INL/CON-23-72053-Revision-0

DICE Conference Presentations

April 2023

Changing the World's Energy Future

Jeren M Browning, Katherine Neis Wilsdon, Ross Kunz

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Idaho Falls, Idaho 83415

http://www.inl.gov

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DICE 2023

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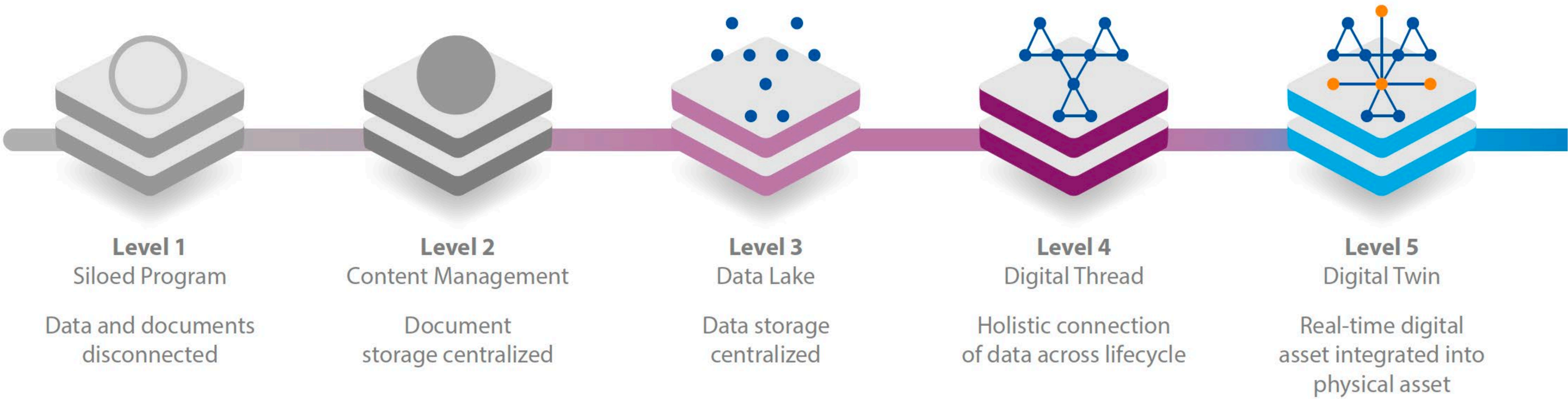
SEARCH:
Digital Twin Analytics

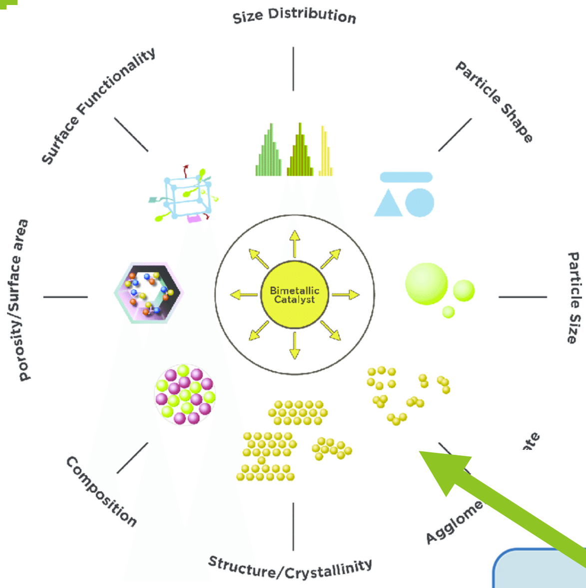
What is Digital Engineering?

Digital engineering transforms the way we **design** and **operate** energy assets:

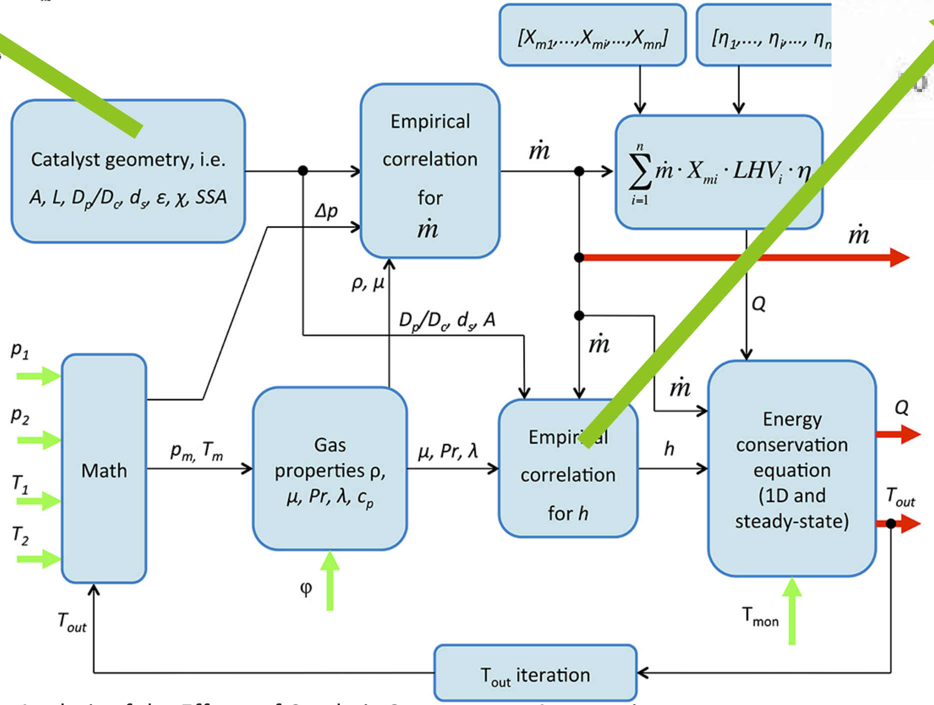
1. Delivers *semi-autonomous design*, *autonomous operation*, and *real-time anomaly detection*
2. Drives research across compute platforms with integrated **human centered visualization**
3. Integrates threads of **data**, **visualizations**, AI/ML, and physics **models** into a cohesive **digital twin**



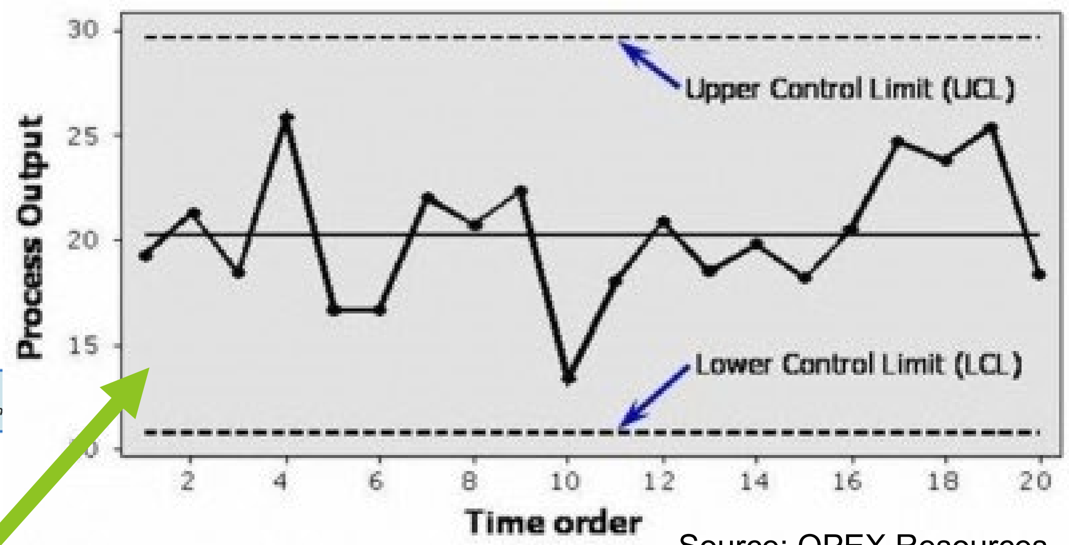
Traditional Operations and Data Science: Micro to Macro



