

Teaching Data-Centric Process Control (Junior Year) Using Experiential Learning

`ndcbe.github.io/controls`

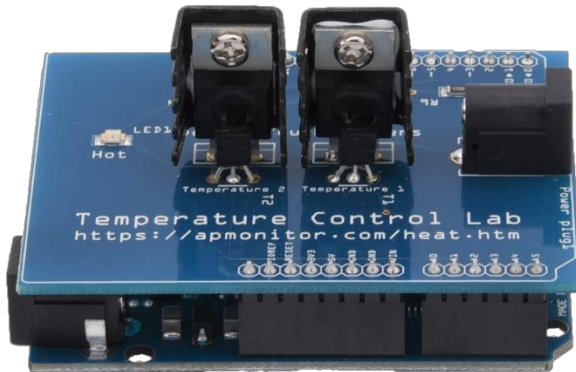


Prof. Alexander (Alex) Dowling
Chemical and Biomolecular Engineering
University of Notre Dame

AICHE Annual Meeting
San Diego, CA
October 30, 2024



*Prof. Jeff Kantor
(1954-2023)*

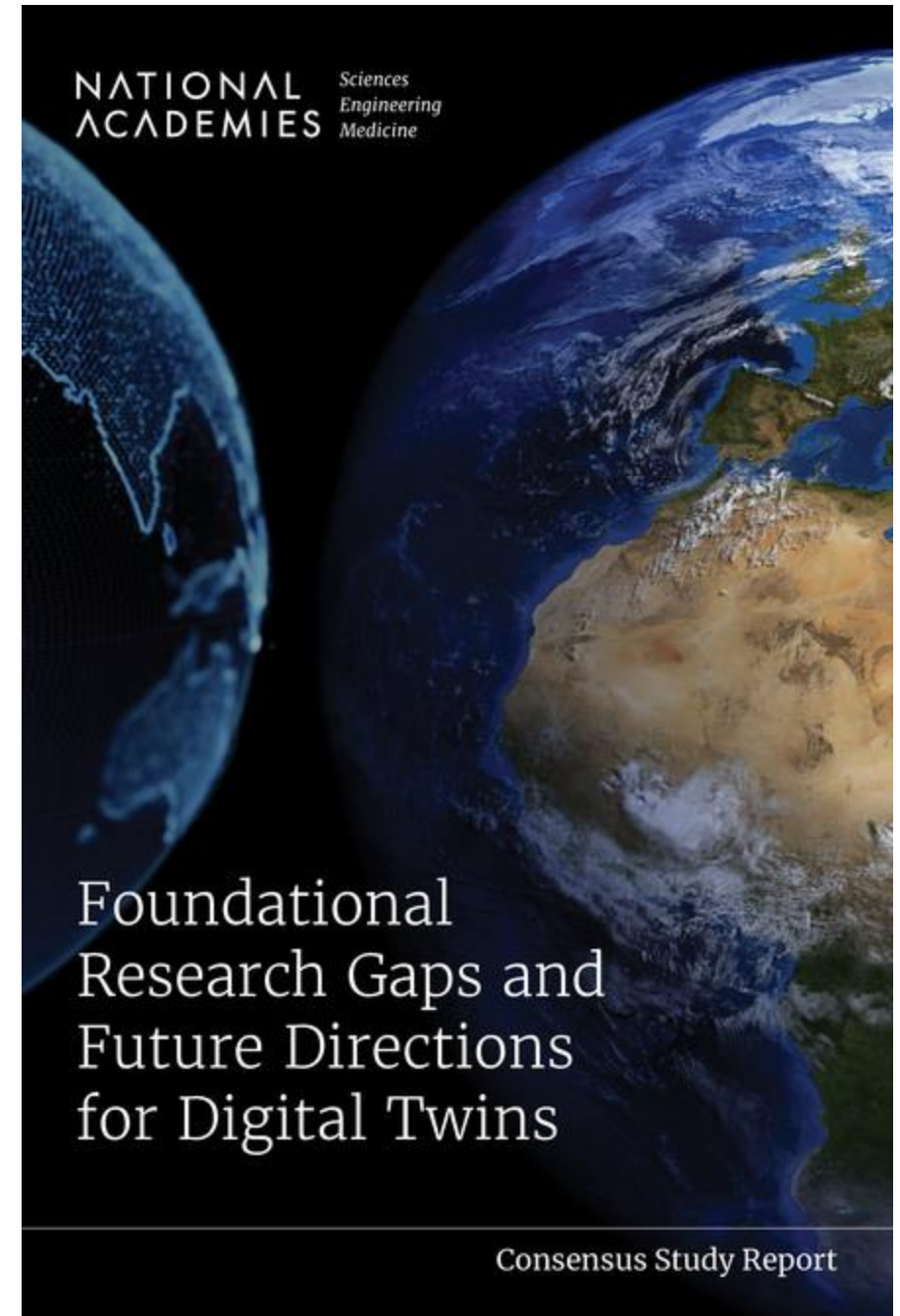
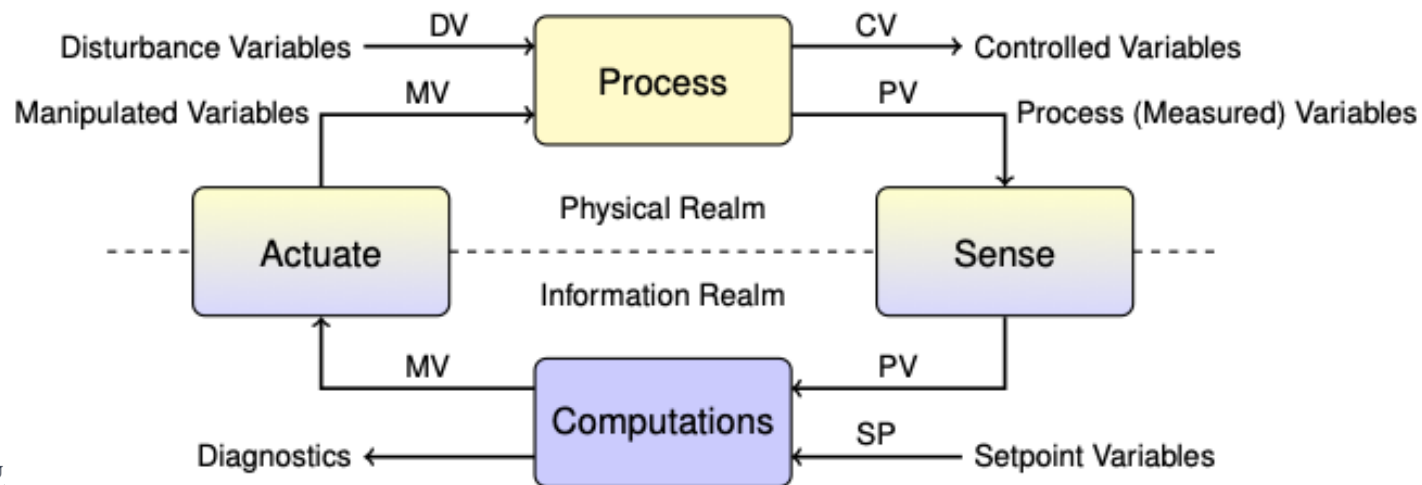


Contributors: Hailey Lynch, Molly Dougher, Maddie Watson, Zhicheng Lu, Daniel Laky

