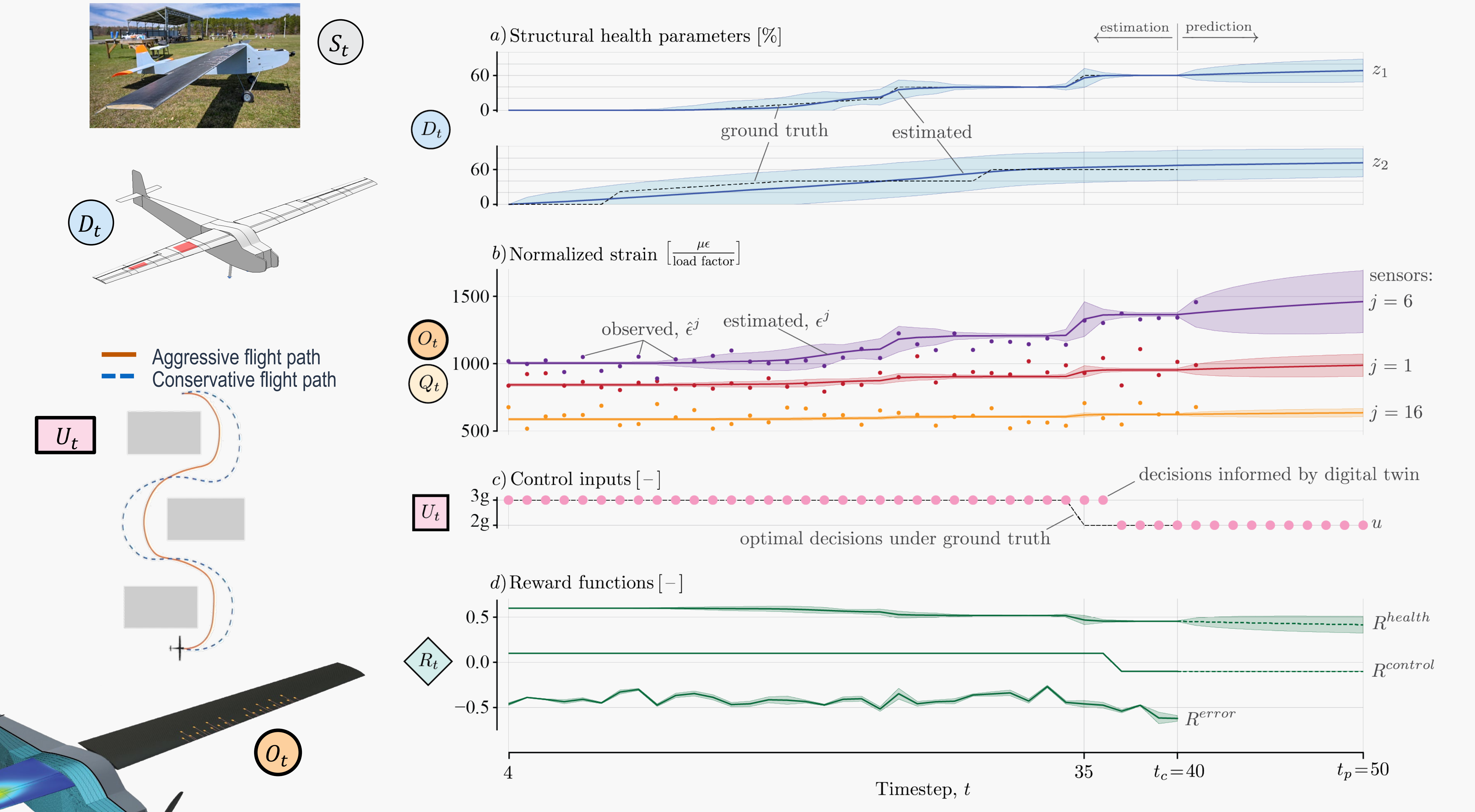
Dynamic evolution and decision-making using the digital twin



- Aircraft undergoes in-flight structural health degradation
- 24 wing-mounted sensors provide noisy strain data O_t
- Digital twin is dynamically updated and used to drive mission re-planning
- Scenarios are simulated in ROS

