A probabilistic graphical model foundation to enable predictive digital twins at scale

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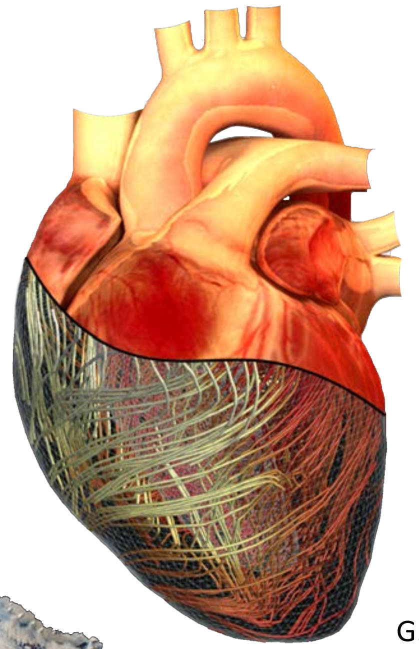
What *is* a digital twin?

"A **digital twin** is a set of computational models that evolve over time to **persistently represent** the **structure, behavior, and context** of a **unique physical asset**, and **informs decisions that realize value**"

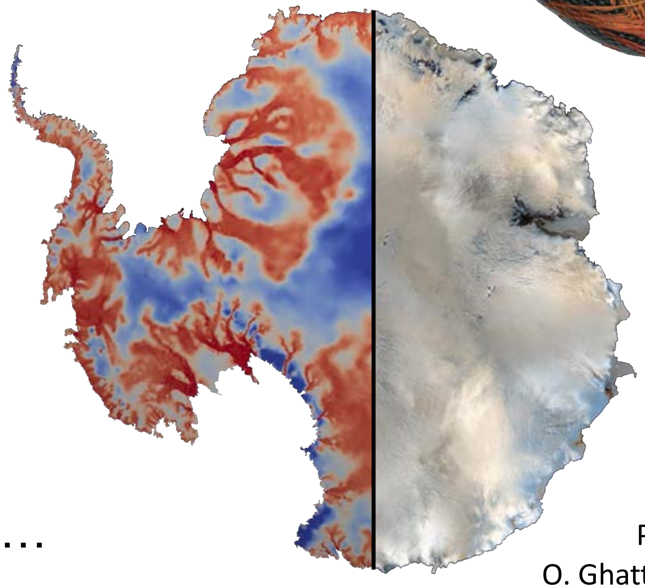
[Digital Twin: Definition & Value – AIAA and AIA Position Paper, Dec. '20]



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

Digital twins have the potential to **underpin intelligent automation** across **engineering, science**, and **society** by enabling:

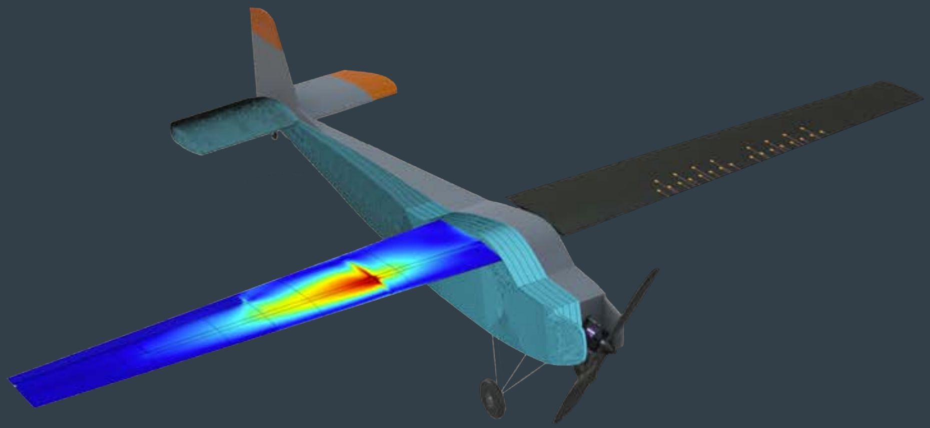
- Asset-specific analysis and prediction
- Data-driven decision making
- Fully integrated asset lifecycles (digital thread)
- Knowledge transfer between assets



PC:
O. Ghattas

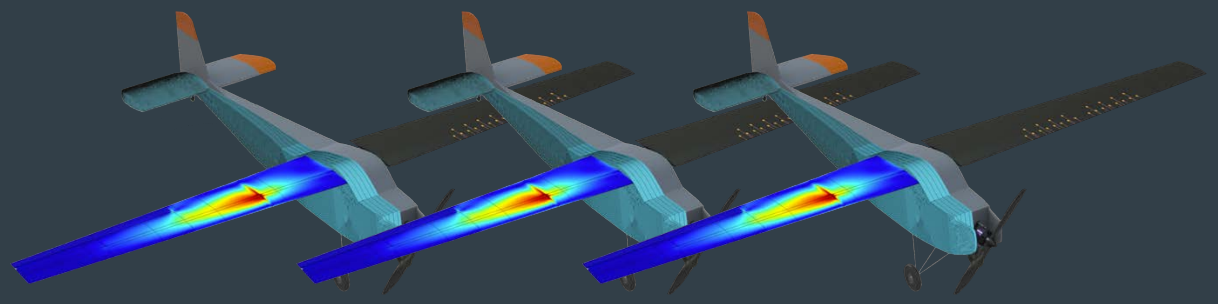
Wide range of proposed applications:
Structural health monitoring, certification, fleet management, manufacturing, healthcare, smart cities, education, climate science, …

DIGITAL TWINS must integrate DATA, MODELS & DECISIONS



Currently, state-of-the-art digital twins are largely the result of **highly specialized**, **application-dependent implementations** that require **considerable expertise and resources**

How can we move toward accessible, robust, and efficient digital twin implementations at scale?



A **rigorous**, **general**, and **unified** **MATHEMATICAL & COMPUTATIONAL FOUNDATION** is needed to **scale up digital twin development and deployment**

This talk:

A Mathematical & Computational Foundation for Digital Twins

1 **Mathematical Abstraction**

Which quantities define an asset-twin system?

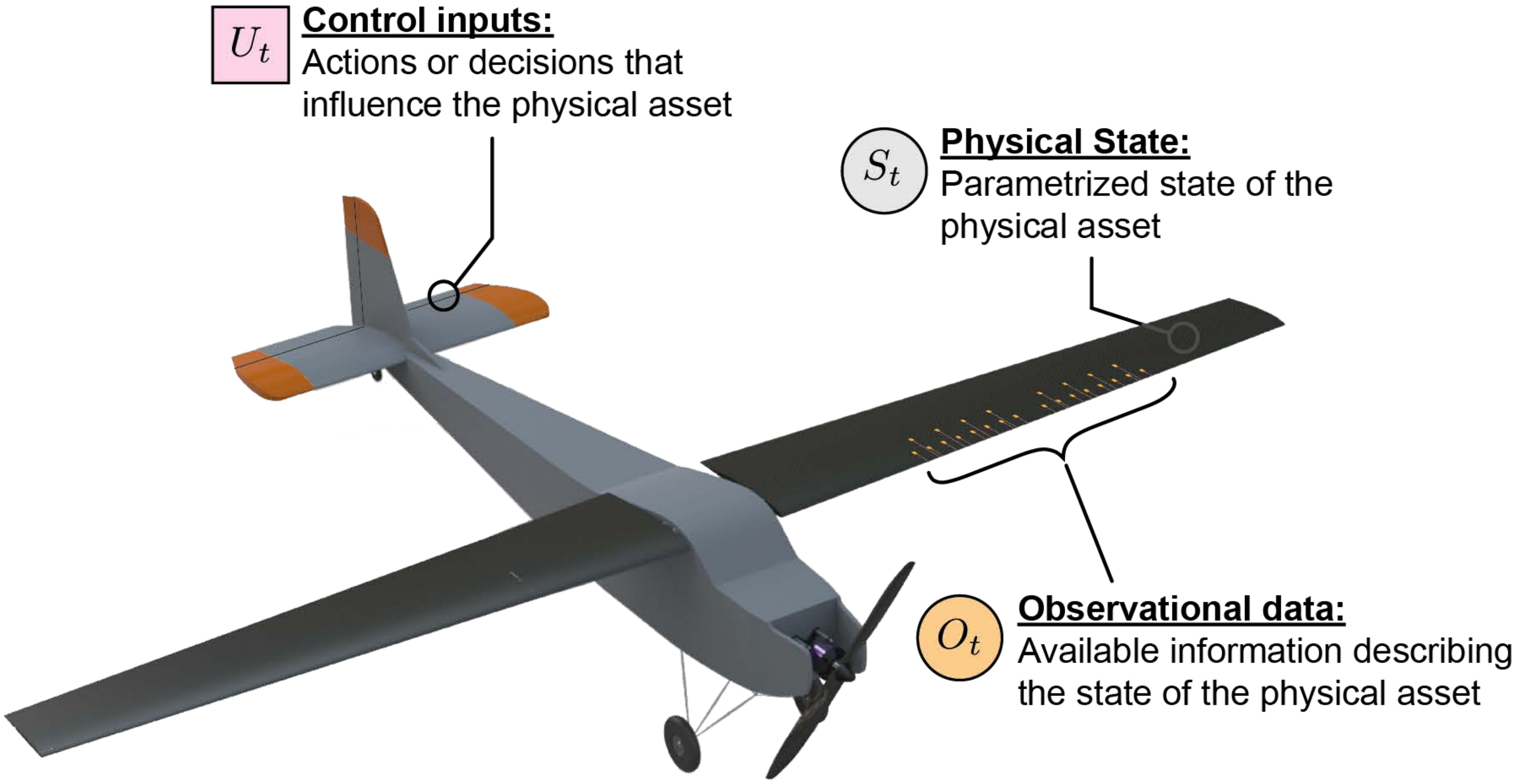
2 **Probabilistic Graphical Model**

How do these quantities interact and evolve?

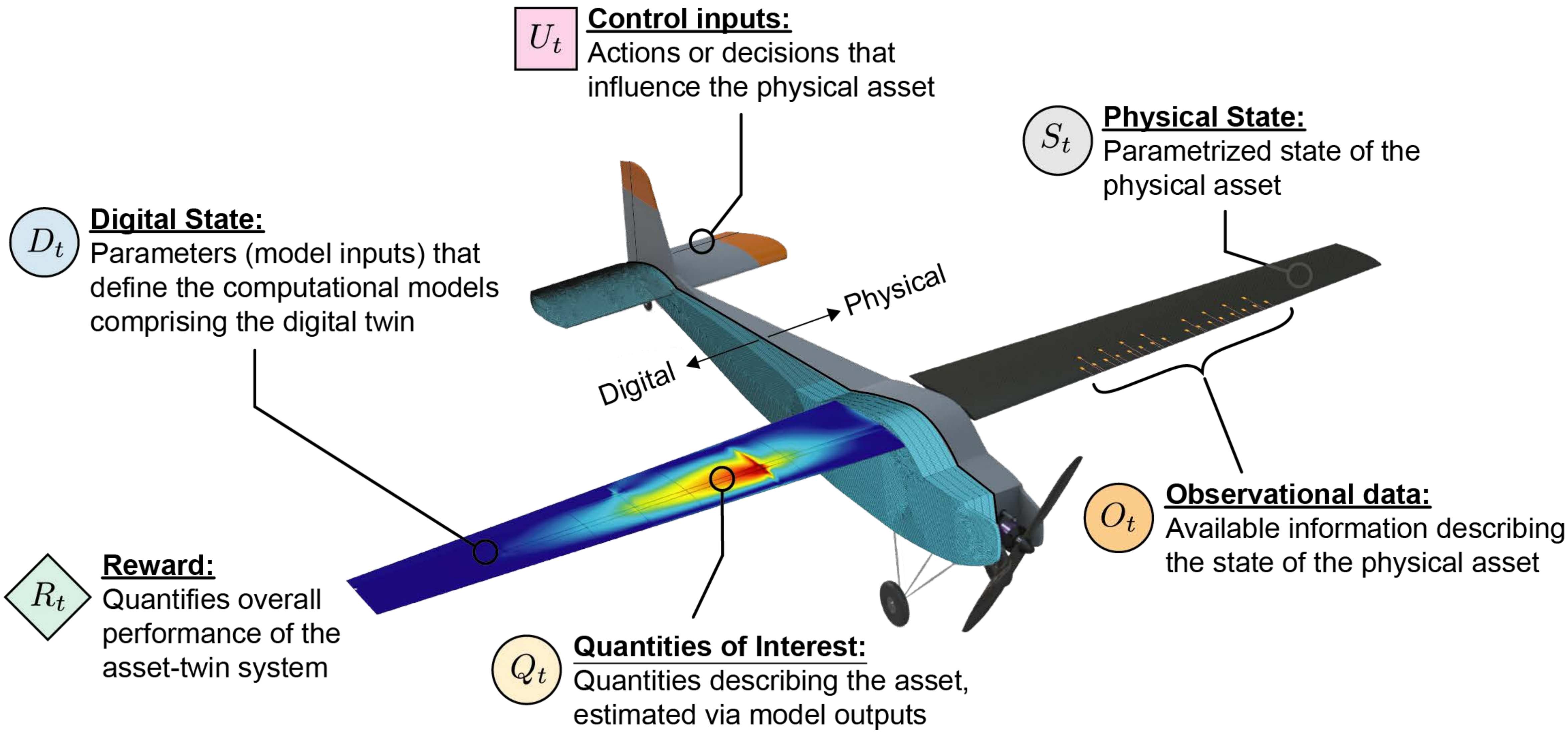
3 **Demonstration: UAV Structural Digital Twin**

Modular, scalable algorithms for Bayesian inference, prediction, and decision-making.

