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Validation Framework of a Digital Twin: A System Identification Approach

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Overview of our Approach

1 **Background & Concepts**

2 **System Identification: A Validation Framework**

3 **Case study**

Background and Concepts

Problem Statement

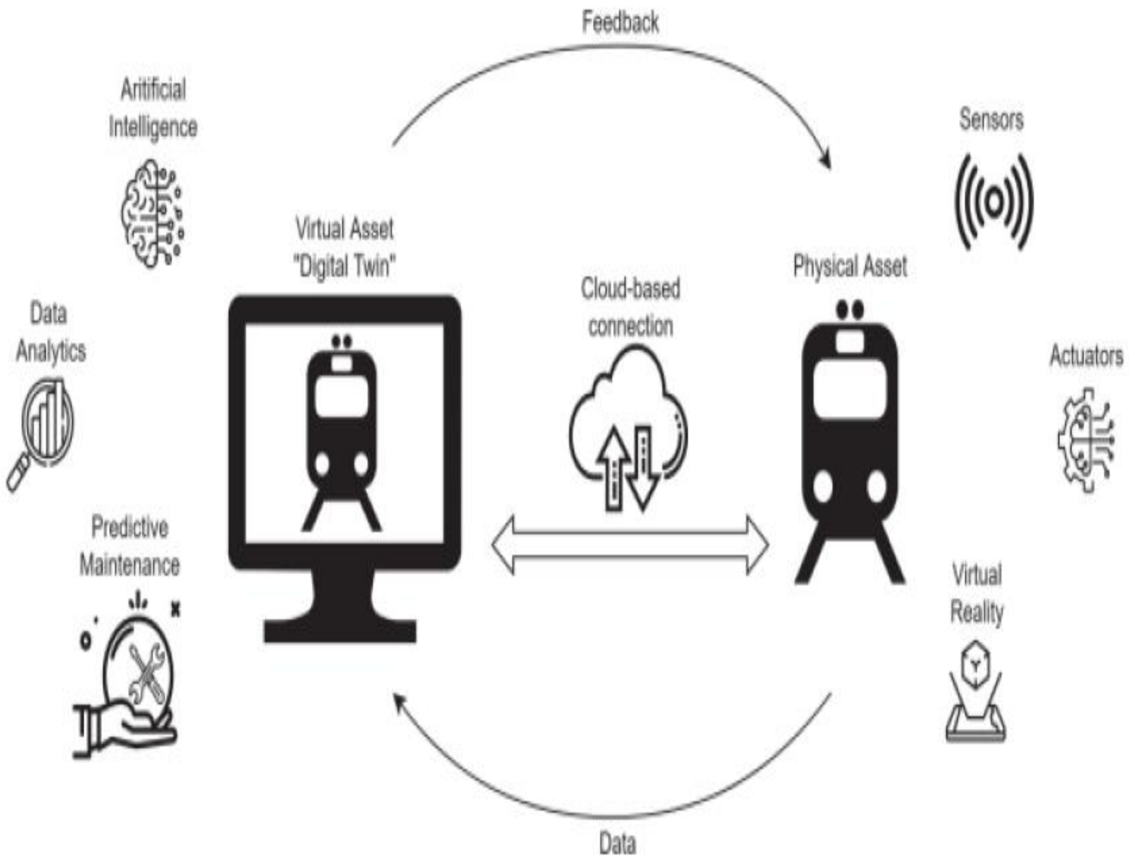
- Recent developments in Machine Learning (ML) algorithms and increasing computational power → AI-Enabled systems
- Can we say that the right system has been built?
- Validation is a critical Systems Engineering (SE) process in answering the question above
- Need to validate system models for AI-Enabled systems wherein their intrinsic dimensions of conceptual, operational and data validity must also be addressed.

Digital Twin as an AI-Enabled System

- AI-enabled systems
  - Consists of software & hardware components, but “also AI algorithms, models, and data” (Pons & Ozkaya, 2019)
  - “cyber-physical systems” exhibiting artificial intelligence (AI) capabilities. (Shadab et al., 2021)

- Digital Twin
  - "high-fidelity model" of a physical asset
  - mimics the actual behavior and operating conditions inherent in the physical asset (Giachetti, 2022)
  - Physical & Virtual assets are linked by sensors exchanging data
  - Data can be analyzed by applying AI techniques and big data analytics (Bešinović, et al., 2021)

- An Intelligent digital twin comprising of a virtual system model of the physical asset with supporting adaptive UI and AI techniques can be classified as an **AI-enabled system**.

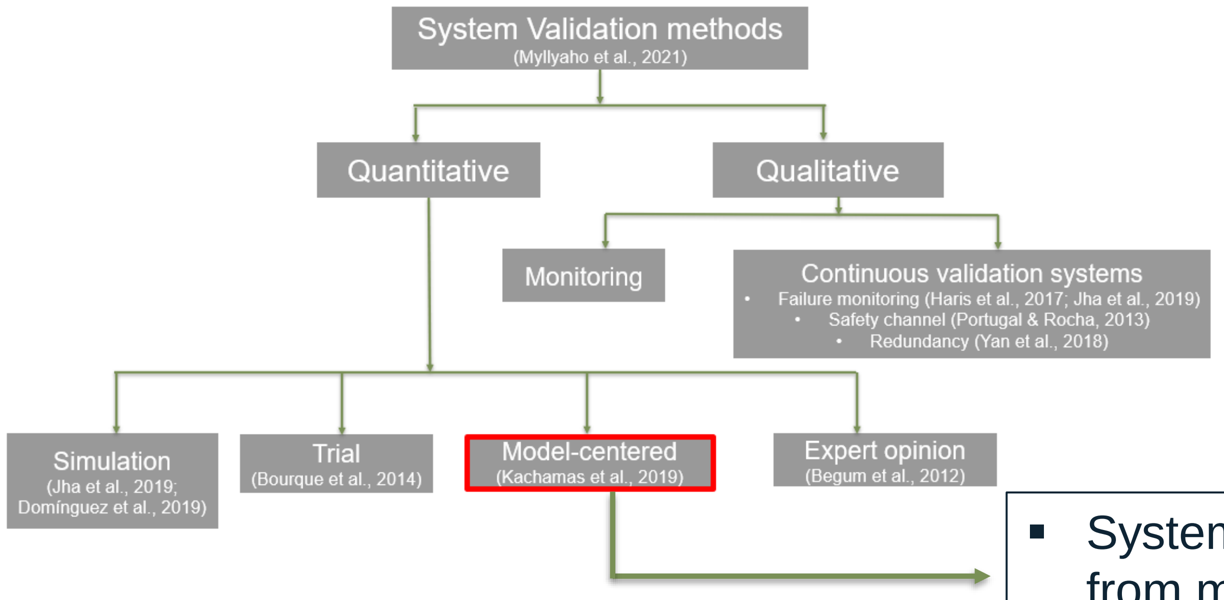


Features of a digital twin (Bhatti, Mohan, & Singh, 2021)

