Optimizing Experiments with Pyomo.DoE

dowlinglab.github.io/pyomo-doe

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PSE Stakeholder Summit
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PYOMO DoE

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Ask us for a Pyomo.DoE pin!

Power of Adaptive Sequential Optimal Experiments

Self-Driving Laboratories

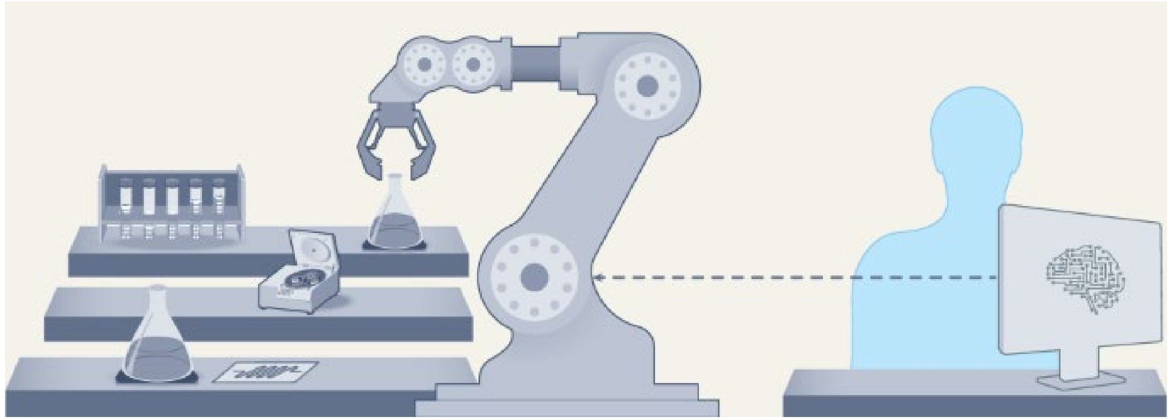
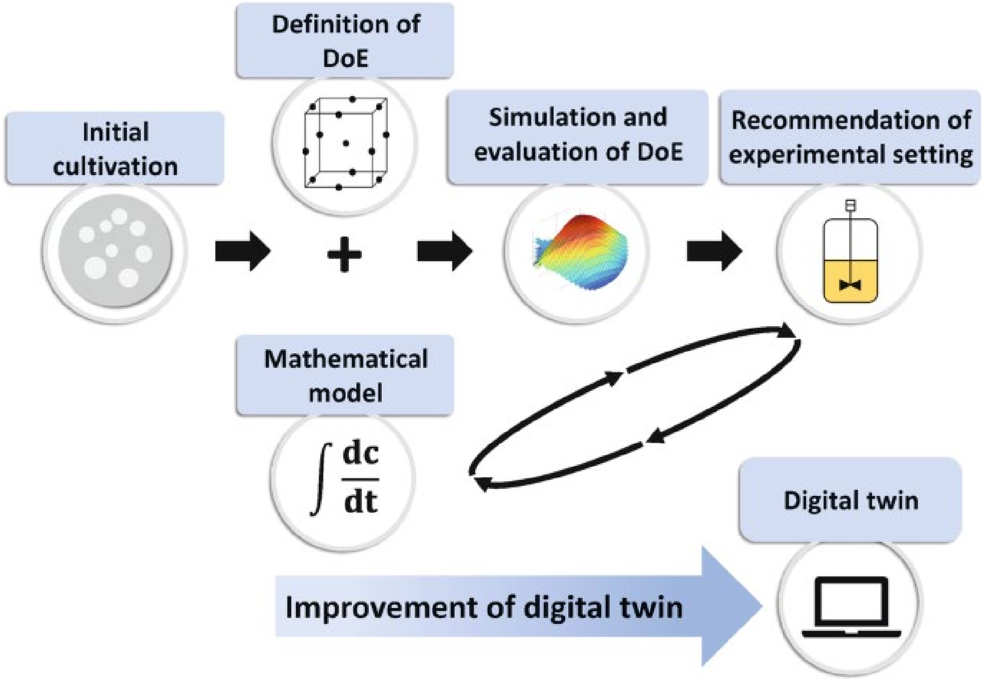


Figure: Abolhasani & Kumacheva (2023), *Nature Syn.*

Epps et al. (2022), *Advanced Materials*
MacLeod et al. (2020), *Science Advances*
MacLeod et al. (2022), *Nature Communications*
Hase, Roch, Aspuru-Guzik (2019), *Trends in Chemistry*
Seifrid et al. (2022), *Acc. Chem. Res.*

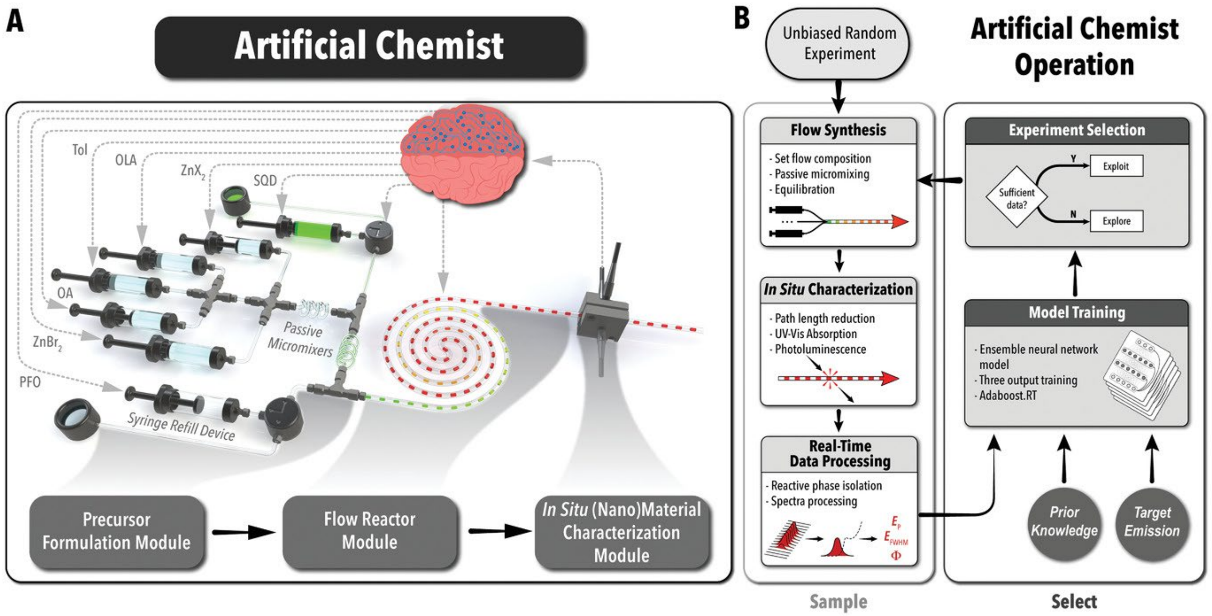
Automation + Model-Based Design of Experiments



Kuchemuller et al. (2020), *Digital Twins*

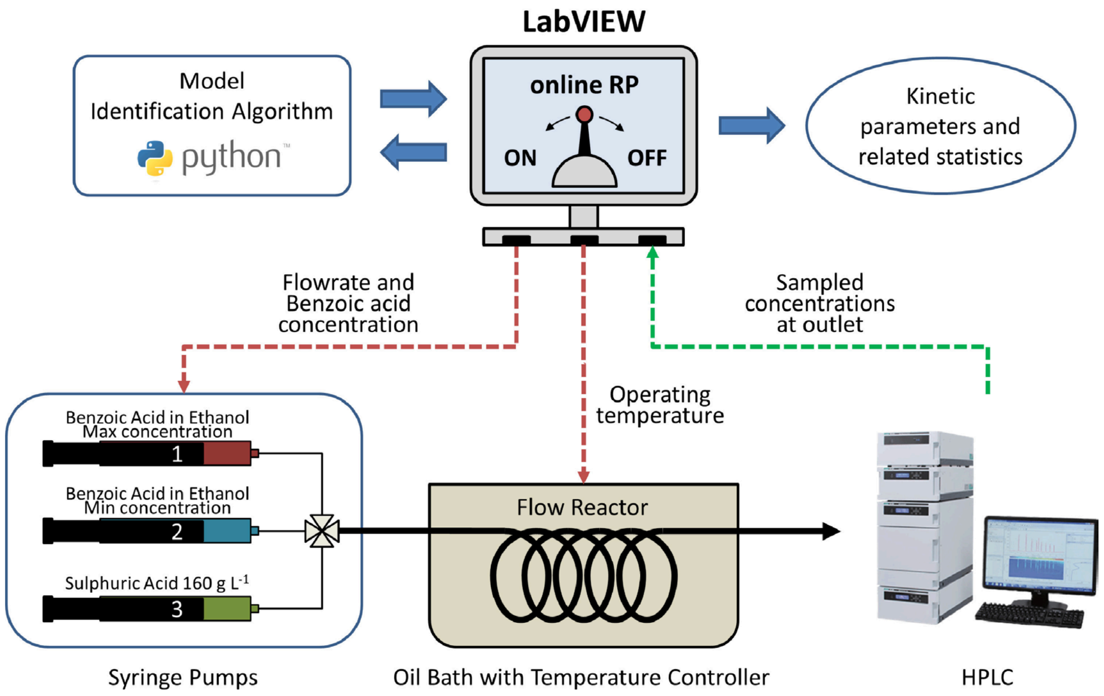
Many Recent Examples of Sequential Optimal Experiments

Quantum Dots
(Machine Learning)



