



Causal Inference: A Bridge Between Simulation Models and Observed Phenomena

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Changing the World's Energy Future

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Causal Inference: A Bridge Between Simulation Models and Observed Phenomena

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Introduction

- **Simulation models** are playing a critical role in the design and operation of complex technological systems
 - Mimic aspects of the real world as closely as possible to correctly capture the evolution and properties of those aspects
- **Starting point:** Set of constituent laws of the considered system
 - Differential equations
 - Algebraic equations
- Development of such equations embraces the purpose of any scientific endeavor
- Causality is at the core of a simulation model's development

“The systematization and abstraction of causal thinking, the search for an understanding of the causal relations among events.” (J. Ismael)

Def. Cause-effect ($A \rightarrow B$). A physical phenomenon such that a change in A leads to a change in B.

Causal Interpretation of Mathematical Models

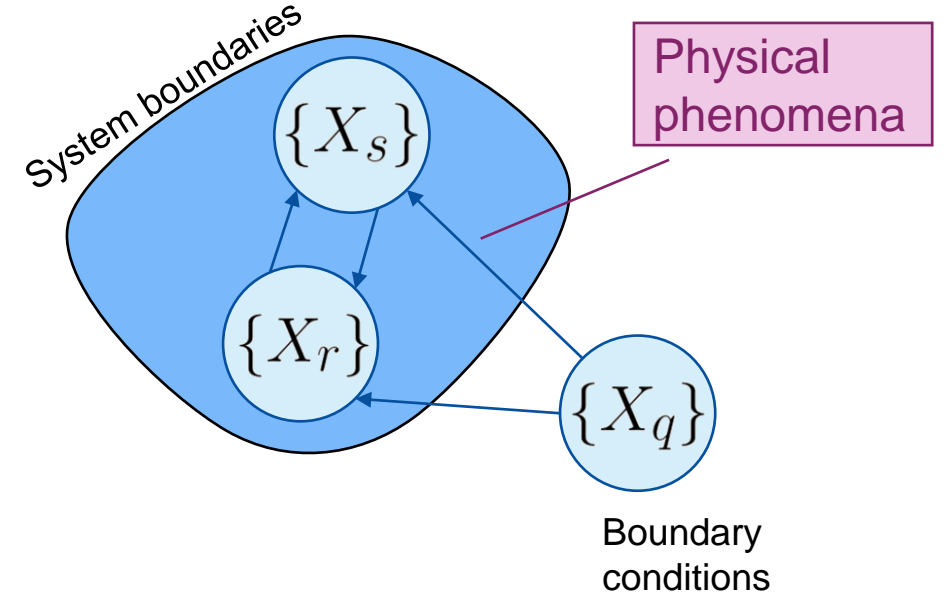
- Focus on set of equations that model system dynamics
 - System described by N variables (X_1, \dots, X_N)

Set of dynamic equations
effect = $f(\text{causes})$

$$\begin{cases} \dot{X}_s = f_s(X_1, \dots, X_N, t), & s \in \Gamma \\ X_r = f_r(X_1, \dots, X_N, t), & r \in \Xi \\ X_q = f_q(t), & q \in \Lambda \end{cases}$$

Set of boundary
conditions (causes)