System validation approaches for AI-Enabled Systems

- System Validation methods (Myllyaho et al., 2021)
  - Quantitative
    - Simulation (Jha et al., 2019; Domínguez et al., 2019)
    - Trial (Bourque et al., 2014)
    - Model-centered (Kachamas et al., 2019)
    - Expert opinion (Begum et al., 2012)
  - Qualitative
    - Monitoring
    - Continuous validation systems
      - Failure monitoring (Haris et al., 2017; Jha et al., 2019)
      - Safety channel (Portugal & Rocha, 2013)
      - Redundancy (Yan et al., 2018)

System validation approaches for AI-Enabled Systems



- System validation (complete AI-enabled system) is *different* from model validation (AI/ML algorithm validation)
- A quantitative method for system validation that aims to sustain the appropriate functioning of the AI model engine concerning the whole AI-enabled system
- Validation type is justified when the system validation process is data-centered and is critical for achieving trust in the system when the model works (Myllyaho et al., 2021)

Research Objectives

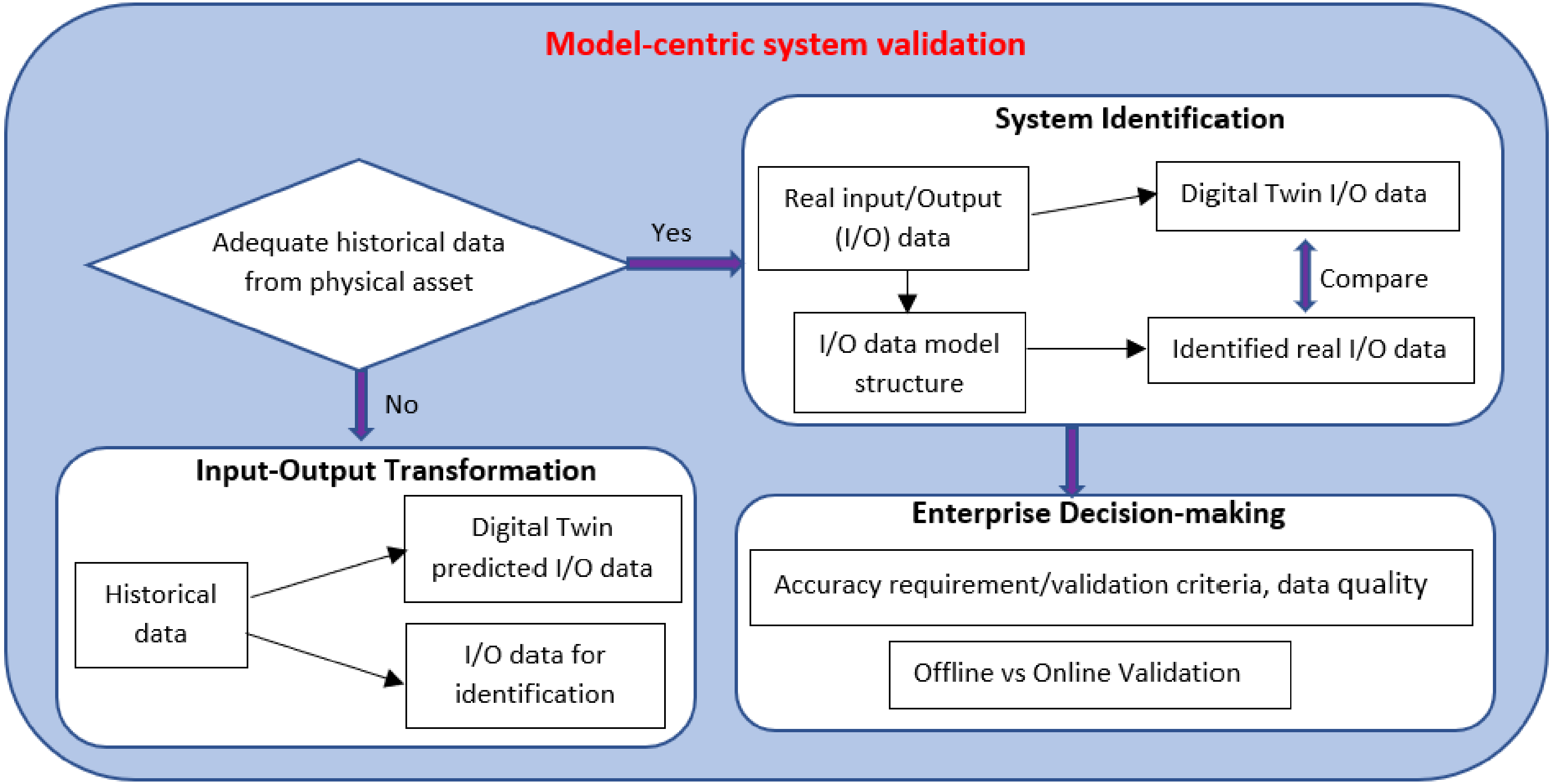
- This work aims to use the system identification technique (model-centric validation approach) to validate a digital twin of a heat-pipe article (an AI-enabled system) at the system level.
- At this level, the digital twin has been successfully built and with one of the stakeholders needs generally concerned with monitoring the physical system towards predicting future failures in the system.
- The exploratory system identification approach helps evaluate historical data from the heat pipe (physical asset) by uncovering unknown system dynamics and mathematical relationships captured within the historical data to understand the asset behavior better.
- Validating the digital twin helps drive the process of validating stakeholders' requirements for the digital twin to mimic the behavior of the heat pipe article.
- The goal of this work is a departure from similar predictive efforts that rely on curve-fitting for extrapolating and making predictions but do not model the system dynamics of the historical data

