ML4ENG - Data efficient and smart design

imec – Ghent University

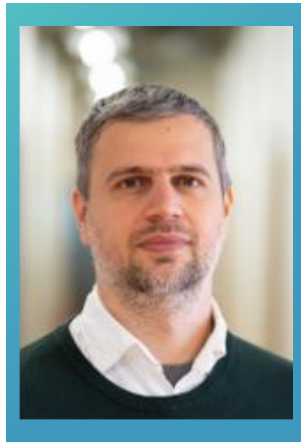
Ivo Couckuyt

ABOUT US

SURROGATE MODELING RESEARCH CLUSTER **(SUMO)**

PROF. DR. IR.
TOM DHAENE

PROF. DR.
DIRK DESCHRIJVER



PROF. DR.
IVO COUCKUYT

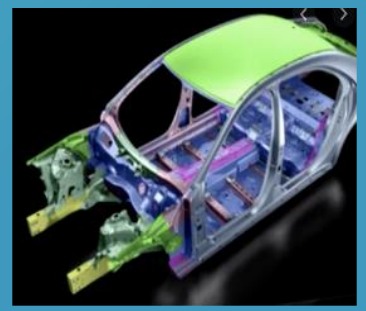
+ 2 POST DOCS,
+ 12 PhDs

https://sumo.ilabt.imec.be

SURROGATE MODELING (SUMO)
Data-Efficient Machine Learning (DE-ML)

- CAD/CAM/CAE design & optimization
- **structural, mechanical, electronic, photonics**

Assist engineers with design **exploration**, optimization and uncertainty quantification



TIME SERIES

- **health, energy, industry**

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SUMO RESEARCH CLUSTER
TOPICS

Machine Learning for Engineer(s)(ing) (ML4ENG)

ENABLING TECHNOLOGIES

- DE-ML: Data-Efficient Machine Learning
- AutoML: Automation in Machine Learning
- PI-ML: Physics-Informed Machine Learning
- X-ML: eXplainable Machine Learning
- UQ: Uncertainty Quantification
- TML: Trust-worthy Machine Learning

APPLICATIONS

- DT: Digital Twins (and siblings)
- Design space exploration
- Design and process optimization
- Generative model-based design
- DM: Multi-Criteria Decision Making
- Verification & Validation (certification)

- Machine learning in healthcare (sleep apnea, sepsis, …)
- Machine learning in biochemistry and biology

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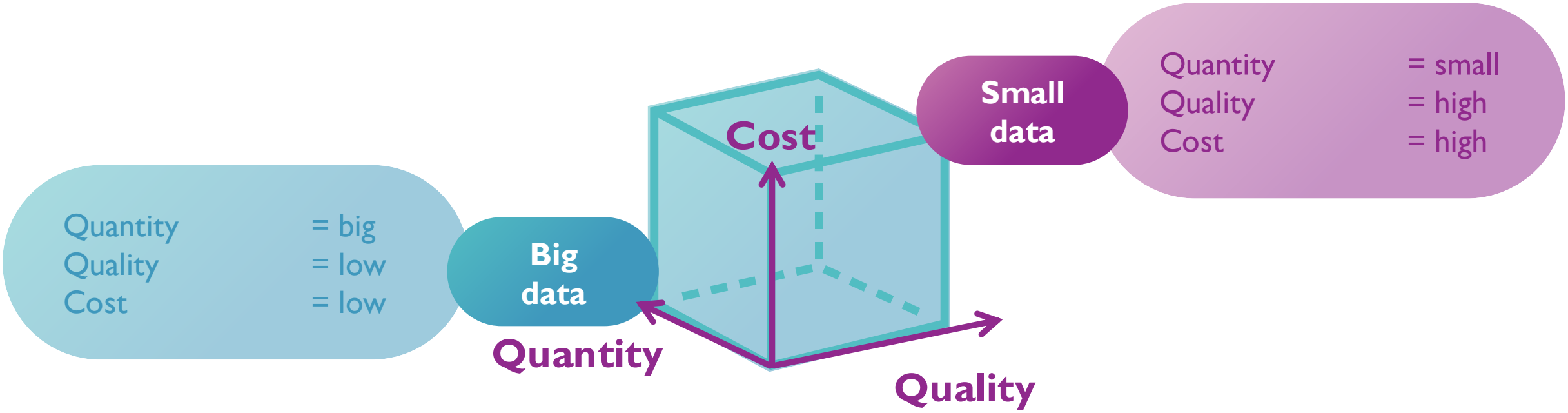
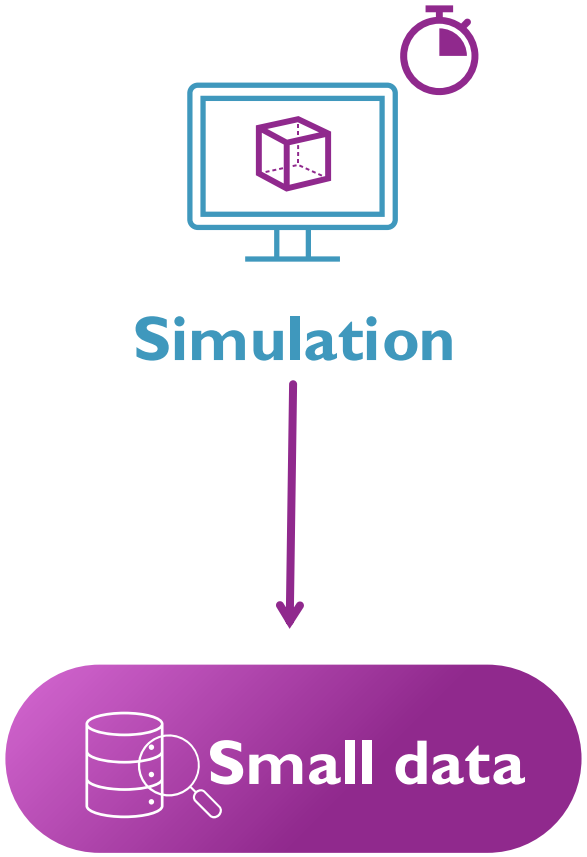
DATA-EFFICIENT MACHINE LEARNING

DATA TAXONOMY



EXAMPLE: COMPUTATIONAL ENGINEERING

- **Physics-based simulations**
  - Finite elements, computational fluid dynamics, etc.
  - Time-consuming
    - **Ford:** ”36-160 hours for 1 crash simulation”
- **Engineering tasks**
  - Design space exploration, optimization, etc.
- **Standard approaches are expensive**
  - Trial-and-error
  - Parameter sweeps
  - Classical optimization methods



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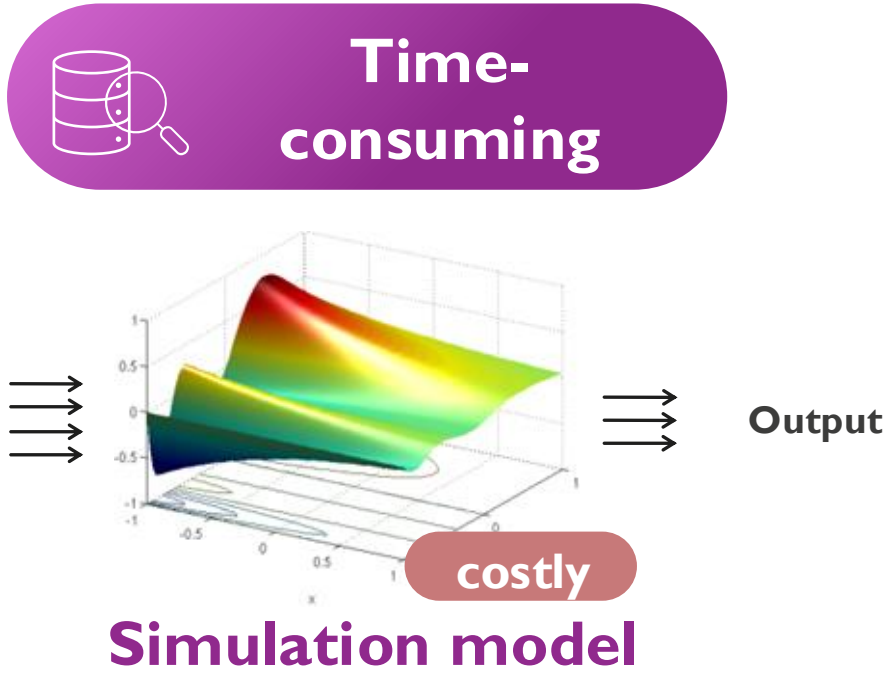


SURROGATE MODELS – WHAT?

automotive | chemistry | aerodynamics | electronics | medical

design variables

width, temperature, angle, frequency, ...

simulation model
lab measurements
Fluent®, HSPICE®, CST®, Comsol®, Abaqus®, ...

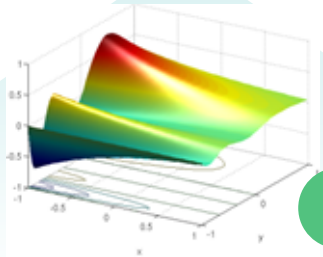
costly

response variables

quality, cost, lift, pressure, stress, ...

SUMO

design variables



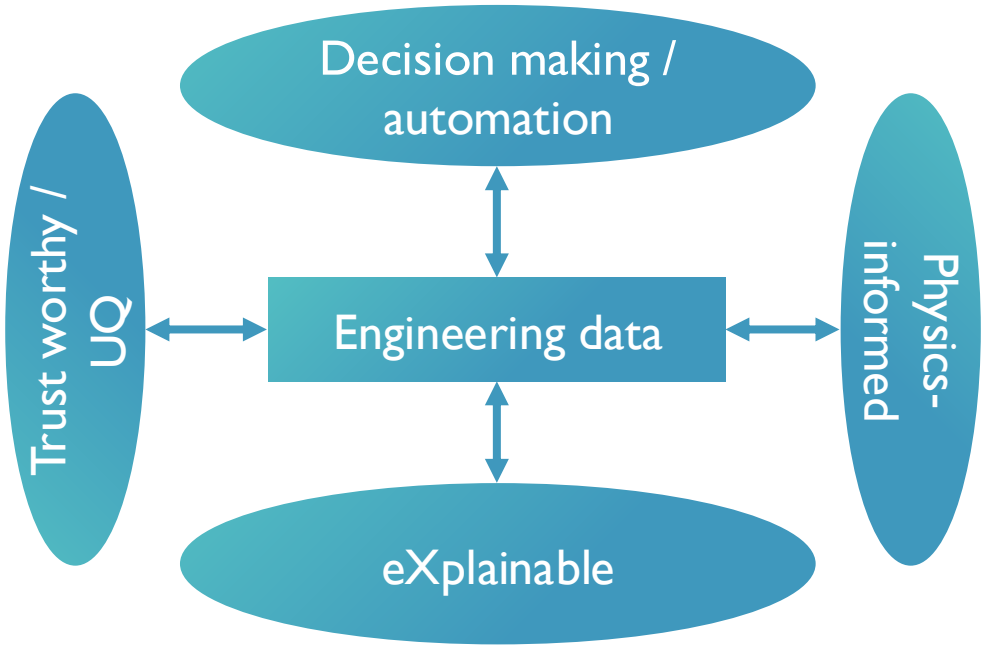
response variables

cheap

surrogate model

Gaussian process, Neural networks, Polynomial, ,...