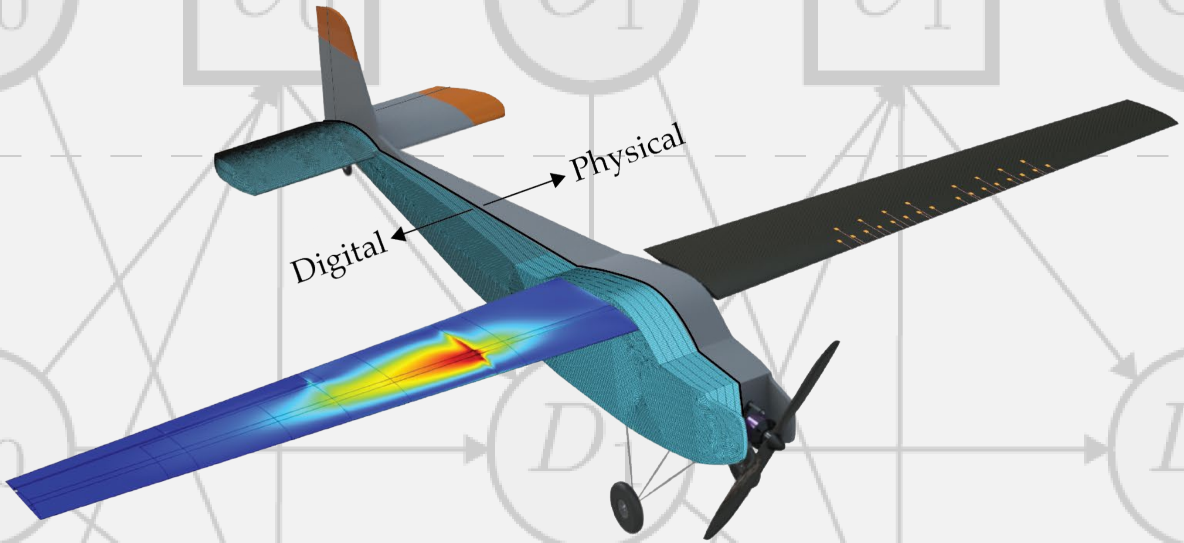


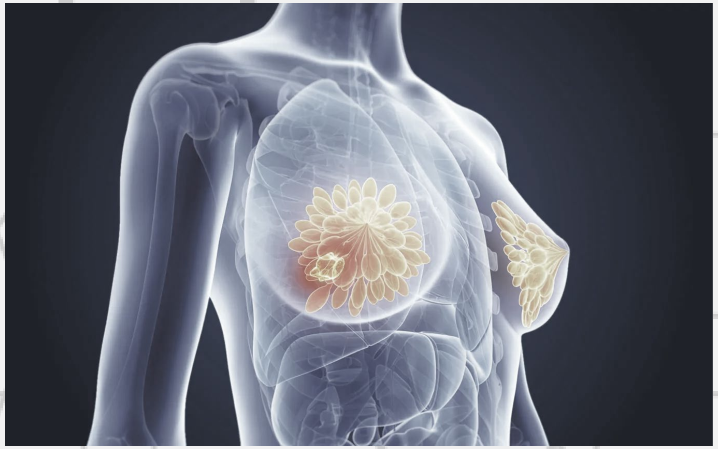
$$p\left(D_0, \dots, D_{t_p}, Q_0, \dots, Q_{t_p}, R_0, \dots, R_{t_p}, U_{t_c+1}, \dots, U_{t_p} \;\middle|\; o_0, \dots, o_{t_c}, u_0, \dots, u_{t_c}\right) \propto \prod_{t=0}^{t_p}\left[\phi_t^{\text{dynamics}}\, \phi_t^{\text{QoI}}\, \phi_t^{\text{eval}}\right] \prod_{t=0}^{t_c} \phi_t^{\text{assim}} \prod_{t=t_c+1}^{t_p} \phi_t^{\text{control}}$$



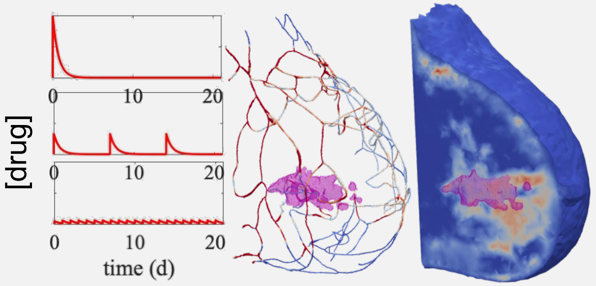
S_t
D_t
Aggressive flight path
Conservative flight path
U_t
O_t
a) Structural health parameters [%]
estimation
prediction
60
0
ground truth
estimated
z_1
z_2
b) Normalized strain $\left[\frac{\mu\epsilon}{\text{load factor}}\right]$
1500
1000
500
observed, $\hat{\epsilon}^j$
estimated, ϵ^j
sensors:
$j = 6$
$j = 1$
$j = 16$
Q_t
c) Control inputs [−]
3g
2g
decisions informed by digital twin
optimal decisions under ground truth
u
d) Reward functions [−]
0.5
0.0
−0.5
R_t
R^{health}
$R^{control}$
R^{error}
4
35
$t_c = 40$
$t_p = 50$
Timestep, t