Source: Supported Gold Nanoparticles as Promising Catalysts



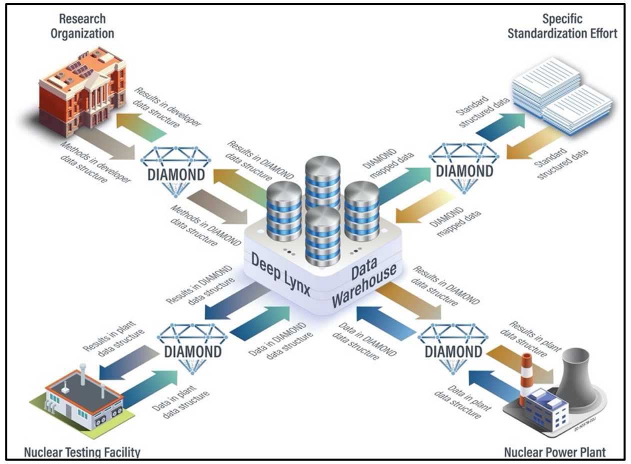
Source: Analysis of the Effects of Catalytic Converter on Automotive Engines Performance Through Real-Time Simulation Models

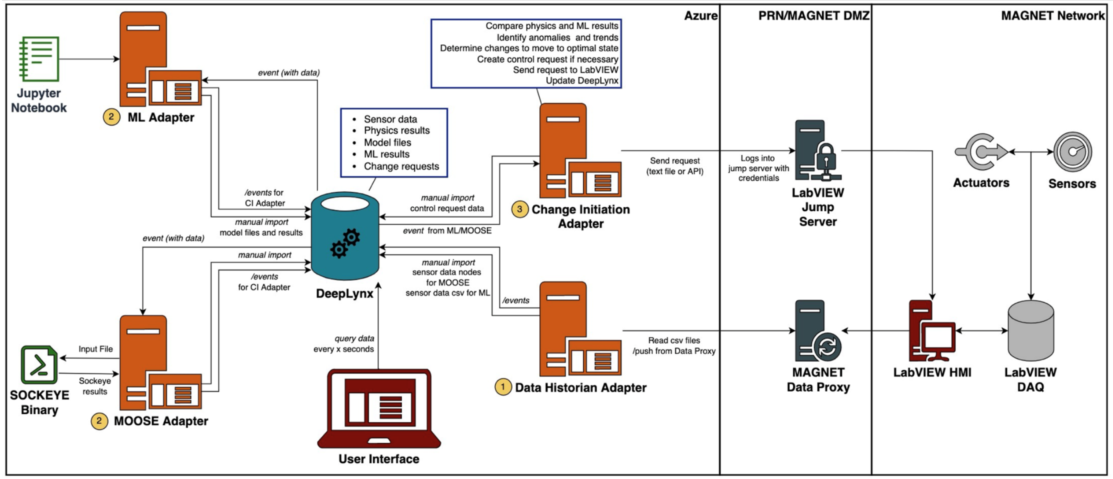


Source: OPEX Resources

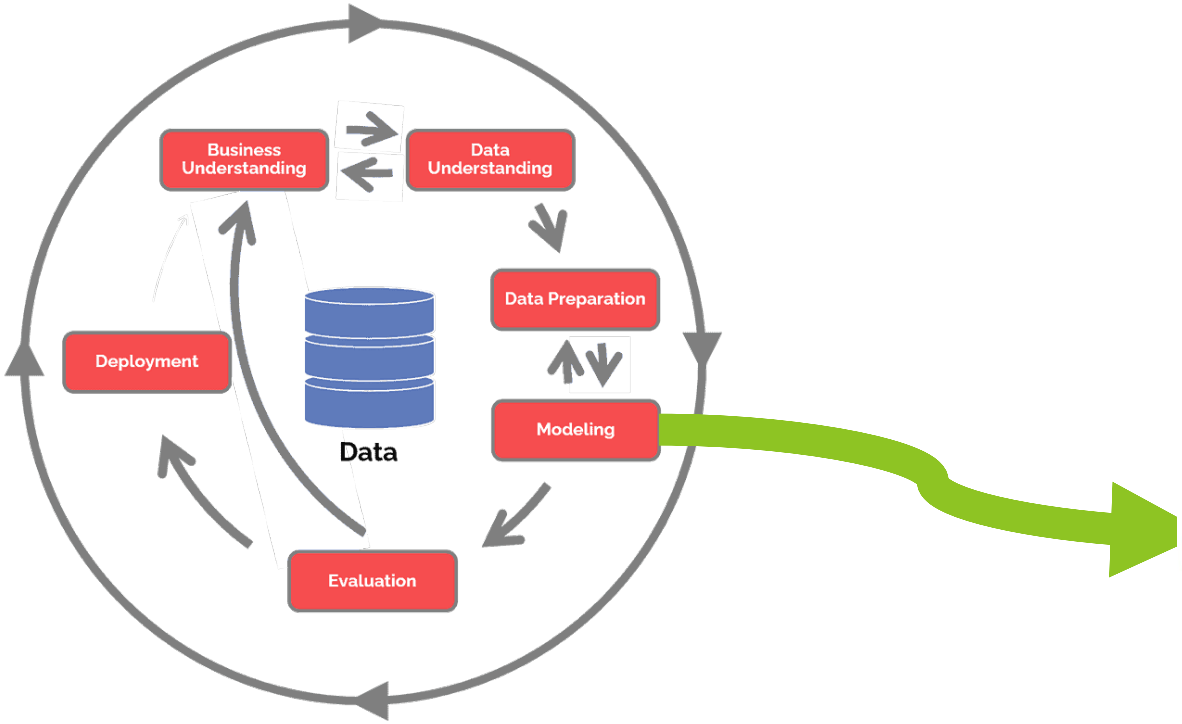
Towards Advanced Analytics / Automation

- **Problems**:
  - Multiple data streams / multiple responses to predict
    - Must handle multiple sensor integration / prediction
  - Real time operations
    - Must be computationally fast (potentially without network connections)
  - Scientific meaning behind measurements
    - Must provide interpretable results

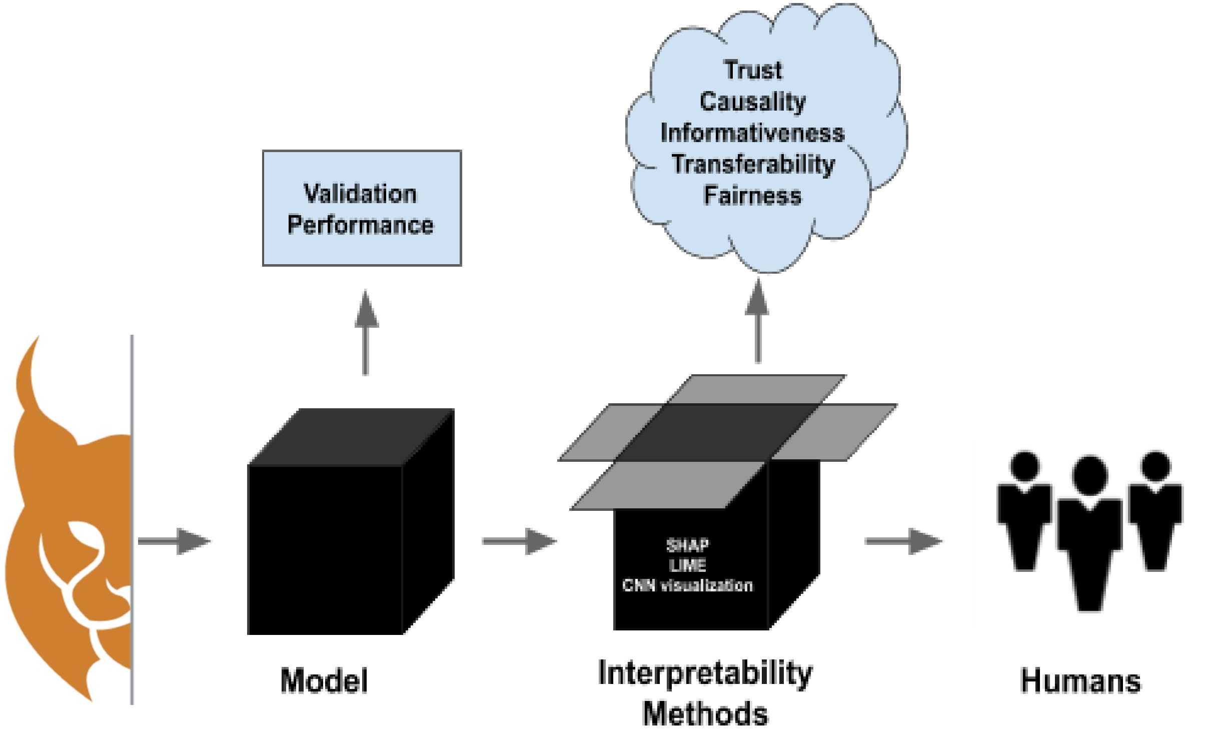




Explainable AI: Scientific Measurements & Interpretability



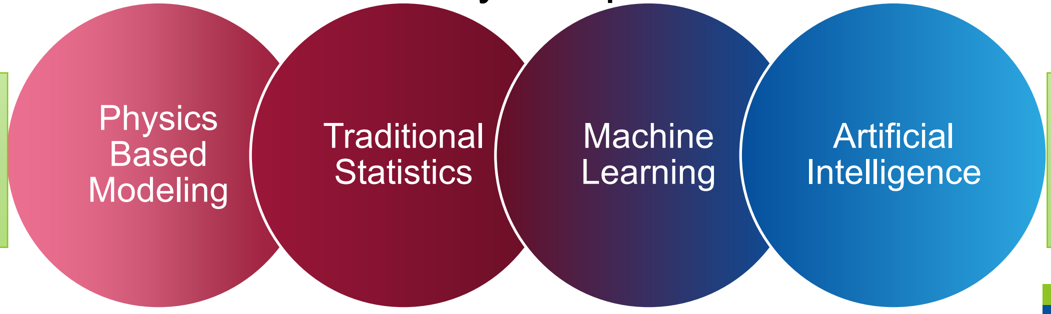
Source: Data Science Process Alliance



Source: ML CMU

Data Analysis Spectrum

- Little to No Data
- Strong Assumptions
- Highly Informative
- High Computation



- Extreme Amounts of Data
- Little to No Assumptions
- Highly Predictive
- High Computation