Set of state equations

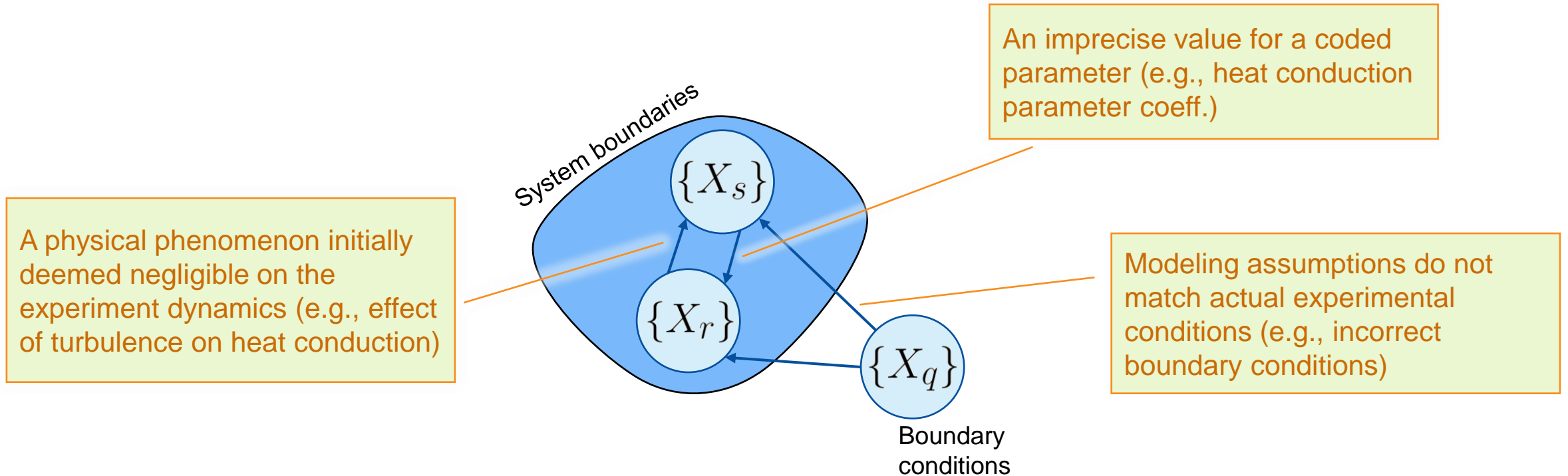


Causal Interpretation of Modeling Choices

- Recall that

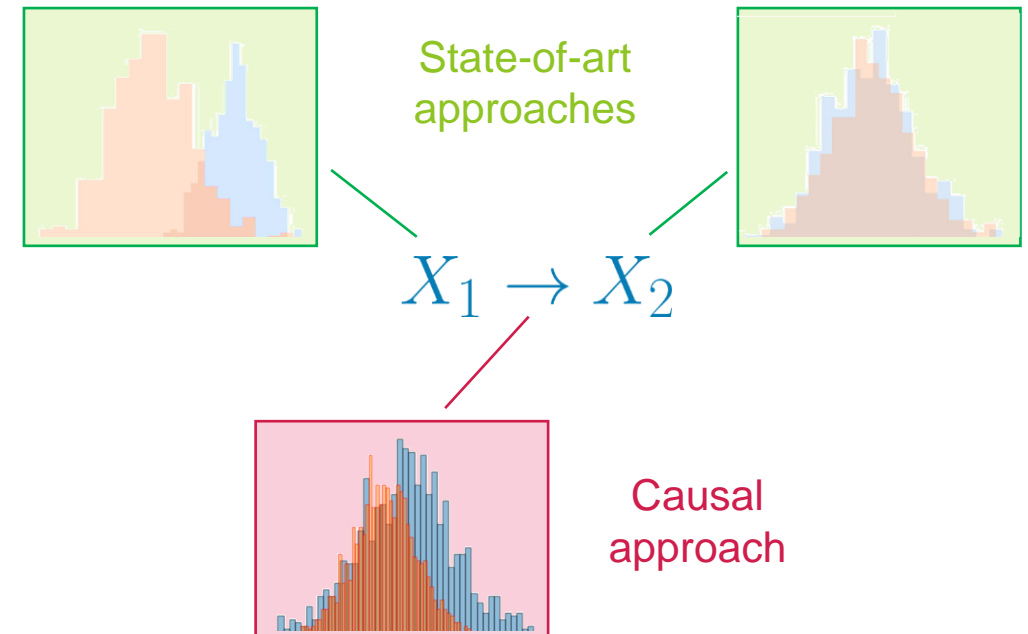
$$\textit{simulation} \cong \textit{reality}$$

- Possible discrepancies between simulation and observed data



Simulation Model Reality Check: Model Validation

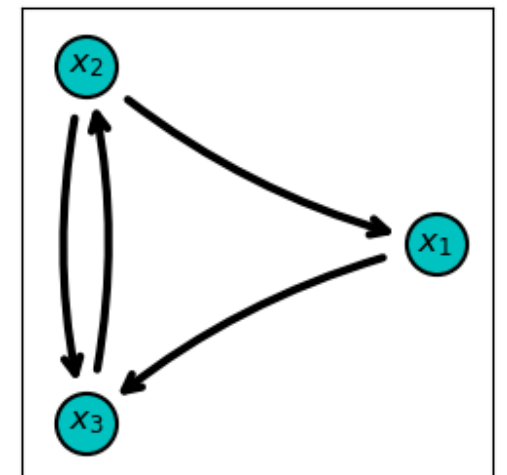
- Current methods for **model validation**
 - Quantitative **statistical comparison between datasets** (i.e., simulated vs. measured data)
 - No explicit consideration of the hypotheses behind them (e.g., boundary conditions) or the structure of the employed models
- Causality is not explicitly considered
- **Different mindset:** Validation approach based on **causal inference**
 - Capture the causal relationships between data elements rather than looking at their associations
 - Compare static properties of the cause-effect relations between variables rather than focusing on the variables themselves