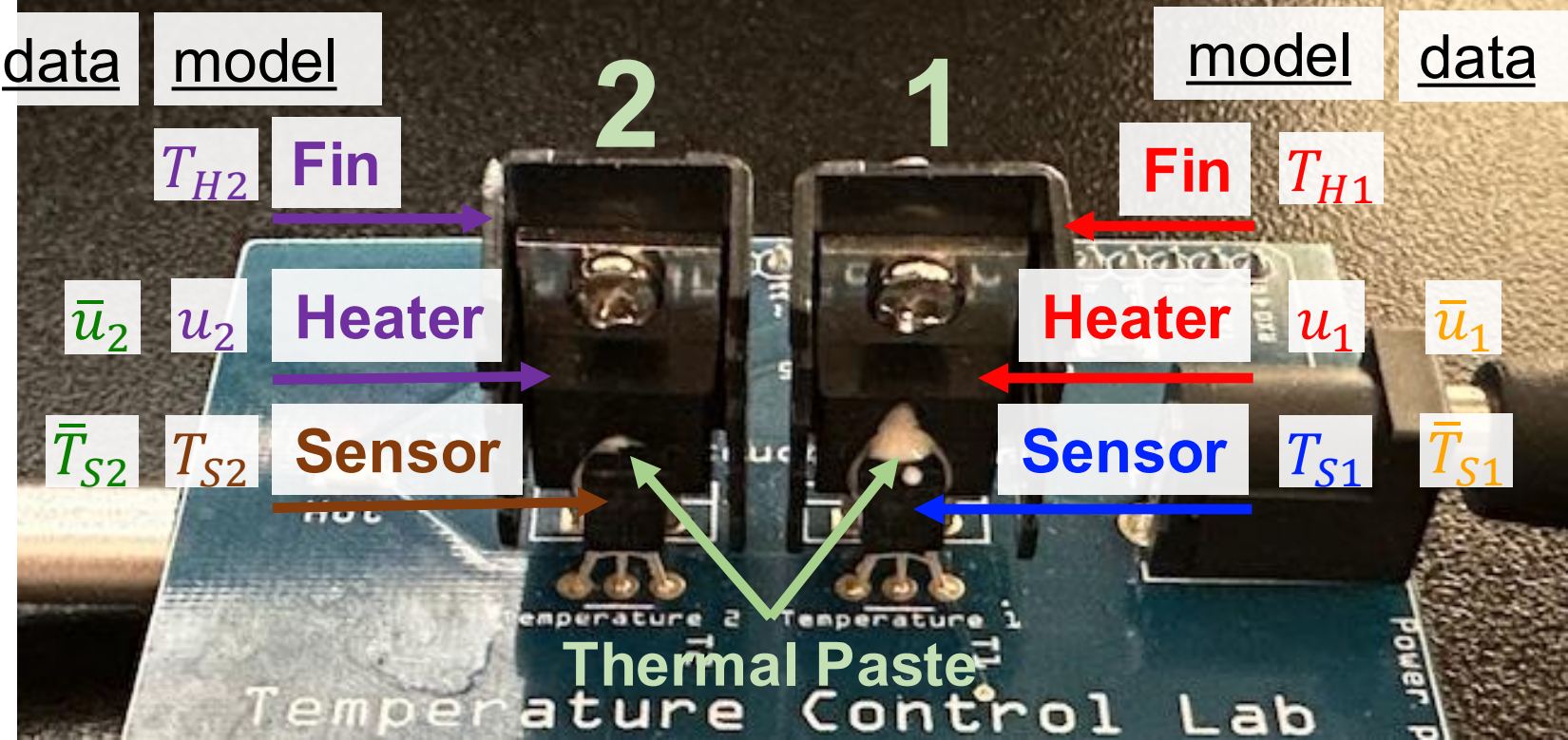
What is a Digital Twin?

A **digital twin** is a set of **virtual information constructs** that mimics the structure, context, and behavior of a natural, engineered, or social **system** (or **system-of-systems**), is **dynamically updated** with data from its physical twin, has a **predictive capability**, and **informs decisions that realize value**. The **bidirectional interaction** between the virtual and the physical is central to the digital twin.

Feedback Control = Sensing + Computations + Actuation



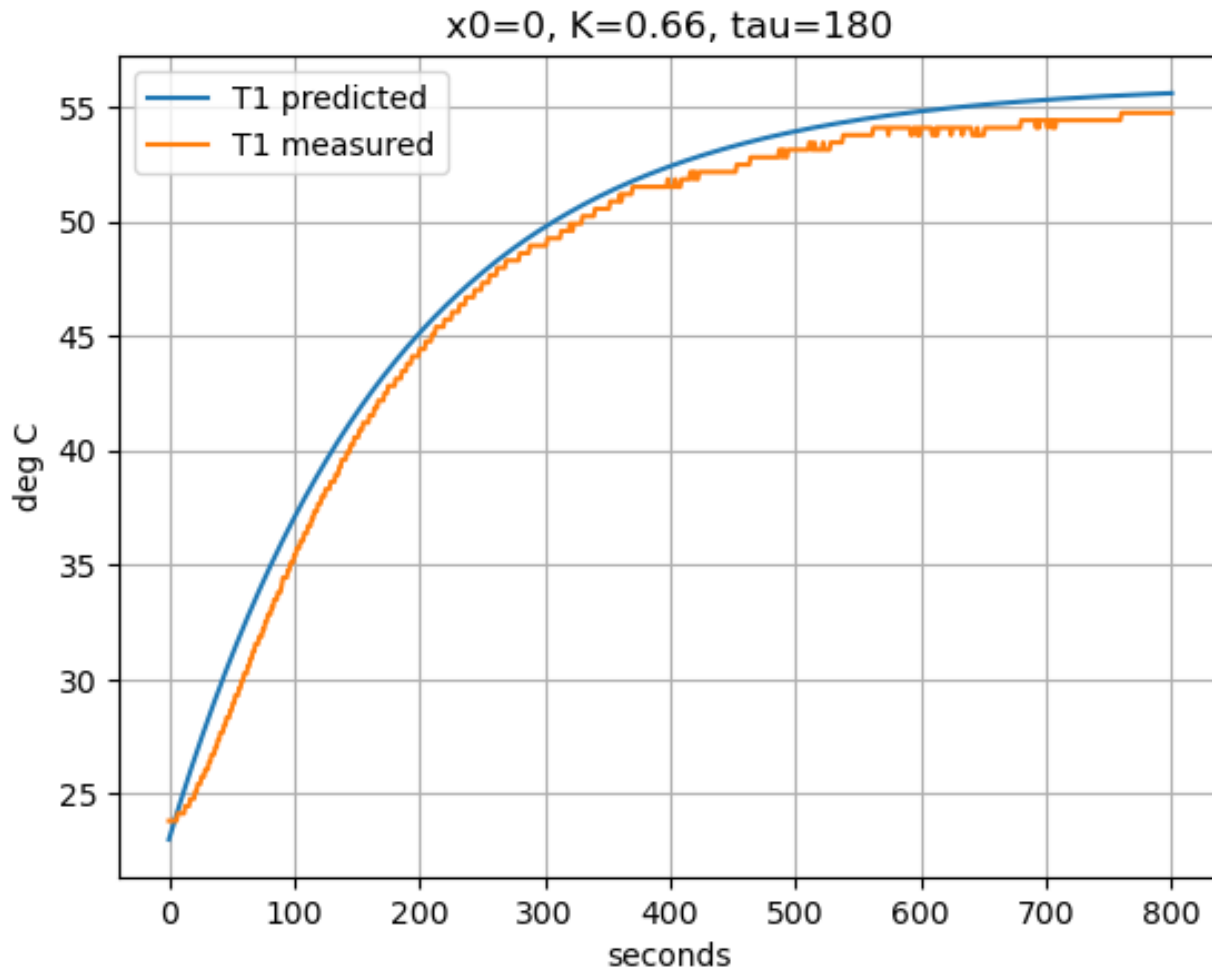
Temperature Control Lab (TC Lab)



$$C_p^H \frac{dT_{H,1}}{dt} = U_a(T_{amb} - T_{H,1}) + U_b(T_{S,1} - T_{H,1}) + \alpha P_1 u_1$$

$$C_p^S \frac{dT_{S,1}}{dt} = U_b(T_{H,1} - T_{S,1}), \quad \theta = (U_a, U_b, C_p^H, C_p^S)^\top$$