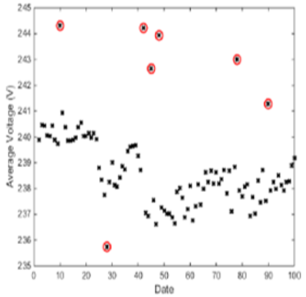
Potential Solution: SEARCH

- Built in connections to Deep Lynx for ease of interaction
- Basic analysis of outliers / imputation / distributions
- Provide an ***initial*** set of analysis for a data scientist
  - Combination of interpretable and more opaque methods
  - No free lunch!
- Dimension reduction and interpolation
- Common set of metrics and permutations of data sets
- Built in documentation of methodologies and generalized interpretation of results
- Written in Rust for computational efficiency

SEARCH: Backend

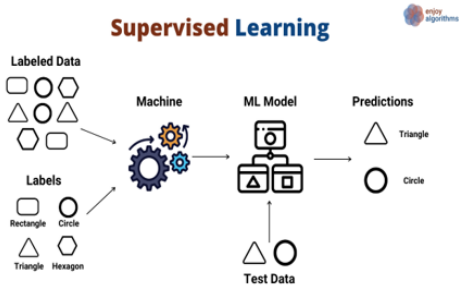
Store: Deep Lynx, CSV, JSON

Explore: Automated Unsupervised Learning



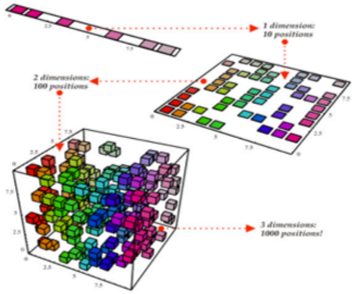
Source: Fast Data Clustering and Outlier Detection using K-Means Clustering on Apache Spark

Assess: Automated Supervised Learning



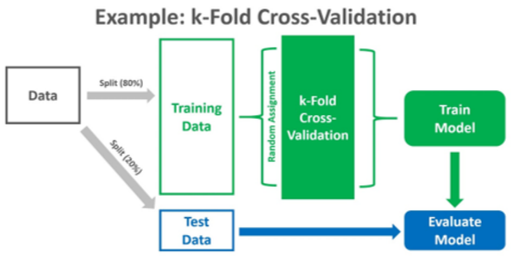
Source: Enjoy Algorithms

Reduce: Dimension Reduction



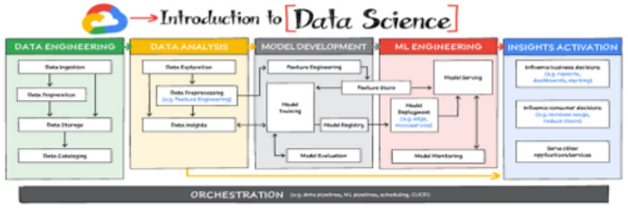
Source: Raft

Confirm: Multiple Iteration Testing



Source: David Caughlin

Holistic: Document Creation and Explanation



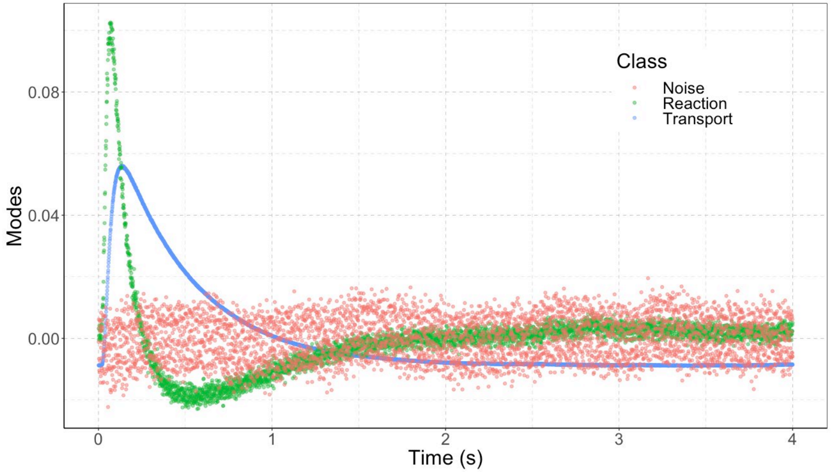
Source: Google Cloud Blog

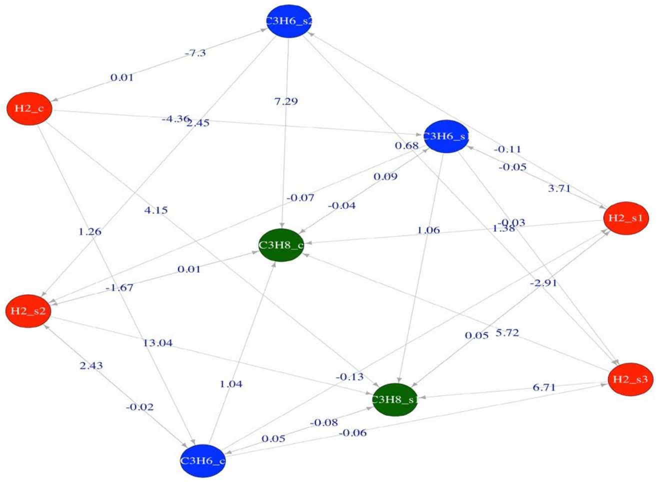
Example Use Case: MAGNET

- Problem:
  - Autonomous prediction and control of heat pipe temperature
- Solution:
  - Local interpretable machine learning with anomaly detection
- Results:
  - 99%+ forecast accuracy over the course of the demonstration
  - Listed as one of the “11 Big Wins for Nuclear Energy in 2022” by DOE https://www.energy.gov/ne/articles/11-big-wins-nuclear-energy-2022
  - Listed as a “Nuclear Milestone” by DOE https://www.energy.gov/ne/articles/idaho-national-laboratory-demonstrates-first-digital-twin-simulated-microreactor