prototyping | optimization | sensitivity analysis | digital twin



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TRUST-WORTHY DIGITAL TWINS

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CERTIFICATION OF DATA-DRIVEN MODELS
TRUST WORTHY SURROGATE MODELS

- **Problem**: Certification of data-driven models for **aircraft systems**
  - Regulatory authorities (EASA + FAA)
  - Nitrogen Generation System (NGS)
    - Measurements and **Monte Carlo simulations**

- **Goal**: Generate trustworthy surrogate models
  - Extensive validation
  - Calibrated uncertainty
  - Explainability
  - …

European Union Aviation Safety Agency

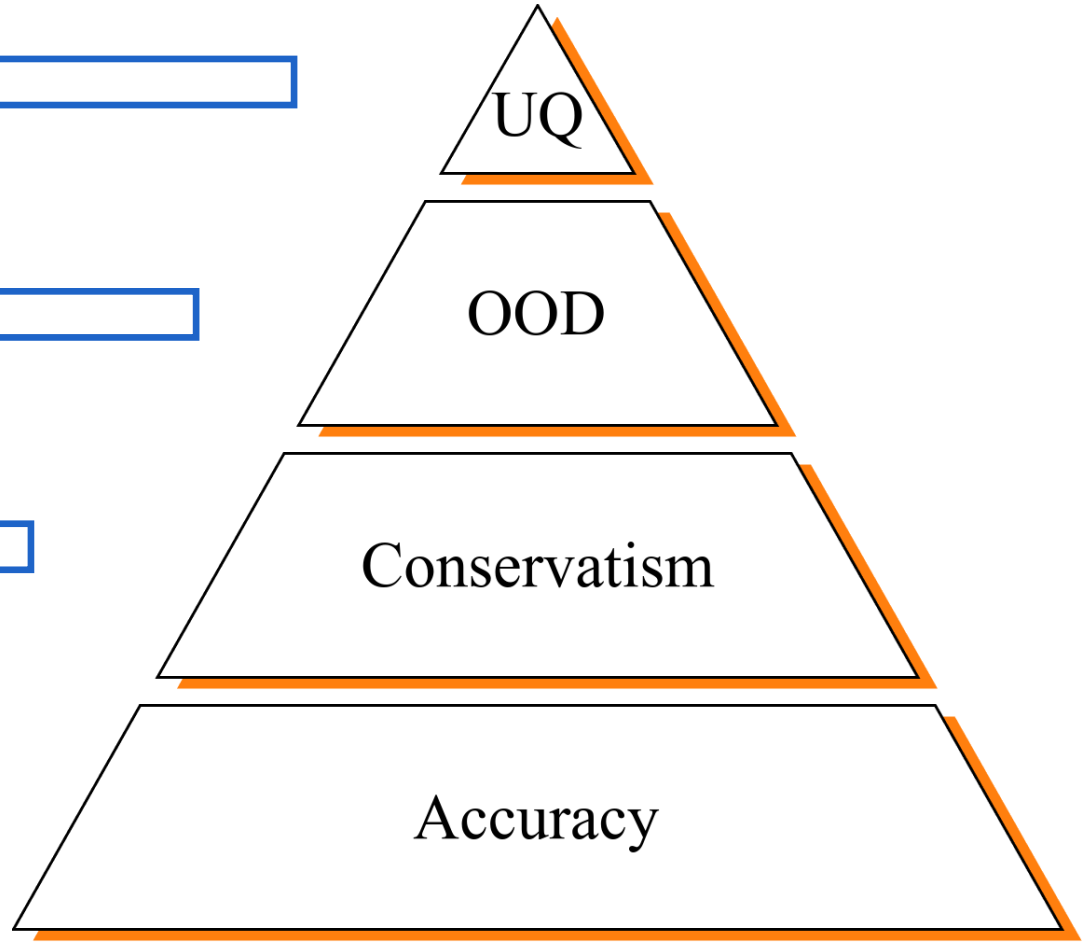
PILLARS OF TRUST-WORTHY MACHINE LEARNING

Uncertainty quantification for improved trust in doubtful cases

Assuring generalization and detection of Out of Distribution points

Tuning for the utility of the application Optimistic vs pessimistic

A high accuracy is the basis



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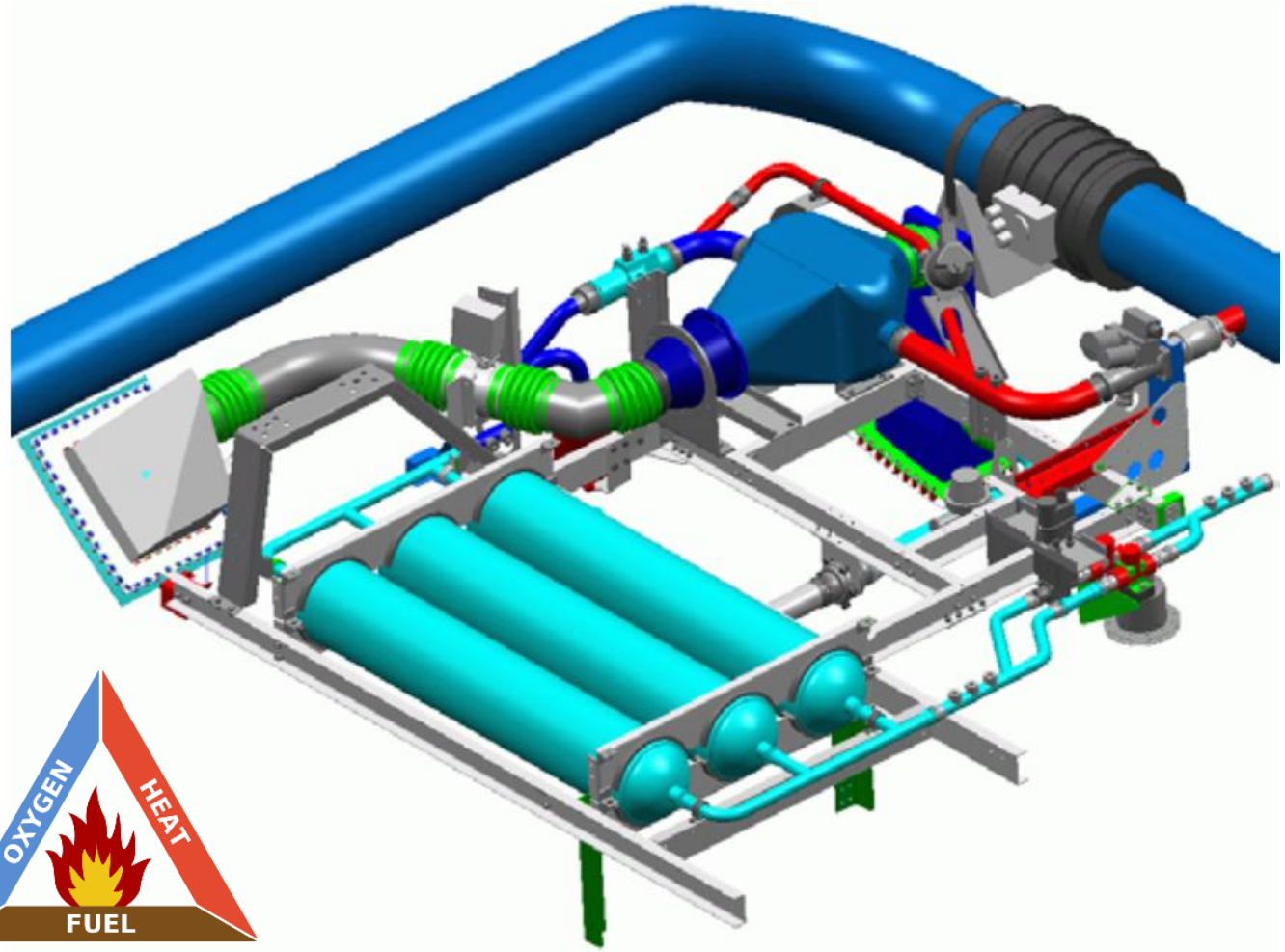
FLAMMABILITY REDUCTION SYSTEM (FRS)

OVERVIEW

- **Reduces oxygen concentration** in fuel tanks to minimize flammability risk.
- Introduces **Nitrogen-Enriched Air** (NEA) with lower oxygen content into the tank.
- Manages oxygen outgassing during ascent and air entry during descent.
- Adjusts **NEA flow and oxygen levels** based on flight phases.



FRS CERTIFICATION

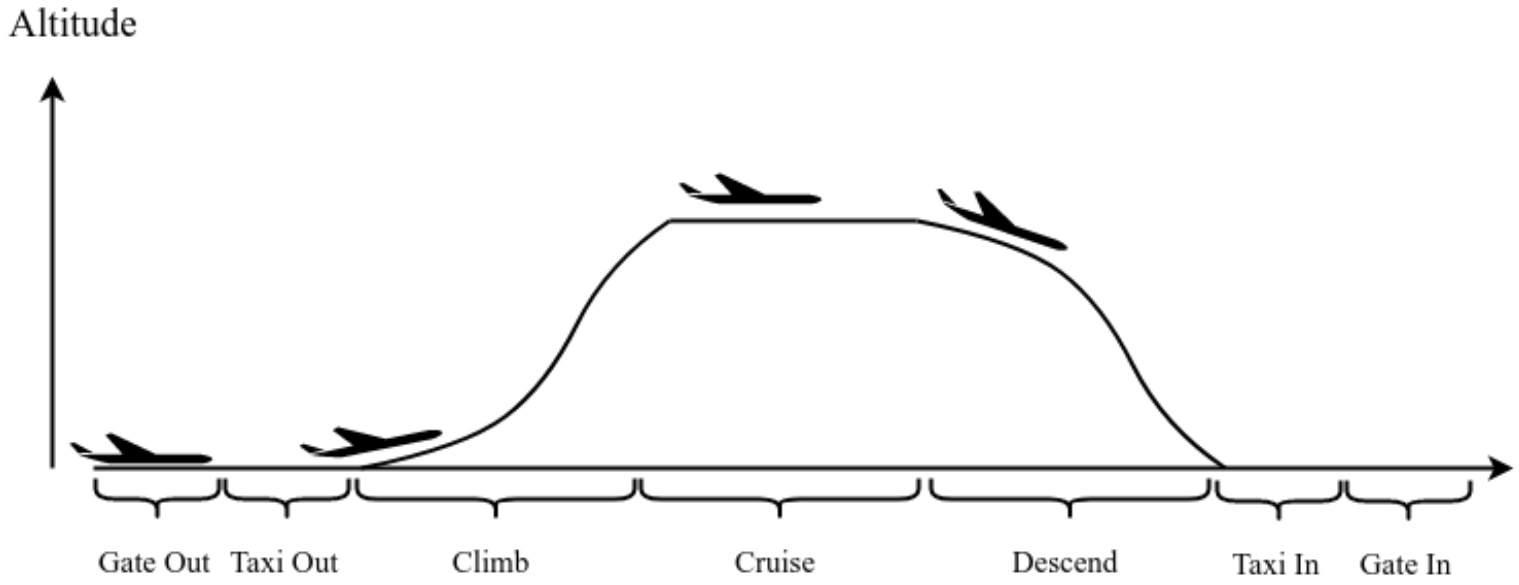
- Certification is done fleetwide through Monte Carlo analysis, rather than examining edge cases
- The acceptable flammability is shown in the following table