Epps et al. (2022), *Advanced Materials*

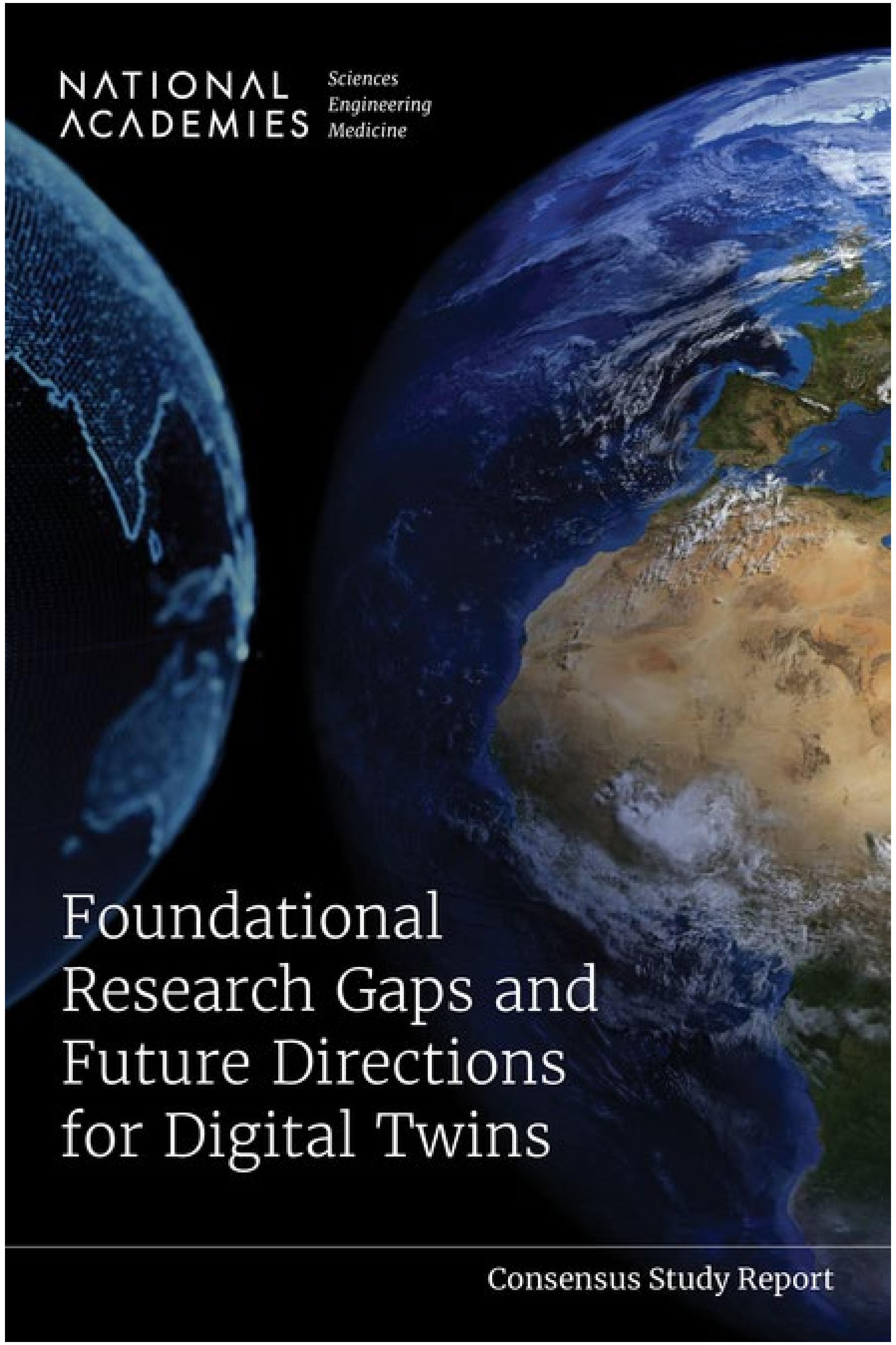
Reaction Engineering
(Science-based Models)



Quaglio et al. (2019), *Comp. & Chem. Eng.*

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.*



Science-based Data Analytics Workflow

Prior Knowledge

Data

Model(s)

Parameter Estimation

Model Discrimination

Sensitivity & Uncertainty Analysis

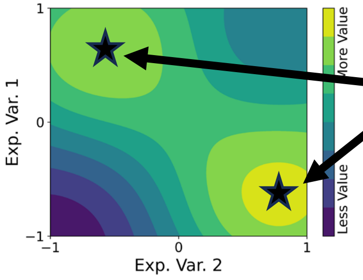
Do I have a good model?

No

Optimize New Experiment(s)

Yes

Model with quantified uncertainty



Optimal new Experiment(s)

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

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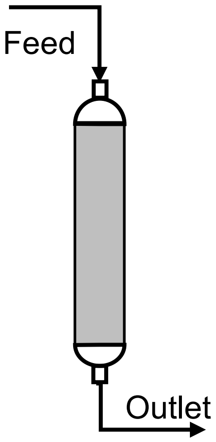
MBDoE Facilitates Collaborations

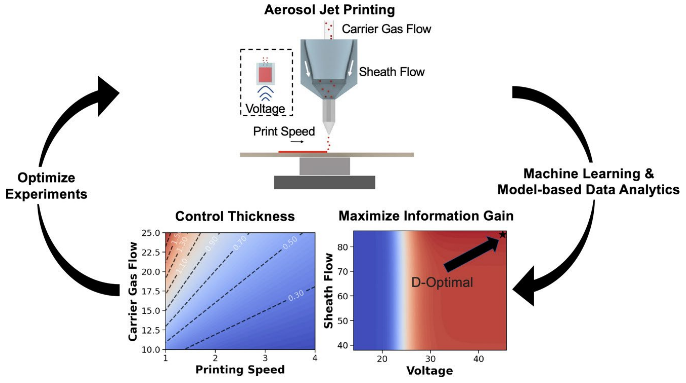
CO_2 Capture



Jialu Wang

Wang, J. and Dowling, A.W. (2022), *AIChE J.* e17813.

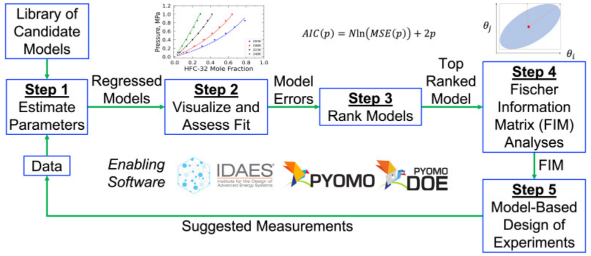
Additive Manufacturing of Thermoelectric Devices



Ke Wang

Wang K., Zhang M., Wang, J., Shang, W., Zhang, Y., Luo, T., Dowling, A.W. (2023), *Digital Chemical Engineering*

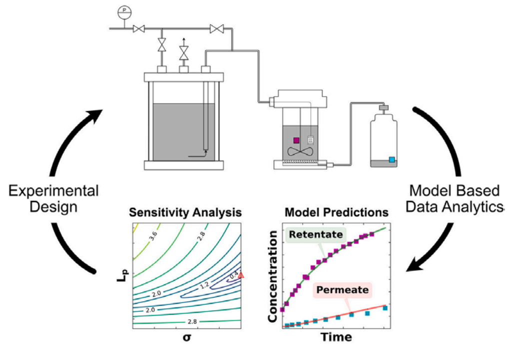
Thermodynamic Modeling (Refrigerants)



Dr. Bridgette Befort

Befort, B.J., Garciadiego, A., Wang, J., Wang, K., Maginn, E.J., Dowling, A.W. (2023), *Fluid Phase Equilibria.*

Rapid/Automated Membrane Characterization



Xinhong Liu

Ouimet, J.A, Xinhong, L., Brown, D.J., Eugene, E.A., Popps, T., Muetzel, Z.W., Dowling, A.W., Phillip, W.A., (2022). *J. Membrane Science.*