System Identification: A Validation Framework

Validation framework for a digital twin

- Challenges to digital twin validation framework development:
  - Model realism :
    - highly dependent on model fidelity
  - Input data uncertainty:
    - arises from sensors taking measurements to range tolerance in specification elements of the product requirements documentation e.g. missing data, and inherent data noise
  - Physical asset system dynamics :
    - Capturing inherent system parameters from data
- Need for a model-centric system validation framework that handles the three challenges identified above
  - Differs from an AI/ML model validation as it is focused on enhancing the ability of the digital twin model to mimic, monitor, and update the physical asset.
    - System identification technique

Validation framework for a digital twin

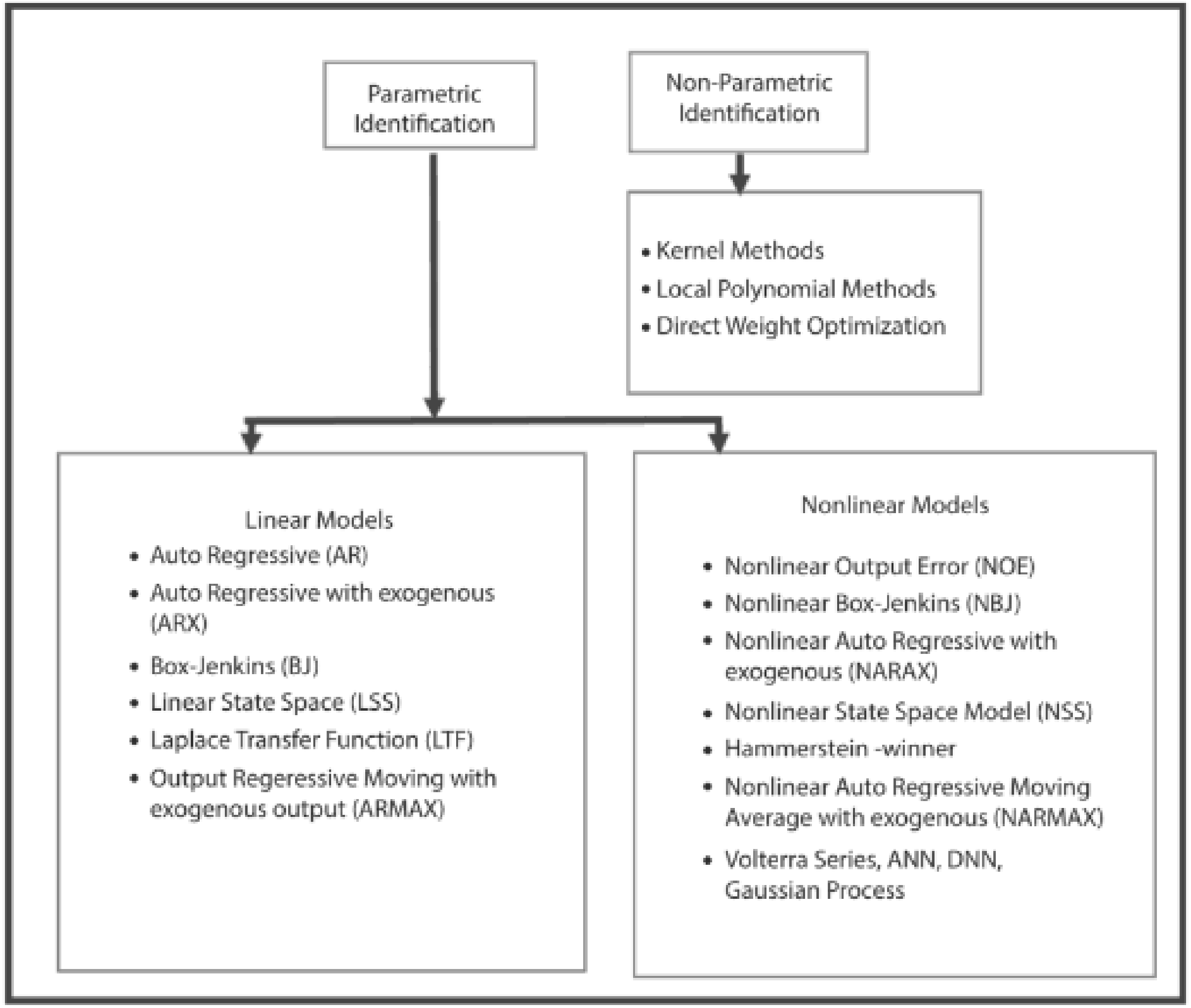


Model-centric validation framework

The System Identification technique

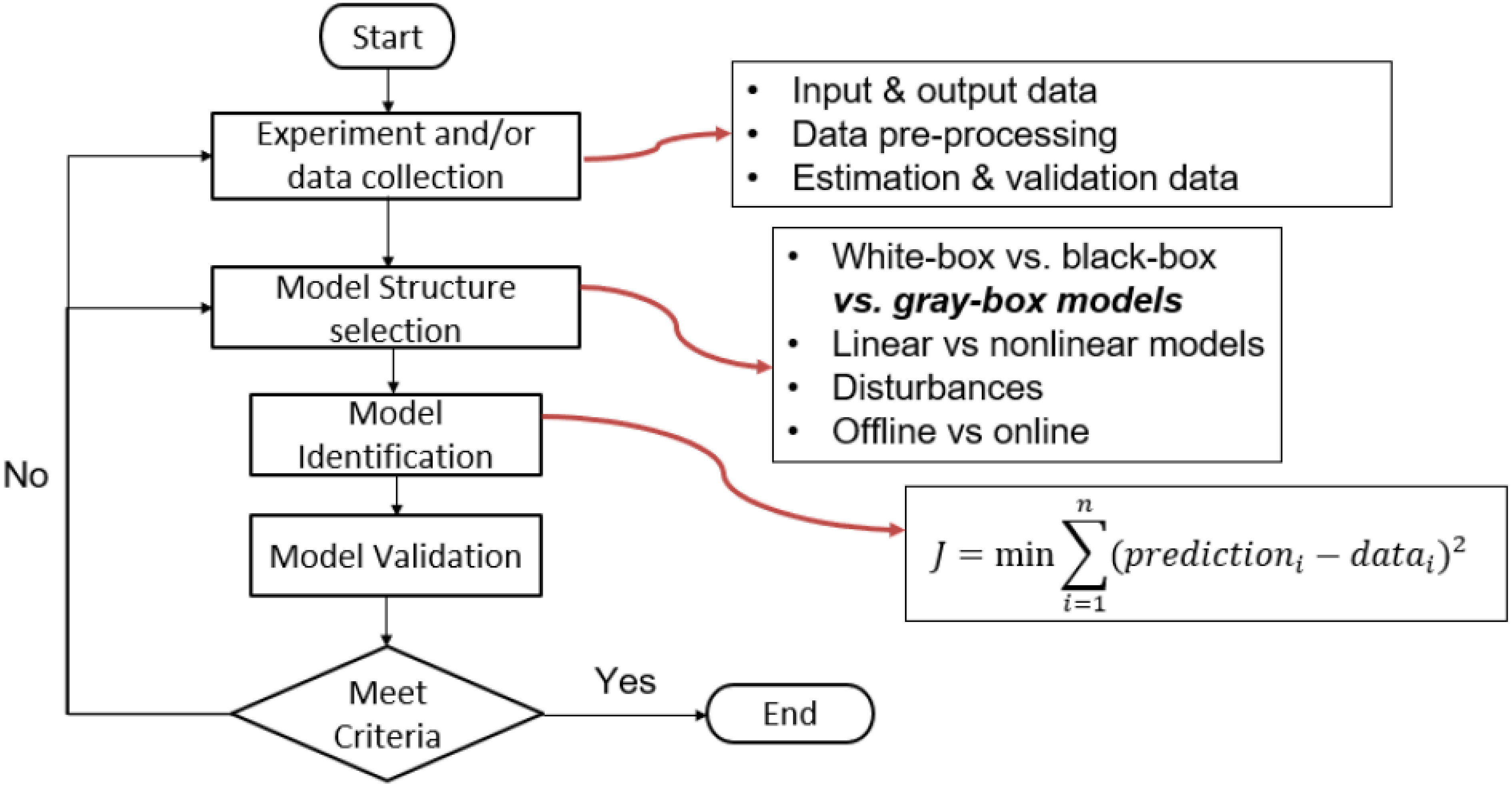
- A data-driven approach that involves building mathematical models of dynamic systems from observed input-output data (Ljung, 2010)

- Digital twin technology is closely related to System Identification