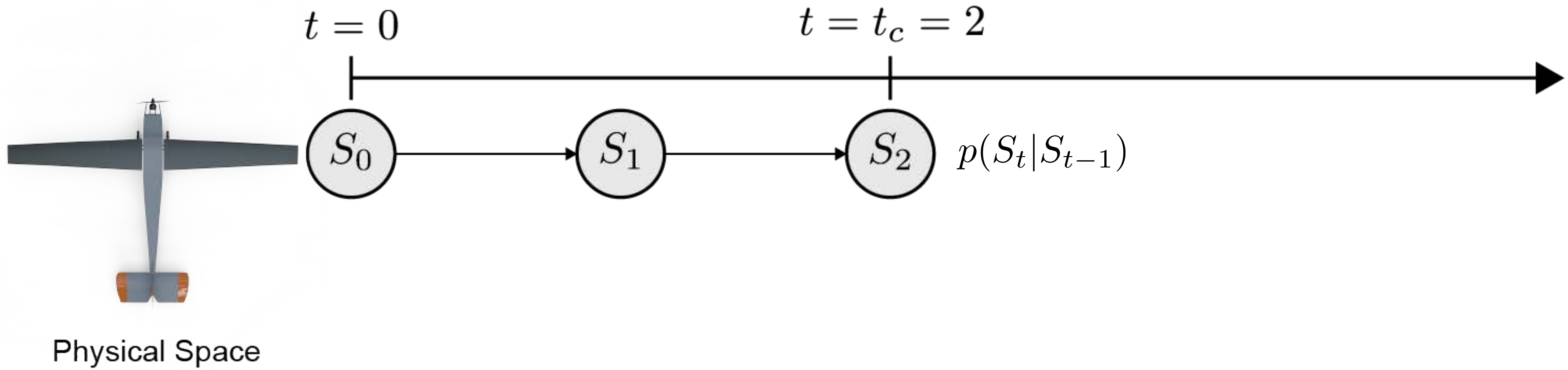
Mathematical abstraction of an asset-twin system



Mathematical abstraction of an asset-twin system



A probabilistic graphical model for the asset-twin system



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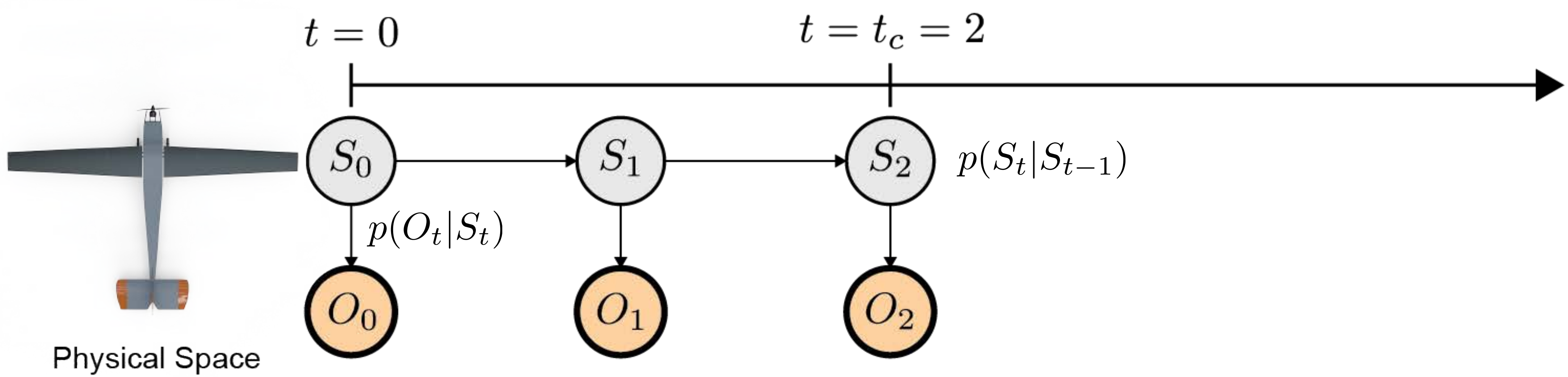

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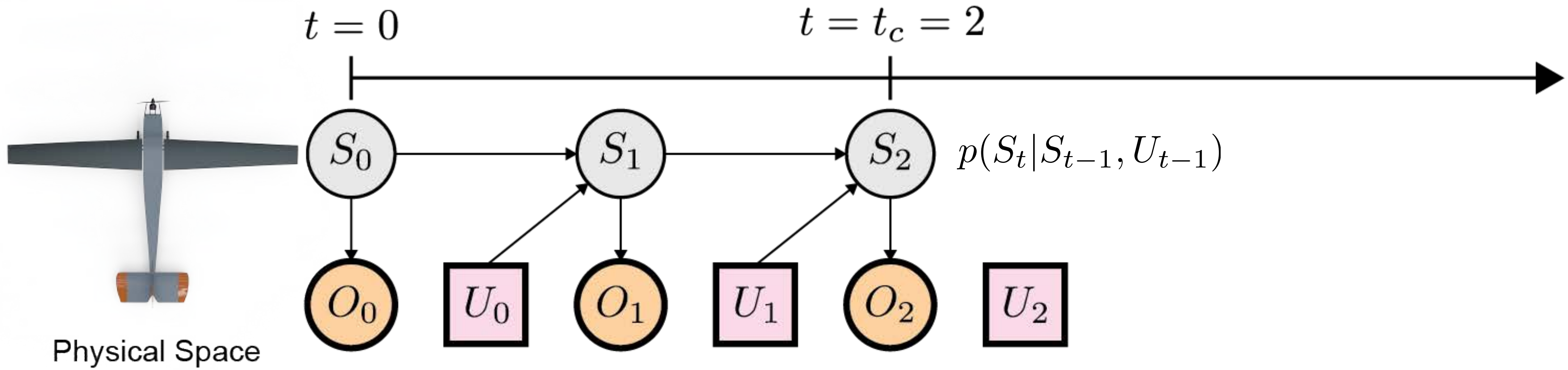

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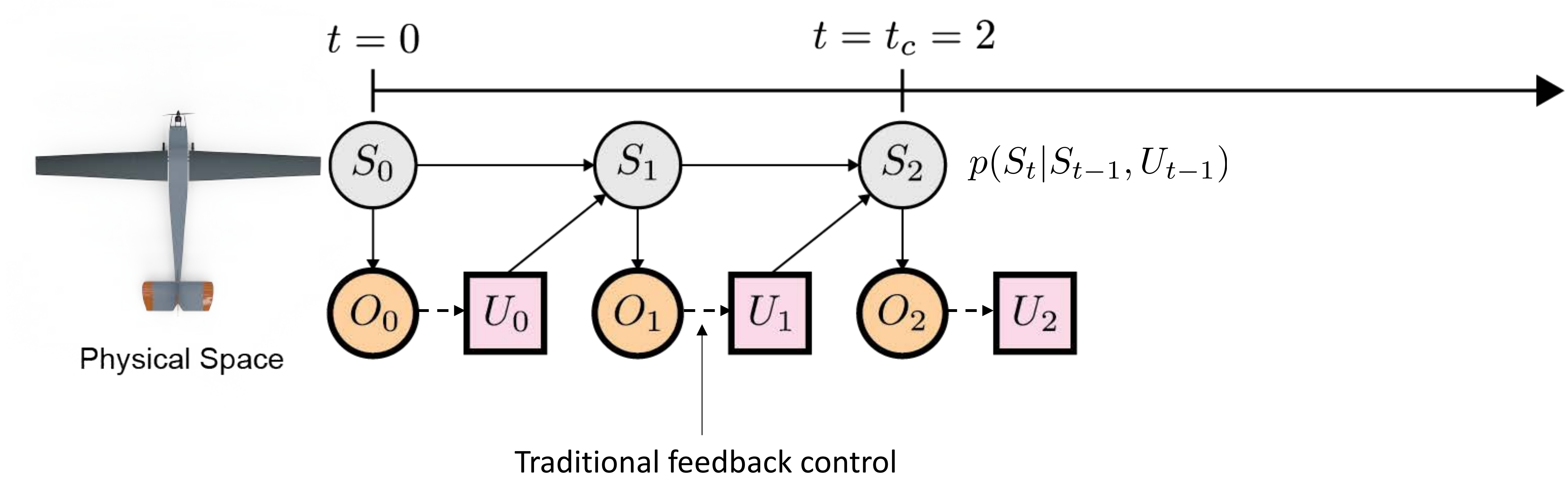

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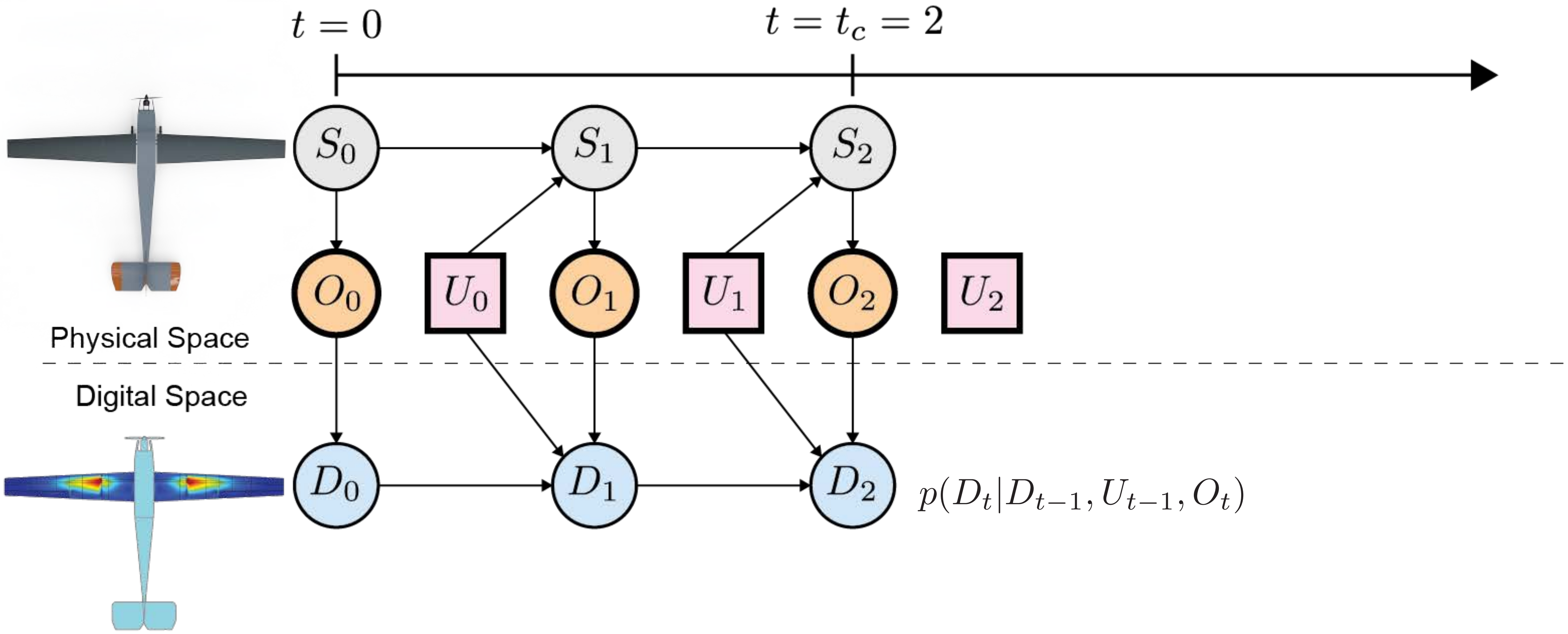

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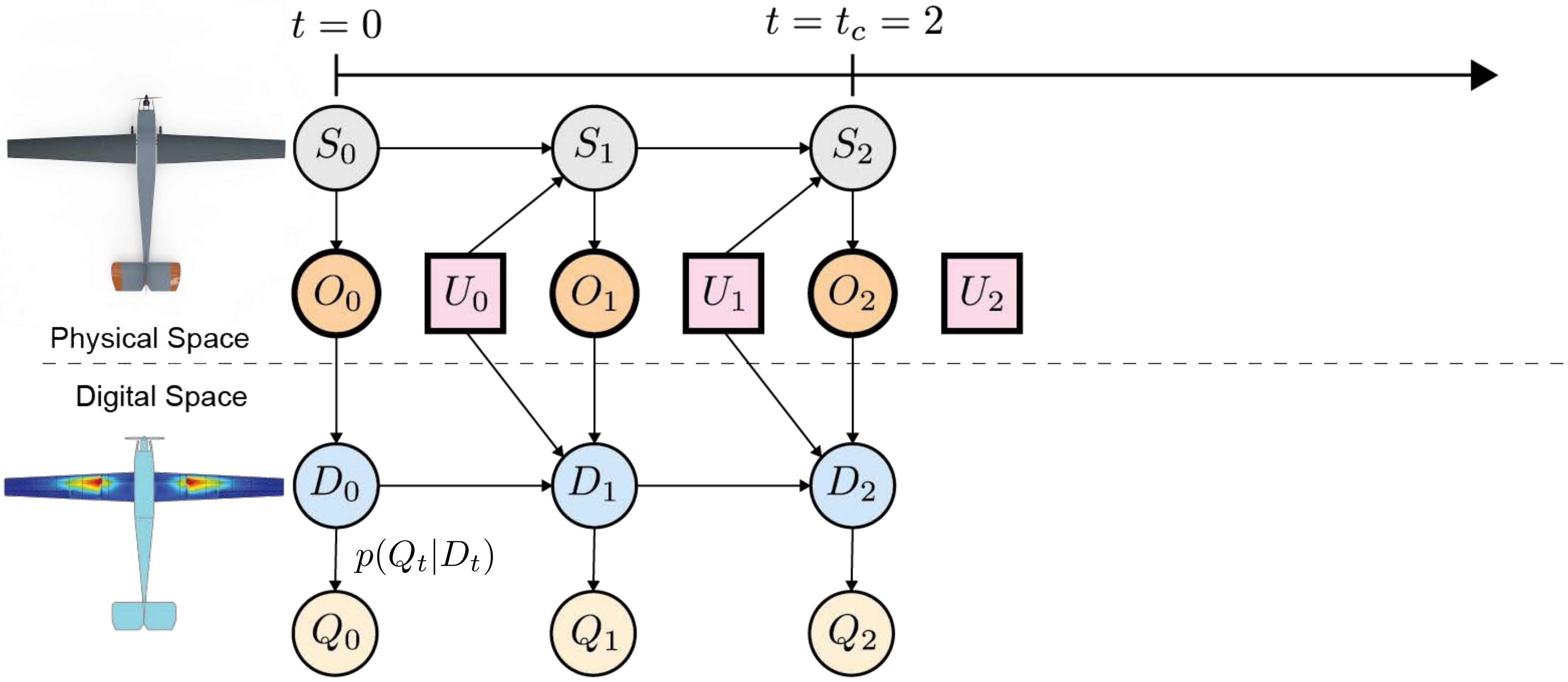

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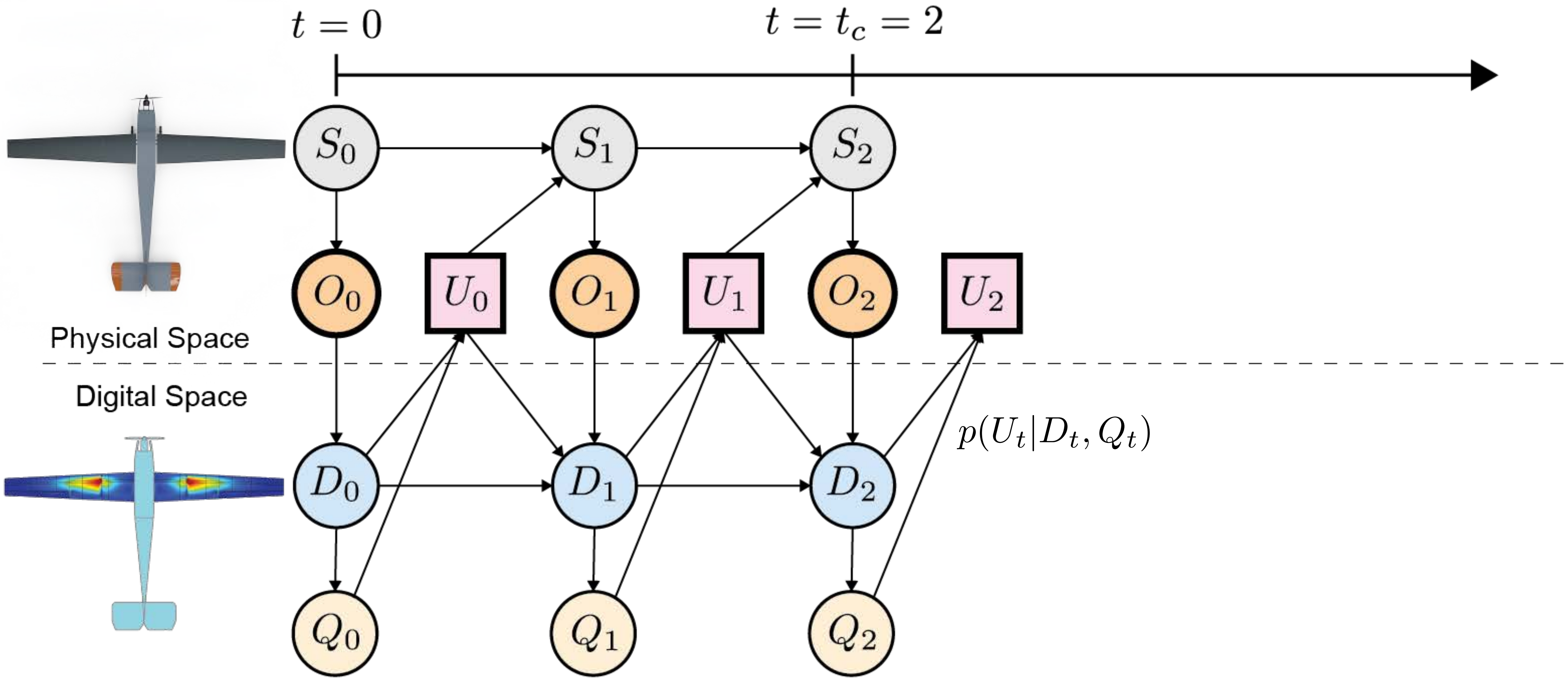