Example Use Case: Dynamic Chemical Engineering

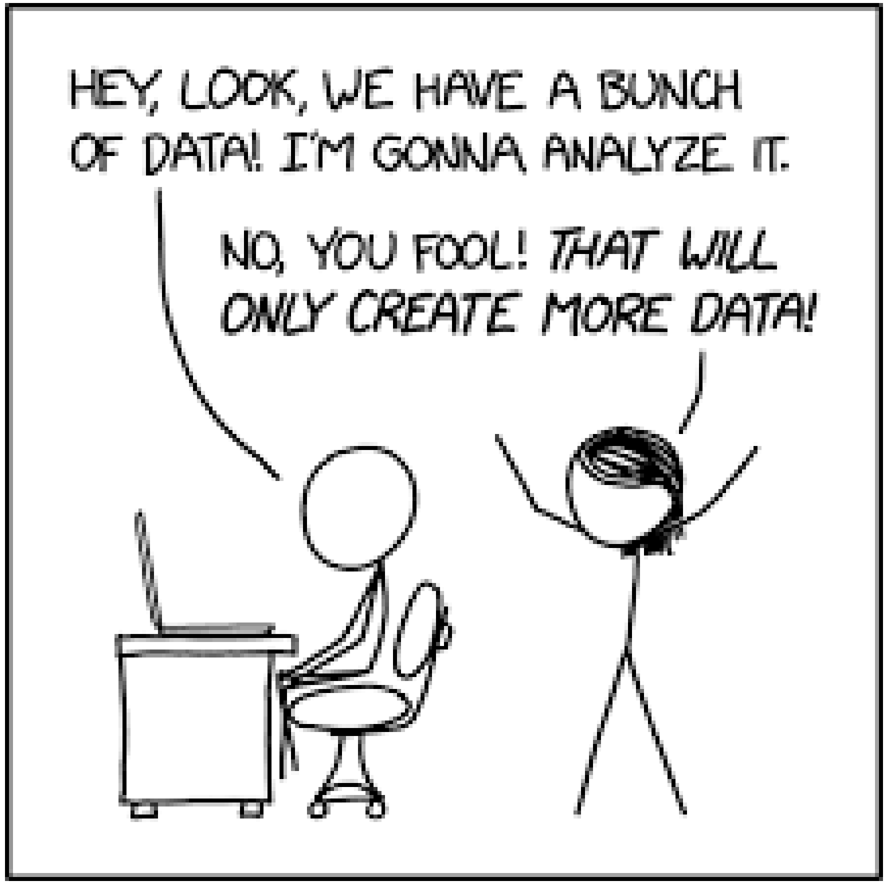
- Problem:
  - There exists a “materials and pressure gap” for understanding industrial applications via first-principles modeling and simulation
  - Need to understand governing equations directly from data
- Proposed solution:
  - Combination of chemical engineering, machine learning, and dynamic systems theory
- Benefits:
  - Data-driven understanding of a process
  - Better connection from first-principles to experiments





Benefits

- A low resource intensive software package based on interpretable machine learning
- Combination of statistics, machine learning, and dynamic control system engineering
- An autonomous prediction of real time operations with human-in-the-loop interactions (subject matter experts and data scientists)



Source: XKCD

Digital Engineering Conference

April 25 & 26 | Idaho Falls

Sandia National Laboratories
PPPL Princeton Plasma Physics Laboratory
Lawrence Livermore National Laboratory
NREL National Renewable Energy Laboratory
Argonne National Laboratory
INL Idaho National Laboratory
NETL National Energy Technology Laboratory
Los Alamos National Laboratory
Jefferson Lab
APL Johns Hopkins Applied Physics Laboratory
Fermilab
MIT Lincoln Laboratory
Oak Ridge National Laboratory

INL Idaho National Laboratory

Jeren Browning
Katie Wilsdon

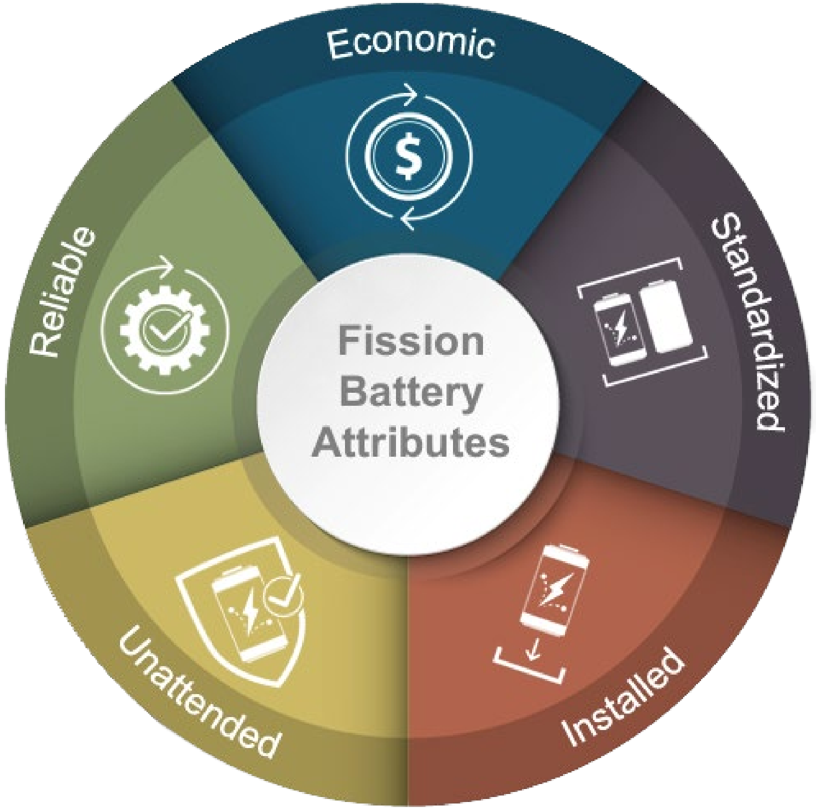
Transformational Digital Twins for Anticipatory and Automated Control

Idaho National Laboratory

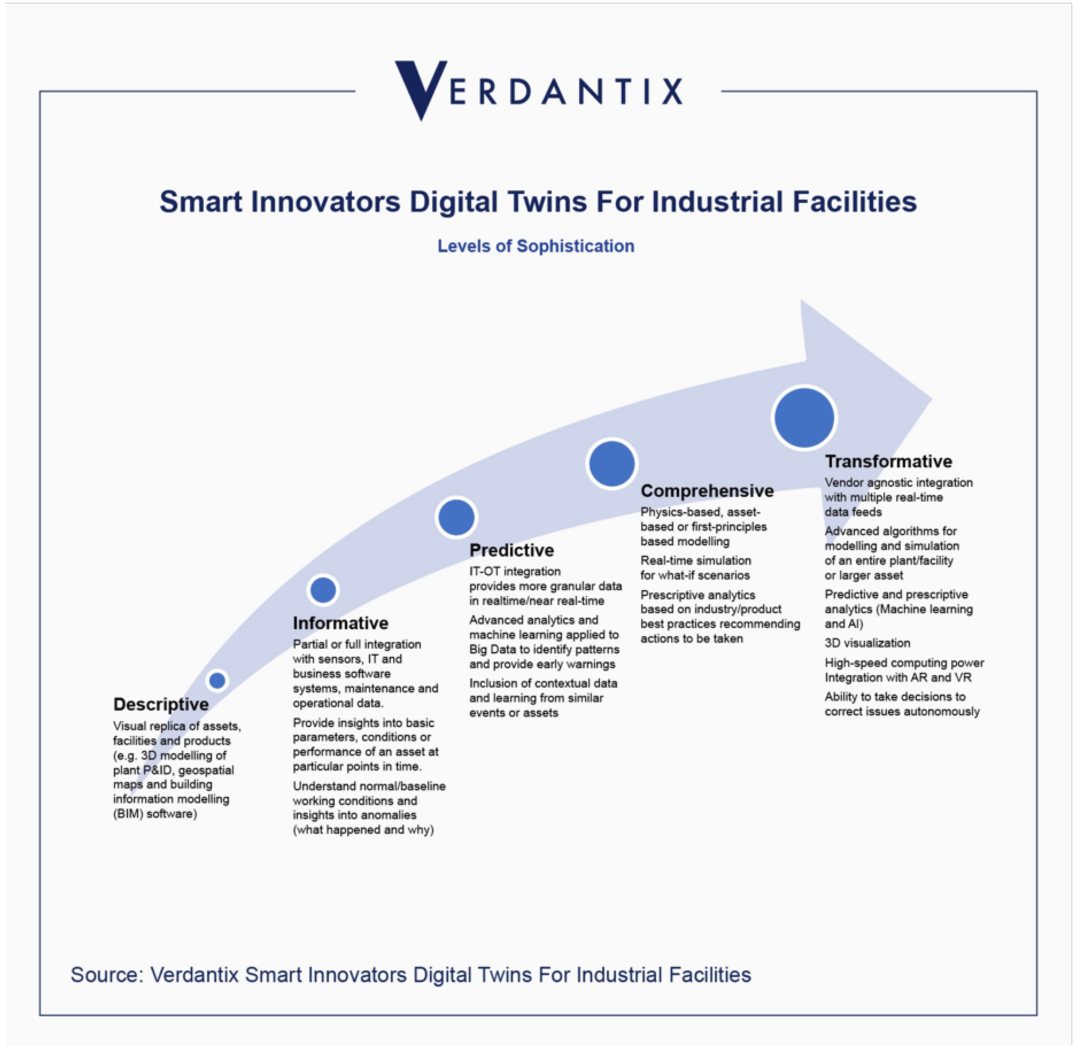
Fission Battery Initiative

- Nuclear energy systems delivered as a “plug-and-play” service
- Five key attributes

Can a digital twin be an enabling technology for <u>unattended</u> fission batteries?