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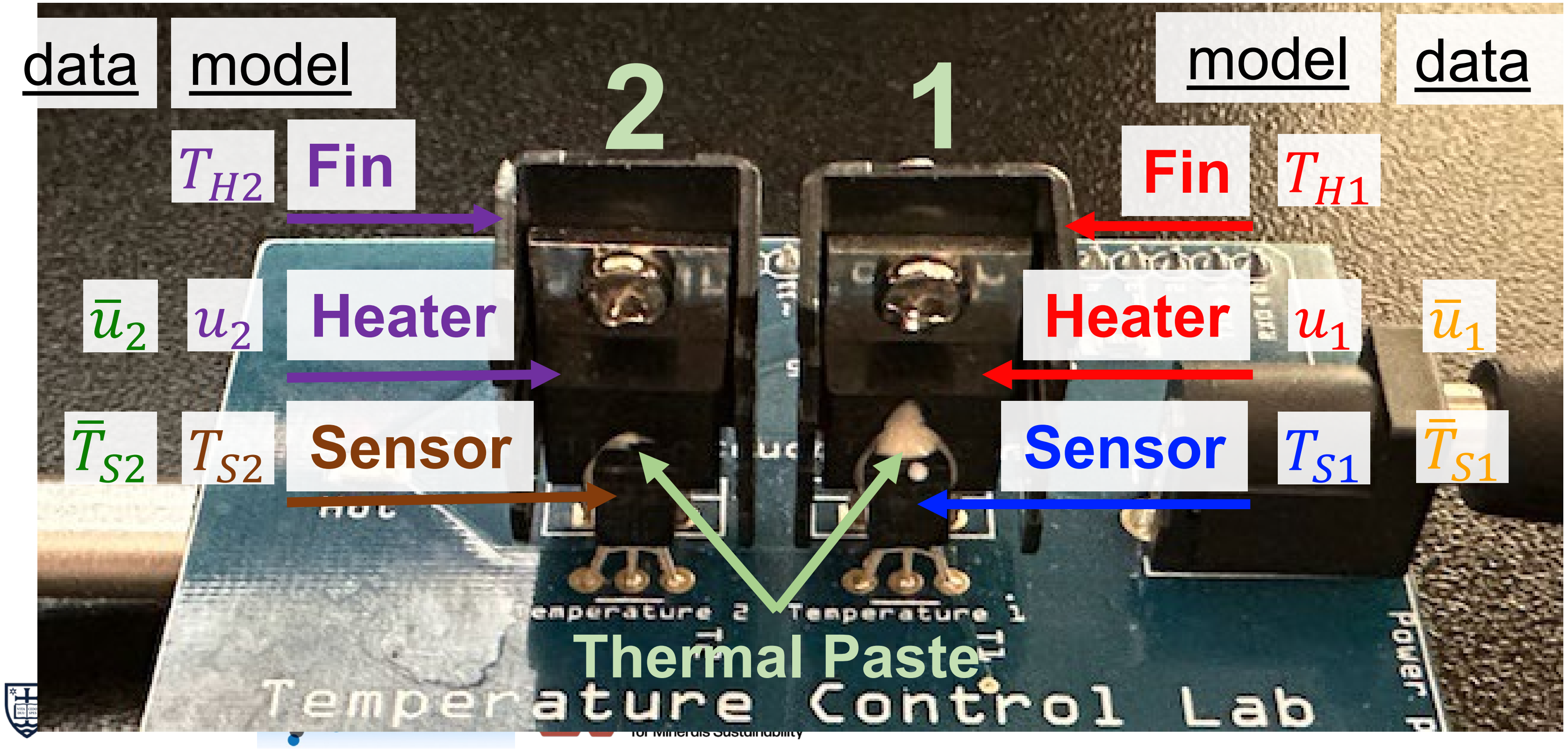
Pyomo.DoE Example: Temperature Control Lab (TC Lab)

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

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

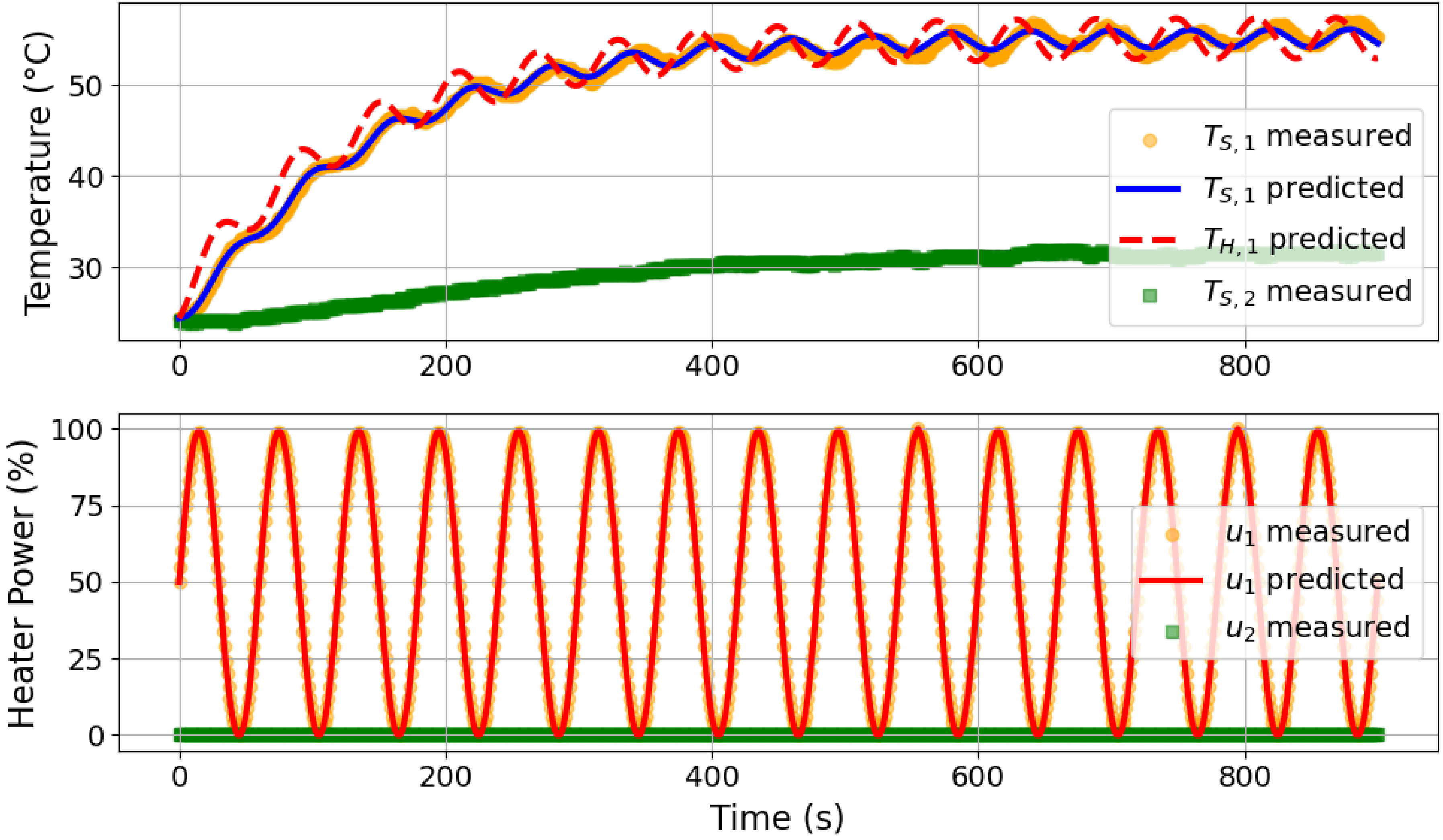
$$C_p^S \frac{dT_{S,1}}{dt} = U_b(T_{H,1} - T_{S,1}), \qquad \theta = (U_a, U_b, C_p^H, C_p^S)^\intercal$$



Thank you to Prof. Jeff Kantor (1954-2023) for the TCLab example and so much more.

TC Lab: Data and Parameter Estimation

Hands-On Tutorial: `dowlinglab.github.io/pyomo-doe`



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TC Lab: Dynamic Optimization in Pyomo

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

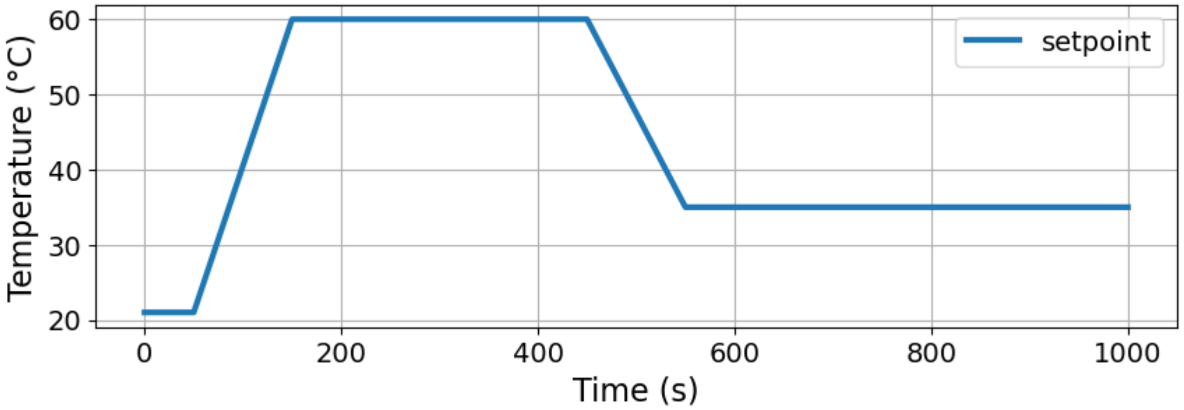
$$\min_{u(t)} \int_{t_0}^{t_f} \| SP(t) - T_H(t) \|^2 \, dt$$

$$\text{s.t.} \quad C_p^H \frac{dT_H}{dt} = U_a(T_{amb} - T_H) + U_b(T_S - T_H) + \alpha P u(t)$$

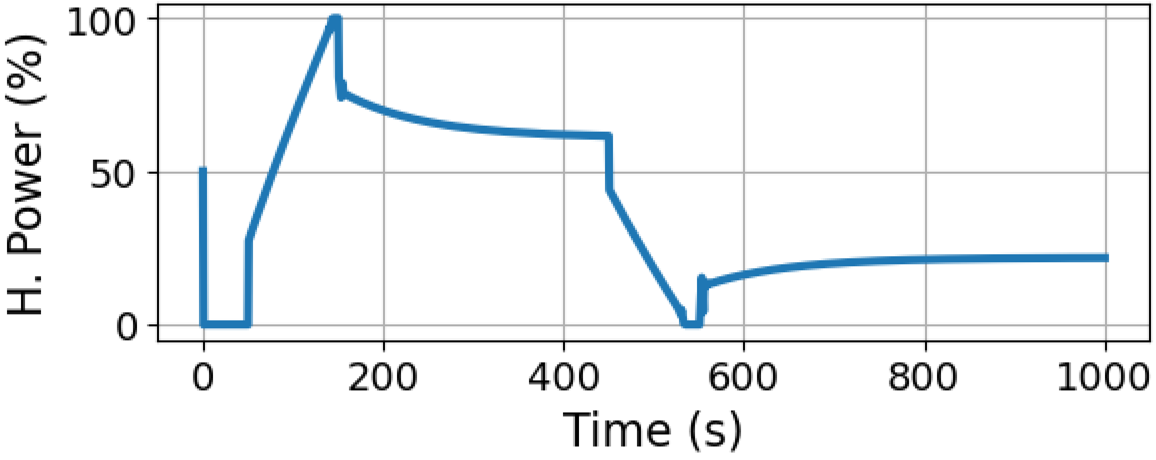
$$C_p^S \frac{dT_S}{dt} = U_b(T_H - T_S)$$