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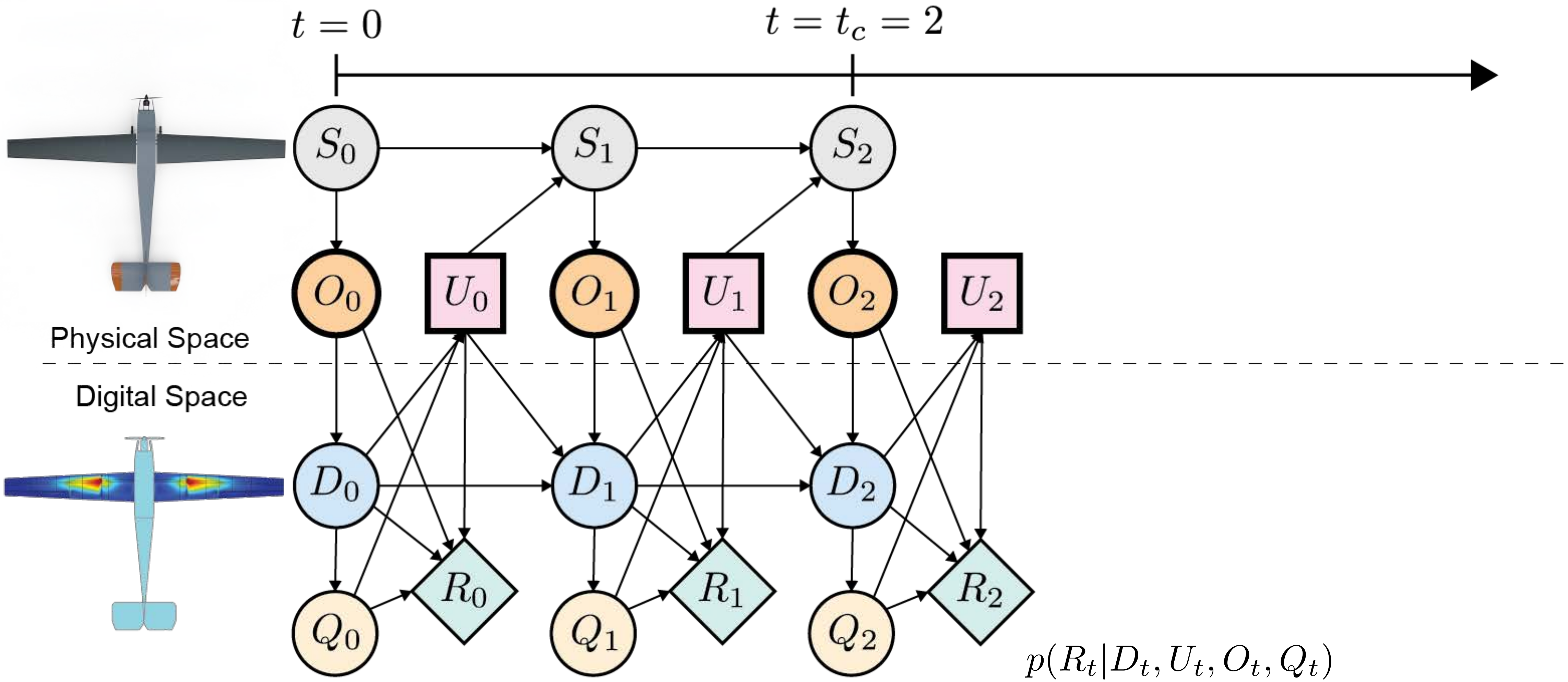

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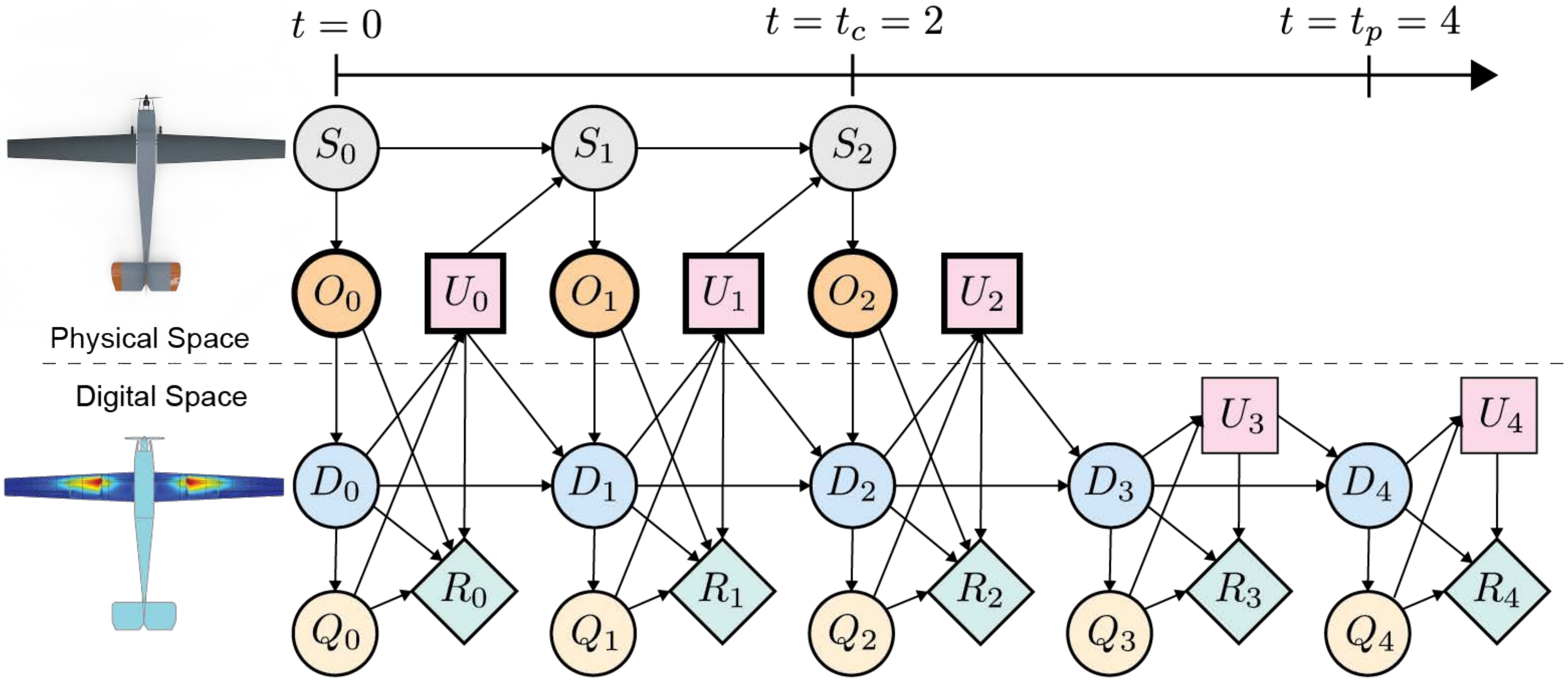
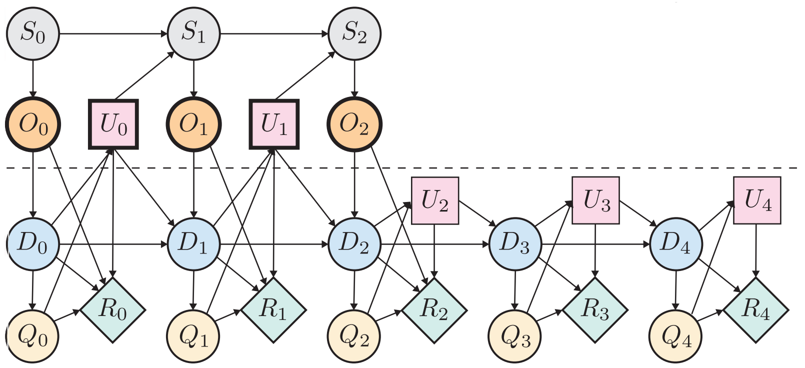


Mathematically defining the models comprising a digital twin

- Assumptions encoded in the model:
  - Markovian dynamics for both physical state and digital state
  - Cannot directly observe physical state
  - Control inputs are informed by digital twin analysis



- Conditional independence structure of the graph admits a factorization of the belief state:

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

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

digital state transition

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

quantities of interest

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

rewards

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

assimilation

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

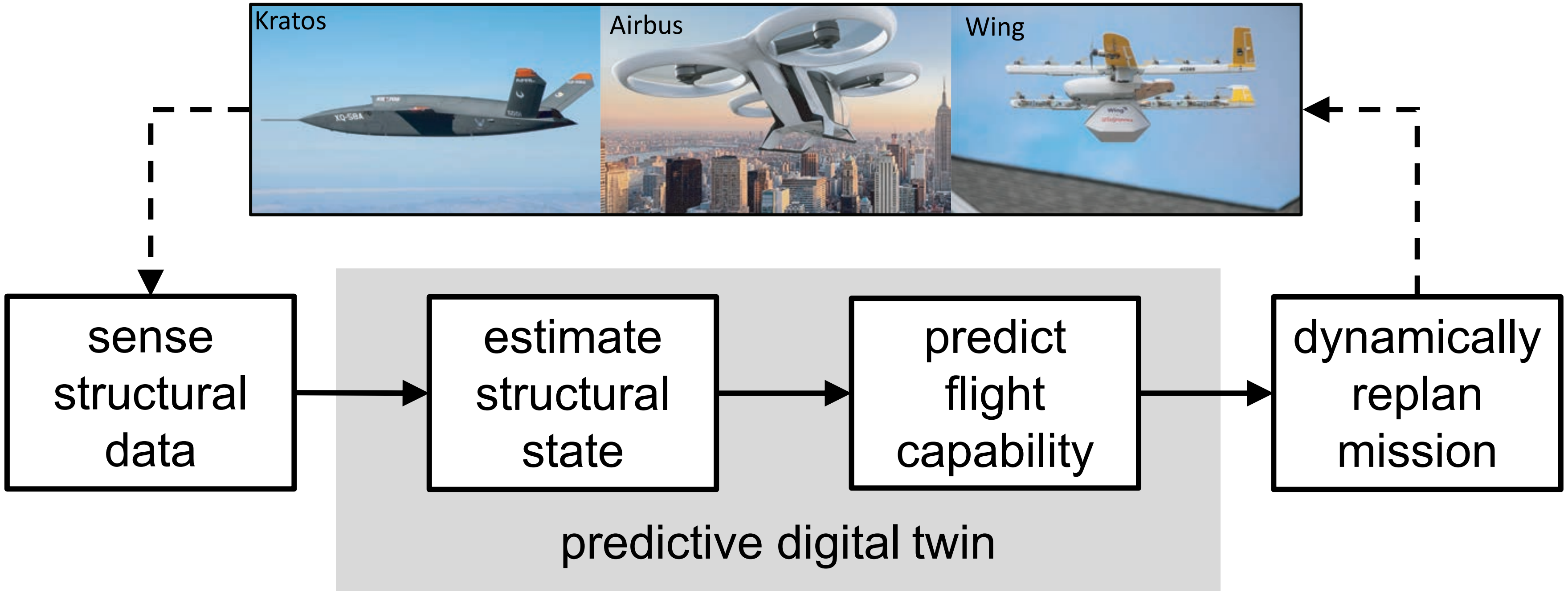
control

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

Unifying digital twin functionality via inference and optimization

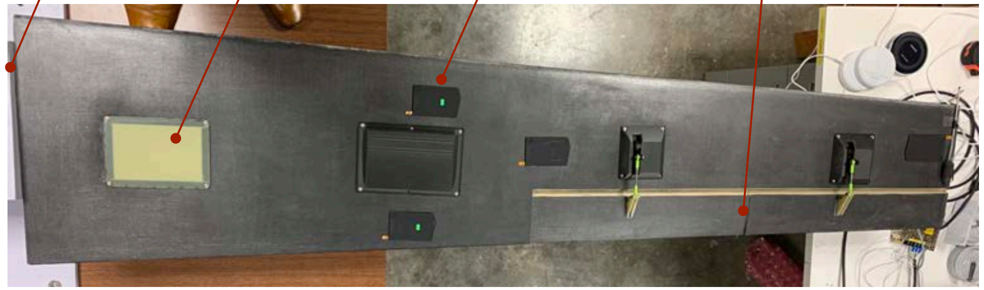
Digital twin use-case	Mathematical formulation via probabilistic graphical model
Automatic monitoring, virtual inspections, simulation-based certification	Data Assimilation: $p(D_{t_c}, Q_{t_c}, R_{t_c} \mid u_0, \ldots u_{t_c}, o_0, \ldots o_{t_c})$
Forecasting, planning, predictive maintenance	Prediction: $p(D_{t_p}, Q_{t_p}, R_{t_p} \mid u_0, \ldots u_{t_c}, o_0, \ldots o_{t_c})$
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: $\phi_t^{\text{dynamics}} = p(D_t \mid D_{t-1}, U_t)$ $\phi_t^{\text{assimilation}} = p(O_t \mid D_t)$ $\vdots$

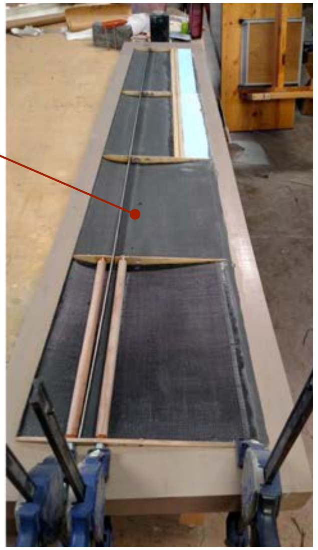
Demonstration:
Creating and evolving a structural digital twin
for a self-aware unmanned aerial vehicle