Table 1 Flammability Exposure Limits, from Title 14 CFR Part 25 Appendix N25.4(d)

Minimum Number of Flights in Monte Carlo Analysis	Maximum Acceptable Monte Carlo Average Fuel Tank Flammability Exposure to Meet 3% Requirements	Maximum Acceptable Monte Carlo Average Fuel Tank Flammability Exposure to Meet 7% Requirements
10,000	2.91%	6.79%
100,000	2.98%	6.96%
1,000,000	3.00%	7.00%

METHODOLOGY
MODEL DATABASE

- 18 Inputs:
  - Altitude
  - Flight Phase
  - …
- 109 Outputs
  - Fuel Temperature
  - Oxygen Concentration
  - ...
- ~12K Flight Profiles



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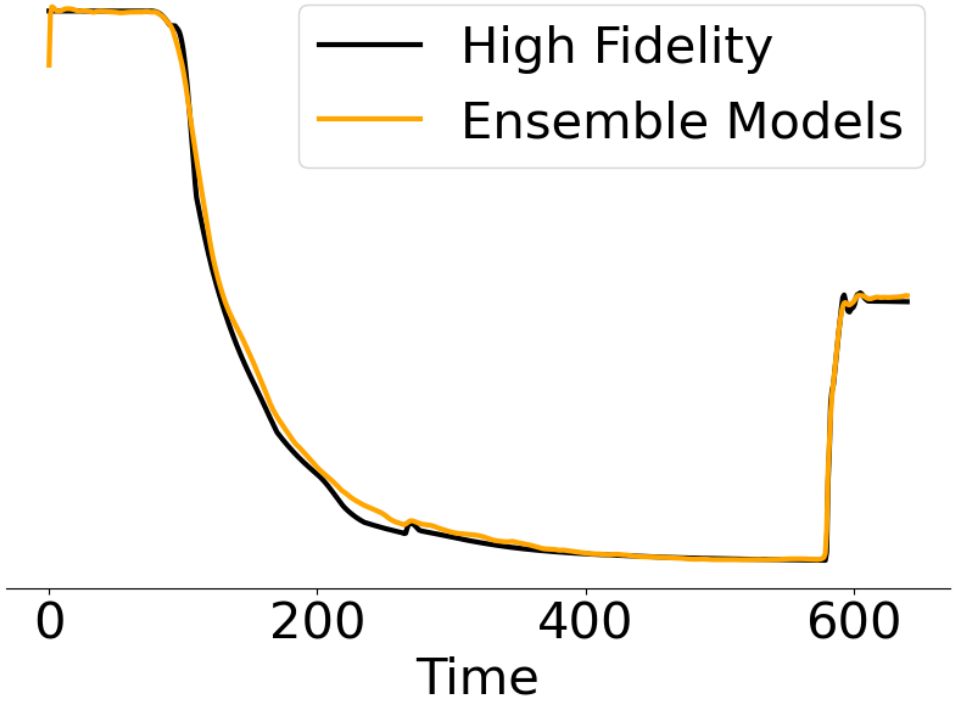
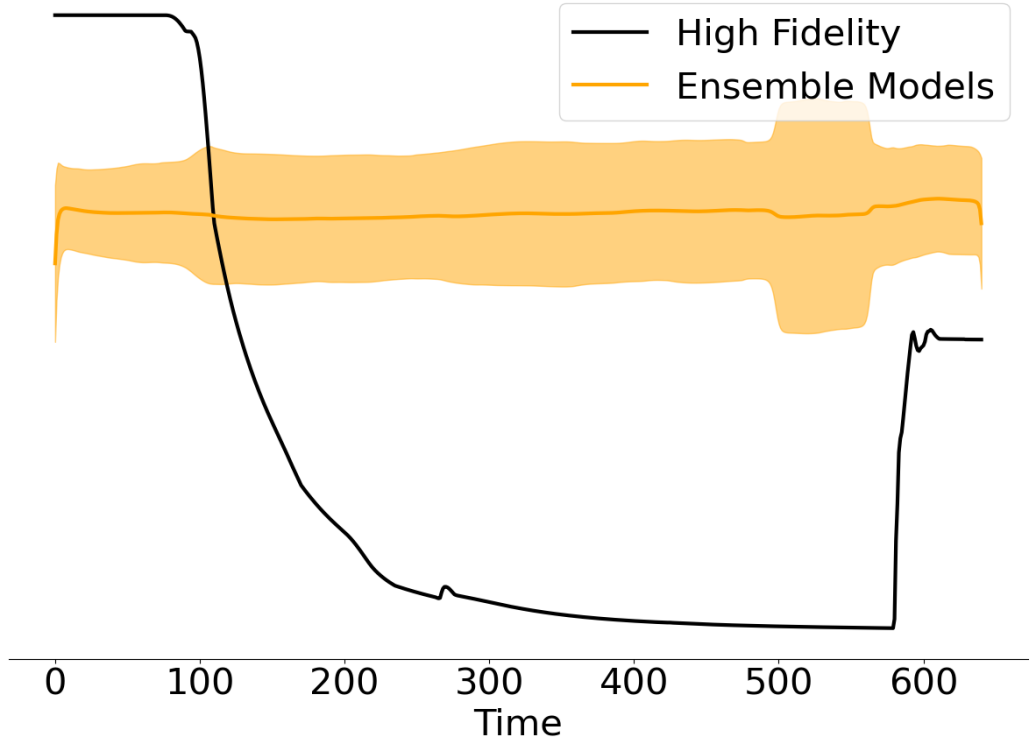
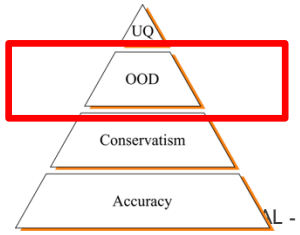
RESULTS - OUT-OF-DISTRIBUTION DETECTION