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

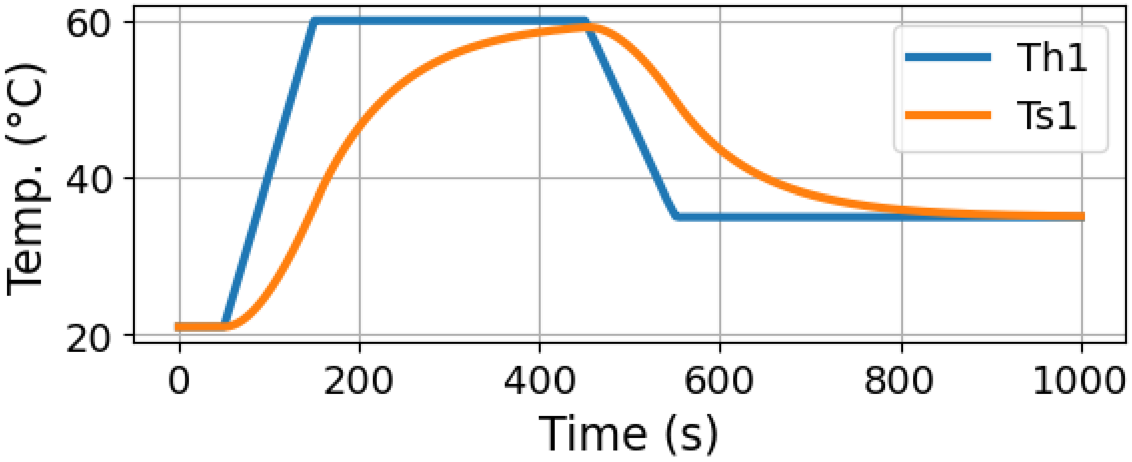
$$T_S(t_0) = T_{amb}$$



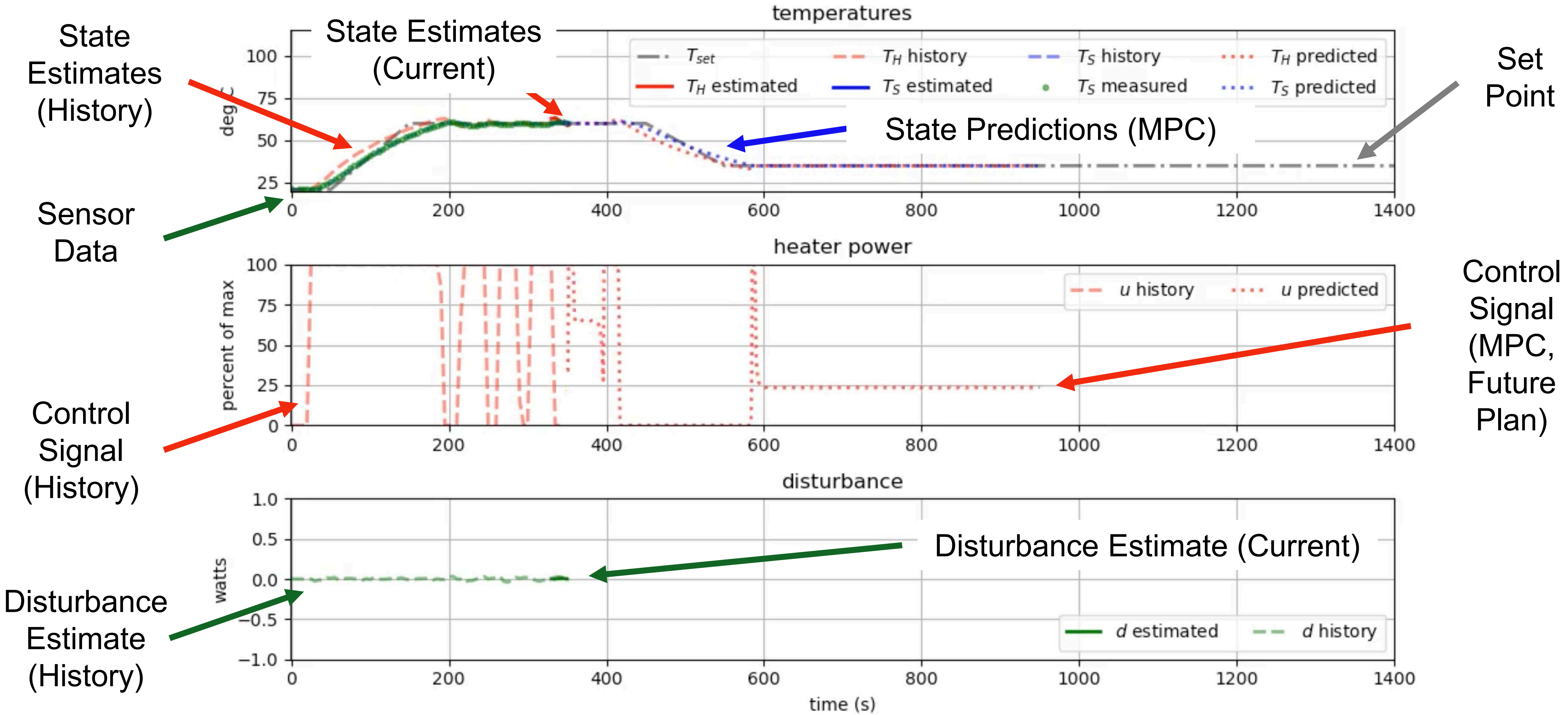
Optimal control profile



T_{h1} matches the setpoint using optimal control



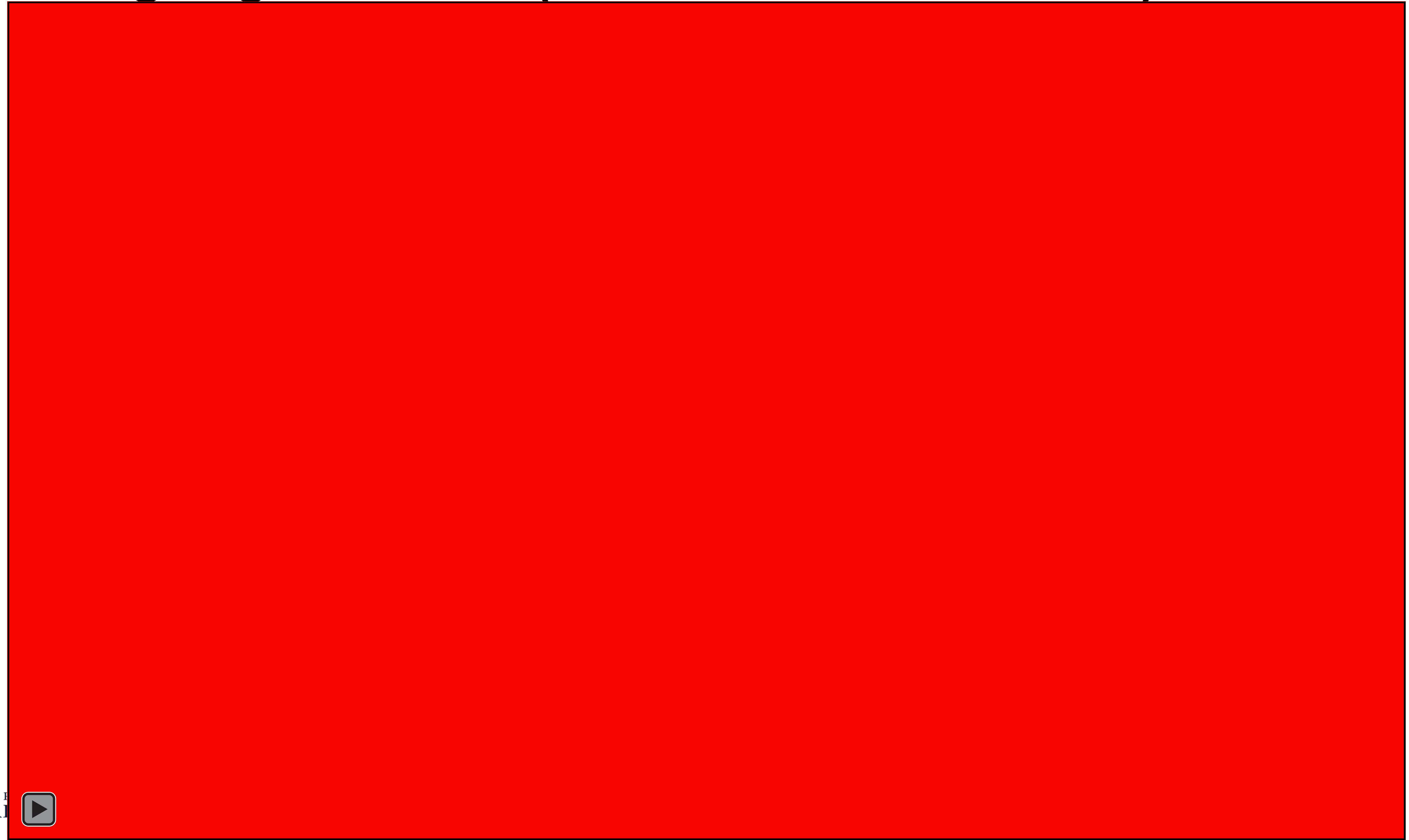
Teaching Digital Twins (MPC, State Estimation)