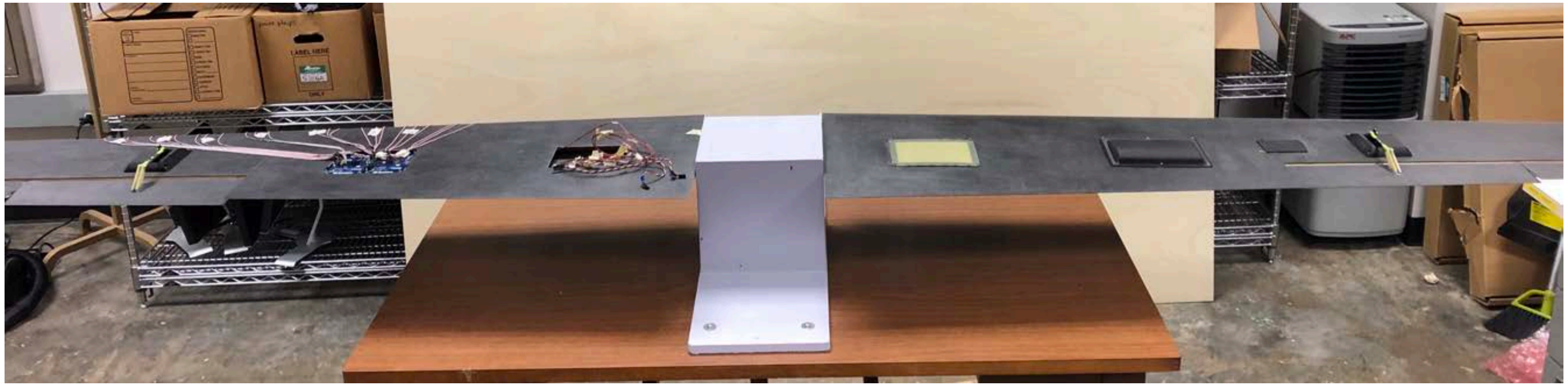


Goal: Create a **digital twin** that adapts to the **evolving structural health** of a UAV, providing **near real-time capability estimates** that **enable dynamic decision making.**

Hardware Testbed:
Customized 12ft Telemaster aircraft







Physics-based 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

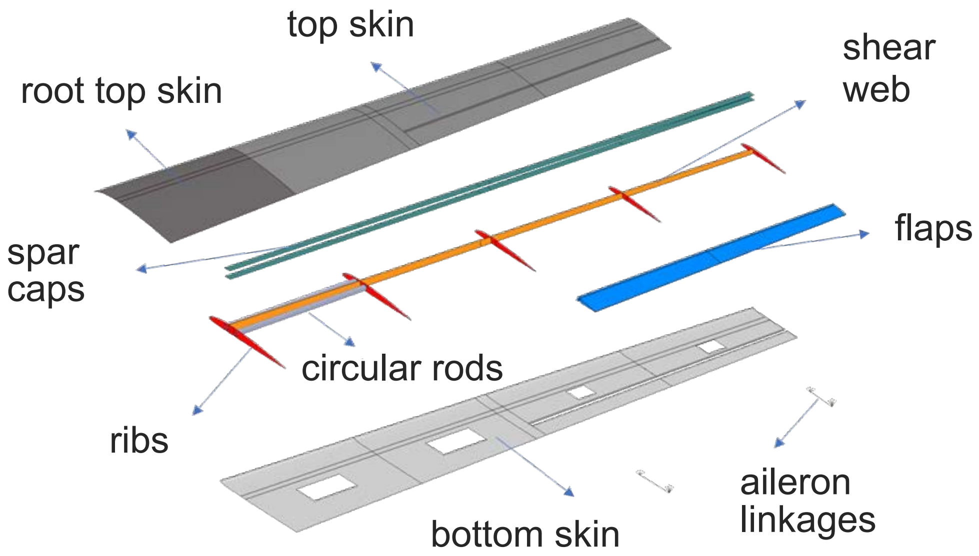
$$\varepsilon = \frac{1}{2}[\nabla u + (\nabla u)^{\top}]$$

strain-displacement equations

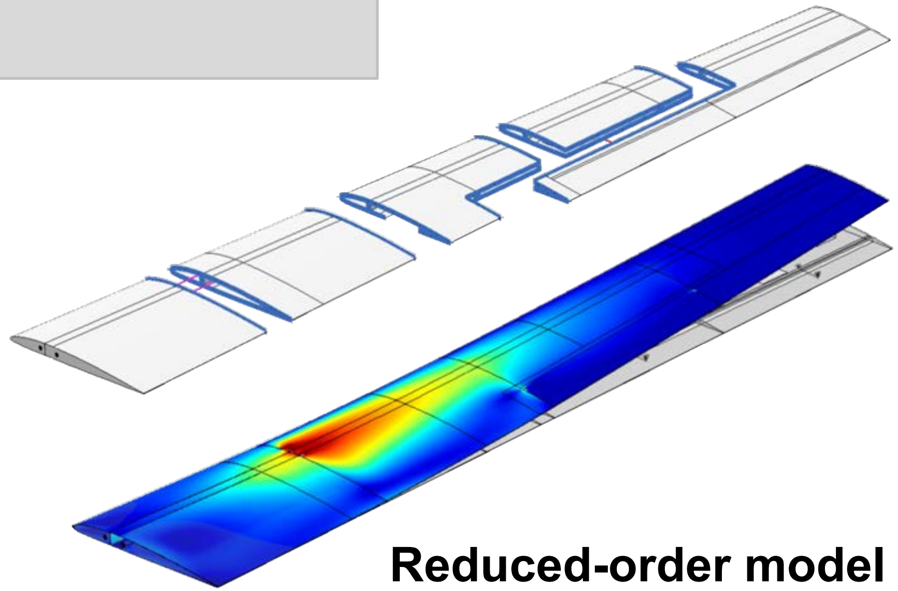
$$\sigma = C : \varepsilon$$

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)

Phase 1: **baseline model** to **calibrated digital twin** via **principled and repeatable Bayesian calibration**

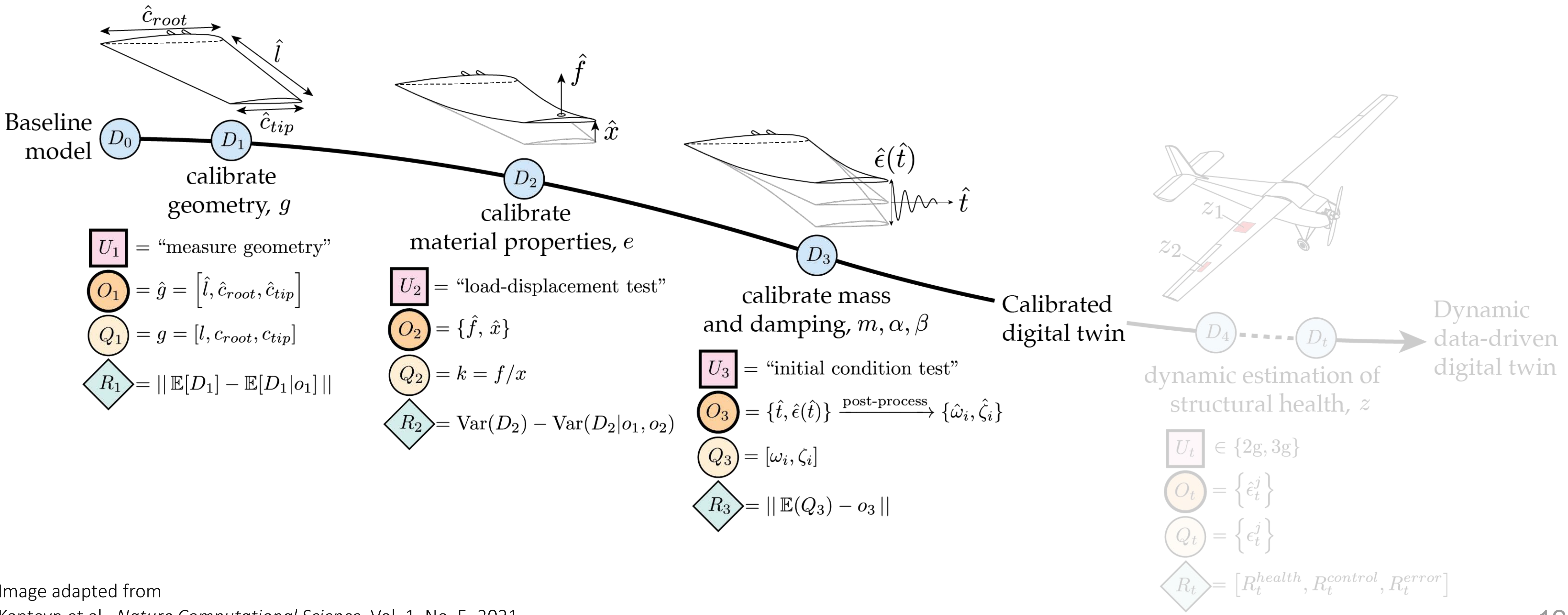


Image adapted from
Kapteyn et al., *Nature Computational Science*, Vol. 1, No. 5, 2021.

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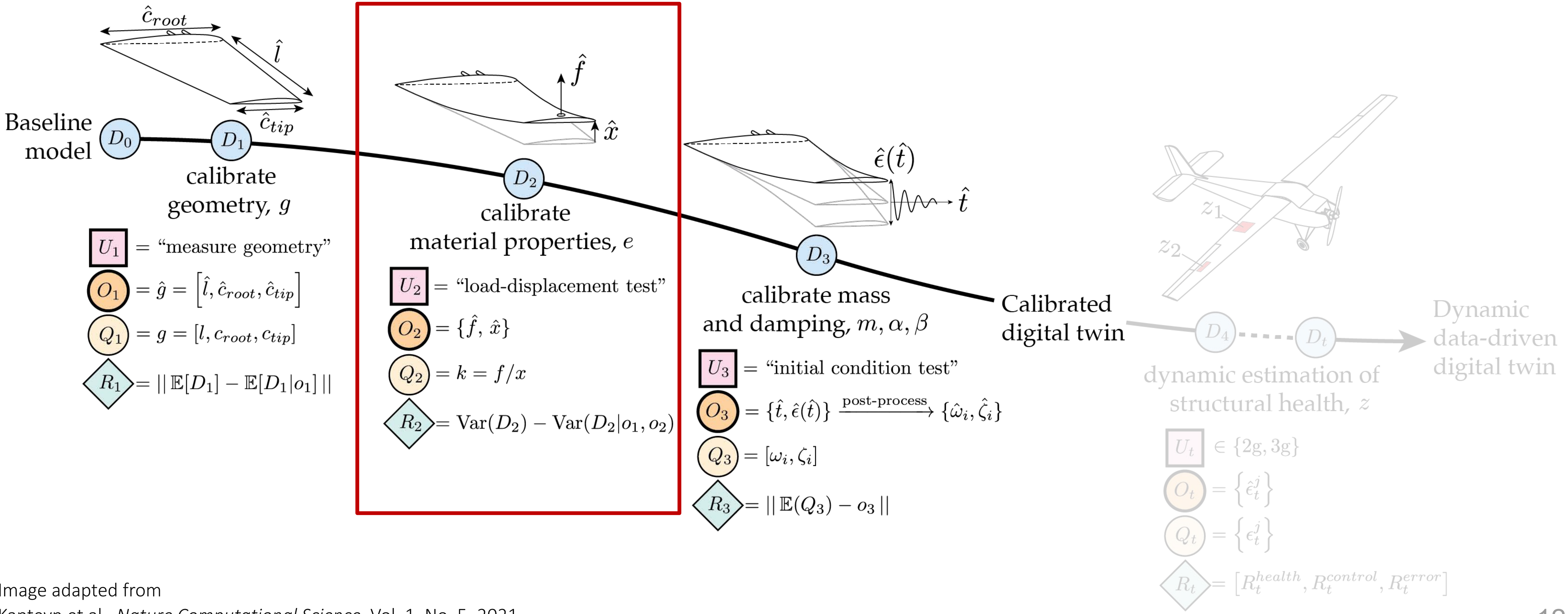

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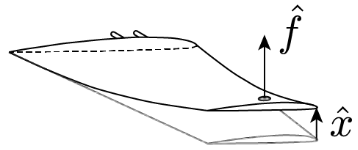
D_2

Digital state
(model input space)



D_2

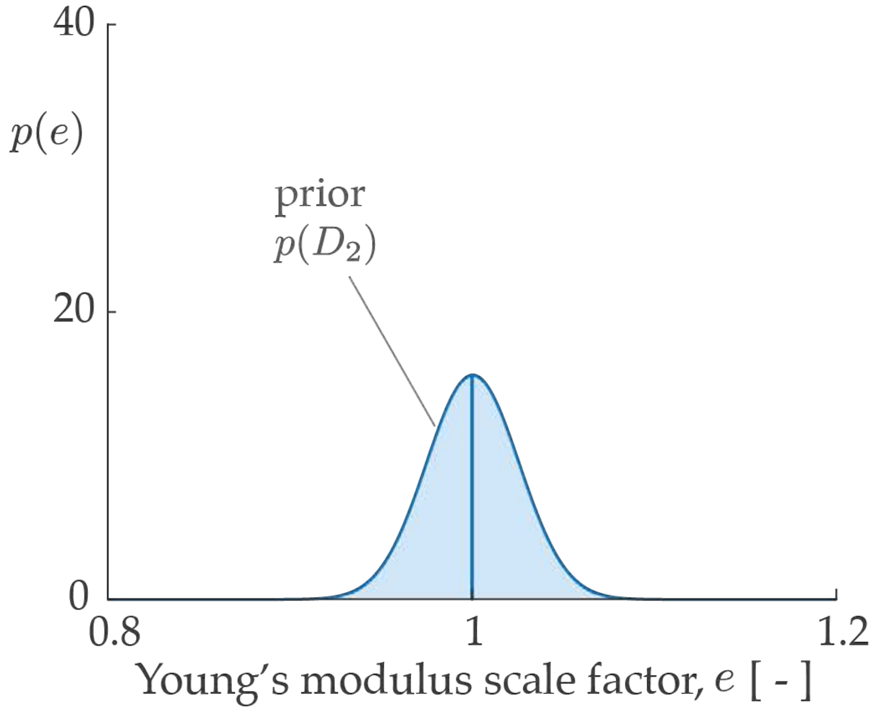
calibrate
material properties, e

U_2 = "load-displacement test"

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

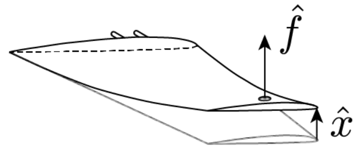
Q_2 = $k = f/x$

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



- Gaussian prior for the Young's modulus (based on UAV material specifications)