  - Application in online identification capabilities
  - Forecast future states and optimize/adapt/control
  - Physical processes are measured and compared to virtual models for validation



Digital twin technology models in System Identification.
Source: Pattanaik & Mohanty (2024)

System Identification process

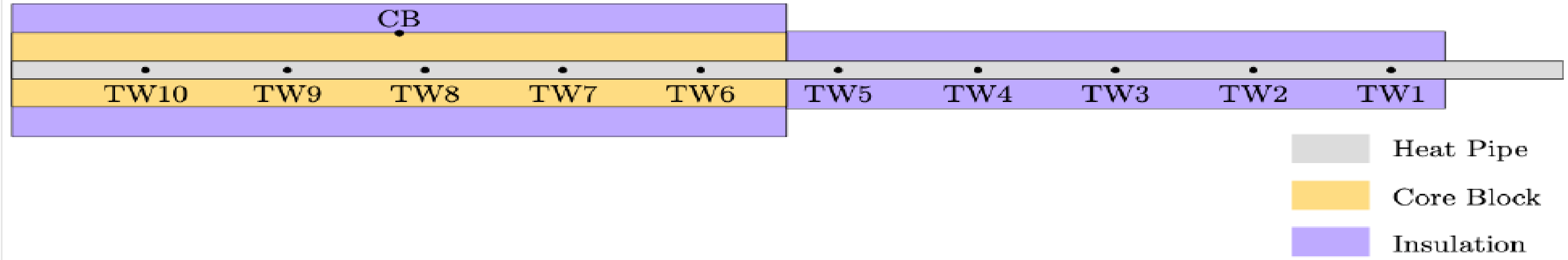


Flowchart for the System Identification technique

Case study: Digital Twin of a Heat-pipe article for a Microreactor Testbed

Case study

- Case study is a digital twin of a single-heat-pipe test article with predictive, self-adjusting capability (Wilsdon et al., 2023)
  - Demonstrated in the Microreactor AGile Non-nuclear Experimental Testbed (MAGNET) at a National laboratory
  - Sodium/stainless steel heat pipe with a mesh screen wick and an unknown quantity of argon gas
  - The heat-pipe article consists of a hexagonal, stainless steel core block containing six cartridge heaters surrounding a single, central heat pipe.
  - Heat pipe is 200 cm long, while the hexagonal block containing the cartridge heaters is 48 cm long.



Axial cross-section of the single-heat-pipe assembly. Source: (Wilsdon et al., 2023)