VALIDITY OF MODEL



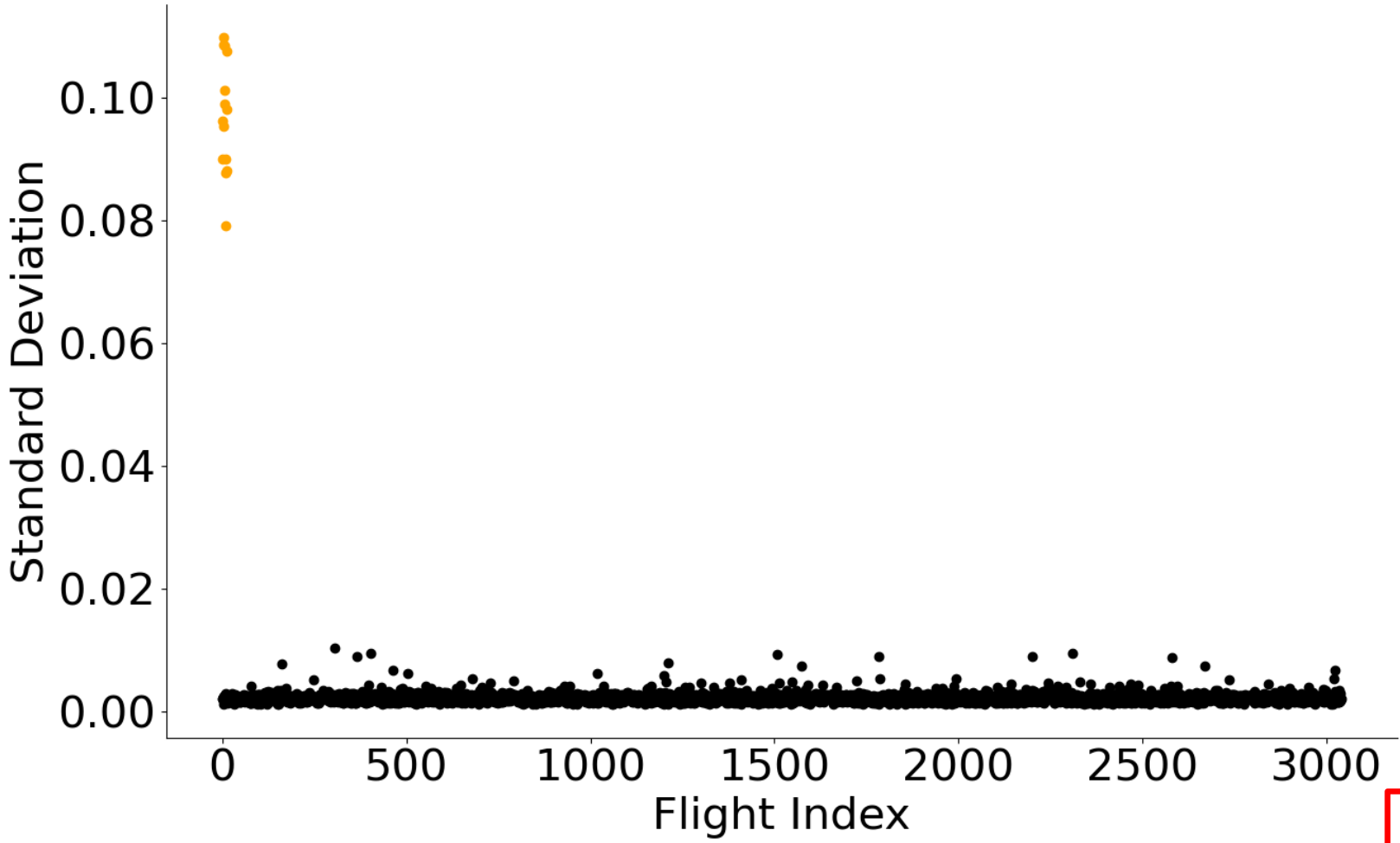


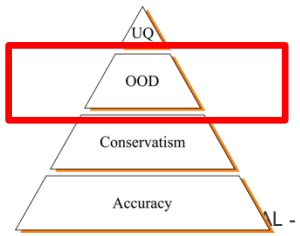


AL - INTERNAL USE

RESULTS - OUT-OF-DISTRIBUTION DETECTION

OUTLIERS

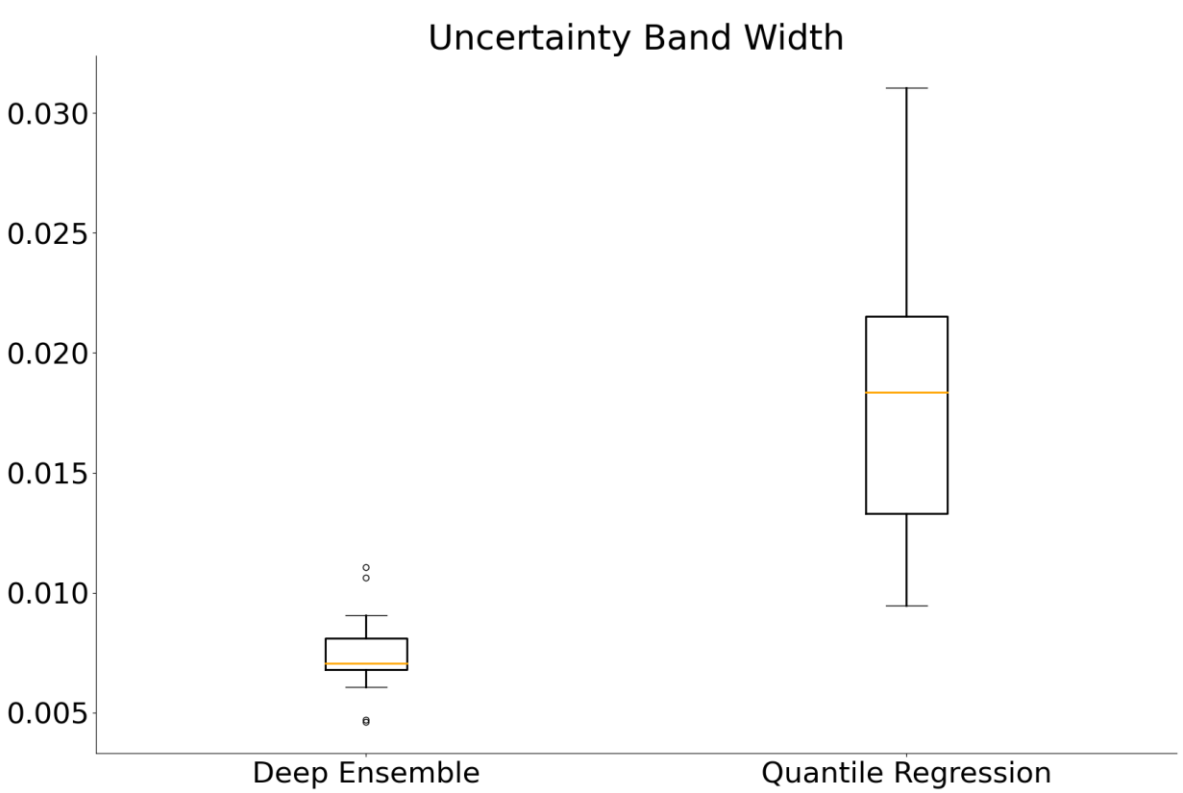


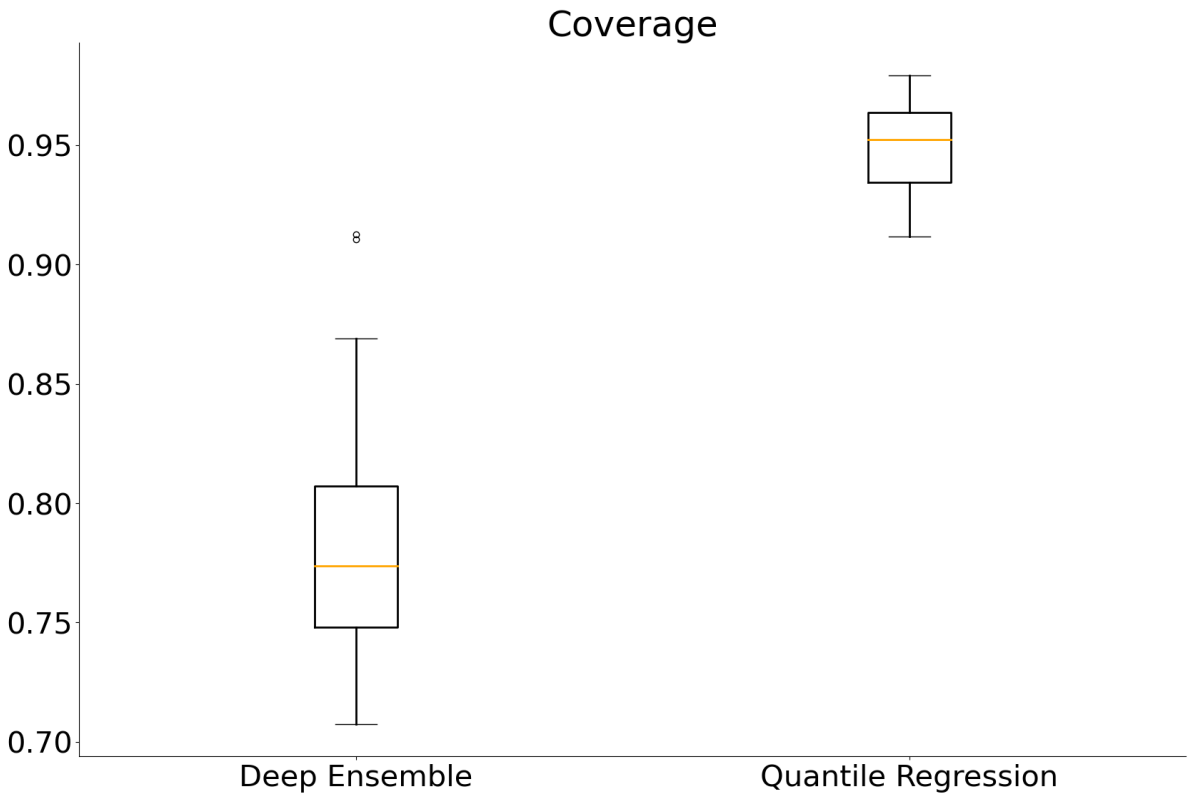


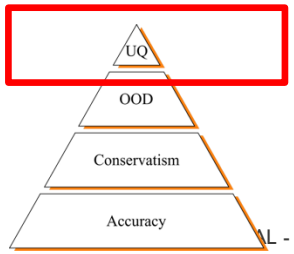
AL - INTERNAL USE

RESULTS – UNCERTAINTY QUANTIFICATION

BANDWIDTH AND COVERAGE

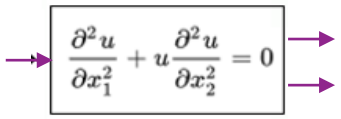






AL - INTERNAL USE

RESULTS - TIMING



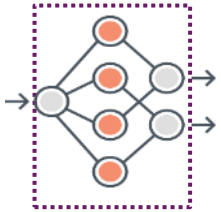


Table 1 Comparison of simulation time for different models for ≈ 12,000 flights

Model	Resource	Simulation Time
Full-Fidelity Model	21x Intel(R) Core(TM) i7-12800H	≈ 100 hrs
Unidirectional LSTM	1x NVIDIA GeForce RTX 2080 TI	< 25 sec
	1x Intel(R) Xeon(R) E5-2620 v3	< 105 sec
Bidirectional LSTM	1x NVIDIA GeForce RTX 2080 TI	< 46 sec
	1x Intel(R) Xeon(R) E5-2620 v3	< 152 sec

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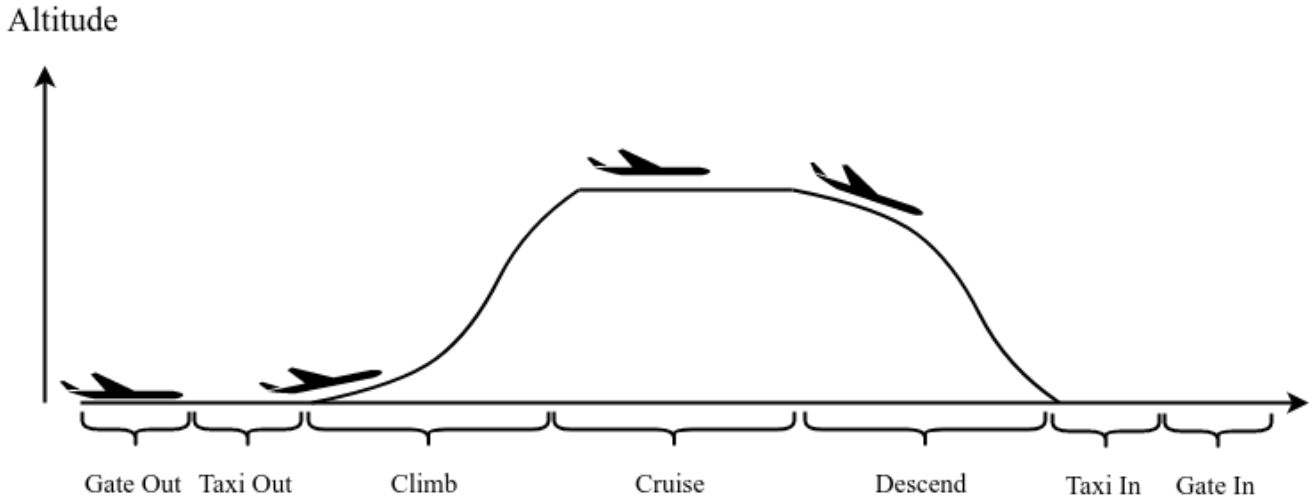
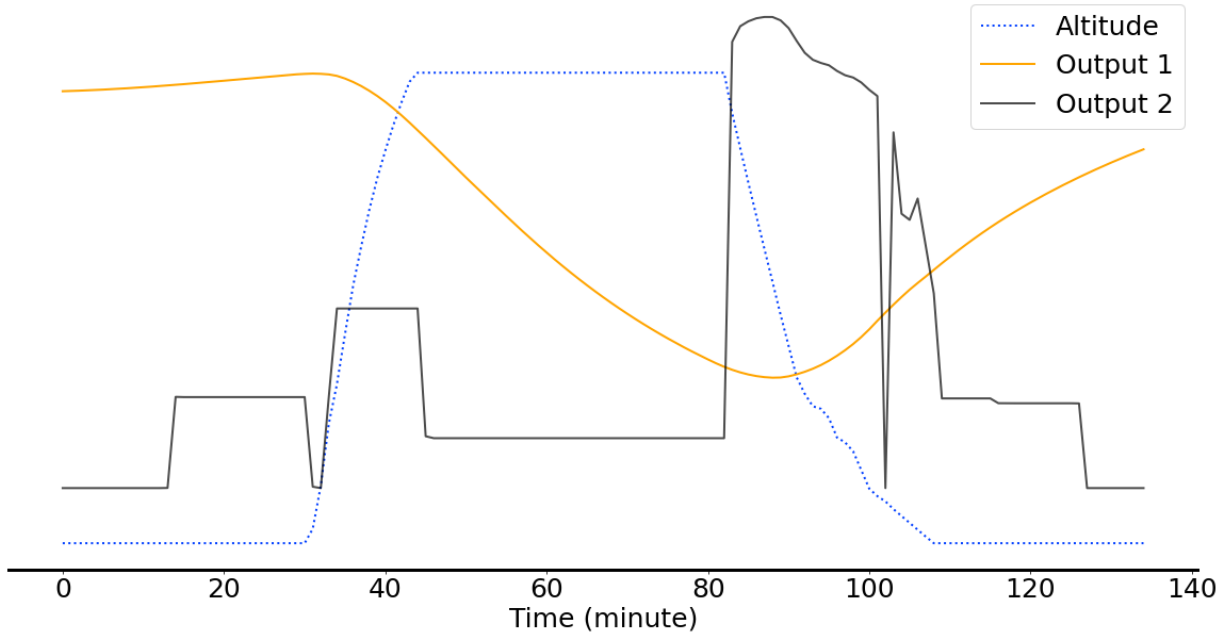
CONCLUSION
OVERVIEW

- **How can we generate trust?**
  - Extensive validation
  - Properly calibrated uncertainty
  - And explainability, etc.
- **Flammability exposure < 3%**
  - For 12000 flights
- Decreasing **evaluation time** from
  - 100 hours to 50-150 seconds
  - **Factor 2000x speed-up!**





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CONCLUSION
FUTURE

Data-driven models for flight testing

- Enable **virtual certification**
  - Persuade EASA/FAA
  - UQ for spatio-temporal models
- Monitor **operational aspects**
  - Continuous airworthiness
  - Detection of temporal drift (aging)
  - Characterization of the operational space
    - UQ for generative models