Lab 1: Step Test and First-Order Model



$$\tau \frac{dx}{dt} = -x + K\bar{u}$$

$$x(t) = \underbrace{x_0 e^{-t/\tau}}_{\text{initial condition } x_0} + \underbrace{(1 - e^{-t/\tau})K\bar{u}}_{\text{input } \bar{u}}$$

$$C_p \frac{dT_1}{dt} = U_a(T_{amb} - T_1) + \alpha P_1 u_1$$

$$x = T_1 - T_{amb}$$

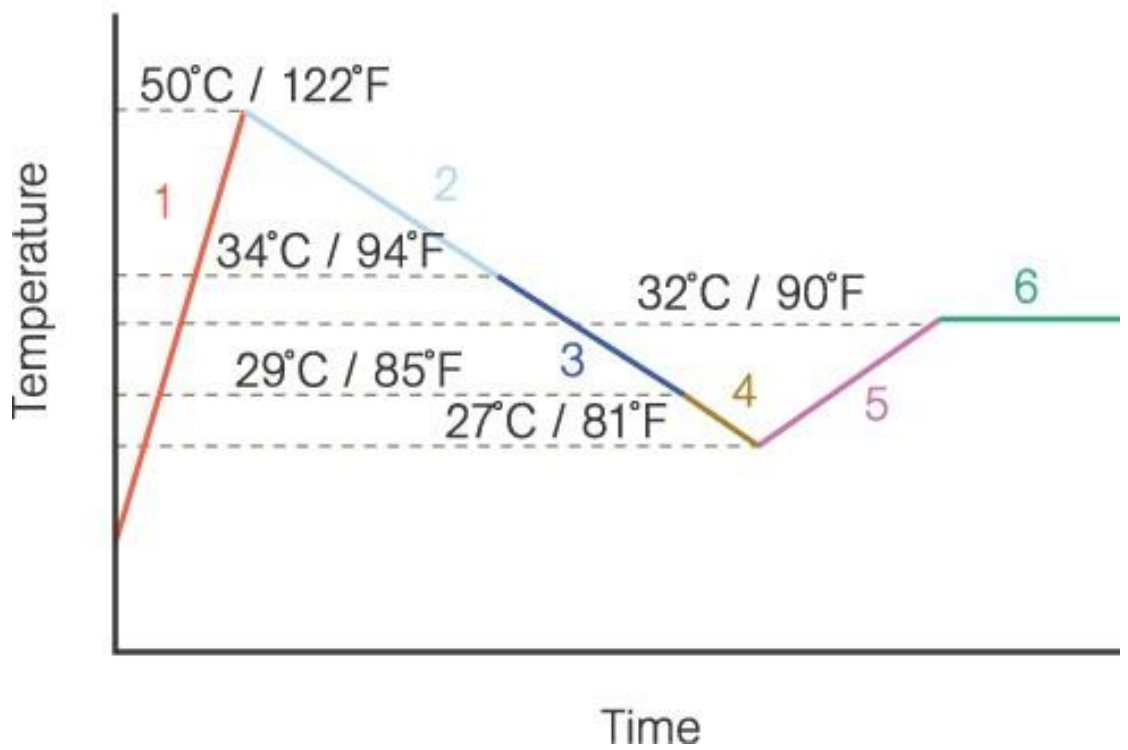
$$\frac{dx}{dt} = \frac{-U_a}{C_p} x + \frac{\alpha P_1}{C_p} u_1$$