D_1



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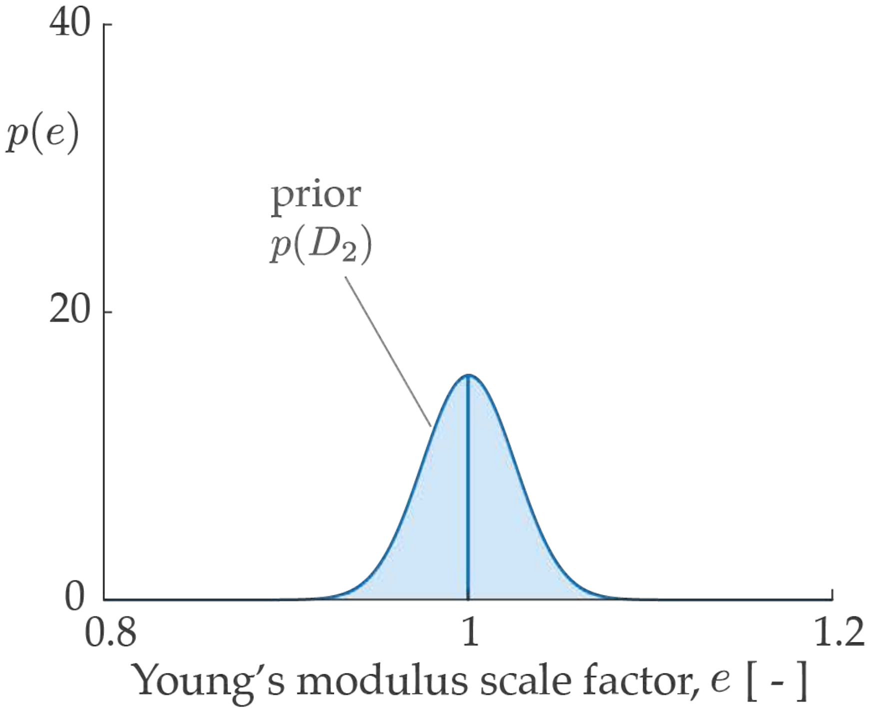
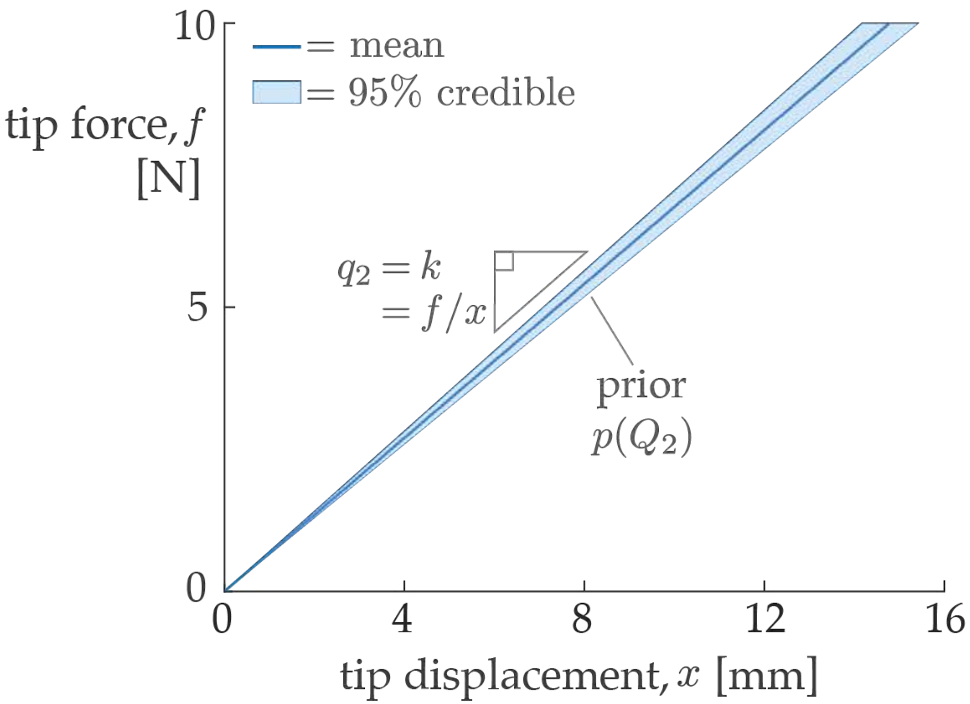
D_2 Digital state (model input space) $\xrightarrow{\text{structural model } \mathrm{K}(\mu)\mathbf{x} = \mathbf{f}}$ Q_2 Quantity of interest (model output space)





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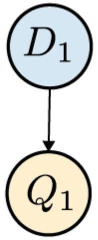

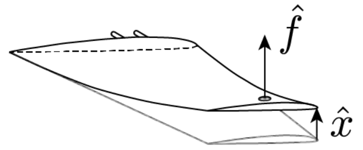

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calibrate material properties, e

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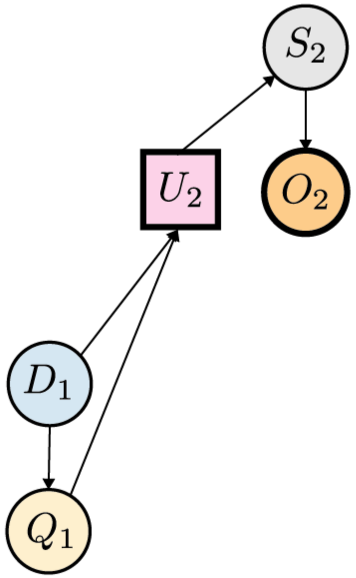


D_2

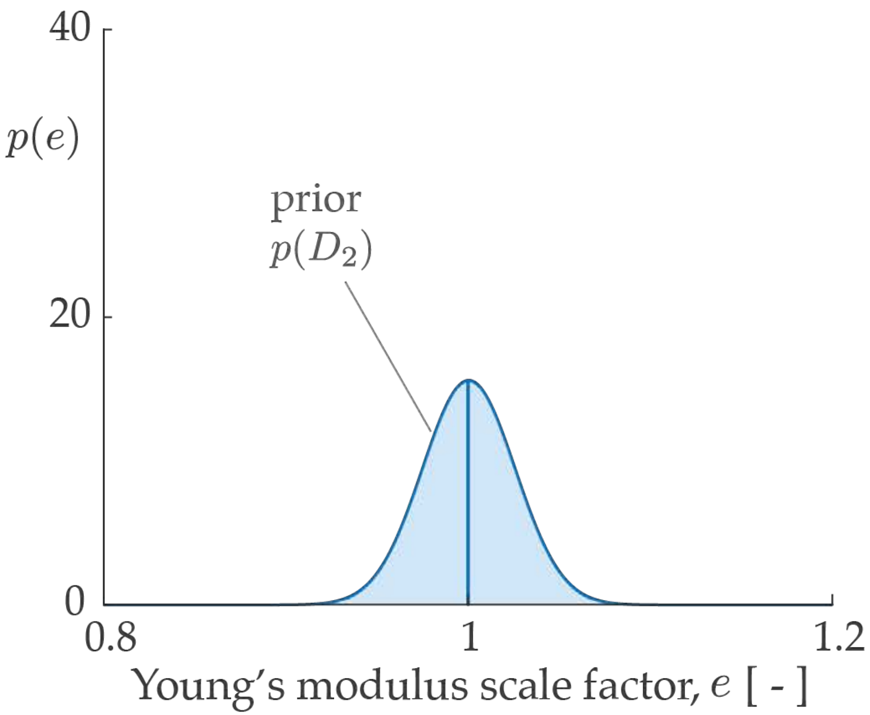
Digital state (model input space)

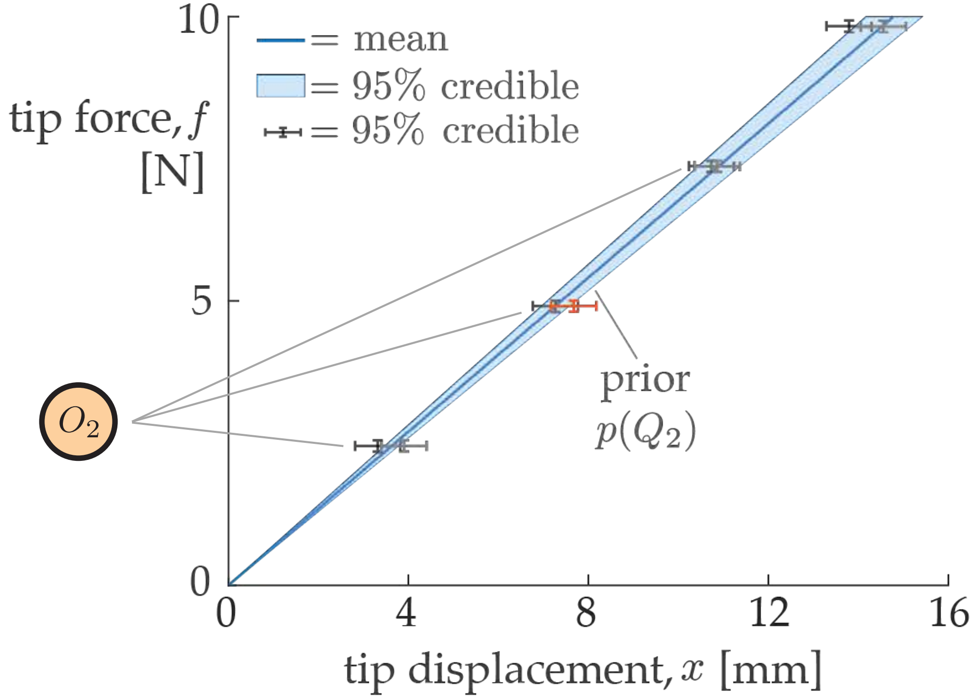
structural model

$\mathrm{K}(\mu)\mathbf{x} = \mathbf{f}$

Q_2

Quantity of interest (model output space)





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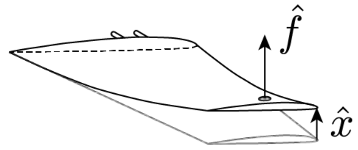

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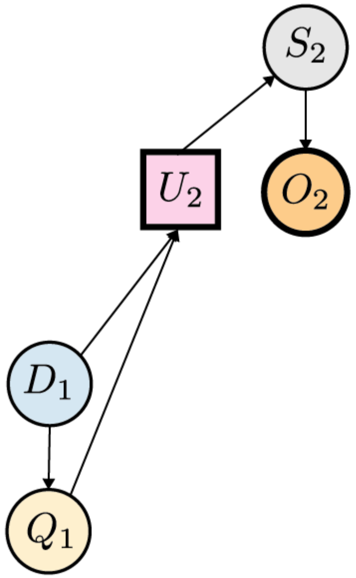
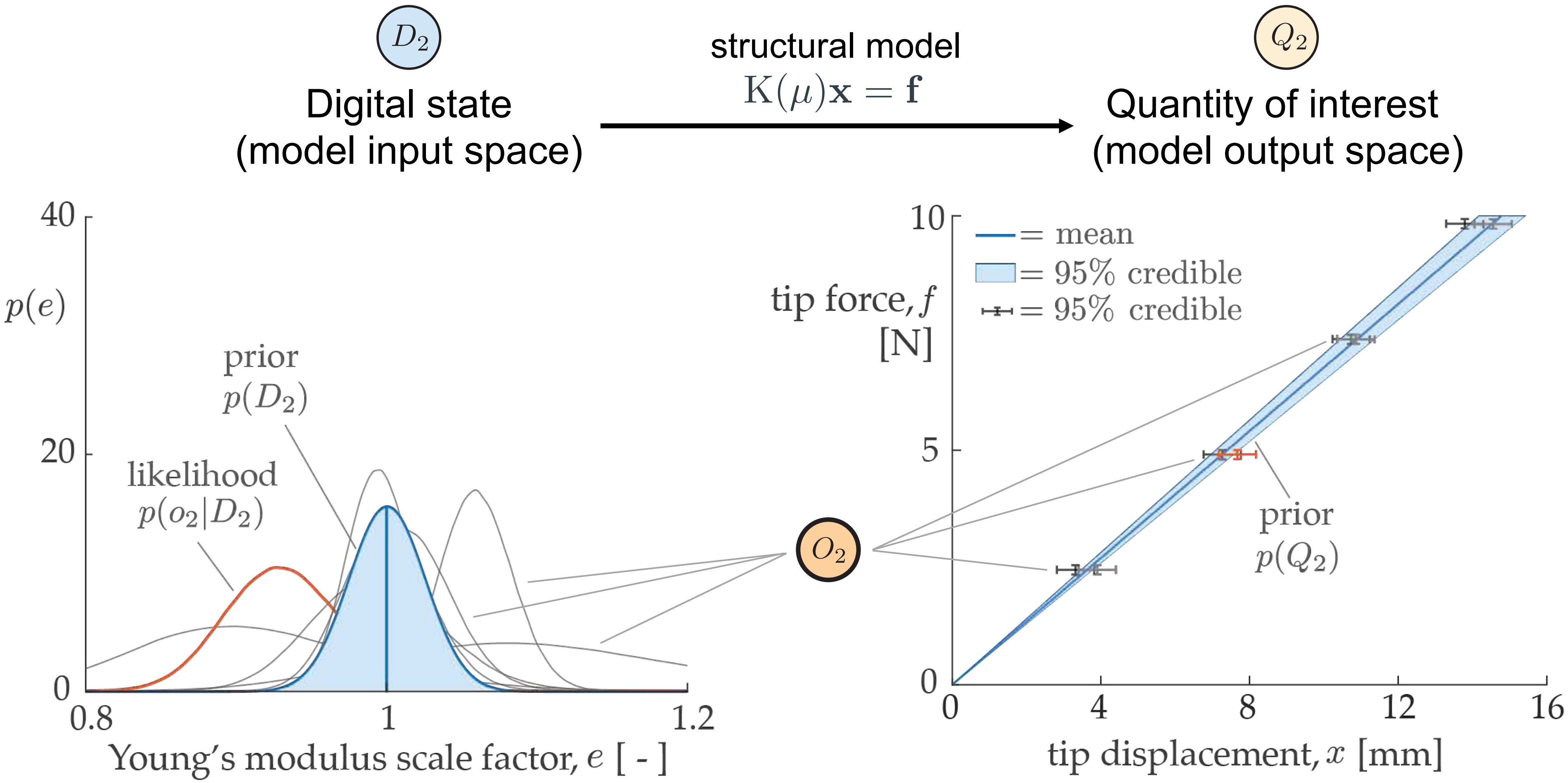
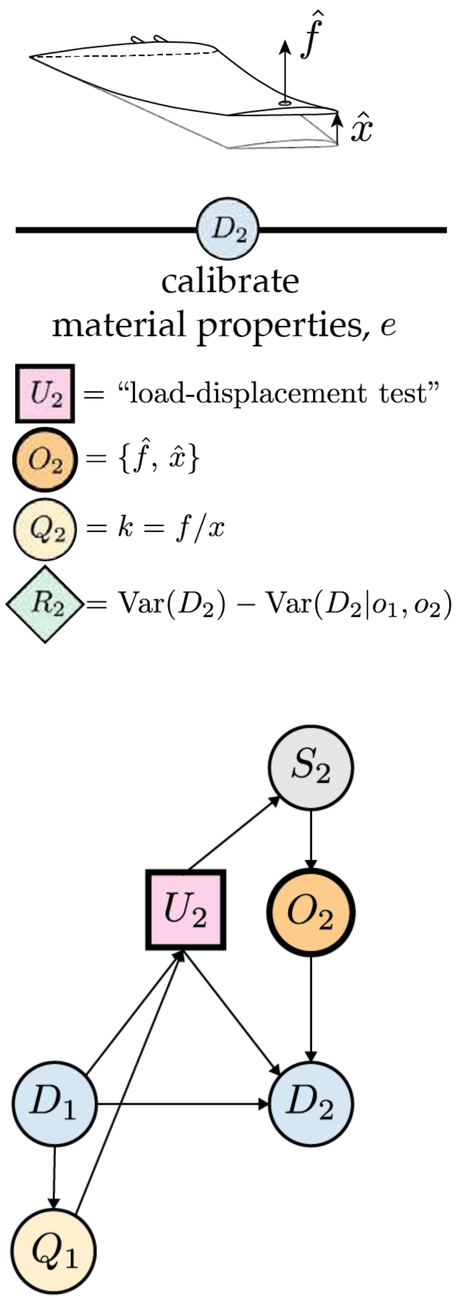
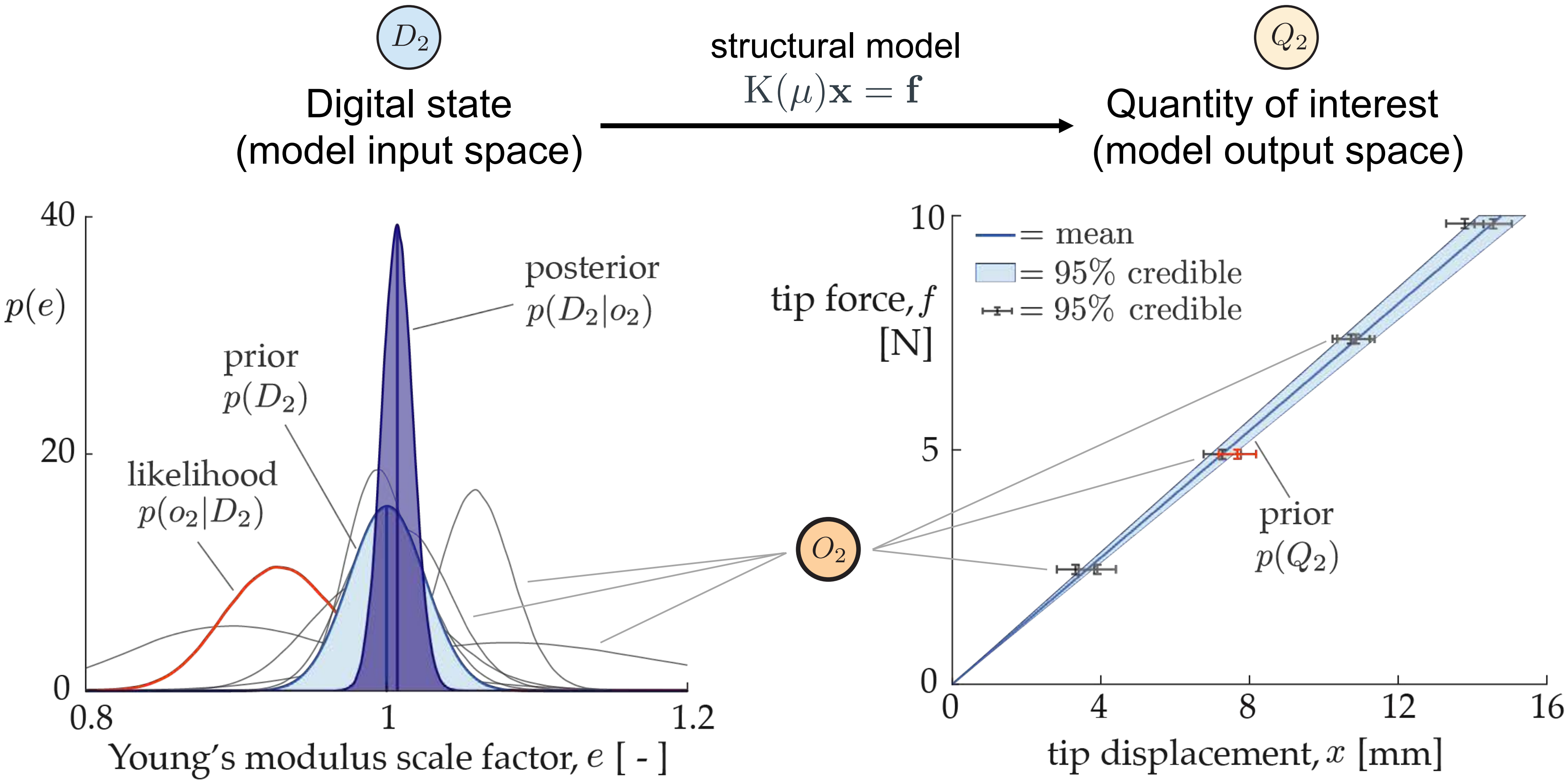