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PROCESS OPTIMIZATION
ADHESIVE BONDING

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INDUSTRIAL ADHESIVE BONDING PROCESSES

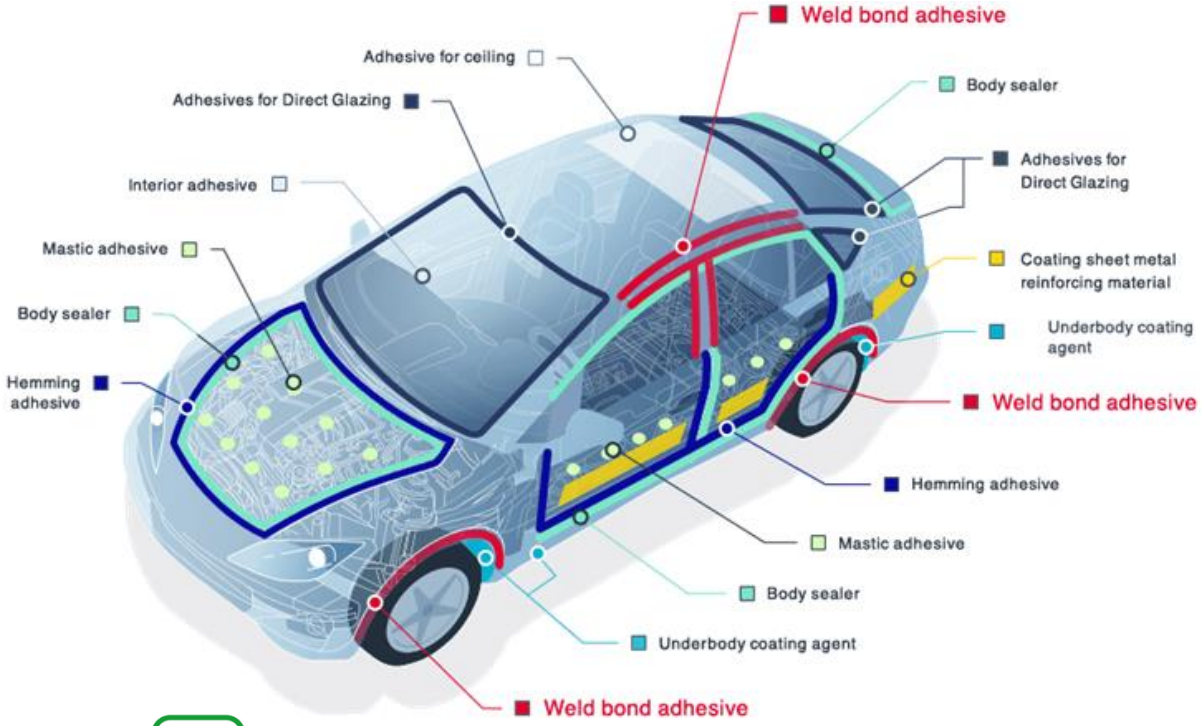
PROBLEM

Need for better fuel efficiency

Results in lighter bodies, new materials

Which tend to be more fragile, more difficult to join

The right bonding process will improve strength



Burned sample

Adhesive failure

Substrate failure

INDUSTRIAL ADHESIVE BONDING PROCESSES

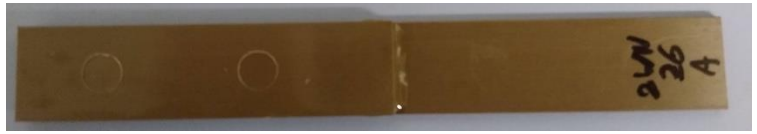
Electronic potting

Material A: Ryton PPS (PolyPhenylene Sulfide)

Material B: Ryton PPS

Adhesive: 2c-epoxy

PPS bonding



Manufacturing industry

Material A: Virgin ABS (Acrylonitrile Butadiene Styrene)

Material B: Recycled ABS

Adhesive: 2c-polyurethane

ABS bonding

How to optimize the bonding process parameters to achieve a high strength but low production cost?

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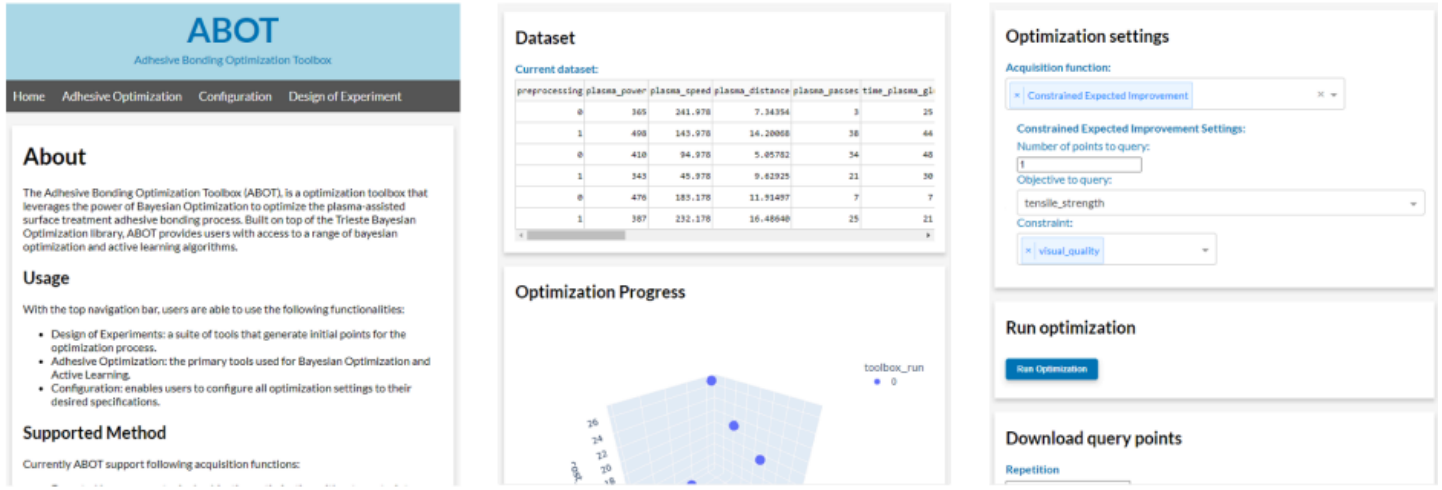
INDUSTRIAL ADHESIVE BONDING PROCESSES
MULTIOBJECTIVE OPTIMIZATION

- **Case:** Minimize cost and maximize break strength
  - Conflicting trade-offs
  - Subject to unknown nonlinear constrains
- **Problem:** Experimentation is complex
  - Expensive, type of failures, noise, …



The Adhesive Bonding Optimization Toolbox (ABOT) developed in the Flanders AI research program.

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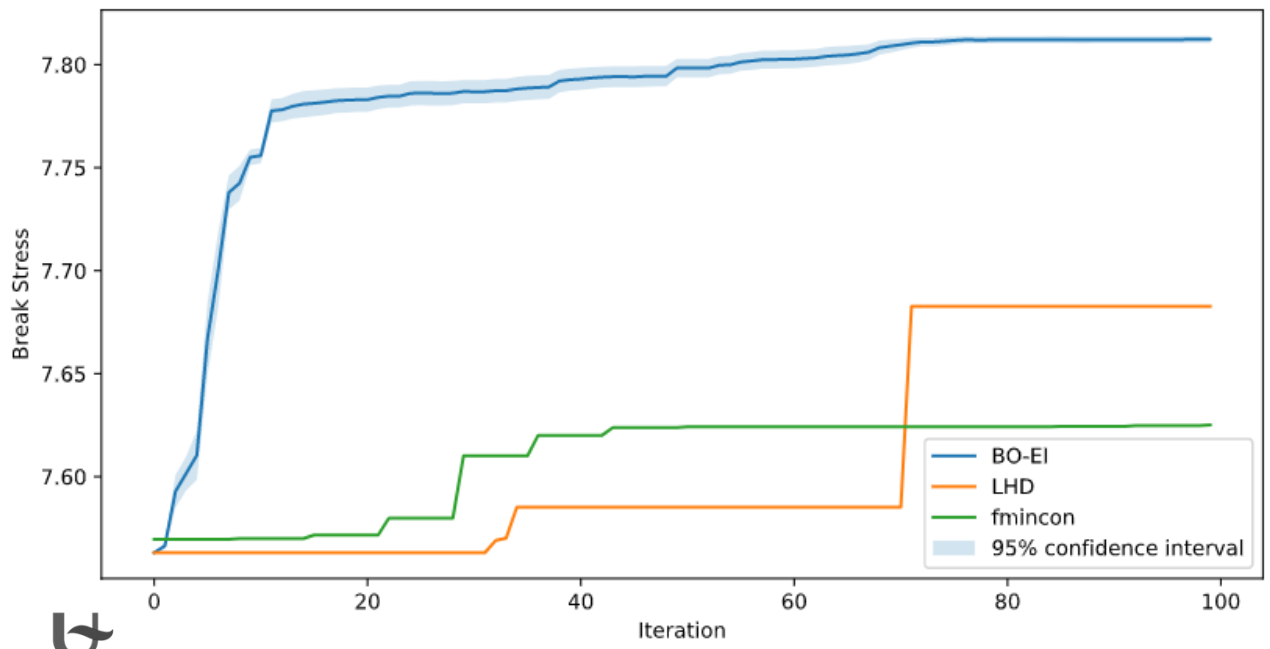
INDUSTRIAL ADHESIVE BONDING PROCESSES

TUNING PROCESS PARAMETERS

- **Problem:** maximize break strength of bonding
  - **Input**: 6 process parameters
  - **Budget**: 100 experiments
- **Results:** **Factor 5x speedup**
  - Standard 489 experiments

Search Domain	
Variable name	**Range**
Preprocessing	[0, 1]
Plasma power	[300, 500]
Plasma distance between nozzle and substrate	[0, 20]
Plasma speed	[5, 250]
real time plasma-gluing	[1, 120]
Number of passes	[1, 50]