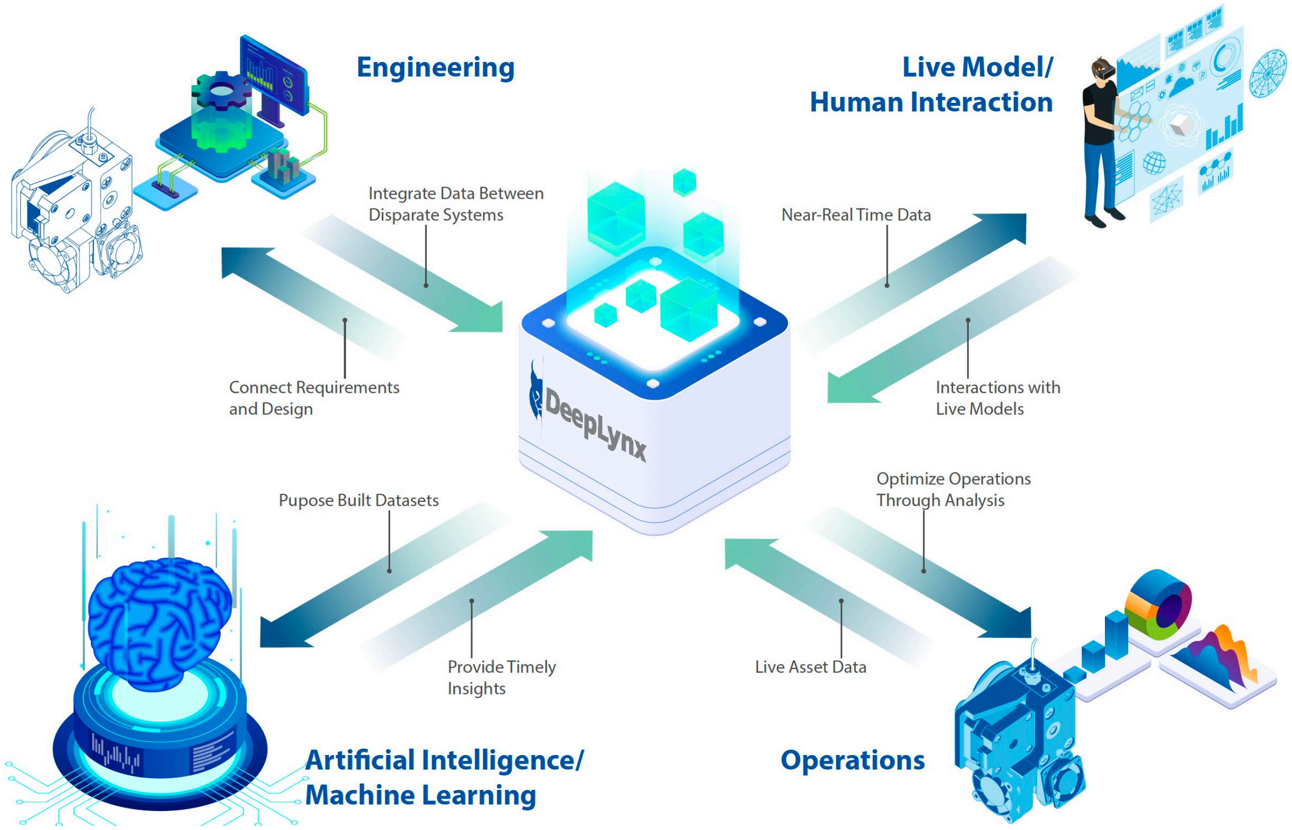
Digital Twin Forms and Levels



1. **Descriptive**: Visual replica
2. **Informative**: Integration with operations (sensor data)
3. **Predictive**: Basic insights through data-driven methods
4. **Comprehensive**: Real-time simulation and prescriptive analytics
5. **Transformative**: Autonomous (automated) operation

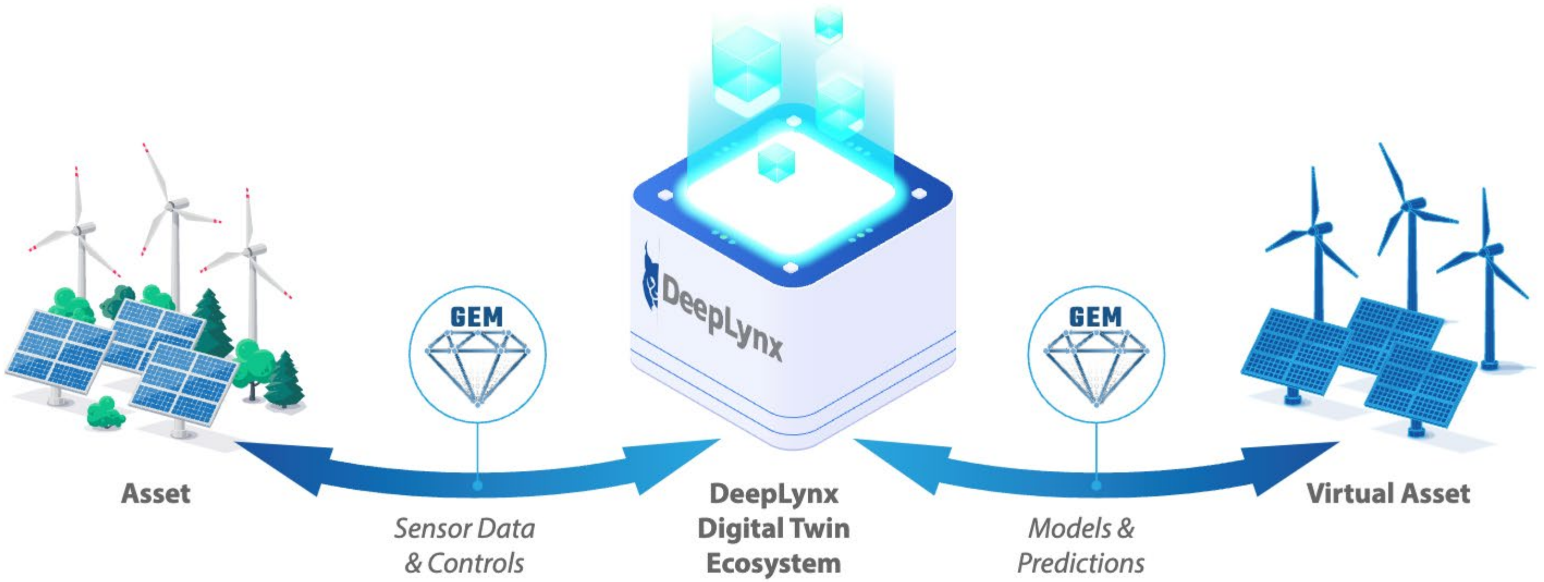
Digital Twin Maturity Model

1. Define architecture and ontology via **Model-Based Systems Engineering** and create the **3D representation**
2. Integrate data into a digital thread **Deep Lynx and Associated Adapters**
3. Provide explainable prediction of asset performance and reliability **Explainable AI**
4. Integrate first-principles models **MOOSE Multi-Physics**
5. Autonomous asset prediction and/or operation for physical assets **Control Adapters**



DeepLynx Data Warehouse

- **Dynamic ontological and time series storage** of digital twin data streams
- **Event system** to push and pull data in real-time around a digital twin
- Heterogeneous architecture (local, cloud, edge)



Integrations with the following data sources:

- AutoDesk Vault (**CAD**)
- AVEVA (**BIM**)
- Hololens (**MR**)
- UNC (**HPC**)
- Lab View **(DAQ)**
- IBM Jazz ELM **(RM)**
- Innoslate **(MBSE)**
- Mathematics **(DiffEq)**
- MOOSE **(Multi Physics)**
- ML Adapter **(AI/ML)**
- Primavera P6 **(Schedule)**
- SERPENT **(Neutronics)**
- RAVEN **(TEA)**
- **And more**