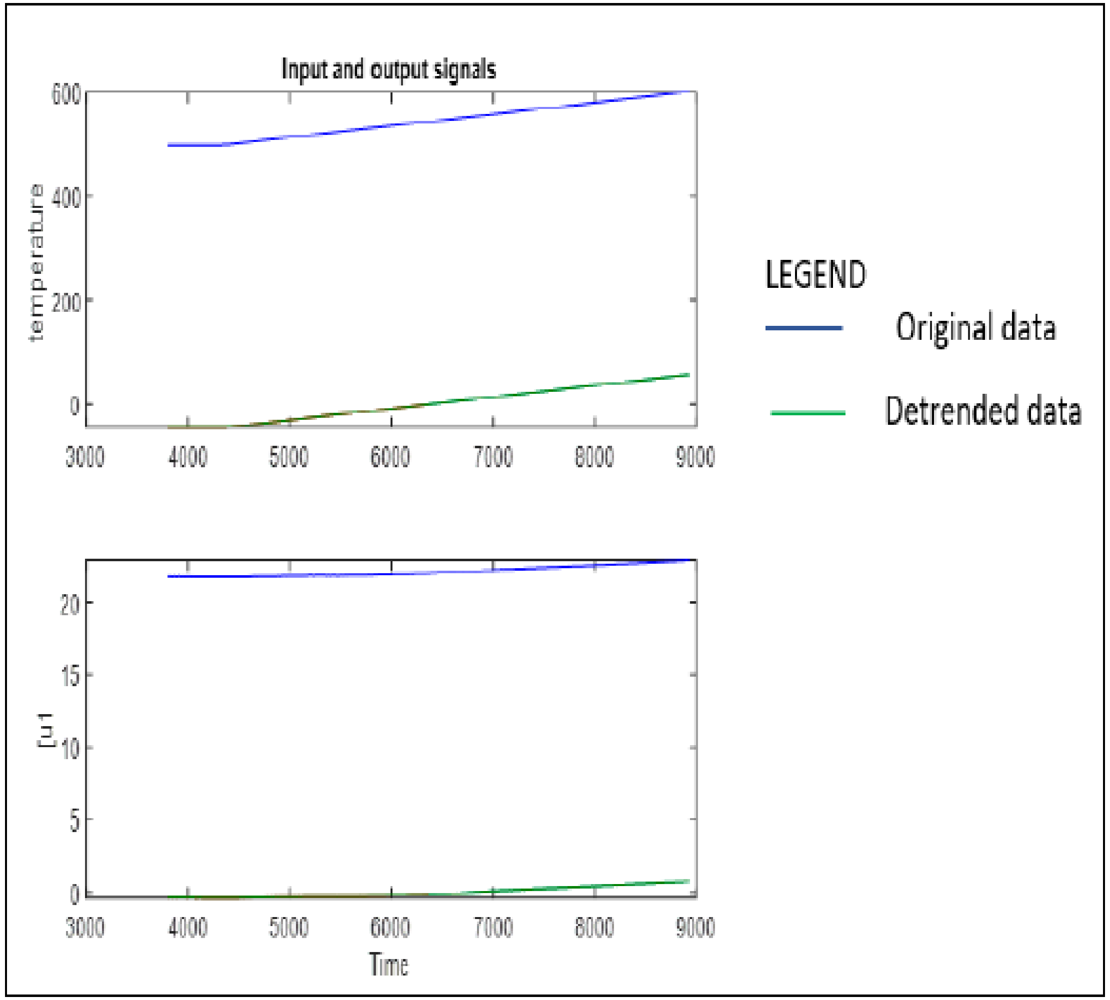
Experiment/Data Collection

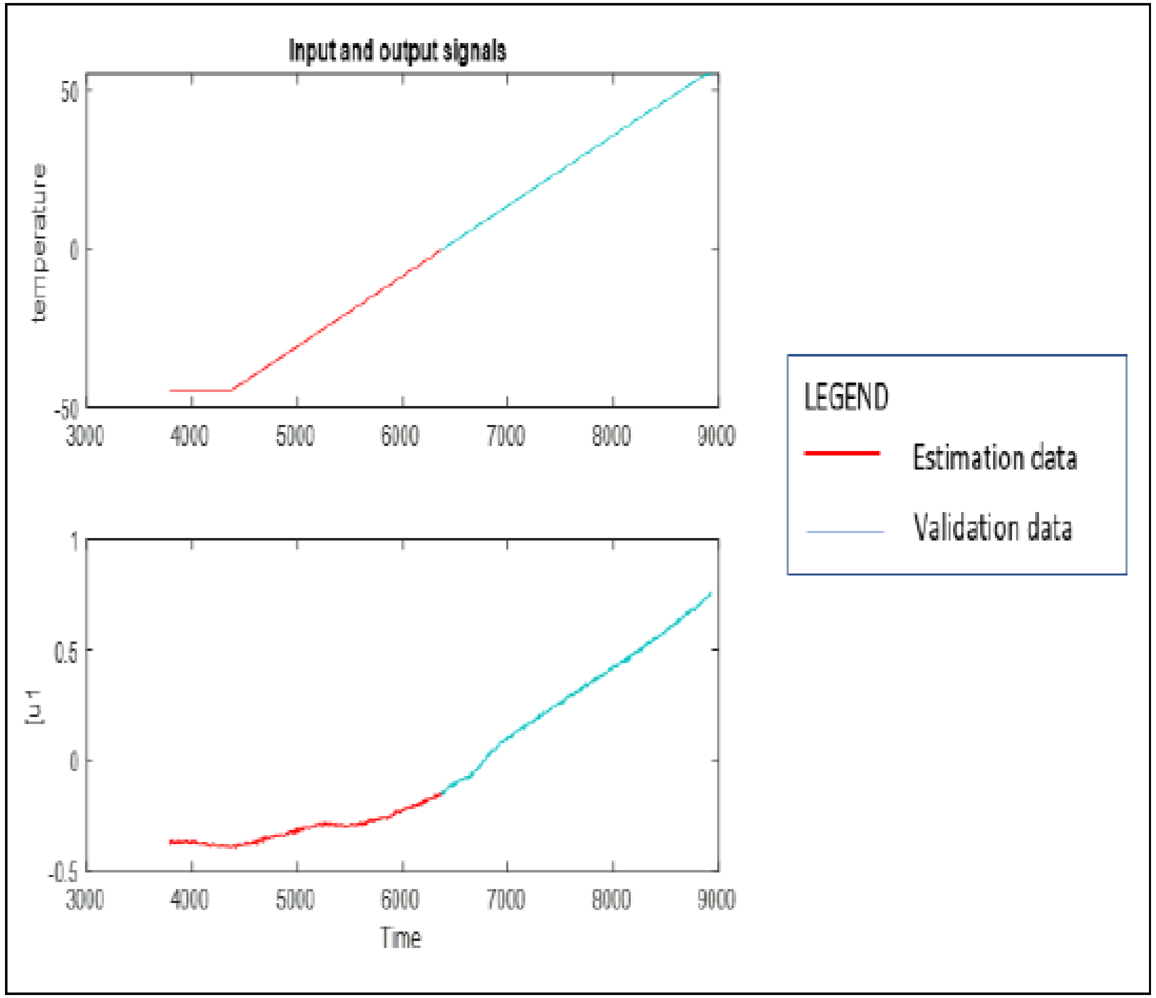
- Input-Output Data (Experimental dataset):
  - Sample size: 5130; start time = 3799 seconds; sample time = 1 second; end time = 8928 seconds
- $temperature = f(u1,\ldots,u10)$ for the thermocouples in heat pipe assembly
  - Output data (single variable) = $temperature$; input data (10 variables) = $u1,\ldots,u10$
- Data pre-processing:
  - detrended the data to remove offsets from the data by subtracting the mean values of the input and the output
  - dataset of 5130 samples is split into two, with the first half set aside for **model estimation** while the other half is used as the **model validation** dataset.