FROM AIRCRAFT
TO CANCER PATIENTS

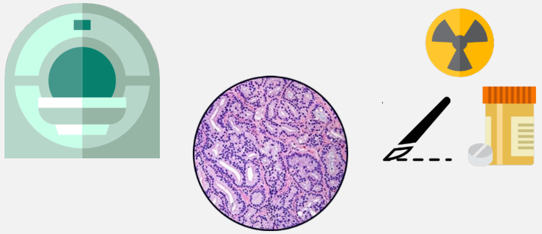


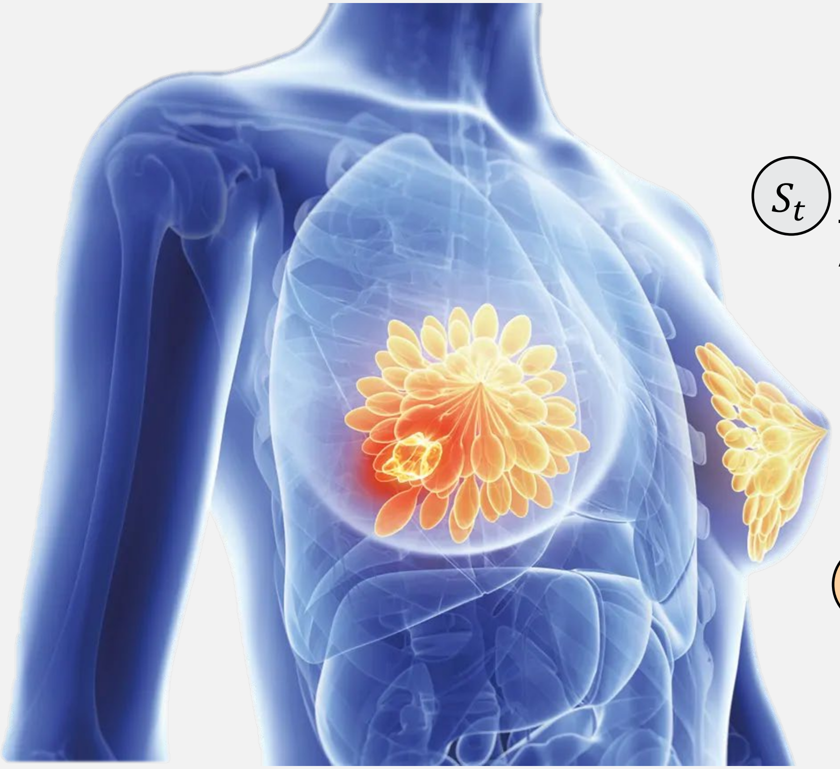


D_t Digital Twin State
Tumor dynamics, mechanics



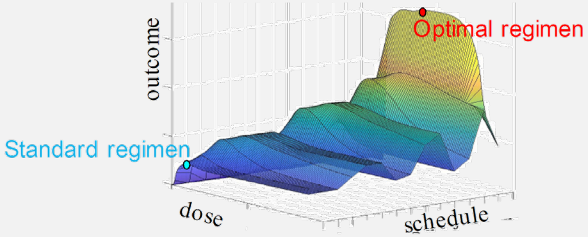
U_t Control inputs
MRI studies, biopsies,
treatment regimens



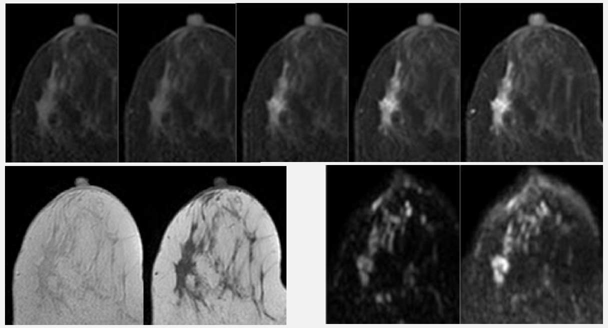


S_t Physical State
Anatomy & morphology,
mechanical & physiological state

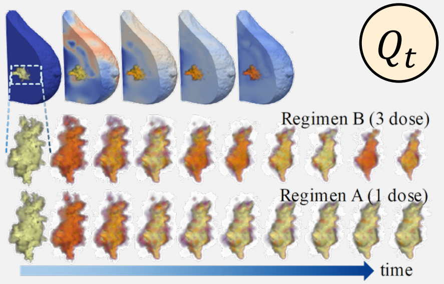
R_t Reward
Patient outcomes:
treatment efficacy, toxicity