MPC = model predictive control

ndcbe.github.io/controls/notebooks/06-TCLab-Model-Predictive-Control.html

Teaching Digital Twins (MPC, State Estimation)

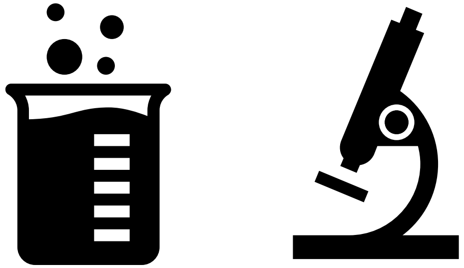


“Experiment” Abstraction Streamlines Closed-Loop Experiment Design

Experiment Inputs (Conditions)

→

Experiment (Physical)



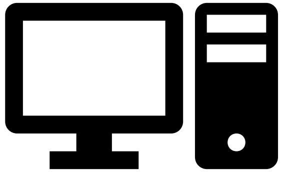
→

Experiment Outputs (Data) + Measurement Uncertainty

ϕ : experimental design vector

→

Experiment (Digital)



$$y_i = f(x, \phi, \theta) + \varepsilon_i$$

→

$\hat{y}$: measurement response variable prediction

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"Experiment" Abstraction Streamlines Closed-Loop Experiment Design

PYOMO - parmest

Known Variables

$\boldsymbol{\phi}$: experimental design vector

$\boldsymbol{y}$: measurement response variable

Experiment

(Digital)

$y_i = f(x, \phi, \theta) + \varepsilon_i$

Unknown Variables

$\boldsymbol{\theta}$: unknown model parameters

$$\min_{\boldsymbol{\theta}} \sum_i (y_i - \hat{y}_i)^2$$

PYOMO DoE

$\boldsymbol{\theta}$: model parameters

Experiment

(Digital)

$y_i = f(x, \phi, \theta) + \varepsilon_i$

$\boldsymbol{\phi}$: experimental design vector

$$\max_{\phi_l \leq \phi \leq \phi_u} \Psi\left(\mathbf{FIM}\left(\boldsymbol{\theta}, \boldsymbol{\phi}\right)\right)$$

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Parameter Estimation and Uncertainty Basics

Assume a model and error structure:

measurement

input variables

observation error (i.i.d.)

$$y_i = m(\boldsymbol{x}_i, \boldsymbol{\theta}) + \epsilon_i \qquad \epsilon_i \sim N(0, \sigma_\epsilon^2)$$

model

parameters

What values of model parameters $\boldsymbol{\theta}$ best fit the data $\boldsymbol{X}$ and $\boldsymbol{y}$?

$$\widehat{\boldsymbol{\theta}} = \arg\min_{\boldsymbol{\theta}} \Psi \coloneqq \frac{1}{2}\sum_i [y_i - m(\boldsymbol{x}_i, \boldsymbol{\theta})]^2$$

best fit estimates

How sensitive are the least-squares objective Ψ to perturbations in $\boldsymbol{\theta}$?

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 \Psi}{\partial \theta_1^2} & \cdots & \frac{\partial^2 \Psi}{\partial \theta_n \partial \theta_1} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 \Psi}{\partial \theta_1 \partial \theta_m} & \cdots & \frac{\partial^2 \Psi}{\partial \theta_m^2} \end{bmatrix} \qquad \boldsymbol{Q}(\boldsymbol{\theta}) = \begin{bmatrix} \frac{\partial m(x_1, \boldsymbol{\theta})}{\partial \theta_1} & \cdots & \frac{\partial m(x_1, \boldsymbol{\theta})}{\partial \theta_m} \\ \vdots & \ddots & \vdots \\ \frac{\partial m(x_n, \boldsymbol{\theta})}{\partial \theta_1} & \cdots & \frac{\partial m(x_n, \boldsymbol{\theta})}{\partial \theta_m} \end{bmatrix}$$

Hessian matrix $\quad \boldsymbol{H} \approx \boldsymbol{Q}^T \boldsymbol{Q} \quad$ sensitivity matrix

How does measurement uncertainty ϵ propagate into uncertainty about the regressed parameters $\hat{\theta}$?

covariance matrix for $\widehat{\boldsymbol{\theta}}$ $\qquad \boldsymbol{V}_{\widehat{\boldsymbol{\theta}}} \approx \sigma_\epsilon^2 \boldsymbol{H}^{-1} \approx \sigma_\epsilon^2 (\boldsymbol{Q}^T \boldsymbol{Q})^{-1}$

Fisher information matrix for $\widehat{\boldsymbol{\theta}}$ $\qquad \boldsymbol{M}_{\widehat{\boldsymbol{\theta}}} \approx \boldsymbol{V}_{\widehat{\boldsymbol{\theta}}}^{-1} \approx \frac{1}{\sigma_\epsilon^2} (\boldsymbol{Q}^T \boldsymbol{Q})$

Bard (1974)
Bates and Watts (1988)
Pirnay, Lopez-Negrete, Biegler (2012)

Extensions not shown: sophisticated error structures, Bayesian or MLE inference, …