$$\frac{dx}{dt} = -\frac{1}{\tau} x + \frac{K}{\tau} \bar{u}$$

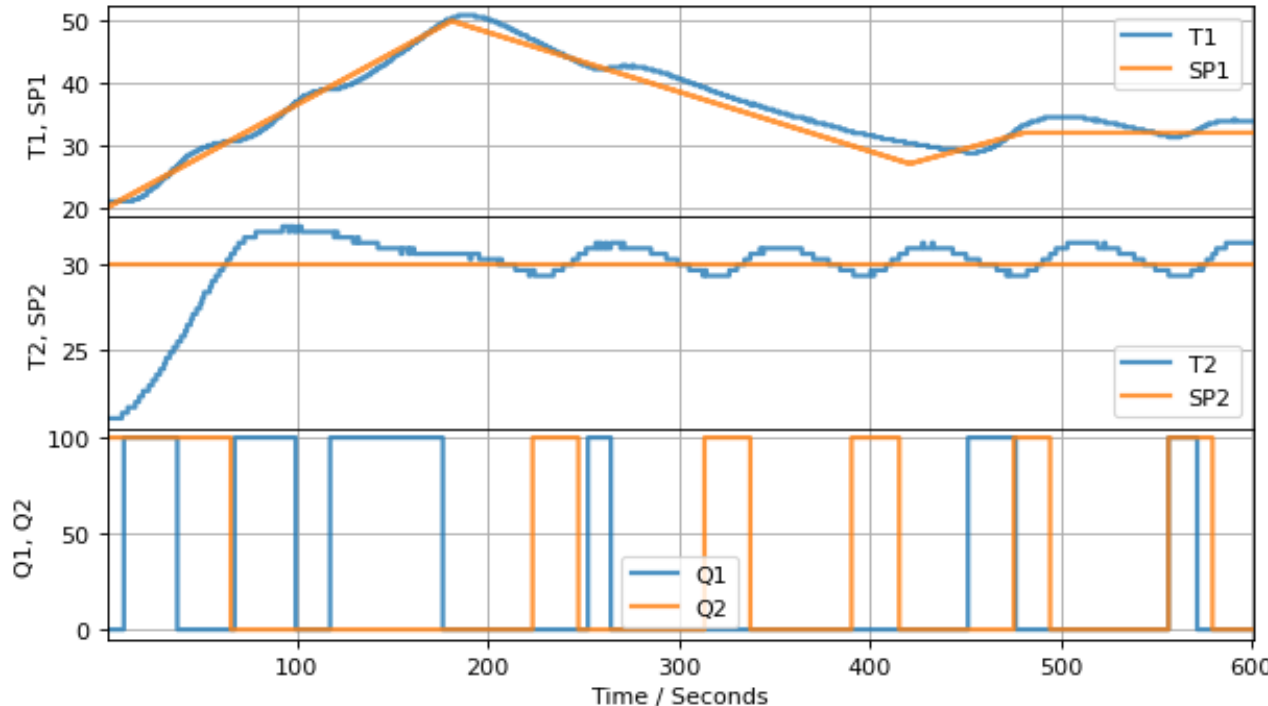
Important skill: read τ and K from plot

Lab 2: Relay (On/Off) Feedback Control

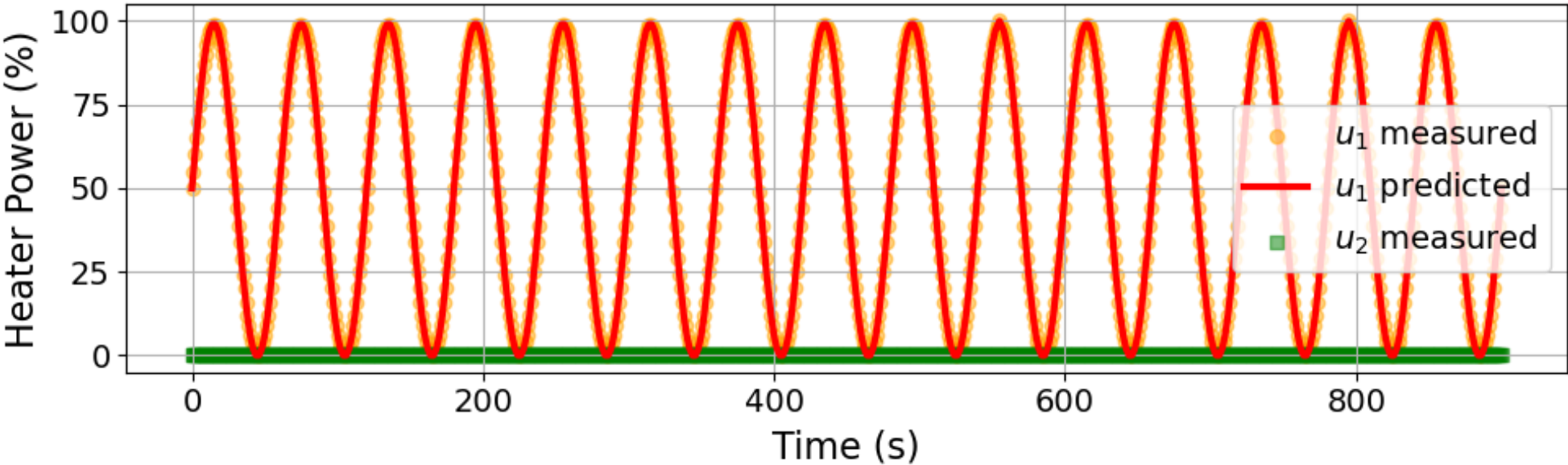
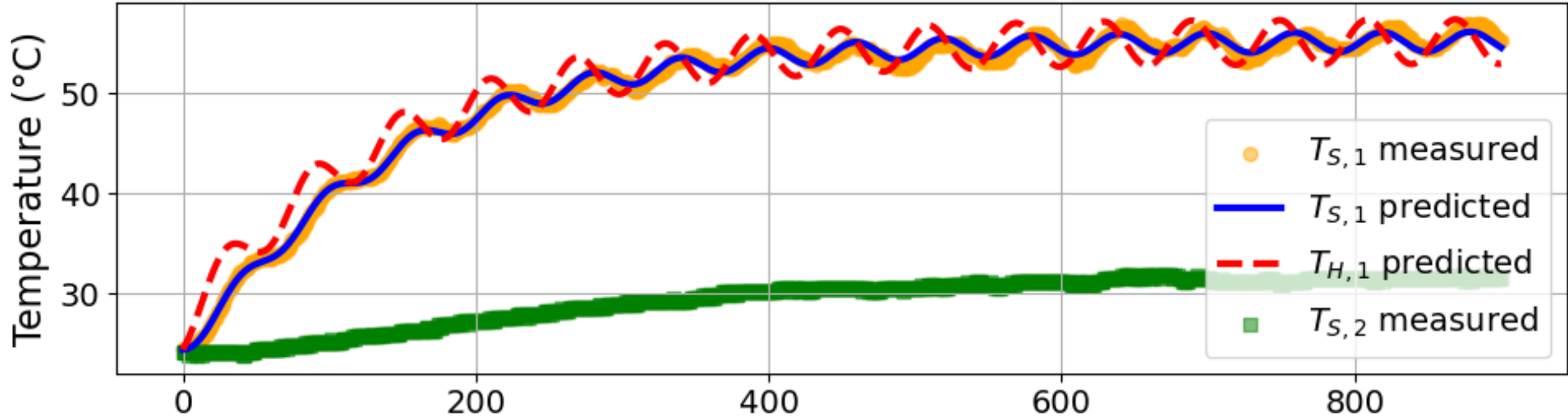
Dark Chocolate Tempering Curve



$$U_k = \begin{cases} U^{max} & \text{if } T_k \leq T_k^{SP} - d \\ U^{min} & \text{if } T_k \geq T_k^{SP} + d \\ U_{k-1} & \text{otherwise} \end{cases}$$



Labs 3: Data Collection and Parameter Estimation



Lab 4: Proportional Integral Control

Main idea: use mathematical model from Lab 3 to tune the controller

Control Law
$$u_1(t) = \bar{u}_1 + K_P(T_{set} - T_{S,1}(t)) + K_I \int_0^t (T_{set} - T_{S,1}(t')) dt'$$

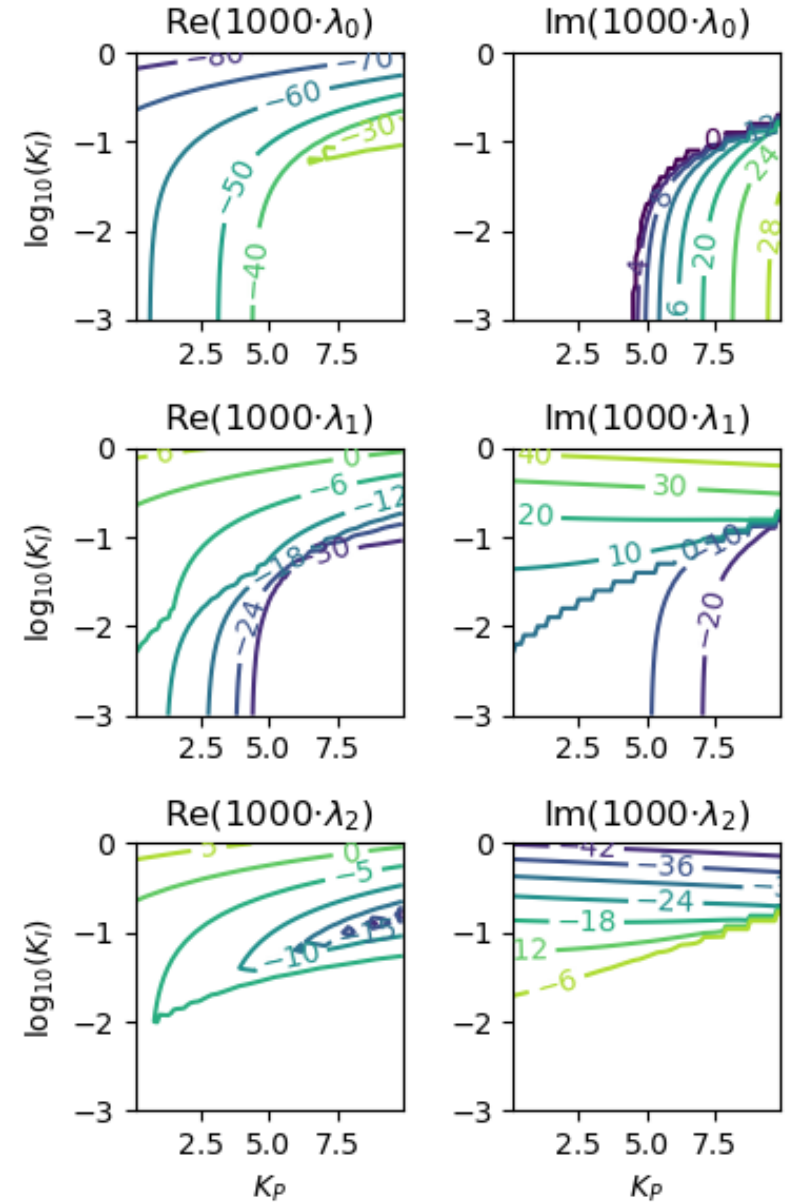
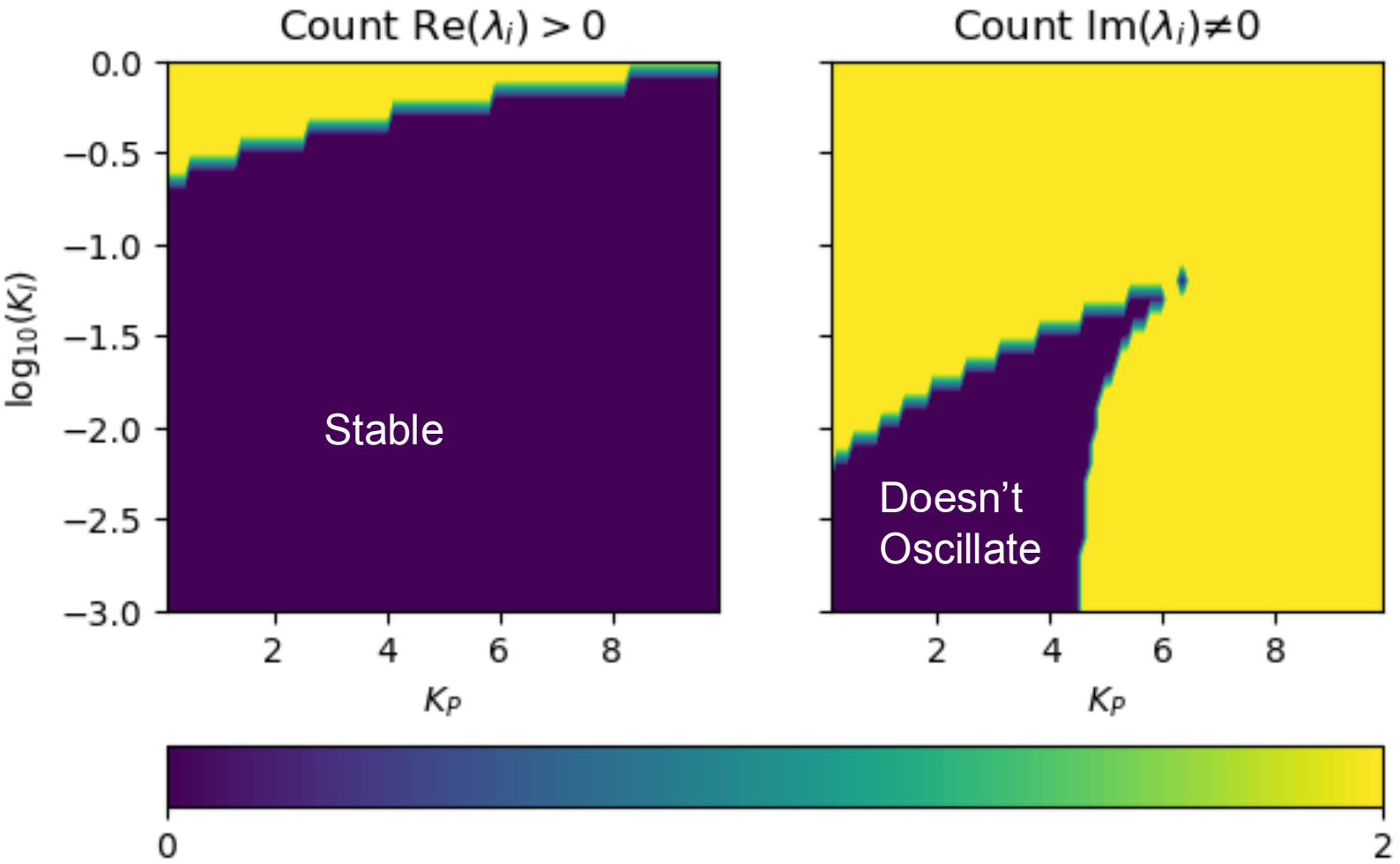
Closed-Loop
Dynamics