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



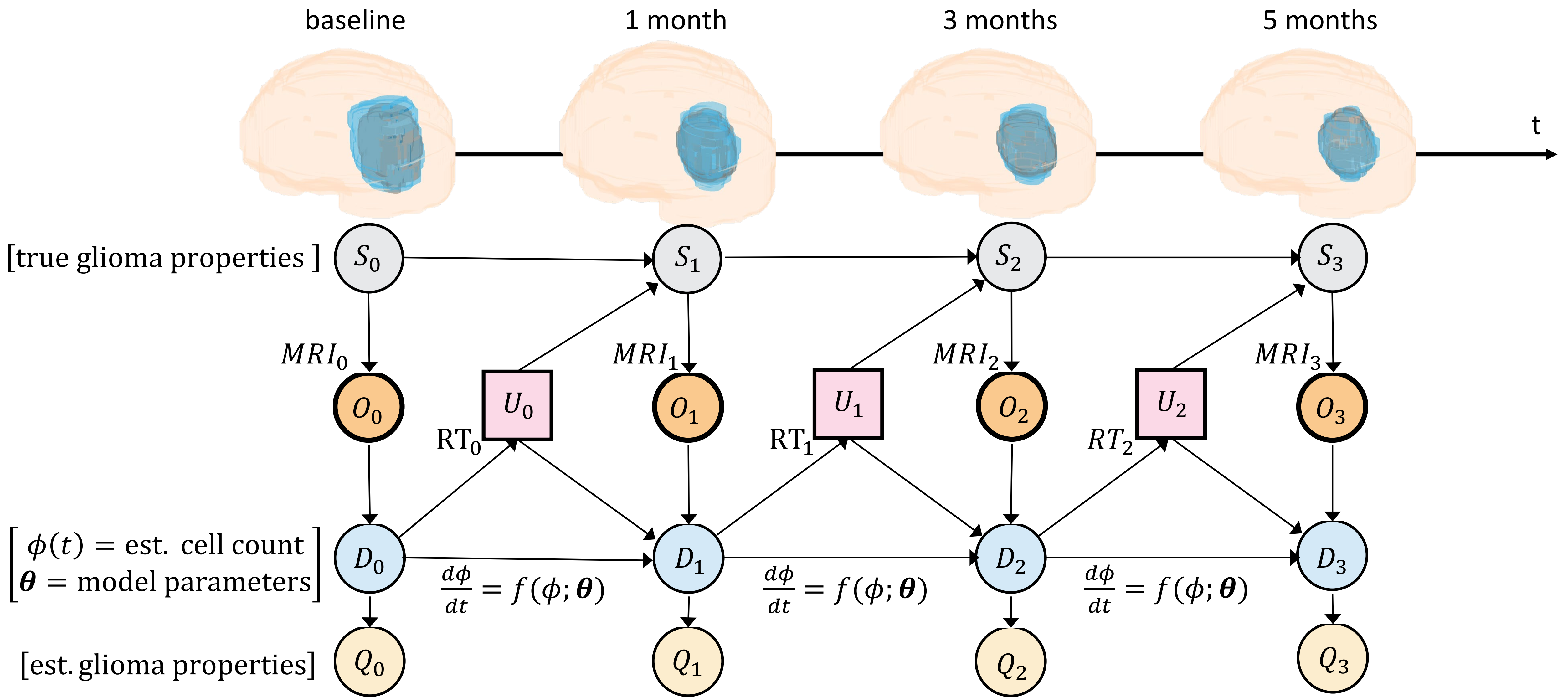
Q_t Quantities of Interest
Distribution of therapies,
tumor shape, cell density



THE CENTER FOR COMPUTATIONAL ONCOLOGY

Cancer Patient Digital Twin

Collaboration with Oden Institute Center for Computational Oncology (T. Yankeelov)



Challenges for **PREDICTIVE DIGITAL TWINS** for complex systems across science, medicine & engineering

1 Predictive modeling for complex systems at scale

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, optimization, planning & control

4 Scalable algorithms for updating, prediction & control

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

5 Optimal sensing strategies

Integrated sensor design, optimal experimental design (active learning), intelligent adaptive data acquisition

Data-driven decisions

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

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