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:
```

$$
\begin{array}{c|cccc|c}
U_a & [[-9.89752804e-01 & -1.35949591e-01 & 4.36702406e-02 & \boxed{-7.52086327e-05}] & U_a \\
U_b & [8.63262440e-04 & -2.26164575e-01 & -6.85698047e-01 & \boxed{-6.91857665e-01}] & U_b \\
1/C_p^H & [1.42671125e-01 & -9.31600001e-01 & 3.33329462e-01 & \boxed{-2.56487437e-02}] & 1/C_p^H \\
1/C_p^S & [5.79584008e-03 & -2.49977462e-01 & -6.45602485e-01 & \boxed{7.21578207e-01}]] & 1/C_p^S
\end{array}
$$

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Difficult to uniquely estimate $U_b C_p^S$ with this experiment!

Model-Based DoE Optimization Formulation

$$\max_{\boldsymbol{\varphi}} \quad \Psi[\, \boldsymbol{M}(\, \hat{\boldsymbol{\theta}}, \boldsymbol{\varphi}\,)\,]$$

$$\text{s.t.} \quad \left.\begin{array}{c} \left.\begin{array}{c} \dot{\boldsymbol{x}}(t) = \boldsymbol{f}(\, \boldsymbol{x}(t), \boldsymbol{z}(t), \boldsymbol{u}(t), \overline{\boldsymbol{w}}, \hat{\boldsymbol{\theta}}\,) \\ \boldsymbol{g}(\, \boldsymbol{x}(t), \boldsymbol{z}(t), \boldsymbol{u}(t), \overline{\boldsymbol{w}}, \hat{\boldsymbol{\theta}}\,) = \mathbf{0} \\ \boldsymbol{y}(t) = \boldsymbol{h}(\, \boldsymbol{x}(t), \boldsymbol{z}(t), \hat{\boldsymbol{\theta}}) \end{array}\right\} \text{DAE System} \\ \left.\begin{array}{c} \boldsymbol{f}^{\mathbf{0}}(\dot{\boldsymbol{x}}(t_0), \boldsymbol{x}(t_0), \boldsymbol{z}(t_0), \boldsymbol{u}(t_0), \overline{\boldsymbol{w}}, \hat{\boldsymbol{\theta}}) = \mathbf{0} \\ \boldsymbol{g}^{\mathbf{0}}(\, \boldsymbol{x}(t_0), \boldsymbol{z}(t_0), \boldsymbol{u}(t_0), \overline{\boldsymbol{w}}, \hat{\boldsymbol{\theta}}) = \mathbf{0} \\ \boldsymbol{y}^{\mathbf{0}}(t_0) = \boldsymbol{h}(\, \boldsymbol{x}(t_0), \boldsymbol{z}(t_0), \hat{\boldsymbol{\theta}}) \end{array}\right\} \text{Initial Conditions} \end{array}\right\} \boldsymbol{m}(\, \boldsymbol{x}(t), \boldsymbol{y}(t), \boldsymbol{z}(t), \boldsymbol{u}(t), \overline{\boldsymbol{w}}, \hat{\boldsymbol{\theta}}\,) = \mathbf{0}$$

$\boldsymbol{y}$	Measurements (model responses)
$\hat{\boldsymbol{\theta}}$	Estimated parameters
$\boldsymbol{x}$	Time-dependent differential state variables
$\boldsymbol{z}$	Time-dependent algebraic state variables
$\boldsymbol{u}$	Time-varying control variables
$\overline{\boldsymbol{w}}$	Time-invariant control variable

Fisher information matrix (FIM):

$$\boldsymbol{M} \approx \boldsymbol{V}_{\hat{\boldsymbol{\theta}}}^{-1} \approx \sigma_\epsilon^{-2} \boldsymbol{H} \approx \sigma_\epsilon^{-2} \boldsymbol{Q}^T \boldsymbol{Q}$$

MBDoE Decisions:

$$\boldsymbol{\varphi} = (\, \boldsymbol{u}(t), \boldsymbol{x}(t_0), \boldsymbol{z}(t_0), \overline{\boldsymbol{w}}, \mathbf{t}\,)$$

Franceschini, G., & Macchietto, S. (2008). Model-based design of experiments for parameter precision: State of the art. *Chemical Engineering Science*, *63*(19), 4846-4872.

Alphabetic Design Criteria Measure Information Content

Figure adapted from: Franceschini, G., & Macchietto, S. (2008). *Chem. Eng. Sci.*, *63*(19), 4846-4872.

A-optimality

max trace(**M**)

enclosing box volume

poor choice for highly correlated **θ**

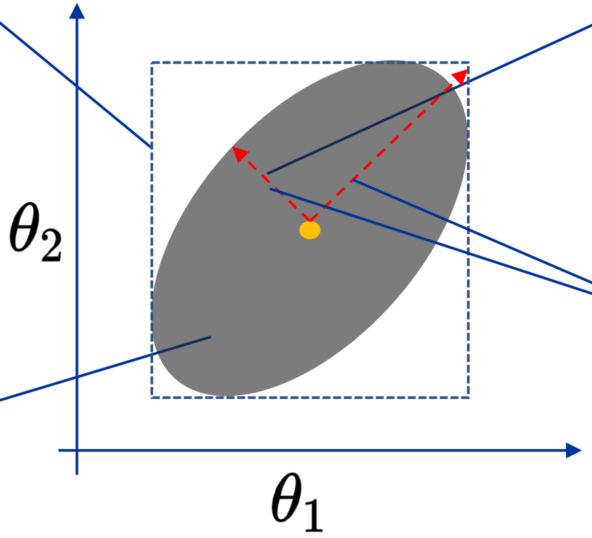
D-optimality

max det(**M**)

ellipsoid volume

robust to linear transformations

confidence ellipsoid for covariance matrix **V** = **M**$^{-1}$



E-optimality

max min(eig(**M**))

major axis

recommended if M is ill-conditioned

ME-optimality

min κ(**M**) = max(eig(**M**)) / min(eig(**M**))

ratio of major to minor axes

recommended if **M** is ill-conditioned

Model Discrimination

Hunter, W.G. and Reiner, A.M., 1965. Designs for discriminating between two rival models. *Technometrics*, *7*(3), pp.307-323.

Buzzi-Ferraris, G. and Forzatti, P., 1983. A new sequential experimental design procedure for discriminating among rival models. *Chemical engineering science*, *38*(2), pp.225-232.