$$\underbrace{\frac{d}{dt} \begin{bmatrix} T_{H,1}^* \\ T_{S,1}^* \\ I \end{bmatrix}}_{\mathbf{x}} = \underbrace{\begin{bmatrix} -\frac{U_a+U_b}{C_p^H} & \frac{U_b-\alpha P_1 K_P}{C_p^H} & \frac{\alpha P_1 K_I}{C_p^H} \\ \frac{U_b}{C_p^S} & -\frac{U_b}{C_p^S} & 0 \\ 0 & -1 & 0 \end{bmatrix}}_{\mathbf{A}} \underbrace{\begin{bmatrix} T_{H,1}^* \\ T_{S,1}^* \\ I \end{bmatrix}}_{\mathbf{x}}$$

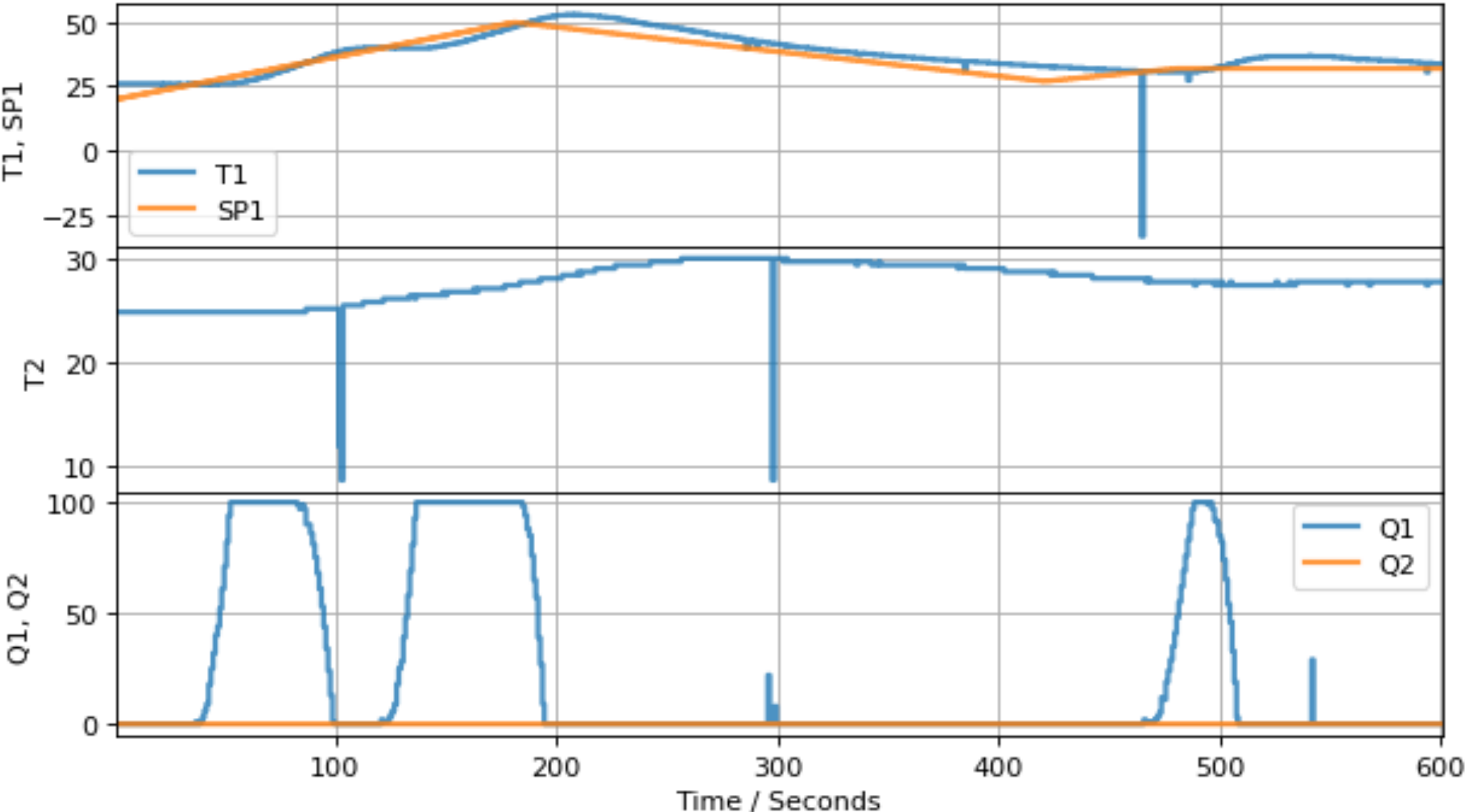
$$\underbrace{\begin{bmatrix} T_{S,1}^* \end{bmatrix}}_{\mathbf{y}} = \underbrace{\begin{bmatrix} 0 & 1 & 0 \end{bmatrix}}_{\mathbf{C}} \underbrace{\begin{bmatrix} T_{H,1}^* \\ T_{S,1}^* \\ I \end{bmatrix}}_{\mathbf{x}}$$

Adjust K_P and K_I to
tune eigenvalues of \mathbf{A}

Lab 4: Proportional Integral Control (Stability Analysis)