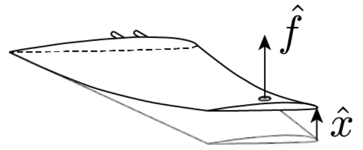


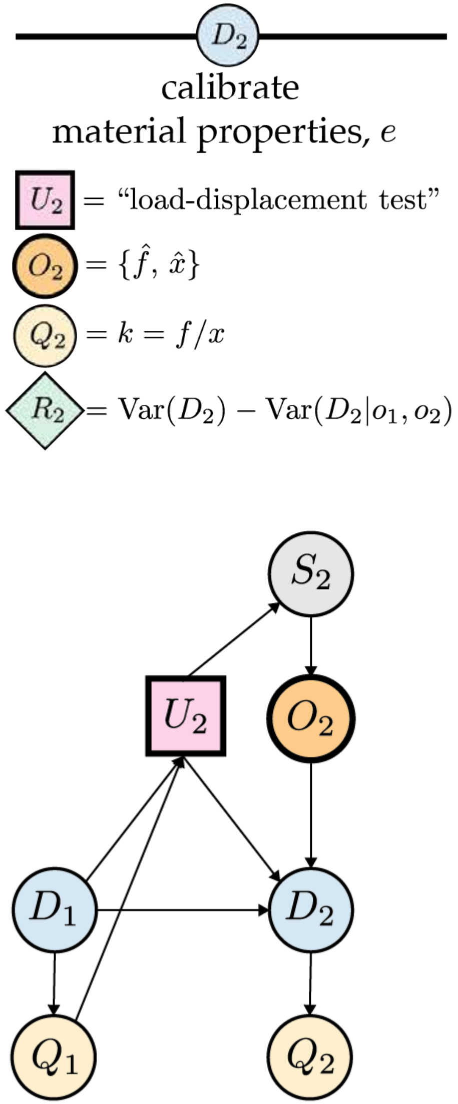
- Gaussian prior for the Young's modulus (based on UAV material specifications)
- Likelihood (non-Gaussian) estimated by sampling + kernel density estimation

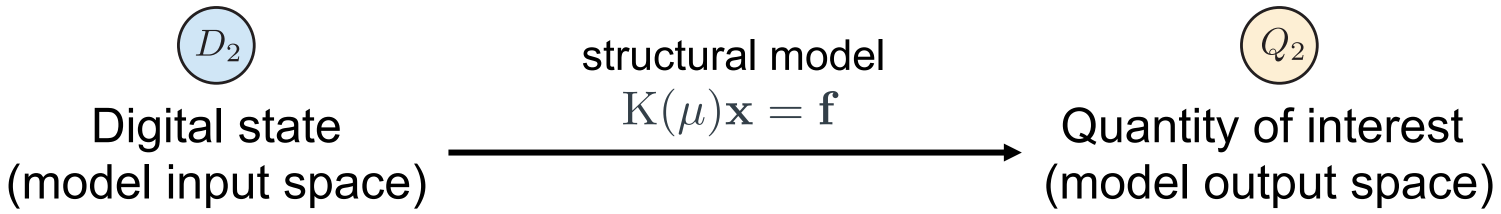


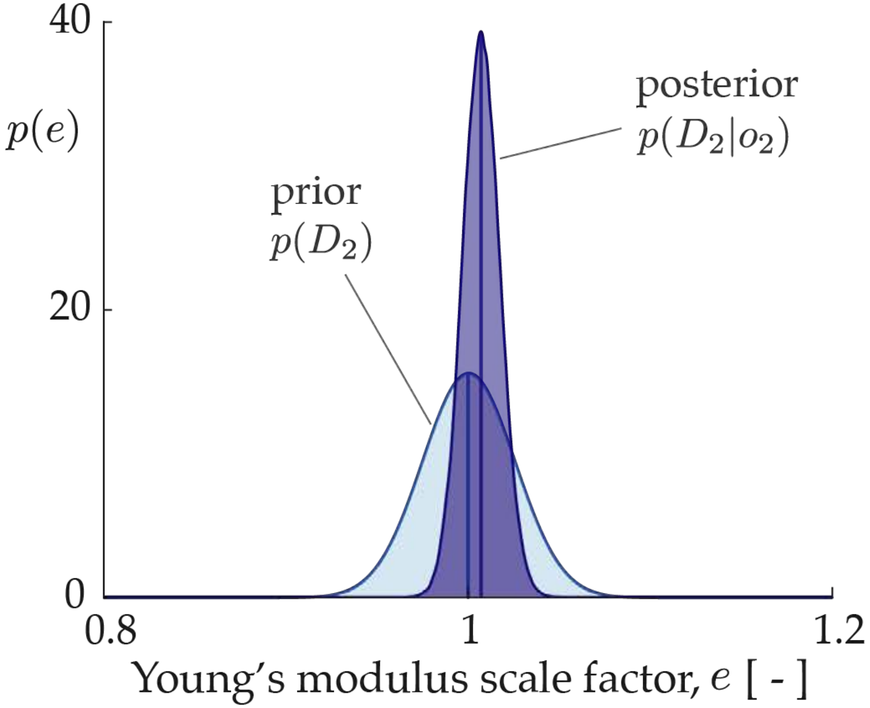


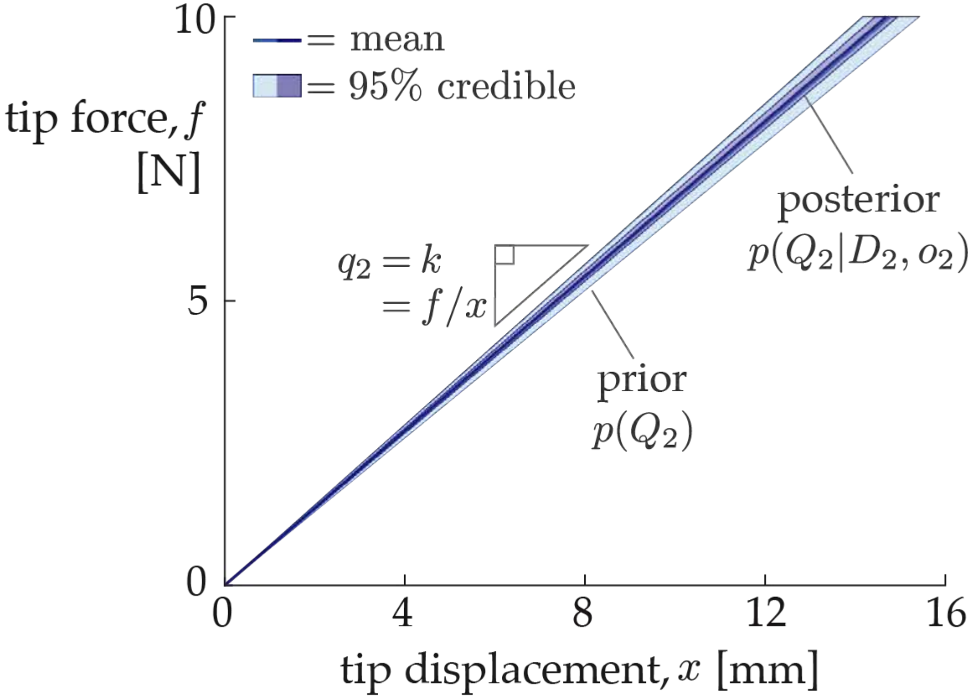
- Gaussian prior for the Young's modulus (based on UAV material specifications)
- Likelihood (non-Gaussian) estimated by sampling + kernel density estimation
- Bayesian update via particle filter ➞ posterior calibrated to as-manufactured UAV