Method: System Identification

- Multiple Input Single Output (MISO) system Identification
  - 10 input variables (temperature for ten thermocouples)
  - 1 output variable (heater temperature)
- Black-box modeling
  - Goal: derive insights from the dataset without prior knowledge of the heat pipe behavior
- Tool/Software: MATLAB System Identification Toolbox
  - MATLAB toolbox for processing system identification technique
  - Experimental data is loaded into the system identification toolbox in MATLAB

System Identification: Data Collection





Plots of the u1-temperature channel. The left side shows detrending. The right side shows the estimation and validation data

System Identification: Model Selection

- Check if input-output data model is linear:
  - Quick Start feature in the System Identification app (4 available linear models)
    - arxqs: Fourth-order autoregressive (ARX) model

$$y(t)+a_1y(t-1)+\cdots+a_{na}y(t-n_a)=b_1u(t-n_k)+\cdots+b_{nb}u(t-n_k-n_{b+1})+e(t)$$

where y(t) represents the output at time t

u(t) represents the input at time t,

n_a is the number of poles,

n_b is the number of b parameters (equal to the number of zeros plus 1)

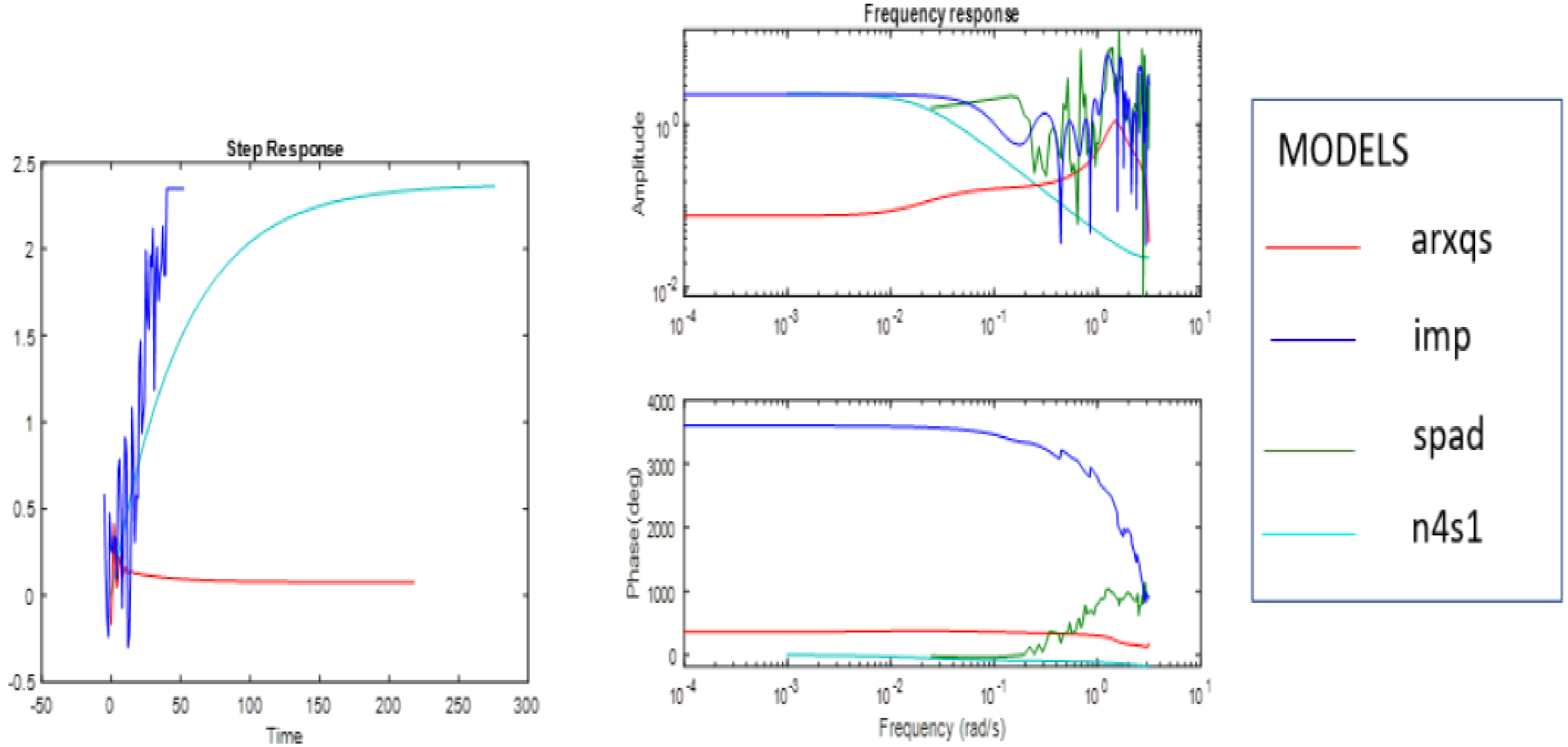
n_k is the number of samples before the input affects the output of the system,

e(t) is the white-noise disturbance.