Ferraris, G.B., Forzatti, P., Emig, G. and Hofmann, H., 1984. Sequential experimental design for model discrimination in the case of multiple responses. *Chemical engineering science*, *39*(1), pp.81-85.

Joint Parameter Precision and Model Discrimination

Alberton, A.L., Schwaab, M., Lobão, M.W.N. and Pinto, J.C., 2011. Experimental design for the joint model discrimination and precise parameter estimation through information measures. *Chemical Engineering Science*, *66*(9), pp.1940-1952.

Galvanin, F., Cao, E., Al-Rifai, N., Gavriilidis, A. and Dua, V., 2016. A joint model-based experimental design approach for the identification of kinetic models in continuous flow laboratory reactors. *Computers & Chemical Engineering*, *95*, pp.202-215.

Galvanin, F., Cao, E., Al-Rifai, N., Dua, V. and Gavriilidis, A., 2015. Optimal design of experiments for the identification of kinetic models of methanol oxidation over silver catalyst. *Chimica Oggi-Chemistry Today*, *33*(3), pp.51-56.

Pankajakshan, A., Waldron, C., Quaglio, M., Gavriilidis, A. and Galvanin, F., 2019. A Multi-Objective Optimal Experimental Design Framework for Enhancing the Efficiency of Online Model Identification Platforms. *Engineering*, *5*(6), pp.1049-1059.

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Pyomo.DoE Formulation: MBDoE as 2-Stage Program

max $\log\det\big(\mathbf{M}(\hat{\boldsymbol{\theta}}, \boldsymbol{\varphi})\big) = 2\sum_{i=1}^{N_p} \log L_{ii}$ D-optimality

s.t. $\mathbf{M} = \sum_{r}\sum_{r'} \tilde{\sigma}_{r,r'} \mathbf{Q}_r^{\mathrm{T}} \mathbf{Q}_{r'}$

Stage 1

$\mathbf{M} = \mathbf{L}\mathbf{L}^{\mathrm{T}}, \quad L_{ii} \geq \epsilon$ Cholesky factorization

$q_{r,p}(t) = \frac{y_{r,p}^{+}(t) - y_{r,p}^{-}(t)}{2\,\epsilon_p}$ Central finite difference

$\boldsymbol{m}\big(\boldsymbol{x}_p^{+}(t), \boldsymbol{y}_p^{+}(t), \boldsymbol{z}_p^{+}(t), \boldsymbol{u}(t), \overline{\boldsymbol{w}}, \boldsymbol{\theta}_p^{+}\big) = \mathbf{0}$

$\boldsymbol{m}\big(\boldsymbol{x}_p^{-}(t), \boldsymbol{y}_p^{-}(t), \boldsymbol{z}_p^{-}(t), \boldsymbol{u}(t), \overline{\boldsymbol{w}}, \boldsymbol{\theta}_p^{-}\big) = \mathbf{0}$

Two model evaluations

$\boldsymbol{\theta}_p^{+} = \hat{\boldsymbol{\theta}} + \boldsymbol{e}_p \epsilon_p$

$\boldsymbol{\theta}_p^{-} = \hat{\boldsymbol{\theta}} - \boldsymbol{e}_p \epsilon_p$

Up and down perturbations

Stage 2

$\forall p \in \{1, \ldots, N_p\}$

Model Sensitivity

$$\mathbf{Q}_r = \begin{bmatrix} \frac{\partial y_r(t_1)}{\partial \theta_1} & \cdots & \frac{\partial y_r(t_1)}{\partial \theta_{N_p}} \\ \vdots & \ddots & \vdots \\ \frac{\partial y_r(t_n)}{\partial \theta_1} & \cdots & \frac{\partial y_r(t_n)}{\partial \theta_{N_p}} \end{bmatrix} = [\mathbf{q}_{r,1} \quad \cdots \quad \mathbf{q}_{r,N_p}]$$

$$\mathbf{q}_{r,p} = \begin{bmatrix} \frac{\partial y_r(t_1)}{\partial \theta_p} & \cdots & \frac{\partial y_r(t_n)}{\partial \theta_p} \end{bmatrix}^{\mathrm{T}}$$

$\boldsymbol{y}$	Measurements (model responses)
$\mathbf{Q_r}$	Dynamic sensitivity for response *r*
$\boldsymbol{m}(\,)$	DAE model
$\hat{\boldsymbol{\theta}} \in \mathbb{R}^P$	Estimate for parameters
$\mathbf{M} \in \mathbb{R}^{P \times P}$	Fisher information matrix
$\mathbf{L} \in \mathbb{R}^{P \times P}$	Lower triangular Cholesky factorization
ϵ_p	Small perturbation for parameter *p*
$\boldsymbol{e}_p \in \mathbb{R}^P$	Unit vector with “1” in position *p*

Temperature Control Lab (TC-Lab) – Closed-Loop Experimental Design with New Experiment Abstraction

Parameter Estimation

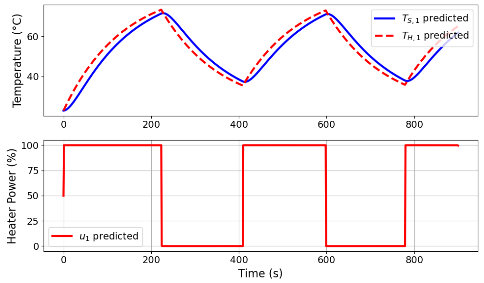
$$C_p^H \frac{dT_{H,1}}{dt} = U_a(T_{amb} - T_{H,1}) + U_b(T_{S,1} - T_{H,1}) + \alpha P_1 u_1$$
$$C_p^S \frac{dT_{S,1}}{dt} = U_b(T_{H,1} - T_{S,1})$$

$$\theta \equiv \{C_P^H, C_P^S, U_a, U_b\}$$