Higher is better

FAIR method

Standard optimization

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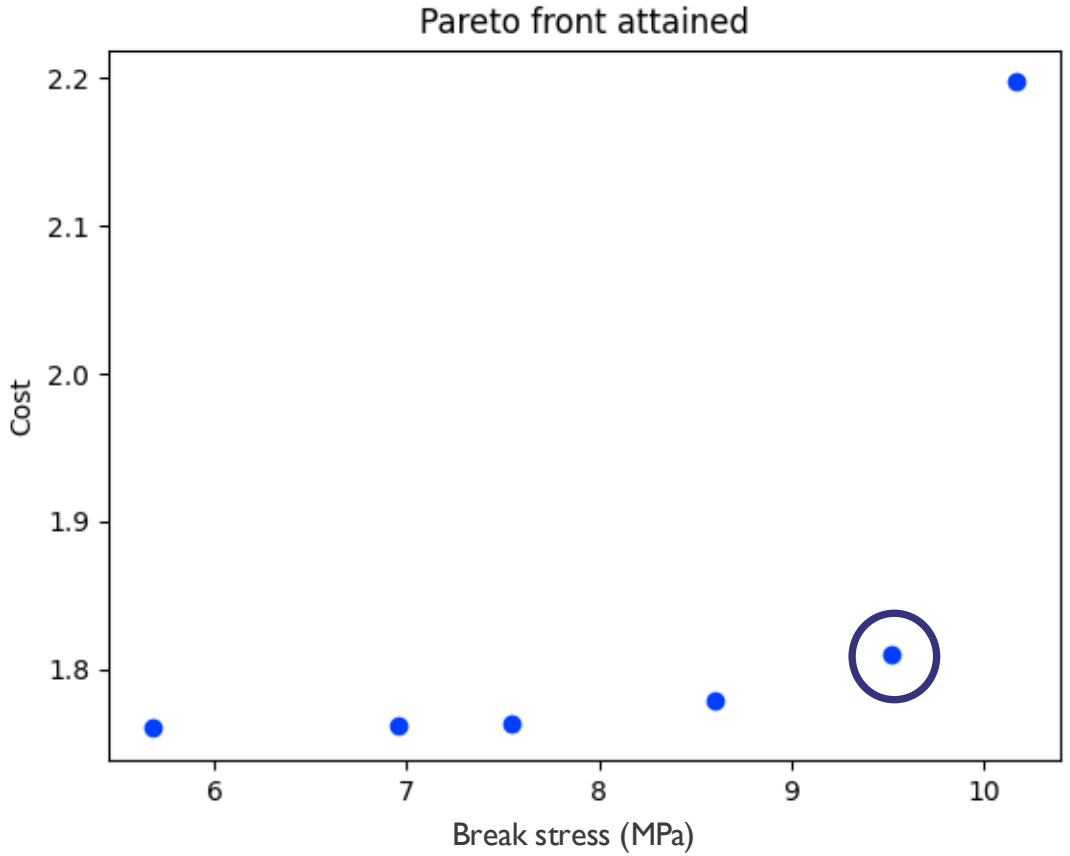
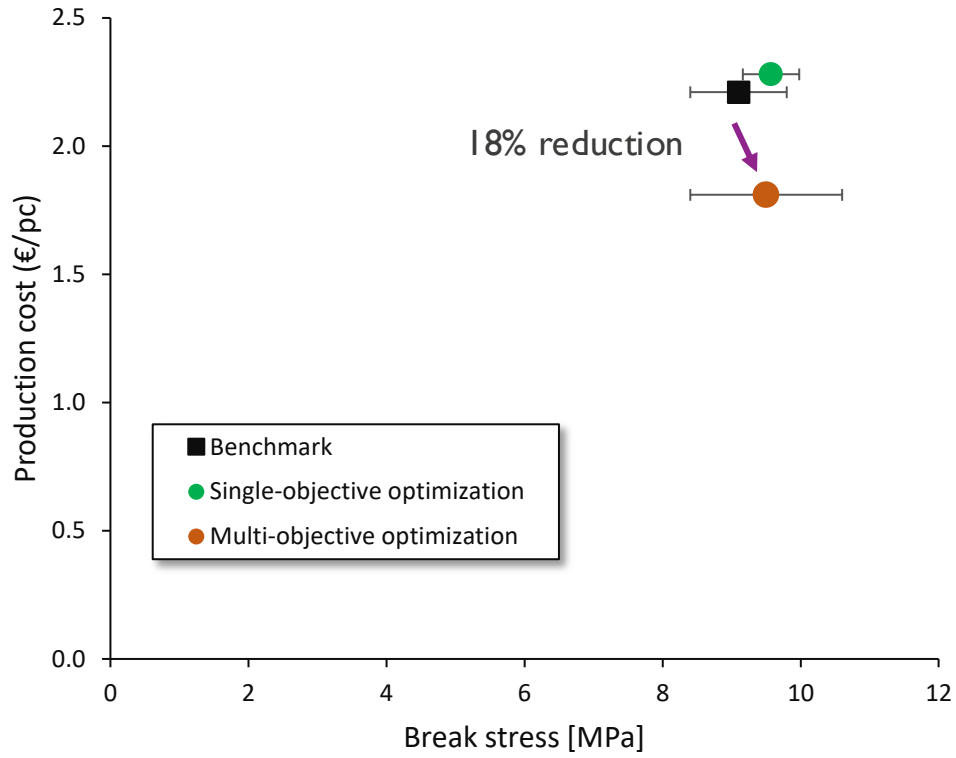
INDUSTRIAL ADHESIVE BONDING PROCESSES
OUTCOME MULTIOBJECTIVE OPTIMIZATION

- **Results:** 18% reduction in production cost feasible for PPS bonding
  - ~100 experiments (+repetitions)





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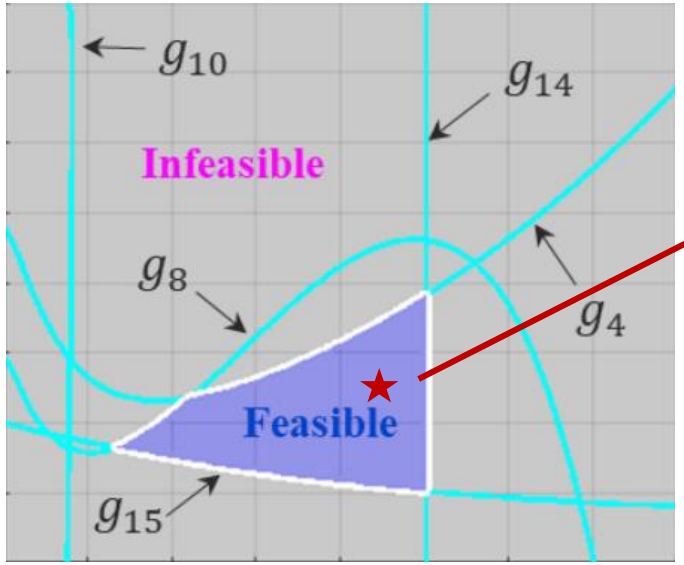
ENGINEERING DESIGN
DESIGN SPACE EXPLORATION AND OPTIMIZATION

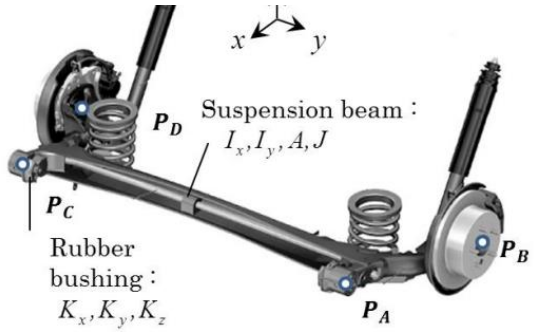
Problem: Explore **feasible designs** in design and testing

Automotive testing

- **Goal**: Identify safe operation conditions

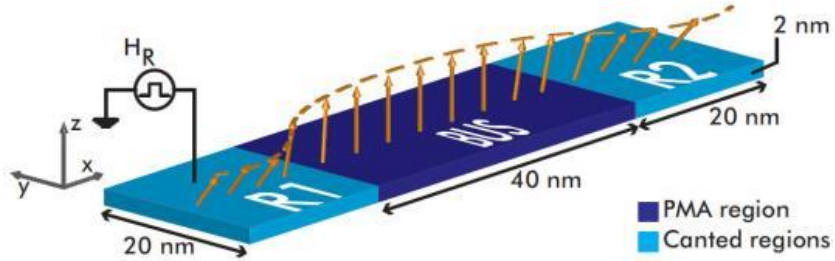


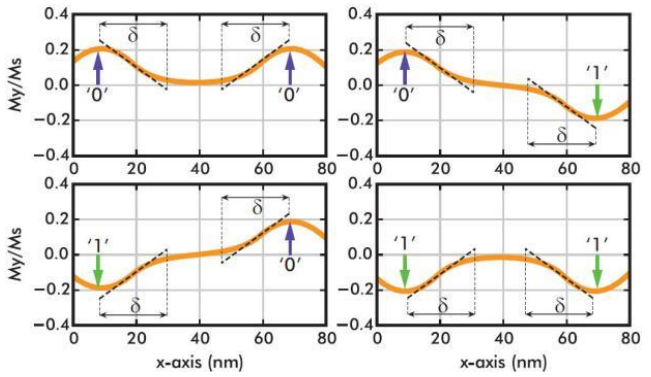
TOYOTA

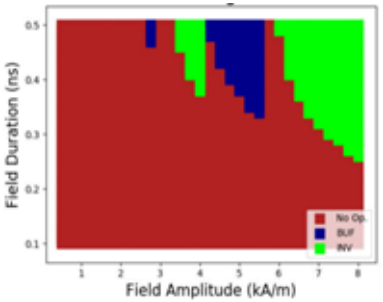


Logic device description

- **Goal**: Design micromagnetic logic device







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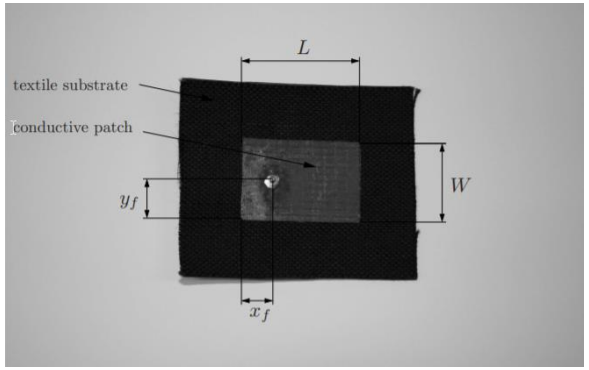
ENGINEERING DESIGN
MULTI-CRITERIA DECISION MAKING

- **Problem**: Design of a **cyclone separator**
- **Goal**: Trade-off between particle size and power
  - With increase of power small particles might get back out
  - Too little power and the bigger particles are not vacuumed
- CFD analysis takes up to 3 days for one design

Approach adopted by

Meta

And…



Antenna design

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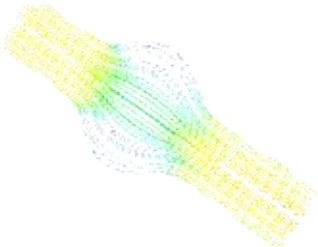

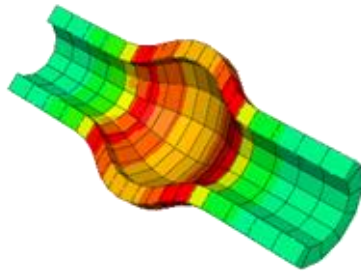

Identify aneurysm

PREFERENCE LEARNING
HUMAN-IN-THE-LOOP OPTIMIZATION

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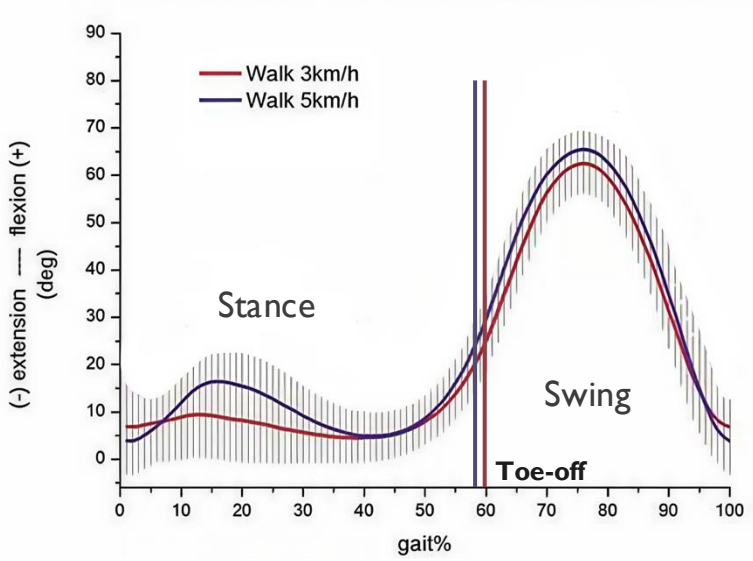
MOTIVATION
CURRENT LOWER LIMB-PROSTHESIS