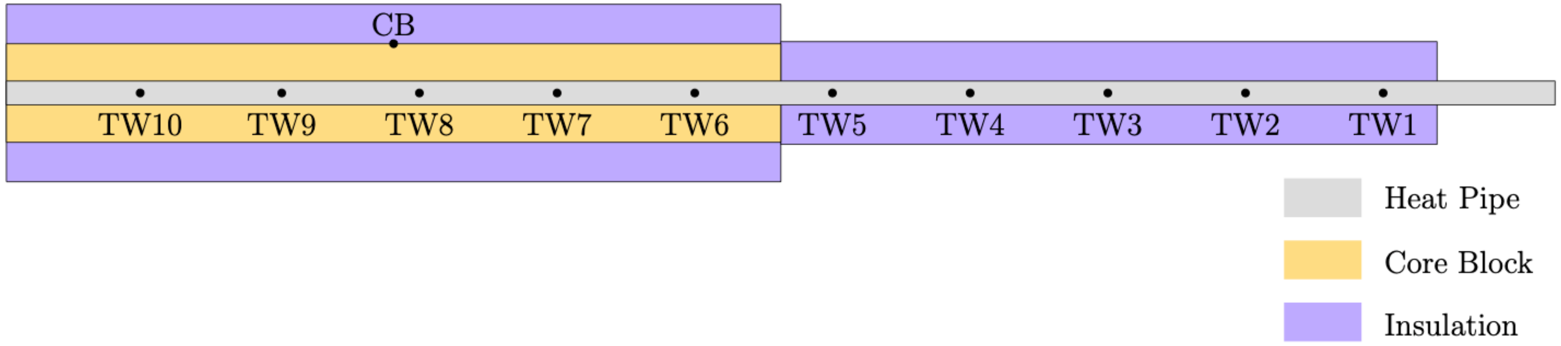
Microreactor AGile Non-Nuclear Experimental Test Bed (MAGNET)

- Thermal-hydraulic and materials performance test chamber for design verification & validation
- Expandable design with integrated power conversion unit (PCU)

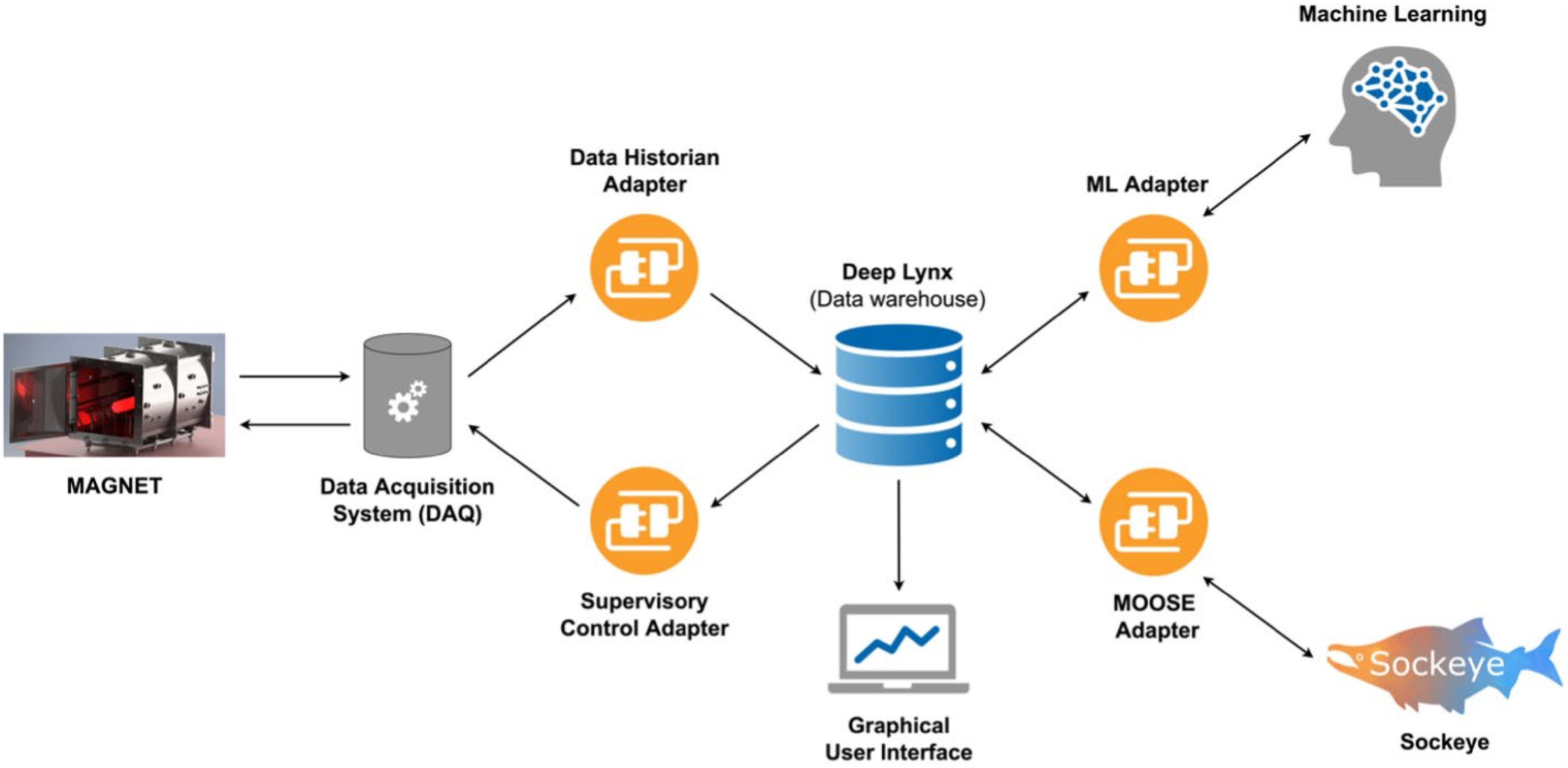
Parameter	Value
Chamber Size	5 ft x 5 ft x 10 ft
Heat Removal	Liquid-cooled chamber walls, gas flow
Connections	Flanged for gas flow and instrumentation feed through and viewing windows
Coolants	Air, inert gas (He, N2)
Gas flow rates	Up to 43.7 ACFM at 290 psig
Design pressure	22 barg
Maximum power	250 kW
Max Temperature	750 C
Heat Removal	Passive radiation or water-cooled gas gap calorimeter

Hypothesis

- The digital twin can:
  - **Predict future temperatures** of heat pipe thermocouples
  - Use predictions to **send control requests** to the HMI
- Experiment Plan:
  1. Manually adjust the temperature set point to an upper or lower limit.
  2. As the heat pipe approaches the limit, the digital twin predicts the temperature will exceed the limit.
  3. The digital twin produces a control request which the HMI can apply to change the temperature set point back to the baseline temperature.