$$y \equiv \{T_{S,1}\}$$
$$\phi \equiv \{u_1\}$$

PYOMO - parmest

PYOMO DoE

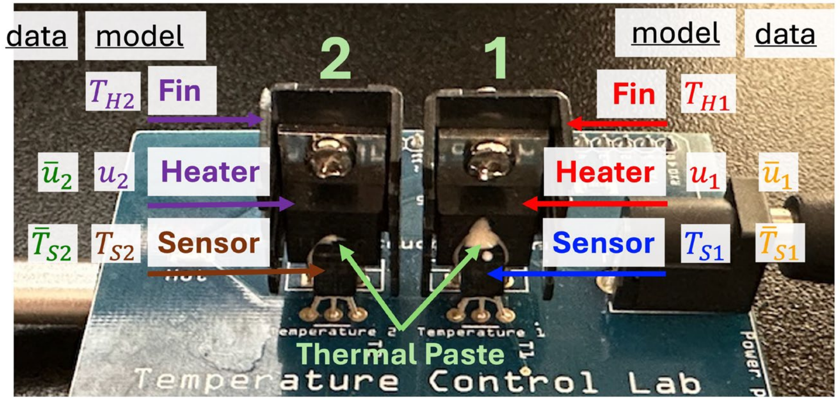
Optimal Experiment Design/Optimal Control



Digital Components

Physical Components

Physical System



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TC Lab: DoE, Exploratory Analysis

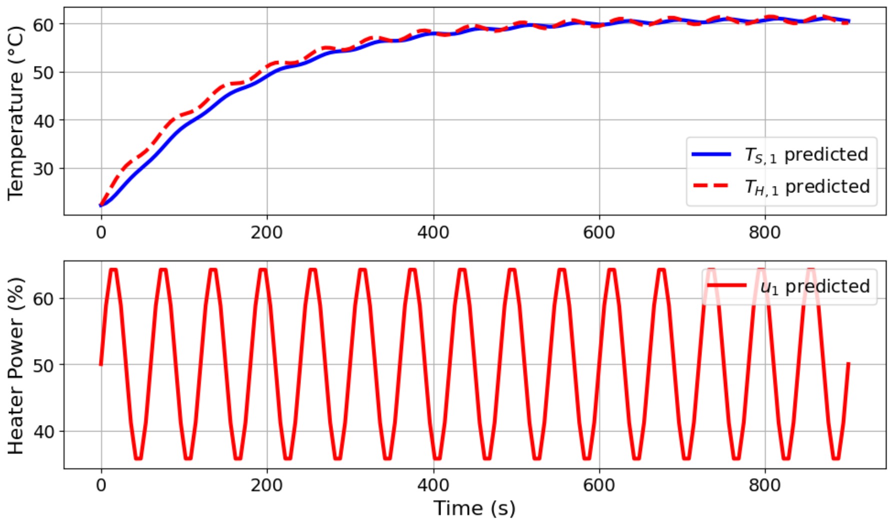
dowlinglab.github.io/pyomo-doe/notebooks/doe_exploratory_analysis.html

Sensitivity of the FIM to experimental design.

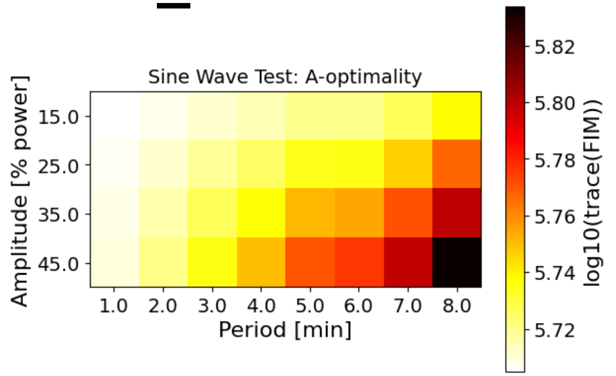
Example: Sine Wave

Vary:

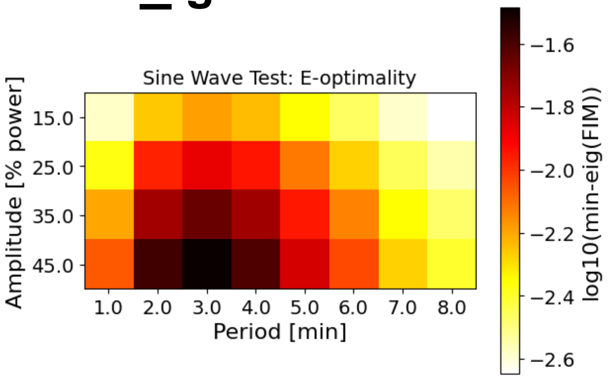
- period (from 1 to 8 minutes)
- amplitude (from 15% to 50%)



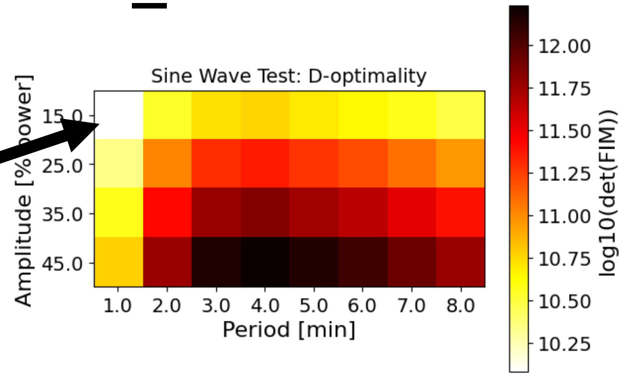
trAce



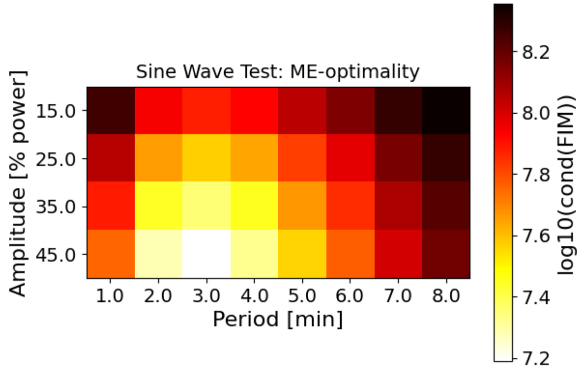
Min. Eigenvalue



Determinant



Condition Number



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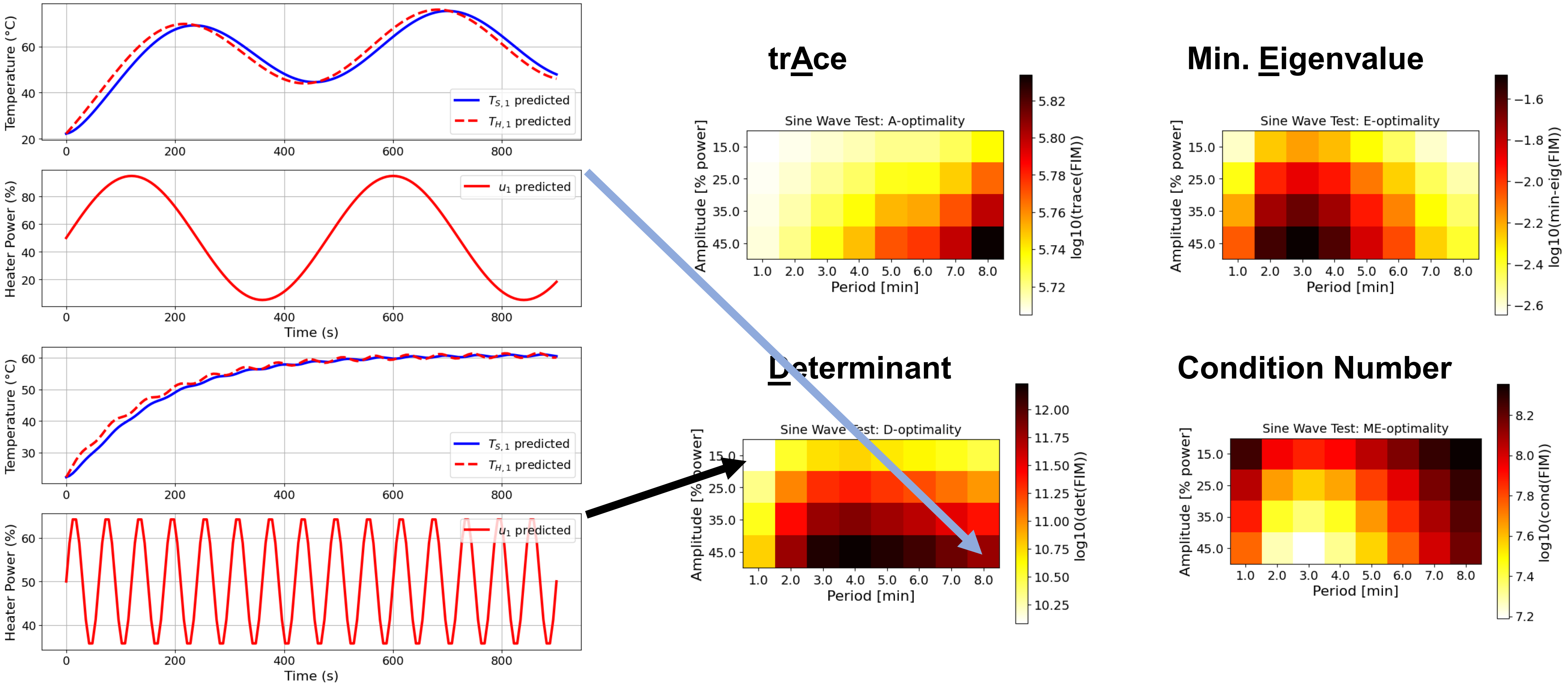
CCSI2 Carbon Capture Simulation for Industry Impact

PROMMIS Process Optimization and Modeling for Minerals Sustainability

TC Lab: DoE, Exploratory Analysis

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



TC Lab: A-Optimal Next Experiment

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

$$\max_{u} \quad \log \operatorname{trace}\left(\mathbf{M}(u) + \mathbf{M}_0\right)$$

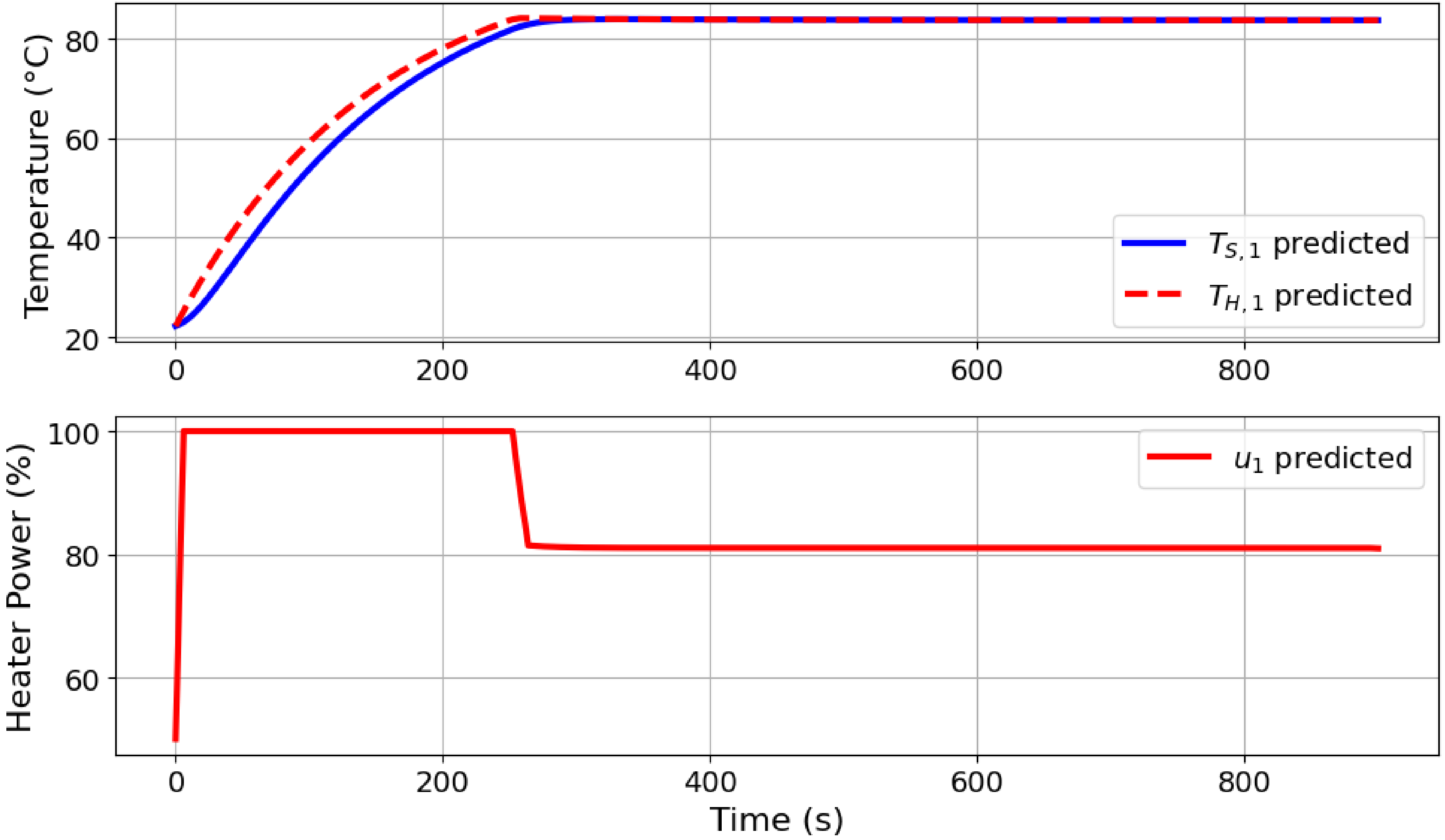
$$\text{s.t.} \quad C_p^H \frac{dT_H}{dt} = \ldots$$

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

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

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

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

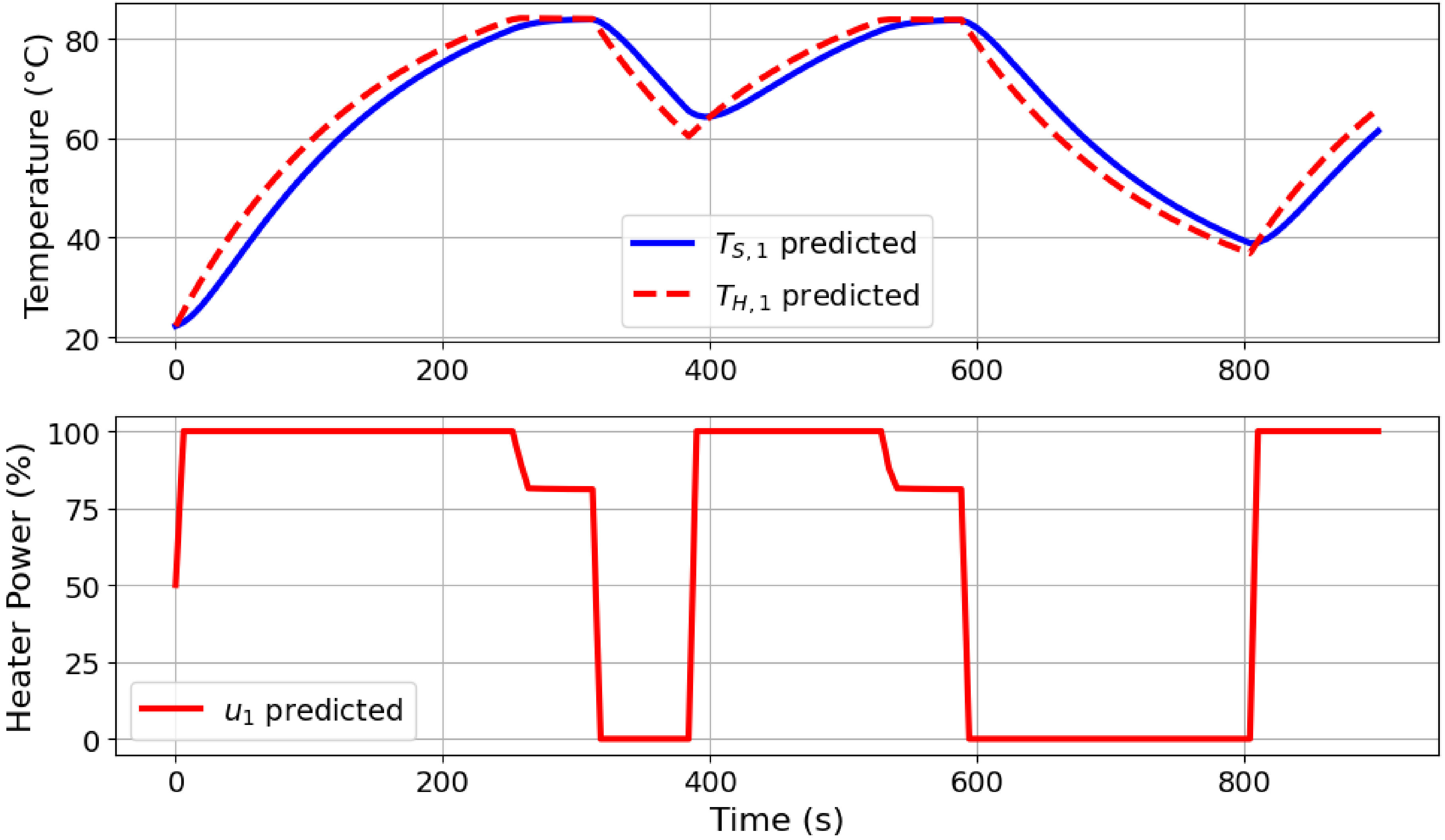


$U_b C_p^S$ is more estimable with two experiments (sine wave test, A-optimal)!

TC Lab: D-Optimal Next Experiment

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

$$
\begin{aligned}
\max_{u} \quad & \log\det(\mathbf{M}(u) + \mathbf{M}_0) \\
\text{s.t.} \quad & C_p^H \frac{dT_H}{dt} = \ldots \\
& C_p^S \frac{dT_S}{dt} = \ldots \\
& 0\% \leq u(t) \leq 100\% \\
& T_H(t_0) = T_{amb} \\
& T_S(t_0) = T_{amb}
\end{aligned}
$$



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

Getting Started with Pyomo.DoE

Documentation: https://pyomo.readthedocs.io/en/stable/contributed_packages/doe/doe.html

Pyomo.DoE

Pyomo.DoE (Pyomo Design of Experiments) is a Python library for model-based design of experiments using science-based models.

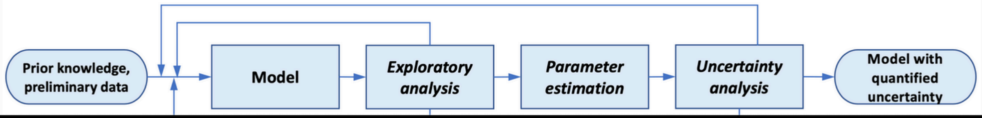
Pyomo.DoE was developed by **Jialu Wang** and **Alexander W. Dowling** at the University of Notre Dame as part of the Carbon Capture Simulation for Industry Impact (CCSI2). project, funded through the U.S. Department Of Energy Office of Fossil Energy.

If you use Pyomo.DoE, please cite:

[Wang and Dowling, 2022] Wang, Jialu, and Alexander W. Dowling. "Pyomo.DOE: An open-source package for model-based design of experiments in Python." AIChE Journal 68.12 (2022): e17813. *https://doi.org/10.1002/aic.17813*

Methodology Overview

Model-based Design of Experiments (MBDoE) is a technique to maximize the information gain of experiments by directly using science-based models with physically meaningful parameters. It is one key component in the model calibration and uncertainty quantification workflow shown below:



ParmEst and Pyomo.DoE Development Plans

Coming soon:

- Improved initialization
- Improved optimization performance
  - NLP decomposition
  - Grey-box objective calculations
- Improved modeling abstraction
  - Multiple experiments (e.g., planning batches)
  - Parameter uncertainty
- More applications, examples, and collaborations
- End-to-end uncertainty workflow (via interface with PyROS)

PYOMO DoE

Acknowledgements

PYOMO DoE

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CCSI² Carbon Capture Simulation for Industry Impact

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