- imp: Finite impulse response (FIR) model
- spad: Frequency response using spa algorithm
- n4s1: State-space model model

$$dy/dx=Ax(t)+Bu(t)+Ke(t); \qquad y(t) = Cx(t)+Du(t)+e(t)$$

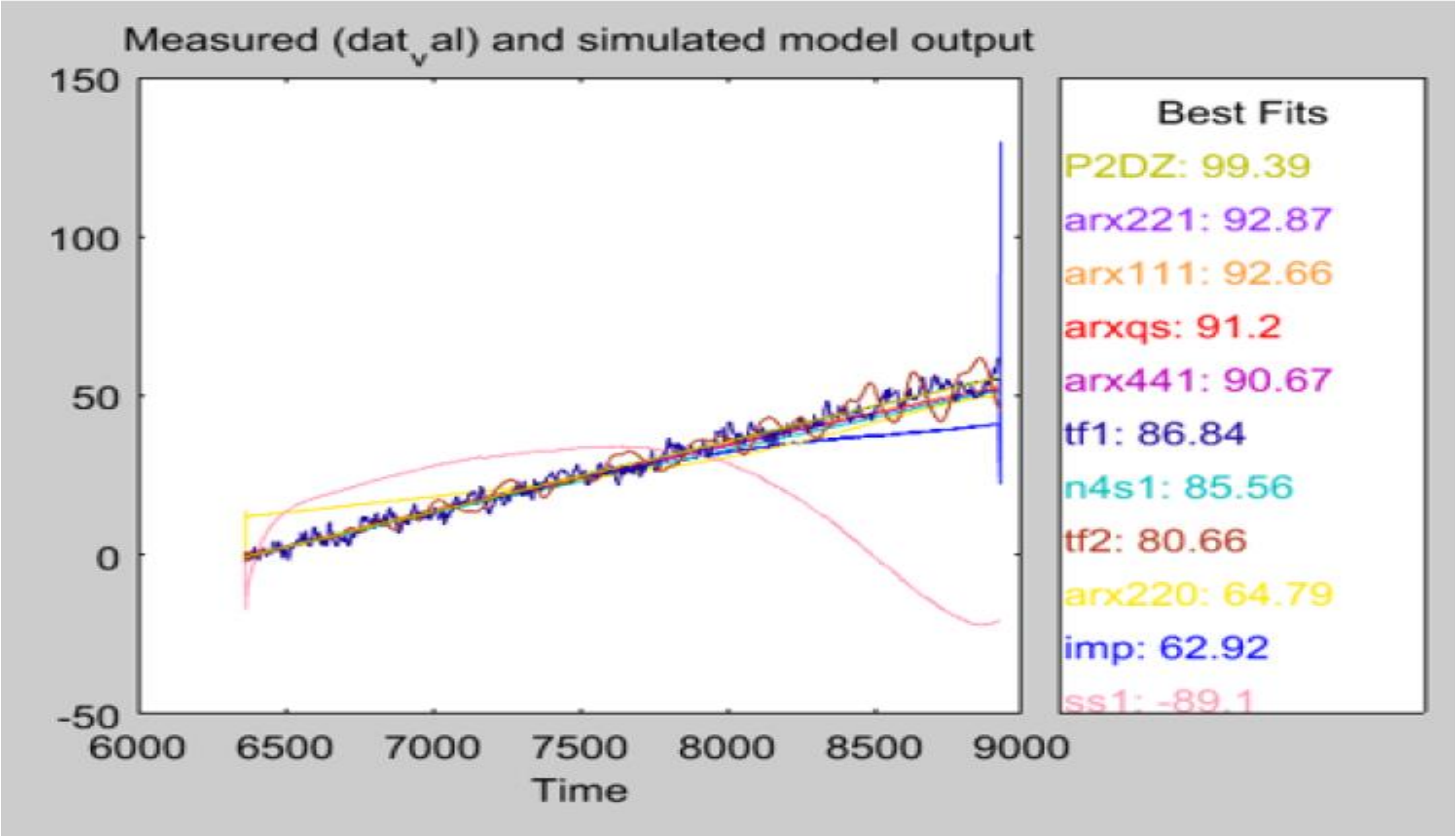
System Identification: Model selection



Plots of the u1-temperature channel. The left side is the step response plot. The right side is the frequency response plot

- Both step response and frequency response plots confirm the lack of agreement among the other model structures and the measured data

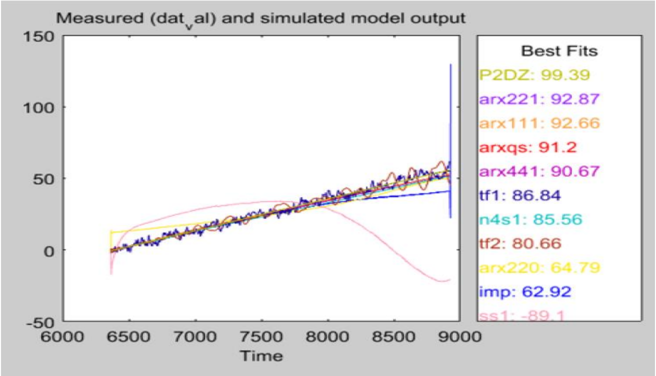
System Identification: Model selection



Model output-plot

- Shows that a linear model sufficiently represents the system's dynamics
- Fourth-order autoregressive (ARX) model provides the best-fit value (91.2) of the model response to the input in the validation data compared to the other QuickStart models.