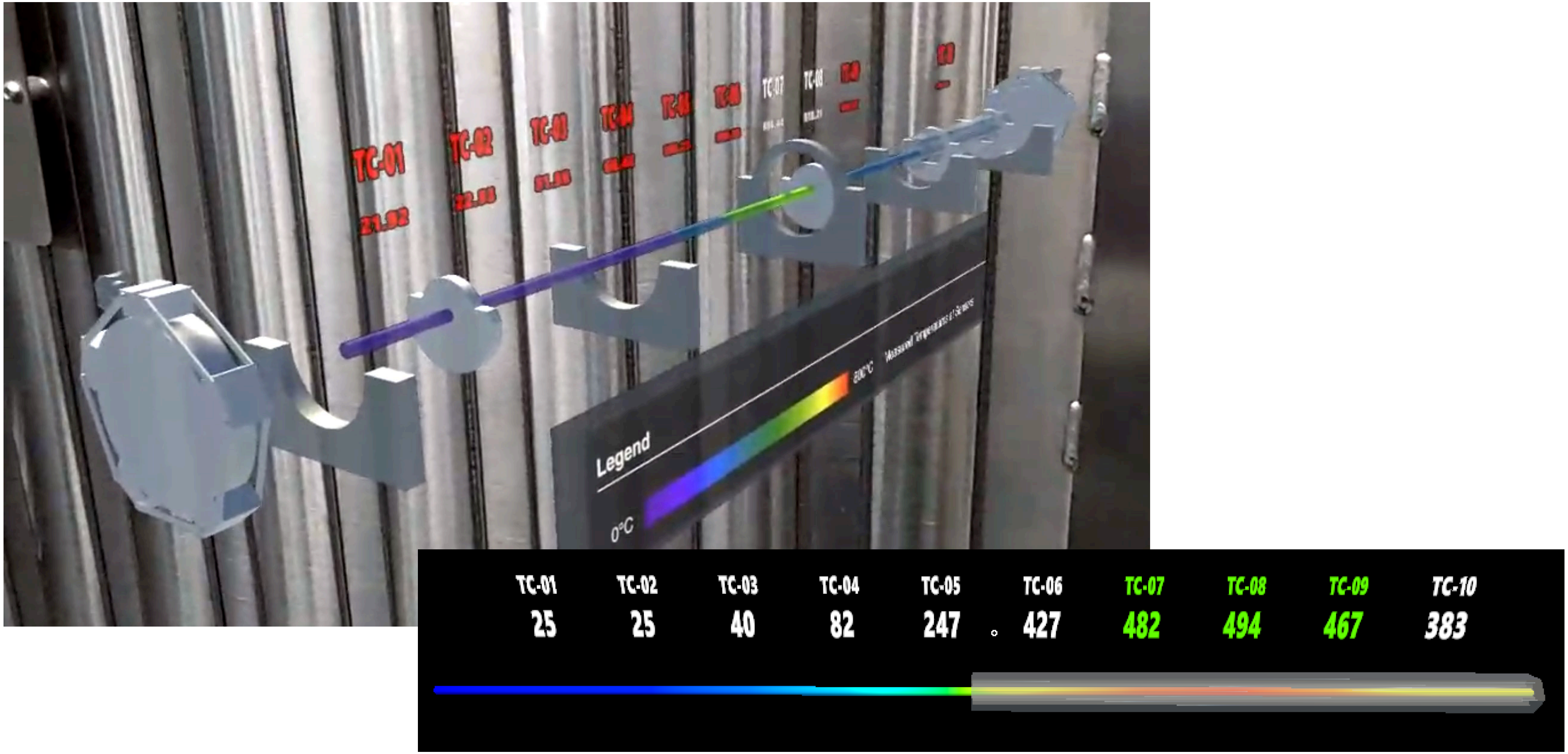
Digital Twin Architecture



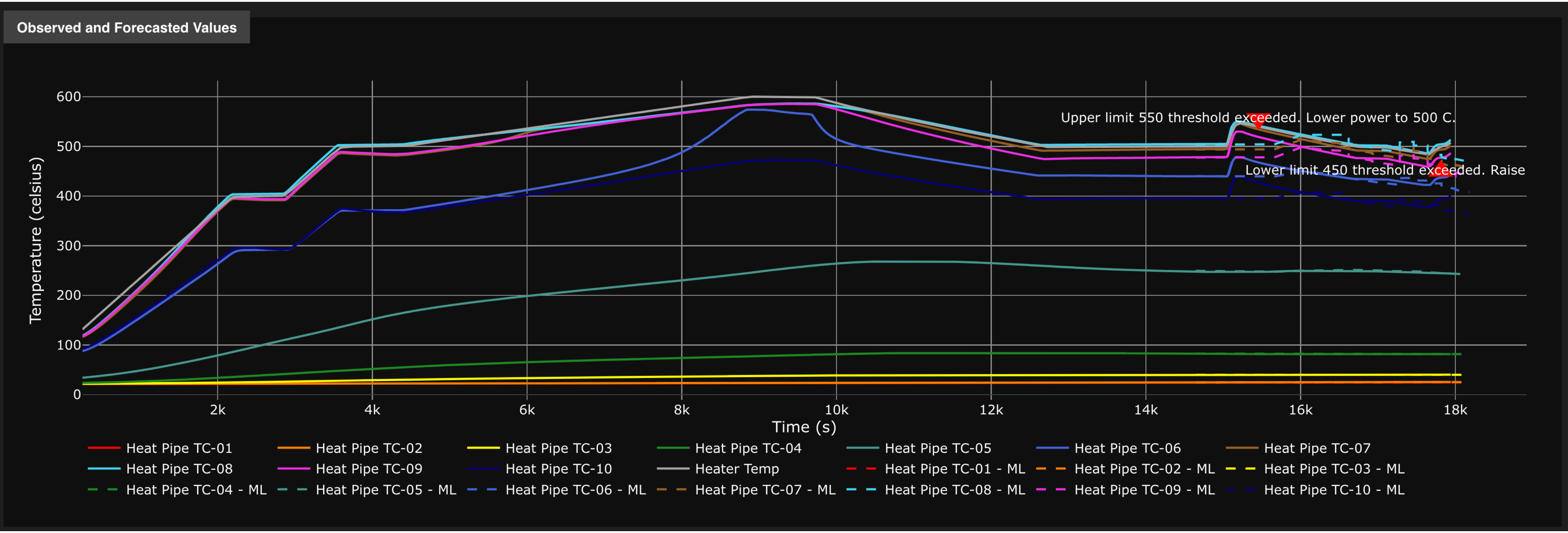
March 30 2022 Test

Video: https://www.youtube.com/watch?v=tRDjY3DZNZM

Live 3D Heat Pipe Model

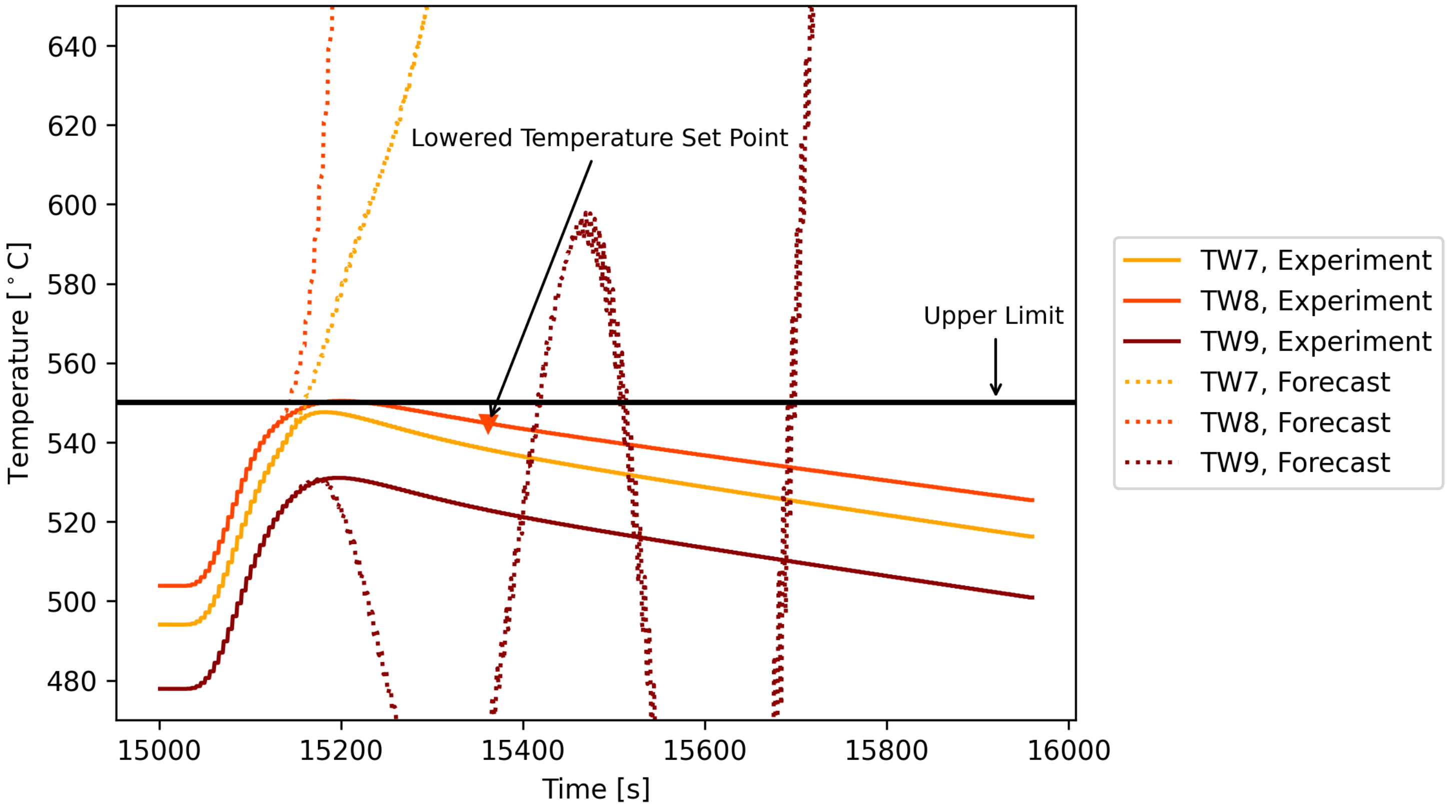


Test Results



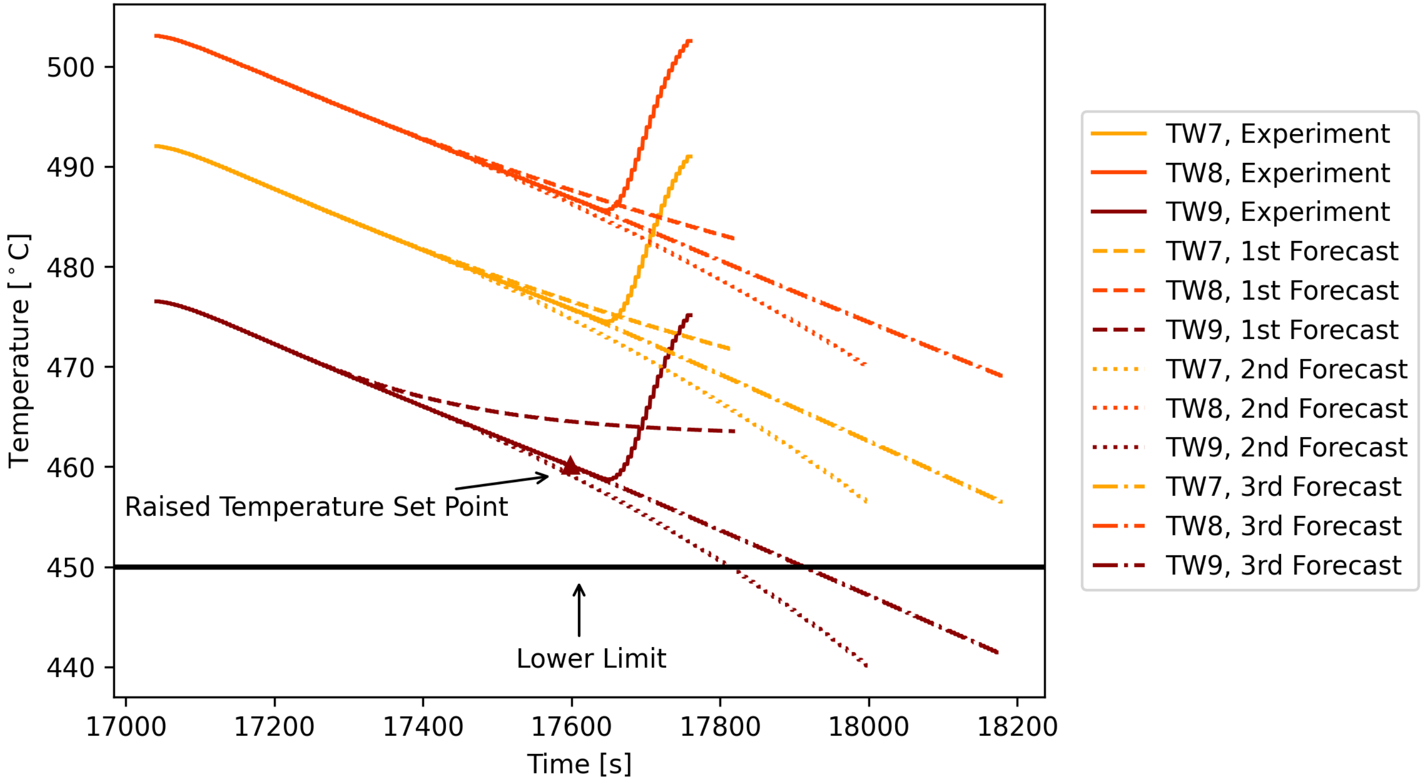
The Upper Limit Test Case

- Result
  - Reached the upper limit before the digital twin could react
- Problem
  - Missing a control for the ramp rate
  - Expected ramp rate of 100°C per hour
  - Rose 50°C in 2 min 20 sec

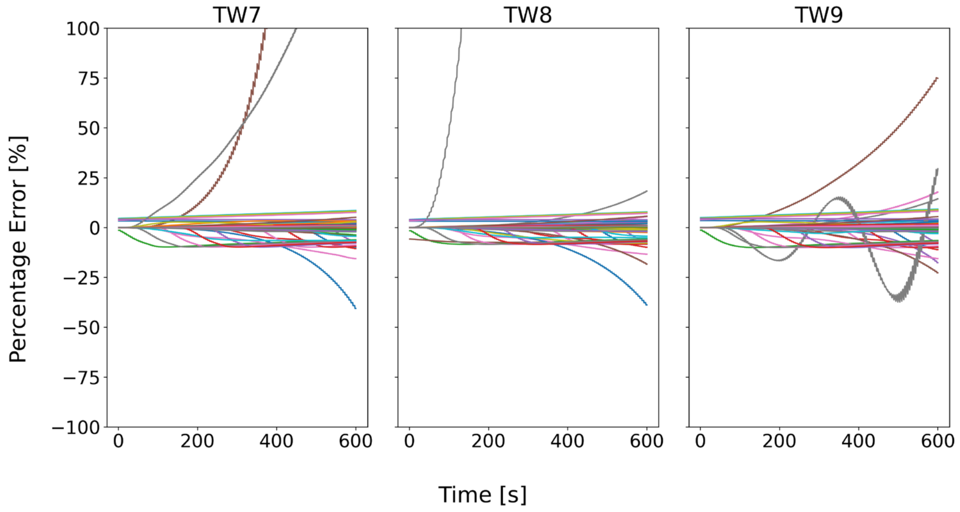


The Lower Limit Test Case

- Result
  - Self-adjusted before reaching the lower limit
  - The digital twin adjusted the temperature set point to baseline when the heater temperature (not shown) reached 483°C



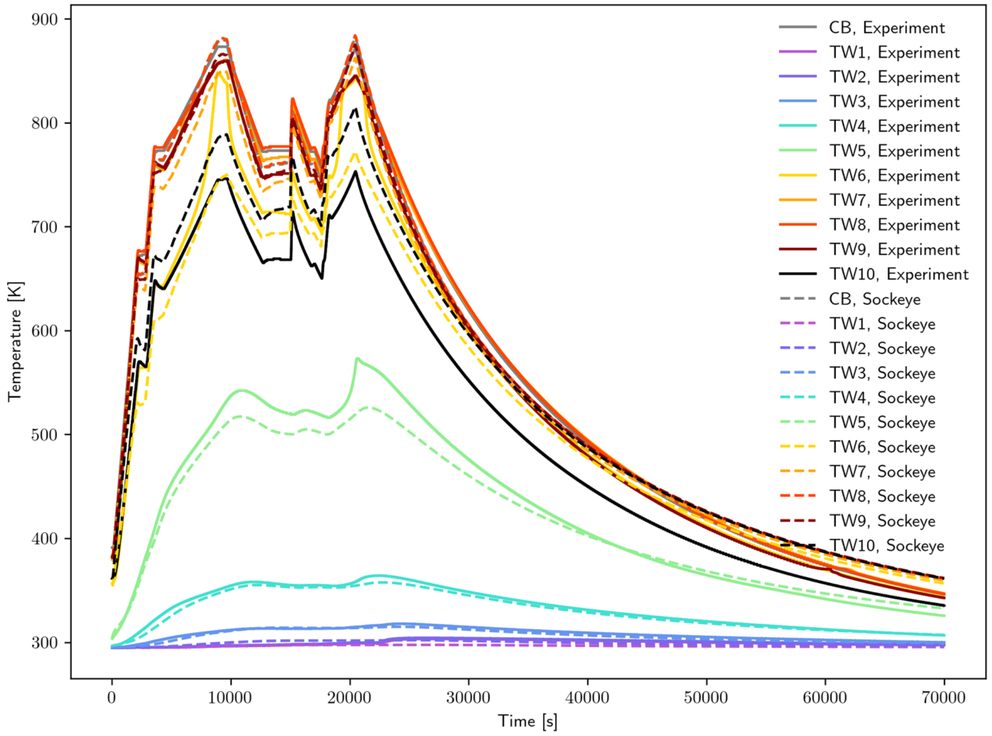
Machine Learning Approach



- Two Stage ML Process
  1. robust variable selection between sensors
  2. multivariate forecasting
- Variable selection
  - ML model: robust elastic-net regression using lasso penalties
  - Determines **relationships between sensors** accounting for any **outliers**
- Multivariate forecasting
  - ML model: vector autoregressive (VAR) model
  - **Extrapolate** the sensor information **in time**
- Result
  - Error: **MAPE < 0.33%** and **RMSE of 2.3 °C** (except for two inflection cases due to ramp rate changes)

Sockeye Multiphysics Results

- Heat Pipe Model
  - 2D heat conduction model: heat pipe cladding and core block
- Experimental Observation
  - **Isothermal operation** was achieved for **two short durations** with only a few thermocouples
- Assumption
  - The vapor core had the thermal conductivity of sodium vapor at 600 K, which is roughly **0.04** W/(m-K)
  - A fully operating heat pipe should have an effective vapor core thermal conductivity of **10^5–10^8** W/(m-K)
- Conclusion
  - This dataset **cannot** be used for the **validation** of operational heat pipe models, only for the heat transfer model of the whole assembly



What’s Next?

- Increase the **intelligence of digital twins**
  - Comprehensive use of sensor and prediction data towards autonomous operation
  - Examine tailored applications of ML and physics predictions
- Build and validate the use of **digital twins for nuclear** (microreactors) and integrated energy systems

Check out the **MAGNET demonstration** during lunch today (12 – 1:30)

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