Passive device

Active device



Average knee kinematics during walking, *Liu et al., 2024*

Personalization is **time-consuming**

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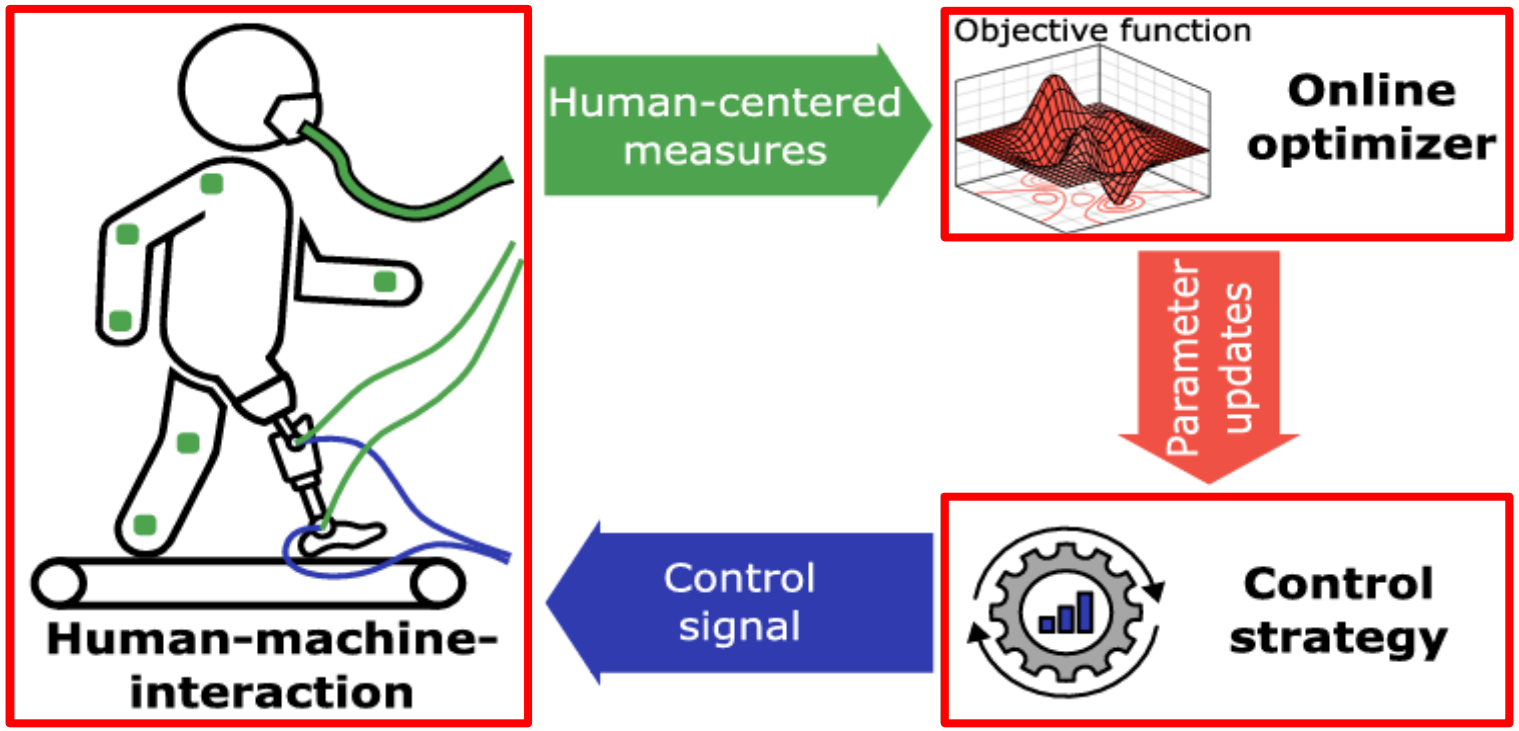
HUMAN-IN-THE-LOOP OPTIMIZATION
OVERVIEW



M. A. Diaz *et al.*, *Human-in-the-loop optimization of wearable robotic devices to improve human–robot interaction: A systematic review,* IEEE Transactions on Cybernetics, 2022

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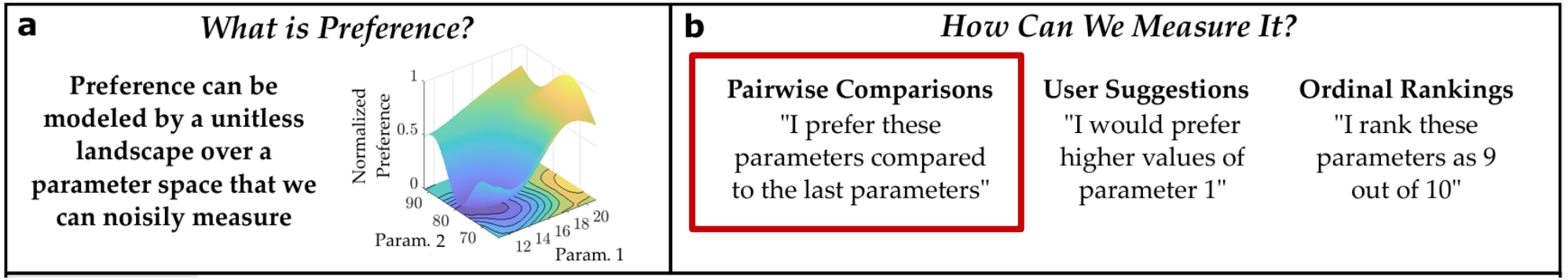
HUMAN-IN-THE-LOOP OPTIMIZATION
OBJECTIVE FUNCTION

Performance analysis metrics:

- "Effort"
- Kinematics
- Comfort, stability, smoothness

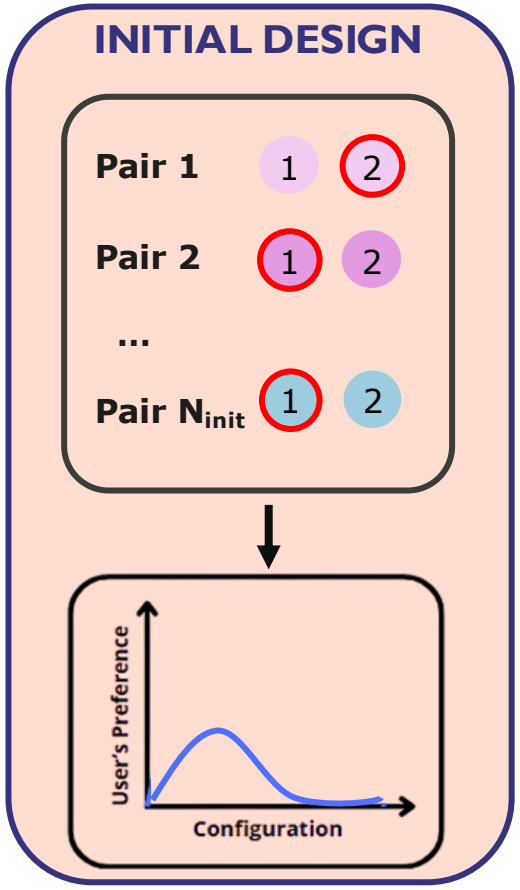
⇒ Preference

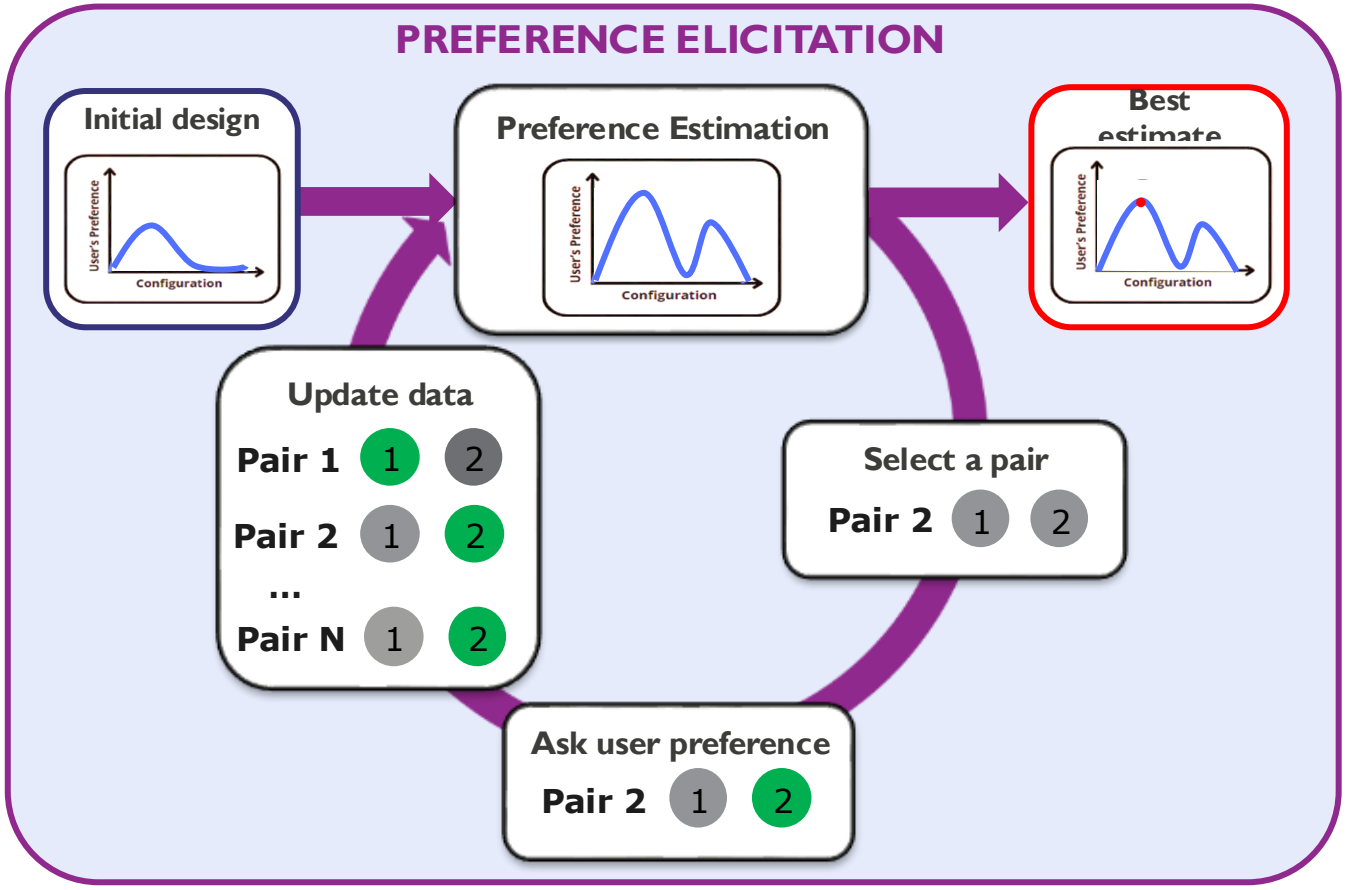
Cognitive load
Fatigue



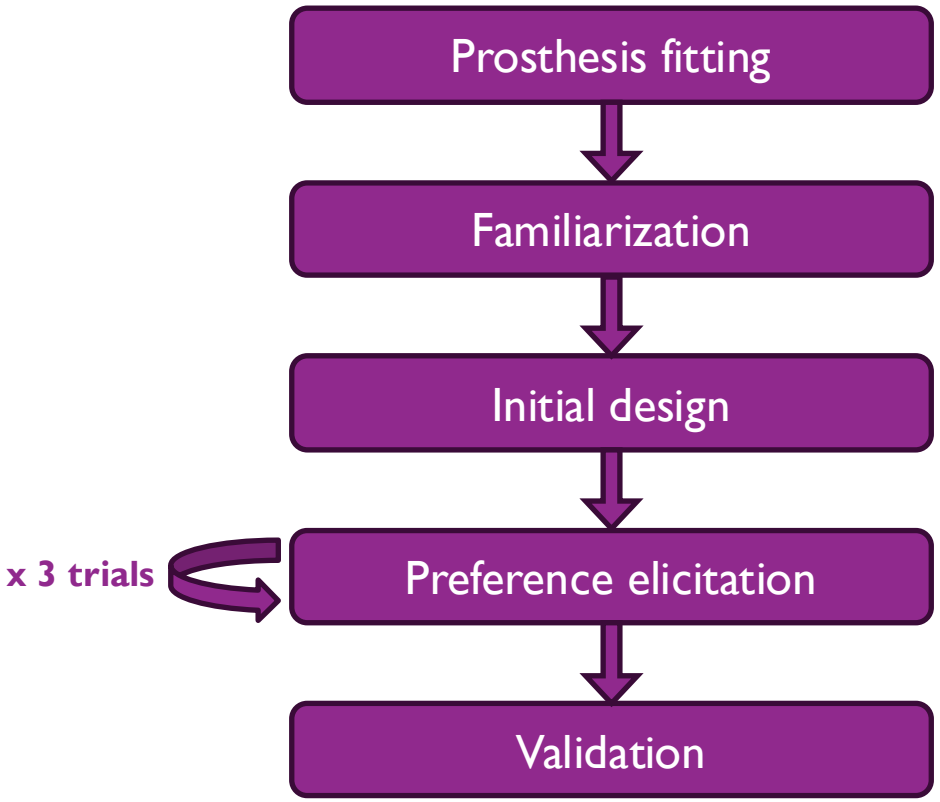
From Ingraham *et al.,* Leveraging User Preference in the Design and Evaluation of Lower-Limb Exoskeletons and Prostheses, 2023

ONLINE OPTIMIZERS
GENERAL FRAMEWORK





PROTOCOL
PROSTHESIS CONTROL TUNING



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RESULTS
PROSTHESIS CONTROL TUNING

	EUBO-Line-CoSpar	*BPE4Prost*	*Ref*
Participants	1 TF, 2 AB	1 TF	6 TF [1], 4 TF [2]
Accuracy	93 %	67 %	83 ± 30 % [1]
Efficiency	10.3 ± 2.5 iterations 8.5 ± 3.6 minutes	35.0 ± 6.2 iterations 21.5 ± 4.7 minutes	46-92 minutes [2]

[1] Tucker *et al.*, 2020; [2] Simon *et al., 2014*

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DECISION MAKING

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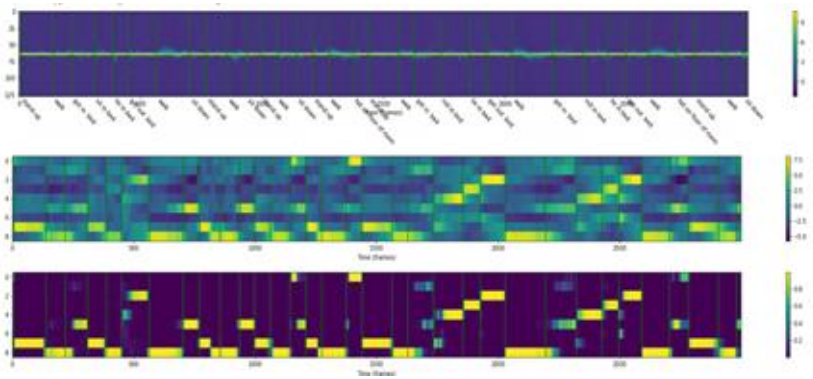
RADAR - PATIENT MONITORING
DECISION SUPPORT

- **Context**: Next-generation high-dimensional radar sensing
  - **Hardware**: Compact, low-power, low-cost
  - **Data-rich**: Speed, distance, …

- **Various use cases:**
  - **Healthcare in Belgium**: Ageing population, shortage of nurses
    - Non-Intrusive Patient Activities Monitoring
  - **Smart Office/Homes**: Gesture and activity recognition, surveillance, heartbeat

- **Result**: compact **surrogates** that provide **trust-worthy decision-making**
  - Solution: bi-directional LSTM with uncertainty quantification
  - Unknown events / Anomaly detection

MARIA MIDDELARES



Class	F1-score
sit down	0.81
stand up	0.86
walk	0.94
fall on the floor	0.86
stand up from floor	0.90
lie in bed	0.68
get in bed	0.83
roll in bed	0.79
get out bed	0.83
sit in bed	0.77

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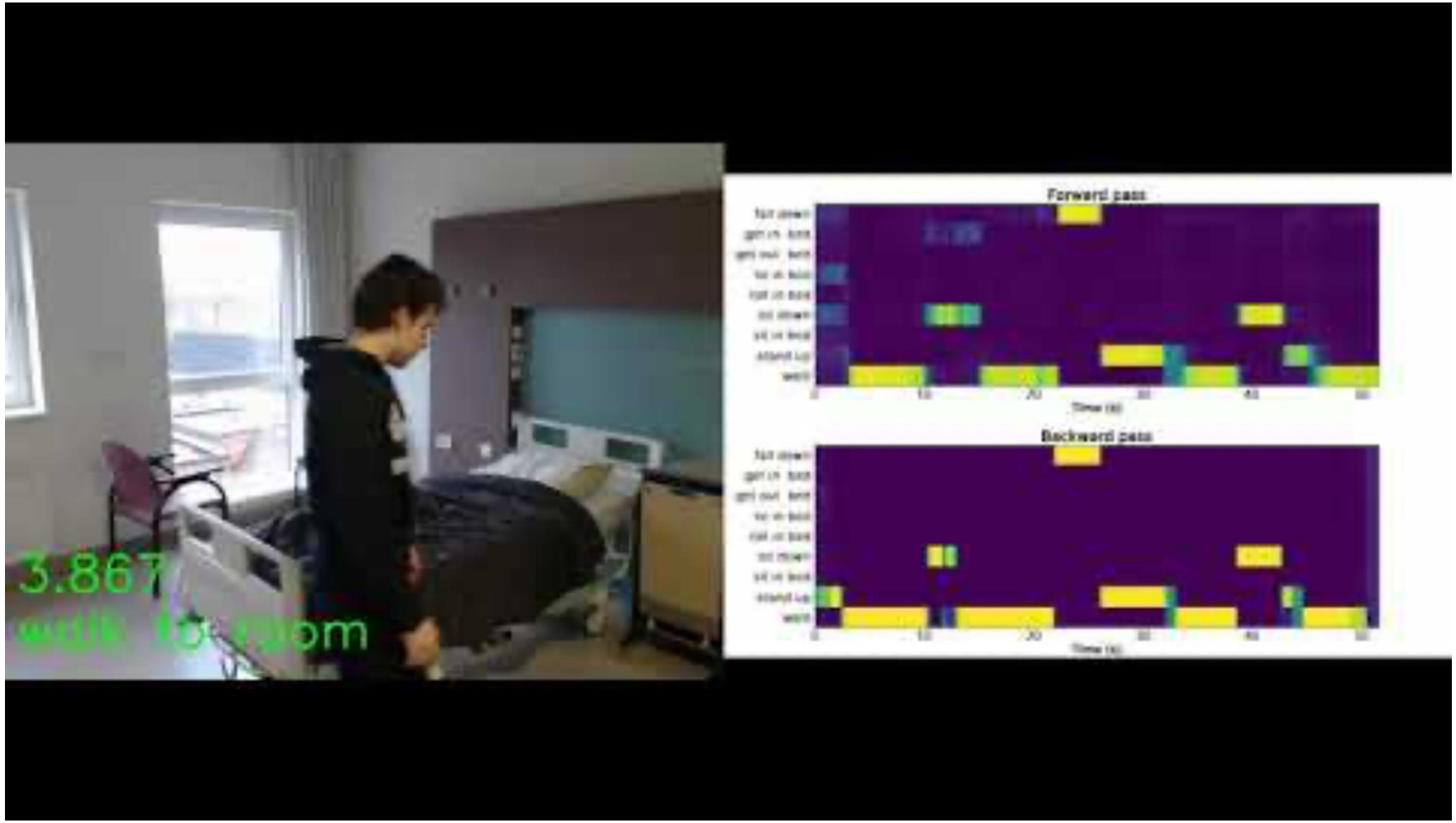
RADAR - PATIENT MONITORING (CONT'D)

DEMO

https://www.youtube.com/watch?v=cW-XpSwrgsI



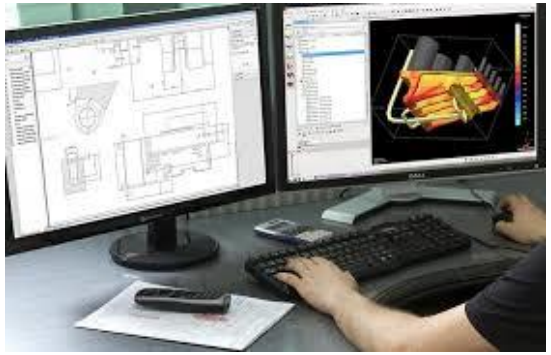
SURROGATE MODELING LAB
MACHINE LEARNING FOR ENGINEERING

- **Research partners**

- **SUMO toolbox**

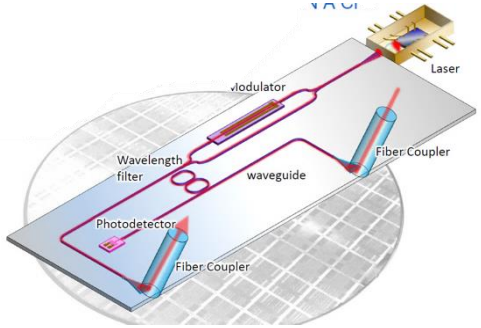
> 5000 downloads

SURROGATES - APPLICATION POTENTIAL



Decision support
- EDA, simulators
- CAE/CAD

Toyota, Siemens, Luceda, Keysight, …



Modeling / Data Science & AI
- Resource-constrained Env.
- Edge-cloud

Atlas Copco, Boeing, BASF, …

Smart Sensing
- Radar
- Industry 4.0/5.0

Roborn, …

Algorithm Engineering

Intel, NXP,
Atlas Copco, ABB, …

embracing a better life

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