- Gaussian prior for the Young's modulus (based on UAV material specifications)
- Likelihood (non-Gaussian) estimated by sampling + kernel density estimation
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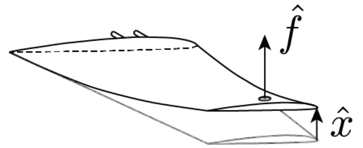
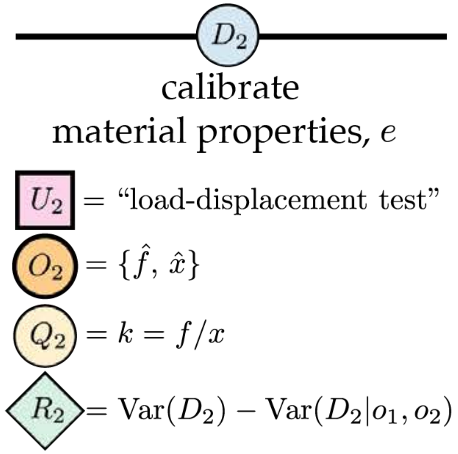
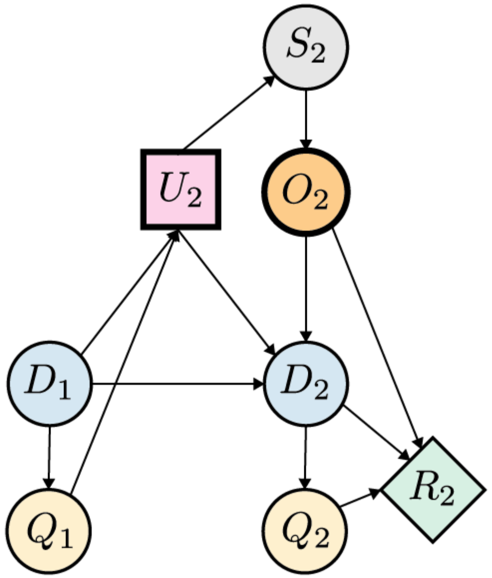
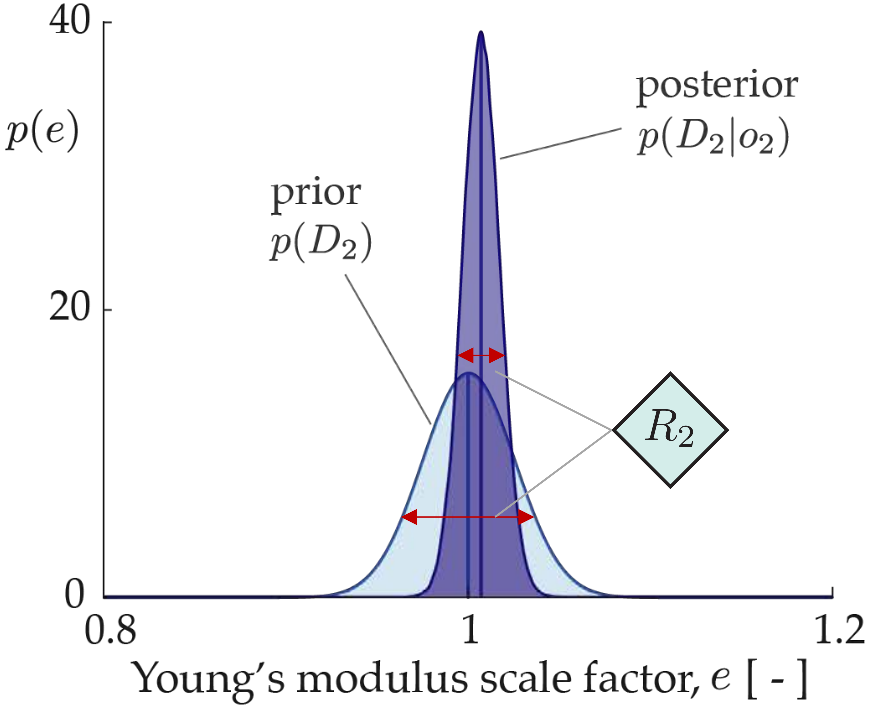
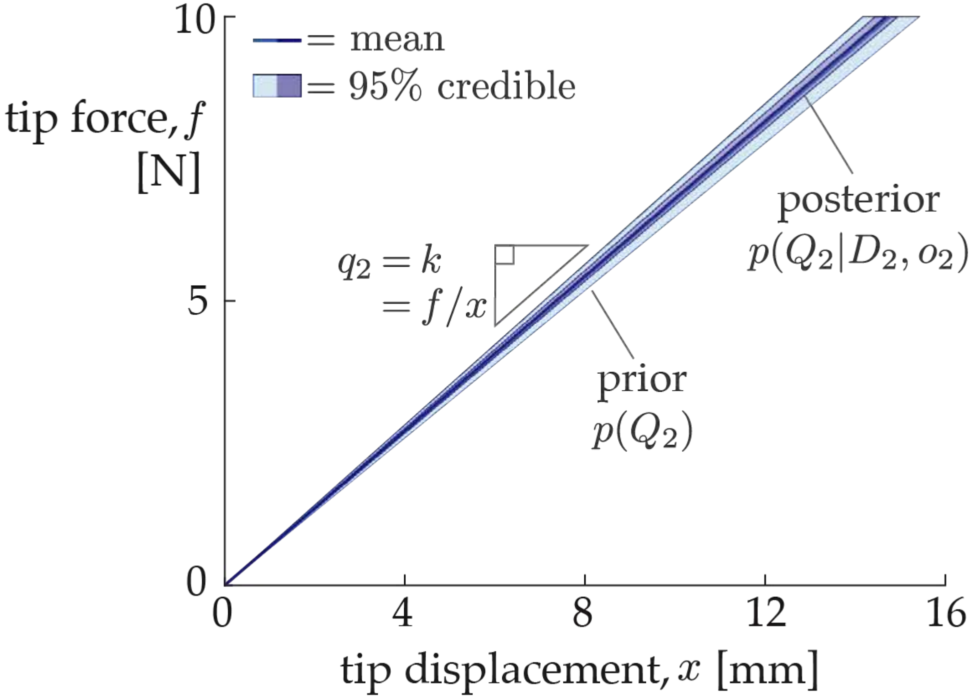
D_2 Digital state (model input space) —— structural model $\mathrm{K}(\mu)\mathbf{x} = \mathbf{f}$ ——→ Q_2 Quantity of interest (model output space)











- Gaussian prior for the Young's modulus (based on UAV material specifications)
- Likelihood (non-Gaussian) estimated by sampling + kernel density estimation
- Bayesian update via particle filter ⟶ posterior calibrated to as-manufactured UAV
- Reward measures reduction in variance achieved via calibration

Phase 2: Leverage the **calibrated reduced-order models** for **data-driven health monitoring** and **self-aware decision making**

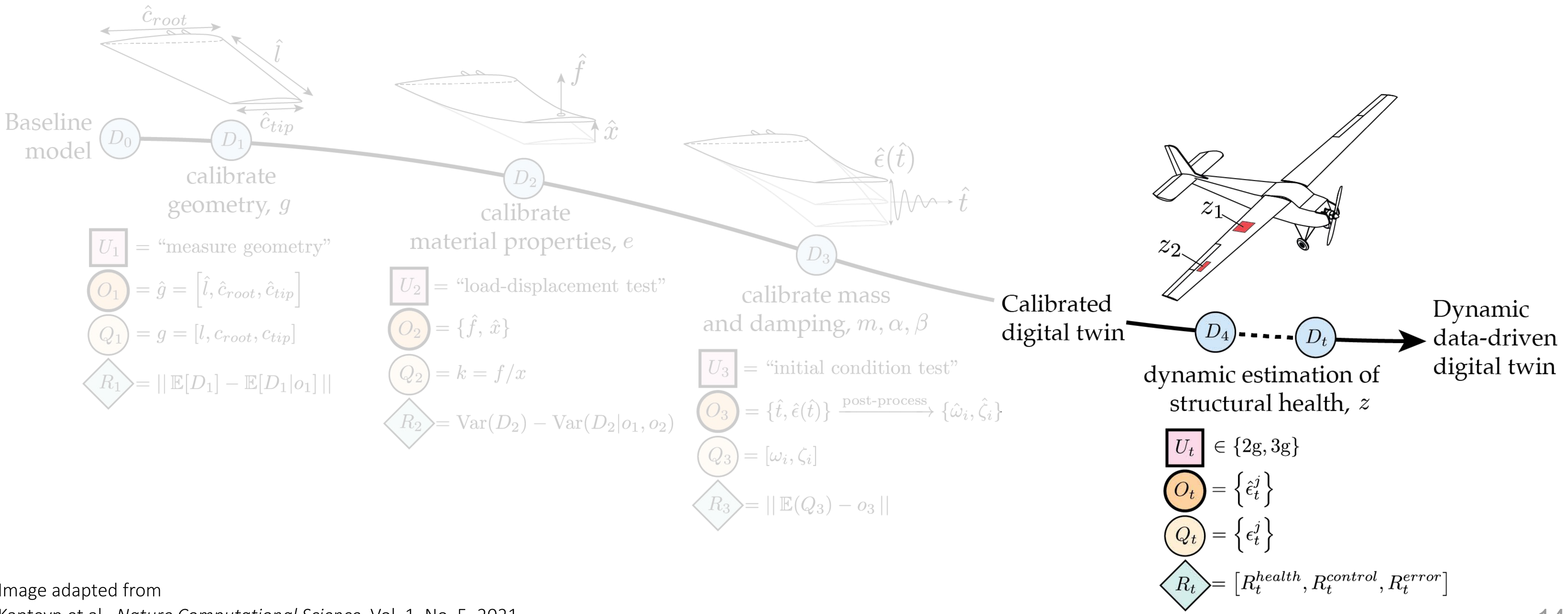
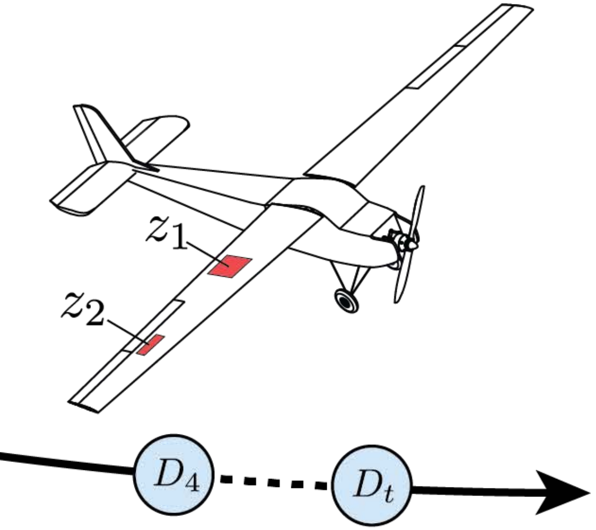


Image adapted from
Kapteyn et al., *Nature Computational Science*, Vol. 1, No. 5, 2021.

Simulated self-aware UAV demonstration



dynamic estimation of structural health, z

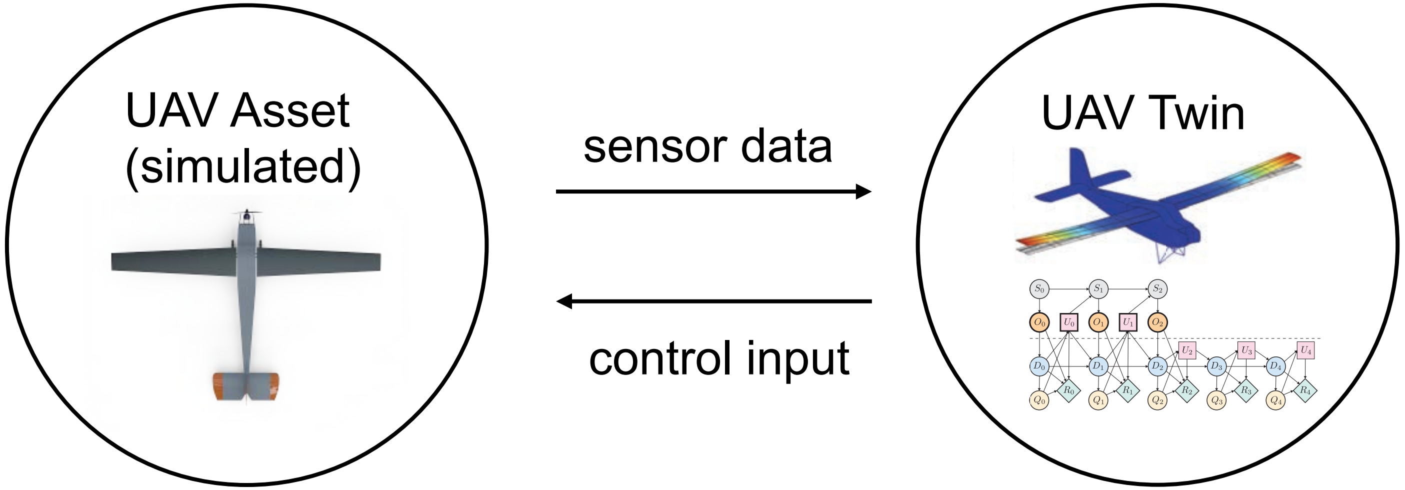
$U_t \in \{2\text{g}, 3\text{g}\}$

$O_t = \left\{\hat{\epsilon}_t^j\right\}$

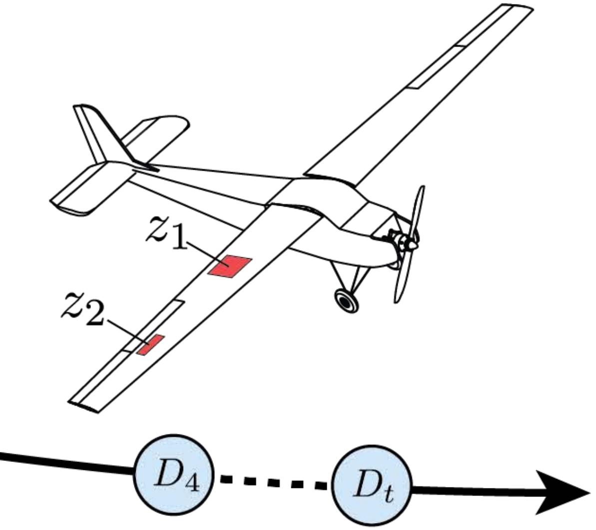
$Q_t = \left\{\epsilon_t^j\right\}$

$R_t = \left[R_t^{health}, R_t^{control}, R_t^{error}\right]$

- Aircraft performs a mission while undergoing in-flight structural health degradation
- 24 wing-mounted sensors provide noisy strain data
- Digital twin is dynamically updated and used to drive mission re-planning
- Scenario is simulated using ROS 2



Dynamic digital twin updating via sequential Bayesian inference



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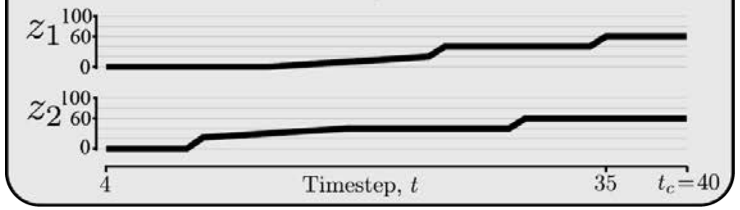
$R_t = \left[R_t^{health}, R_t^{control}, R_t^{error}\right]$

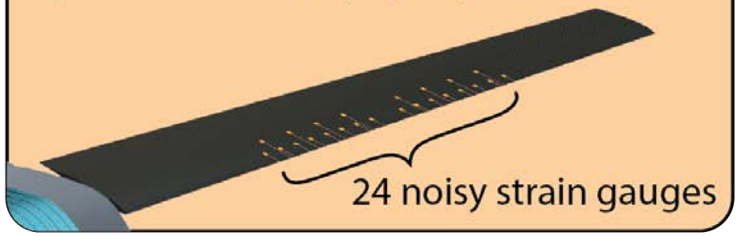
Aircraft undergoes prescribed in-flight structural health degradation (simulated)



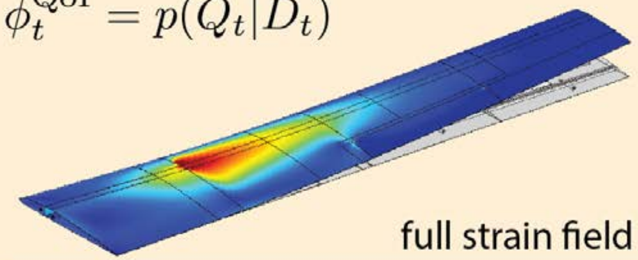
$\phi_t^{\text{dynamics}} = p(D_t | D_{t-1}, u_{t-1})$

$$p(z_i \text{ worsens by } 20\%) = \begin{cases} 5\% \text{ if } u_t = 2\text{g} \\ 10\% \text{ if } u_t = 3\text{g} \end{cases}$$

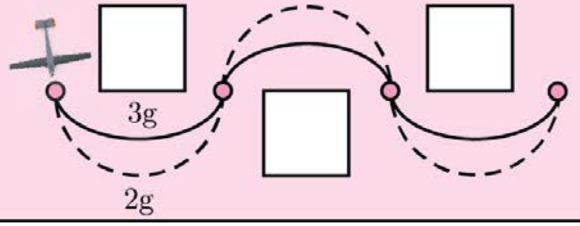
$\phi_t^{\text{assimilation}} = p(o_t | D_t)$