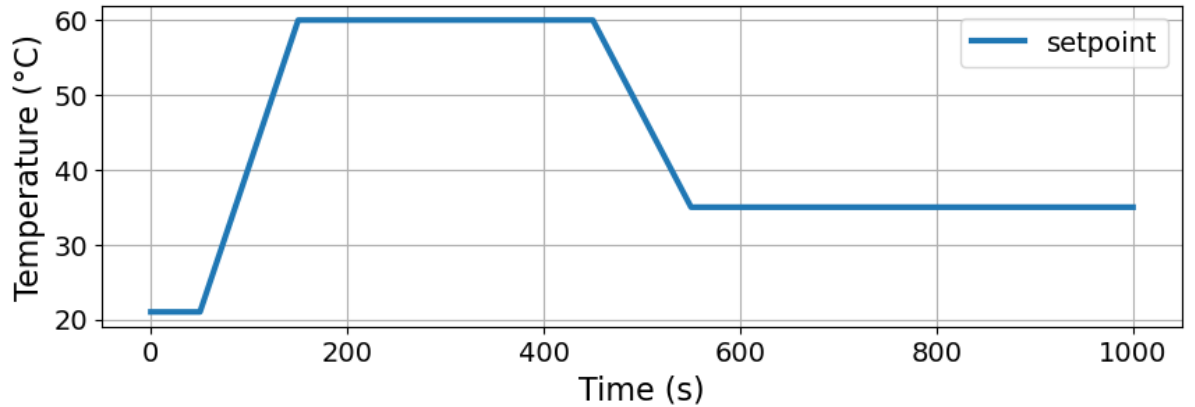


Lab 4: Proportional Integral Control (Hardware Results)

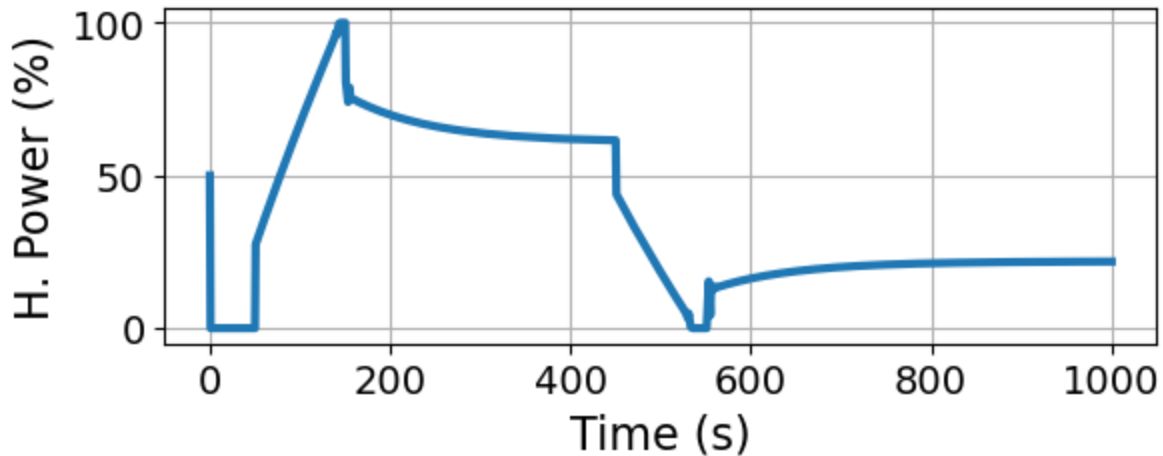


Lab 5: Open-Loop Dynamic Optimization in Pyomo

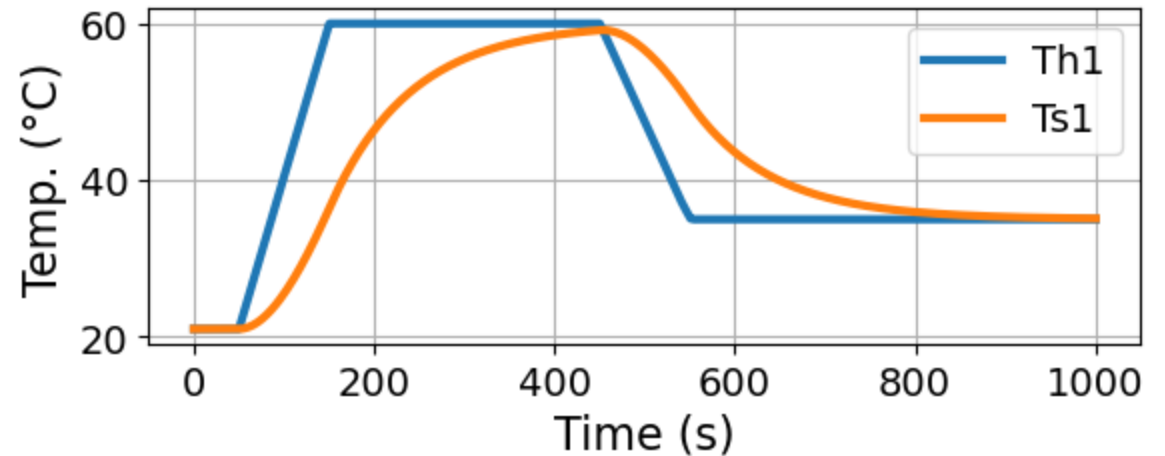
$$\begin{aligned} \min_{u(t)} \quad & \int_{t_0}^{t_f} \| SP(t) - T_H(t) \|^2 dt \\ \text{s. t.} \quad & C_p^H \frac{dT_H}{dt} = U_a(T_{amb} - T_H) + U_b(T_S - T_H) + \alpha P u(t) \\ & C_p^S \frac{dT_S}{dt} = U_b(T_H - T_S) \\ & T_H(t_0) = T_{amb} \\ & T_S(t_0) = T_{amb} \end{aligned}$$