System Identification: Model identification



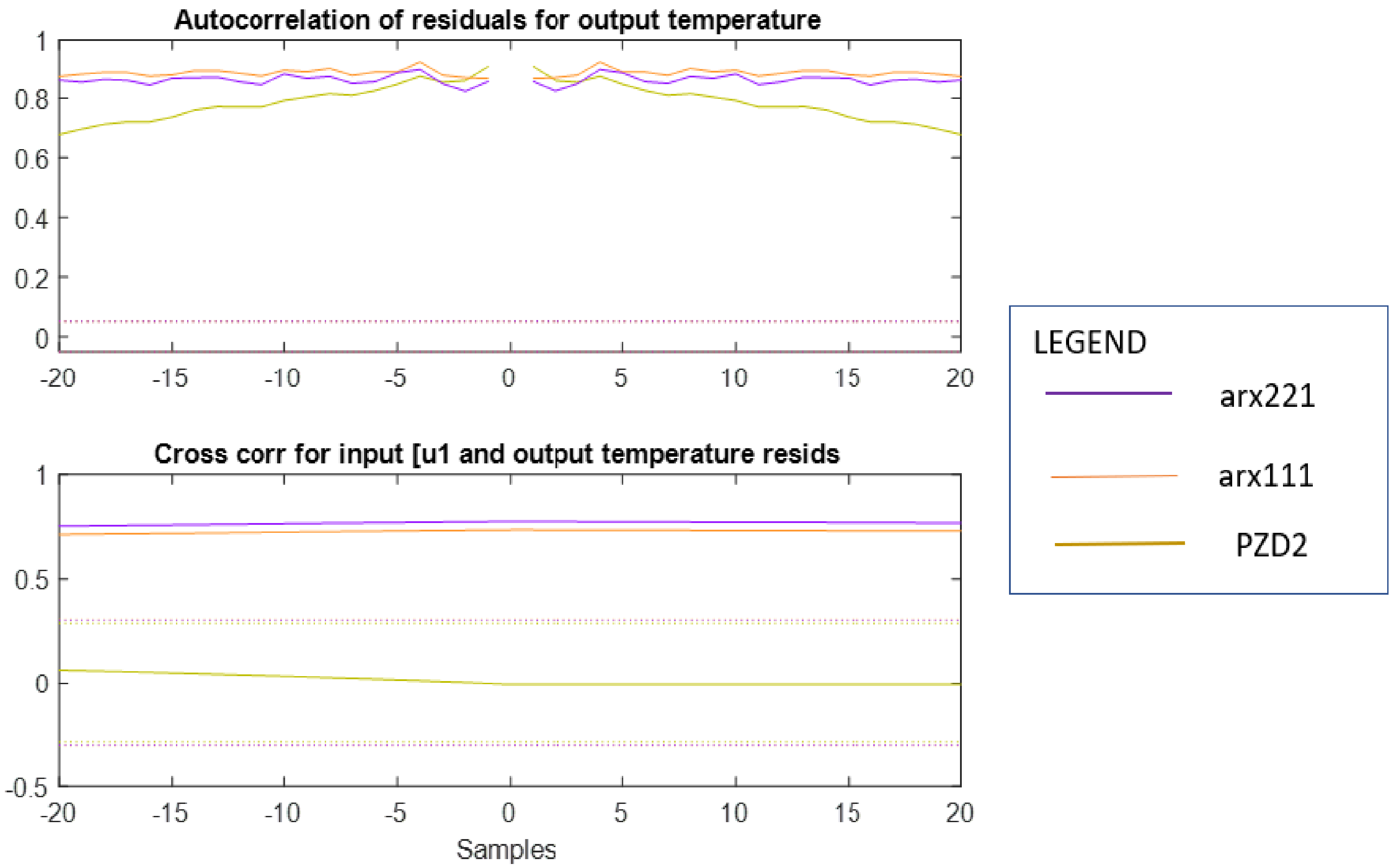
- The fourth-order autoregressive (ARX) models provide the best fit from the model structure selection step
- More complex ARX model structures with varying poles (order), zeros, and delays to get more accurate parametric models were explored
- Also, different linear polynomials, state-space, transfer function, and process models with the number of poles, $n_a = 2$, number of zeros, and $n_b = 1$, were analyzed
- The process model (P2DZ) from the model output-data plot in the previous slide provides the best fit with a value of 99.39

System Identification: Model validation

- Model fitting
  - Validate the best candidate models that perform best in terms of fit (P2DZ, arx221, and arx111) and select the best,
  - Helps uncover if models selected from the model structure selection process are wrong, or the data is influenced by a random disturbance process or a combination of the two.

- Correlation analysis
  - of the residual function was done to ascertain if the errors in our models are random or autocorrelated in some way.
  - Whiteness and Independence test
  - Residual analysis plots for autocorrelation & cross-correlation plots

System Identification: Model validation



Residual analysis plot for the three best models

☑ P2DZ (Process model)

- Possesses the best-fit value (99.39) of the three candidate models
- Only model (of the 3) passing the whiteness and independence test criteria for both autocorrelation and cross-correlation plots.
- Only model (of the 3) satisfying *both* model fitting and correlation analysis tests.

System Identification: Results

- A linear model like the process model (P2DZ) best represents the experimental data from the heat pipe compared to our initially assumed linear models

```
Process model with 10 inputs: y = G11(s)u1 + ...+ G110(s)u10
  From input "[u1" to output "temperature":
                       1+Tz*s
  G11(s) = Kp * ------------------ * exp(-Td*s)
                  (1+Tp1*s)(1+Tp2*s)
```

Mathematical equation output for the Process model (P2DZ)

- Any machine learning algorithm making future predictions for the digital twin can utilize the process model as its prediction model for multivariable forecasting.

Conclusions

- System Identification - model-centric system validation framework can identify the best mathematical model that represents the system dynamics of a physical asset such as a microreactor testbed's heat pipe.
- Model-centric validation helps engineers better understand how well their digital twin model's predictions mirror that of the physical system.
- Digital twin prediction failures (such as in Wilsdon et al. (2023)) can be mitigated by linear and nonlinear models from a model-centric validation approach that accurately captured the dynamics of the physical asset.

Limitations & Future Work

❖ Conclusion

- Study could not fully validate the Digital Twin of the heat pipe article due to the lack of input-output data for the predicted ML data from Digital Twin's ML model.
  - Previous digital twin development only provided ML-forecasted data for the ten thermocouples (input data), not the overall heater temperature (output data)

❖ Future Work

- Need for not just experimental data but also ML-predicted data to conduct extensive system identification and evaluate its predictive ability.
- Current study was more of offline identification. Online identification will provide ‘live’ validation of the digital twin.

Questions

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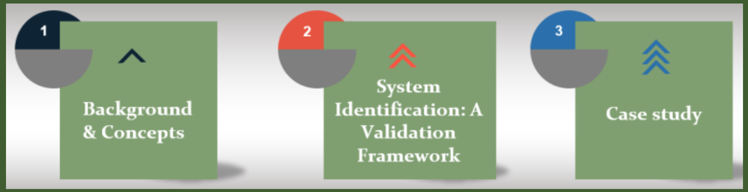

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