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



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



$\phi_t^{\text{evaluation}} = p(R_t | D_t, Q_t, u_t, o_t)$

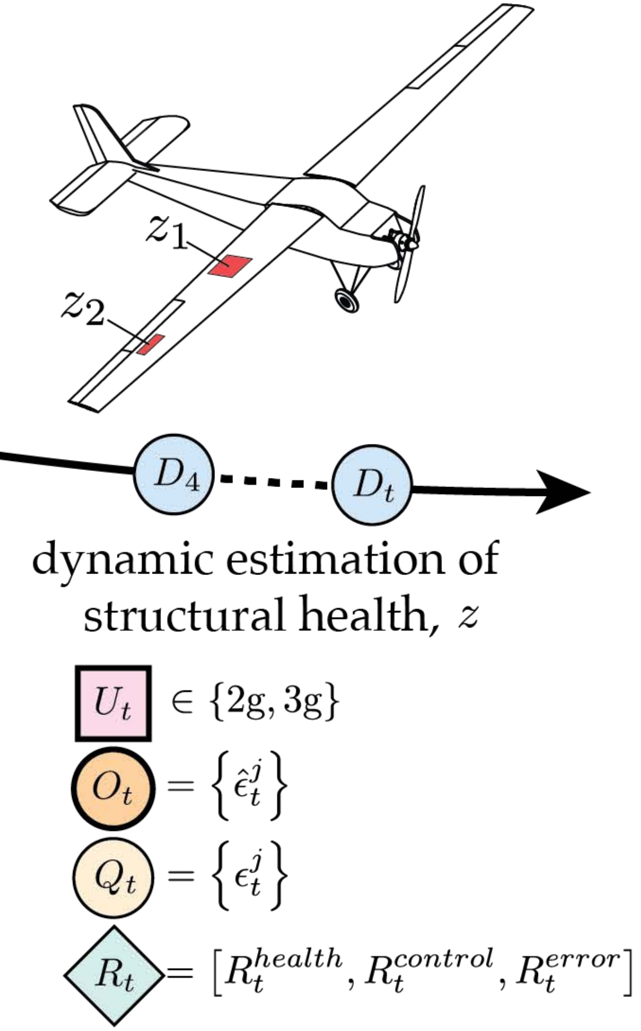
$$r_t^{health}(q_t) = \frac{\epsilon_{\max} - \max(\epsilon_t)}{\epsilon_{\max}}$$

$$r_t^{control}(u_t) = \begin{cases} 0.1 \text{ if } u_t = 3\text{g} \\ -0.1 \text{ if } u_t = 2\text{g} \end{cases}$$

$$r_t^{error}(o_t, q_t) = -||\hat{\epsilon}_t - \epsilon_t||$$

$$p(D_0, \ldots, D_{t_p}, Q_0, \ldots, Q_{t_p}, R_0, \ldots, R_{t_p}, U_{t_c+1}, \ldots, U_{t_p} \mid o_0, \ldots, o_{t_c}, u_0, \ldots, u_{t_c}) \propto \prod_{t=0}^{t_p} \left[\phi_t^{\text{dynamics}} \phi_t^{\text{QoI}} \phi_t^{\text{evaluation}}\right] \prod_{t=0}^{t_c} \phi_t^{\text{assimilation}} \prod_{t=t_c+1}^{t_p} \phi_t^{\text{control}}$$

Planning and optimal control via reinforcement learning



- Control policy maps from the current belief to a control action

$$u_t = \pi\left(p(D_0, \ldots, D_t, Q_0, \ldots, Q_t \mid o_0, \ldots, o_t, u_0, \ldots, u_{t-1})\right)$$

- Maximize expected accumulated reward over prediction horizon

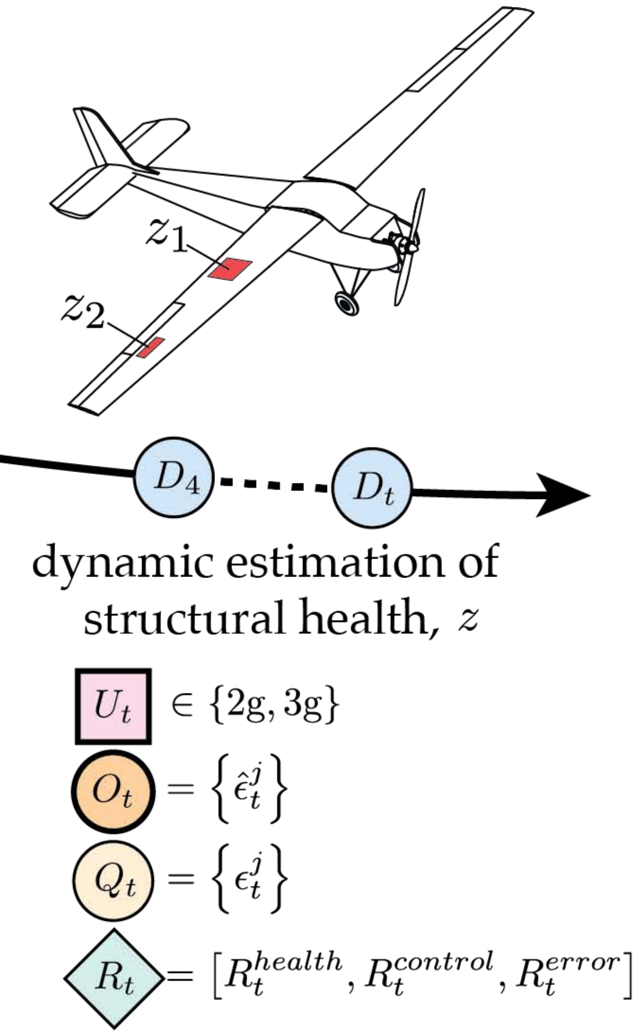
$$\pi^\star = \arg\max_{\pi} \sum_{t=t_c+1}^{t_p} \gamma^{(t-t_c-1)} \mathbb{E}\left[R_t\right]$$

- We use maximum a posteriori estimates d^*, q^* to define (suboptimal) policy

$$u_t = \tilde{\pi}\left(d^\star, q^\star\right)$$

- Solve offline via dynamic programming (value iteration)

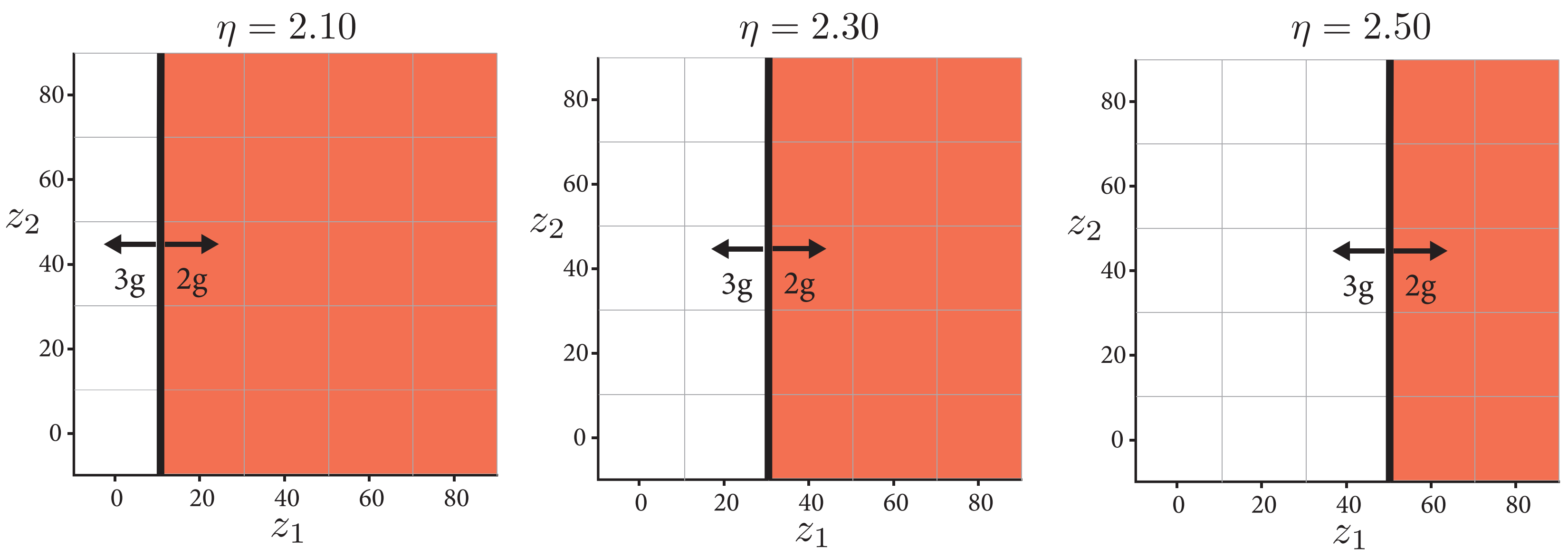
Results: Self-aware control policies



- Multi-objective planning reward function

$$r_t(u_t, q_t) = r_t^{health}(q_t) + \eta r_t^{control}(u_t)$$

tradeoff parameter, η, balances UAV aggression with self-preservation



- Optimal policies only depend on z_1
- Structural model analysis has revealed that z_2 does not affect structural integrity, as measured by $r_t^{health}(q_t)$

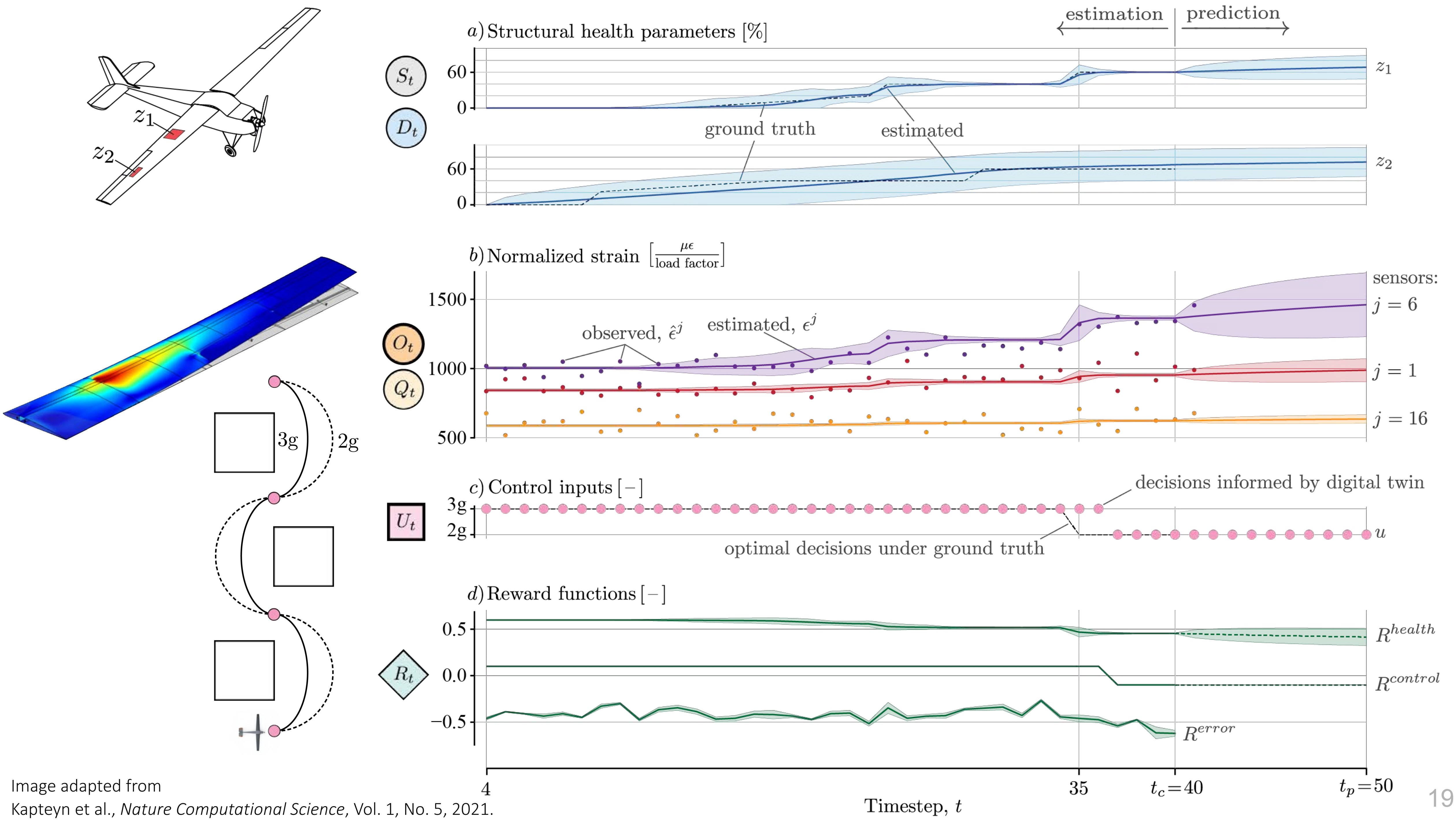


Image adapted from
Kapteyn et al., *Nature Computational Science*, Vol. 1, No. 5, 2021.

Summary & Conclusion

A mathematical and computational foundation to help enable predictive digital twins at scale that is…

- General
  - Define, analyze, compare digital twins across different application areas and different use-cases
- Rigorous
  - Bayesian estimation, end-to-end uncertainty quantification, data-driven learning, principled decision-making
- Flexible
  - Models comprising the digital twin can be physics-based, data-driven, or derived from expert knowledge
- Scalable
  - Principled
  - Repeatable

Many open challenges!
Tailored inference algorithms; active learning; transfer learning; optimal experimental design; model adaptation/enrichment; …

Want to learn more?

Technical papers:

[A Probabilistic Graphical Model Foundation for Enabling Predictive Digital Twins at Scale]
Kapteyn, M., Pretorius, J. and Willcox, K., *Nature Computational Science,* Vol. 1, No. 5, May 2021.

[Data-driven physics-based digital twins via a library of component-based reduced-order models]
Kapteyn, M., Knezevic, D., Huynh, D.B.P., Tran, M. and Willcox, K. *Int. J. Numerical Methods in Eng.,* 2020

Overview articles:

[Creating "digital twins" at scale]
Ham, B., *MIT News*, June 2021

[Digital Twins: Where Data, Mathematics, Models, and Decisions Collide]
Kapteyn, M., and Willcox, K., *SIAM News*, Sept. 2021

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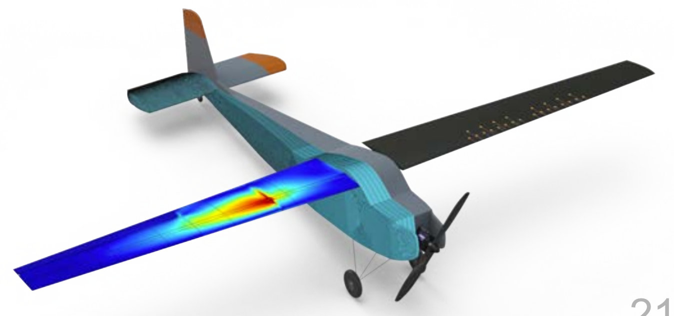

Image credits (slide 9)

[Kratos]
“Kratos’ XQ-58A Valkyrie “Loyal Wingman” Drone Completes its Fourth Flight”
https://defpost.com/kratos-xq-58a-valkyrie-loyal-wingman-drone-completes-its-fourth-flight/
Press Release: 2020-01-28. Accessed: 2021-03-18.

[Airbus]
“Rethinking Urban Air Mobility”
https://www.airbus.com/newsroom/stories/rethinking-urban-air-mobility.html
Published: 2017-06-17. Accessed: 2021-03-18

[Wing]
“Wing Launches America's First Commercial Drone Delivery Service to Homes in Christiansburg, Virginia”
https://www.youtube.com/watch?v=wCTKwkYzVzo&t=43s
Uploaded: 2019-10-18. Accessed: 2021-03-18