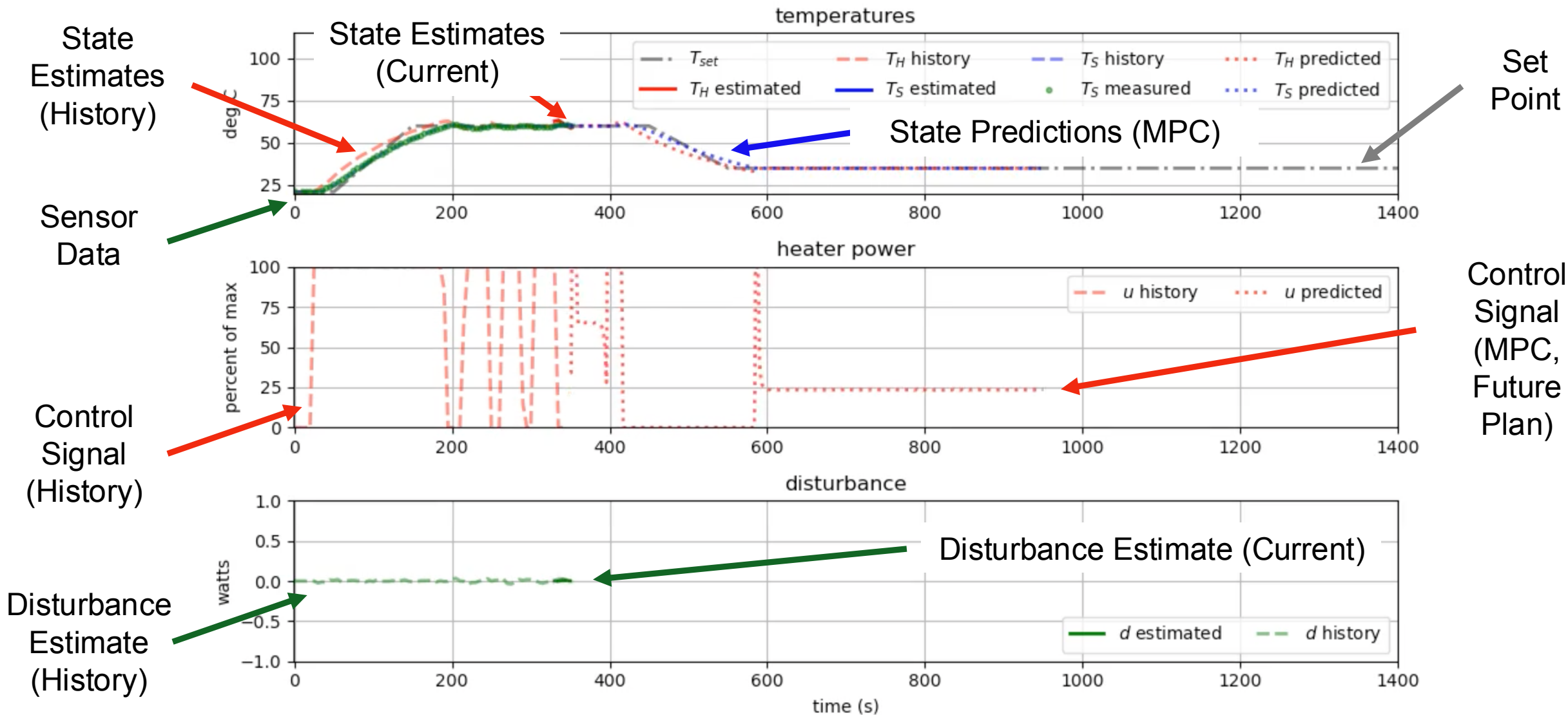
Optimal control profile



T_{h1} matches the setpoint using optimal control

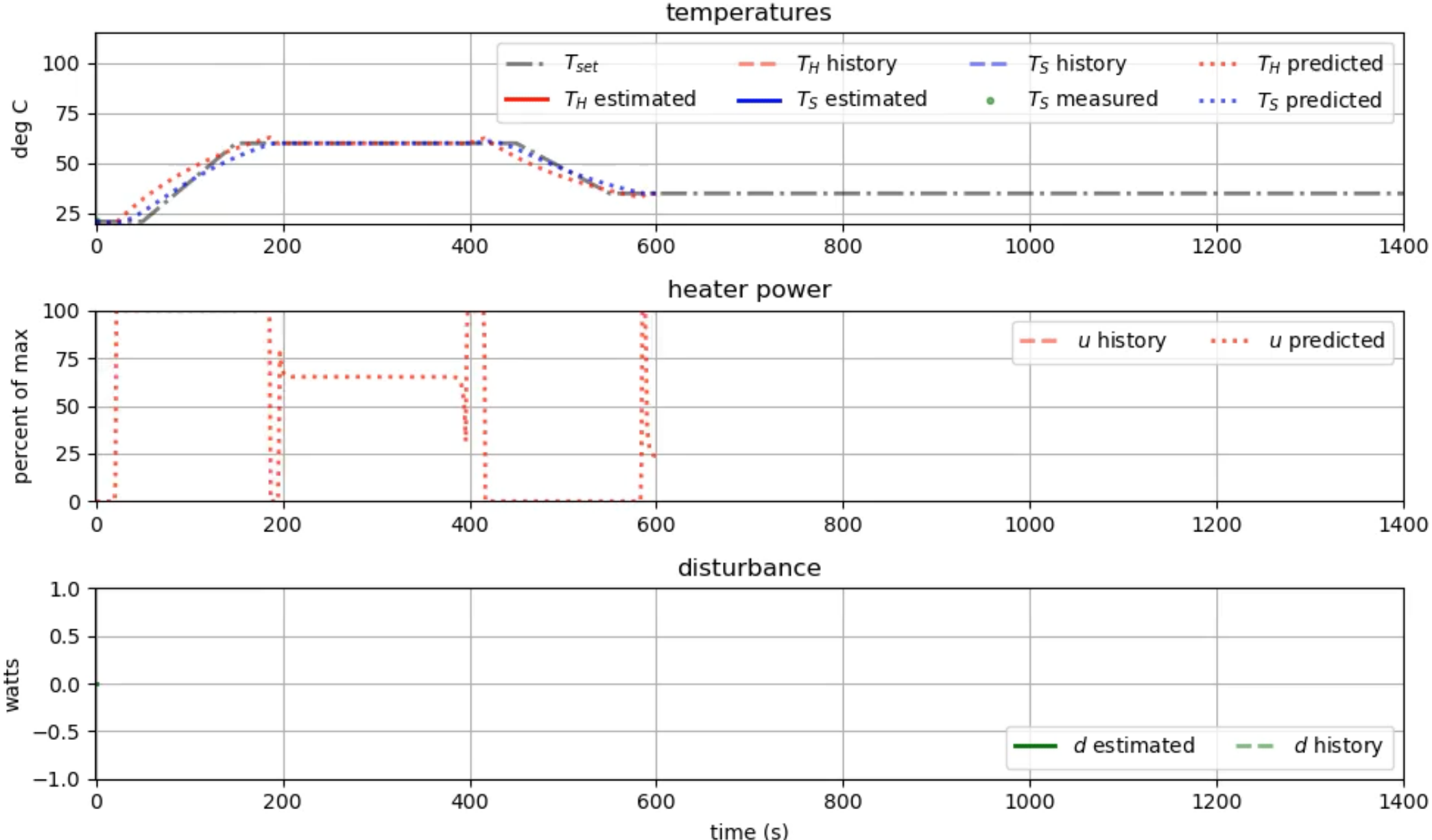


Lab 6: Digital Twins (MPC, State Estimation)



MPC = model predictive control
ndcbe.github.io/controls/notebooks/06-TCLab-Model-Predictive-Control.html

Lab 6: Digital Twins (MPC, State Estimation)



Data-Centric Controls Should Be The Most Fun ChE Core Course!

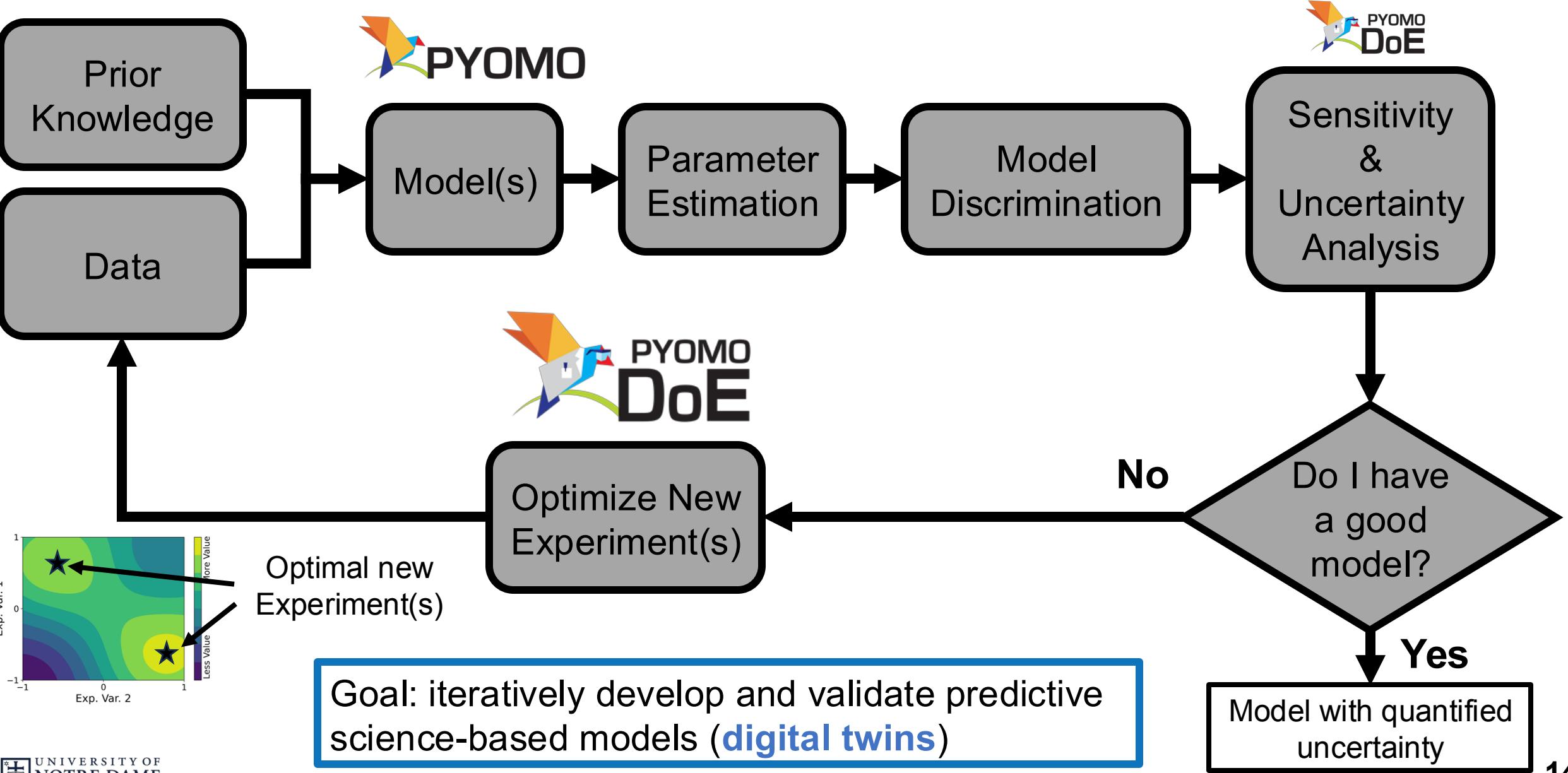
Why this works:

- Hands-on and data-centric
- No Laplace transforms, state-space modeling aligns with ChE core
- Dedicated linear algebra course (sophomore)
- Numerical methods & data analytics in Python (sophomore)
- Homework assignments re-enforce data skills and optimization (decision-making) with Pyomo
- Students get creative with open-ended final project

Ongoing improvements:

- Correlated error structure/lag models
- Four state model (both channels)
- Model-based design of experiments

Science-based (Model-based) Data Analytics Workflow



Goal: iteratively develop and validate predictive science-based models (**digital twins**)

Model with quantified uncertainty

TCLab: Eigendecomposition of the Fisher Information Matrix

ParmEst: dowlinglab.github.io/pyomo-doe/notebooks/parmest.html

FIM: dowlinglab.github.io/pyomo-doe/notebooks/doe_exploratory_analysis.html

FIM:

```
[[517225.40941304    1360.01262476 -66404.72541298   -1002.47319402]
 [   1360.01262476    5004.3737258    12379.2662576    5238.40389773]
 [-66404.72541298    12379.2662576    65481.16908635    14190.01468139]
 [  -1002.47319402    5238.40389773    14190.01468139    5526.94375493]]
```

eigenvalues:

```
[5.26802218e+05  6.26035823e+04  3.83207978e+03  1.61037063e-02]
```

eigenvectors:

U_a	[[-9.89752804e-01	-1.35949591e-01	4.36702406e-02	-7.52086327e-05]	U_a
U_b	[8.63262440e-04	-2.26164575e-01	-6.85698047e-01	-6.91857665e-01]	U_b
$1/C_p^H$	[1.42671125e-01	-9.31600001e-01	3.33329462e-01	-2.56487437e-02]	$1/C_p^H$
$1/C_p^S$	[5.79584008e-03	-2.49977462e-01	-6.45602485e-01	7.21578207e-01]	$1/C_p^S$

Difficult to uniquely estimate U_b and C_p^S with this

single experiment!

TC Lab: D-Optimal Next Experiment

dowlinglab.github.io/pyomo-doe/notebooks/doe_optimize.html

$$\max_u \quad \log \det(\mathbf{M}(u) + \mathbf{M}_0)$$

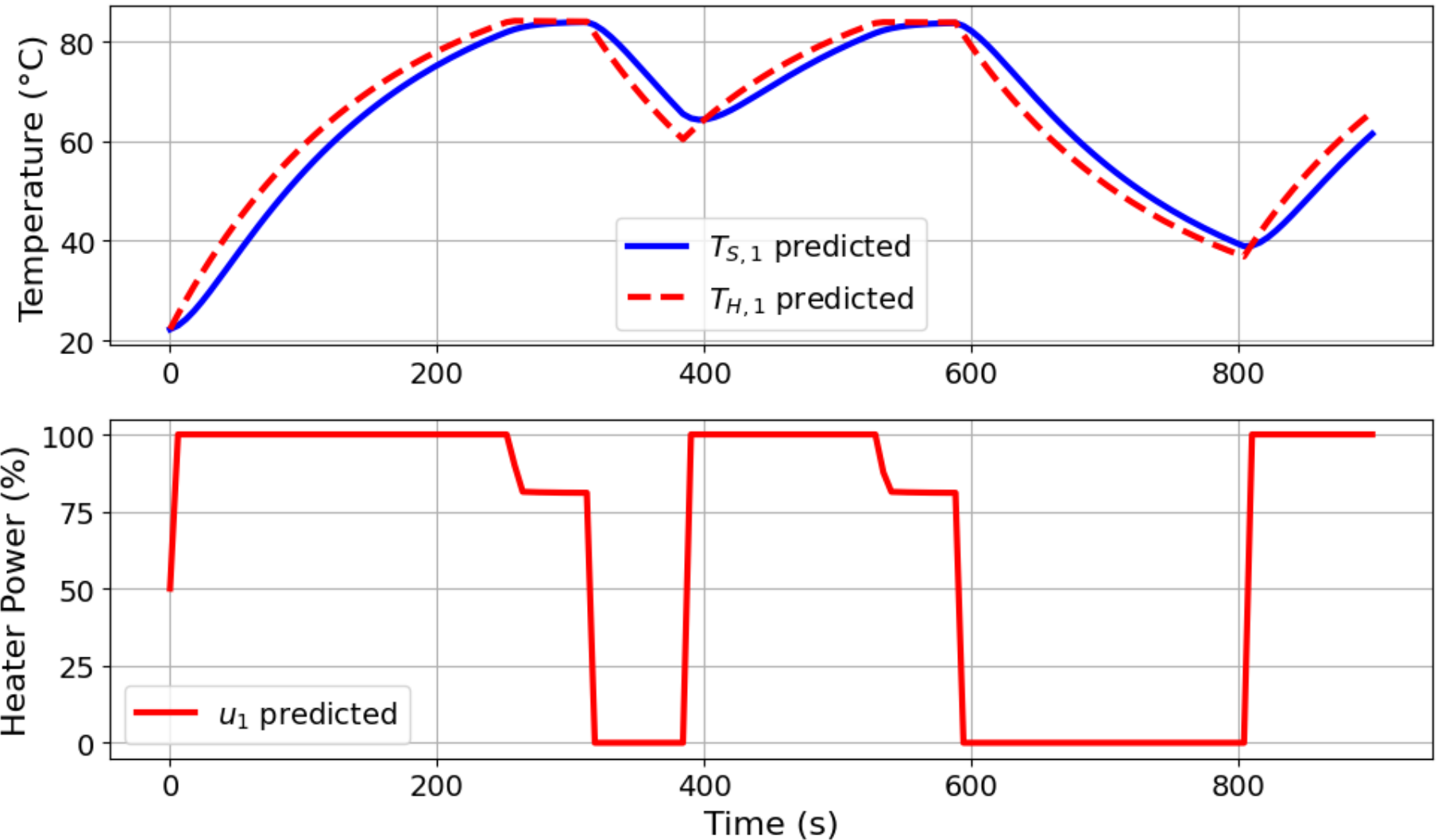
$$\text{s.t.} \quad C_p^H \frac{dT_H}{dt} = \dots$$

$$C_p^S \frac{dT_S}{dt} = \dots$$

$$0\% \leq u(t) \leq 100\%$$

$$T_H(t_0) = T_{amb}$$

$$T_S(t_0) = T_{amb}$$



$U_b C_p^S$ is more estimable with two experiments (sine wave test, D-optimal)! 16