Causal Inference and Causal Discovery

- Classical statistics or machine learning methods
 - Model/construct a probabilistic distribution from historic observations
 - Identify patterns out of this distribution (e.g., to predict the outcome of future observations)
- Causal inference aims to identify the possible mechanisms that might have generated historic observations
- Structural causal models (SCMs): Causal models that can model cycles, interventions, and counterfactuals
 - Given a set of N variables X_n ($n = 1, \dots, N$), an SCM consists of a set of structural equations of the form
$$X_n := h_n(X_{pa_n}) \quad n = 1, \dots, N$$
 - SCM can be visualized in a graphical form: Directed acyclic graph (DAG)
- SCMs and dynamic equations

$$\dot{X}_n(t) = \frac{dX_n(t)}{dt} = f_n(X_1, \dots, X_N) \quad X_n(0) = X_{n,0} \quad n = 1, \dots, N$$



Statistical Methods for Causal inference

Def.: Cause-effect ($A \rightarrow B$). A physical phenomenon such that a change in A leads to a change in B.

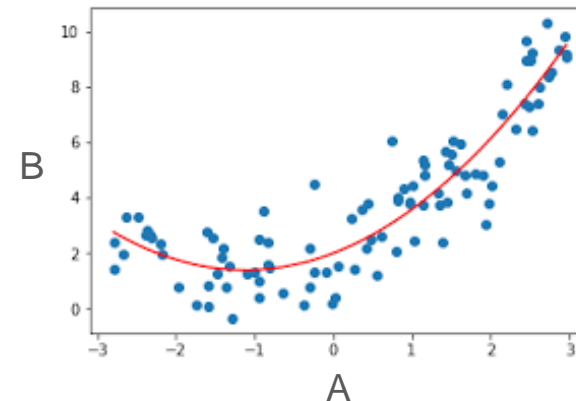
A physical phenomenon

Method: Independence testing

Change in A leads to a change in B

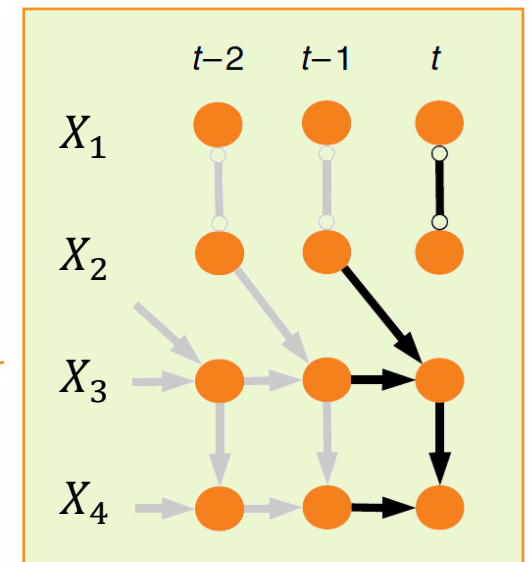
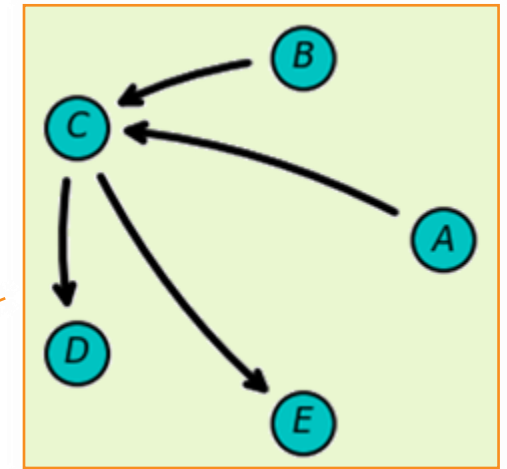
Method: Regression

$$A \perp\!\!\!\perp B \Leftrightarrow Pr(A \cap B) = Pr(A) \cdot Pr(B)$$



Causal Discovery From Time Series Data

- **Input:** Temporal profile of N variables $X(t) = [X_1(t), \dots, X_N(t)]$
- **Independence testing**
 - **PC:** Check for statistical independence
 1. Start with complete undirected graph
 2. Identify the skeleton of the graph: remove $A - B$ if $A \perp\!\!\!\perp B|C$ for some conditioning set (e.g., C)
 - Starting with empty conditioning set and increasing size
 3. Identify “colliders” for each triple $B - C - A$
 - Determine direction of edges: $B \rightarrow C \leftarrow A$
 4. Identify “forks” for the remaining triples
 - Determine direction of edges: $D \leftarrow C \rightarrow E$
 - **PC1:** Modified version of PC applied to time series
 - Conditional independence testing between
 - $X_n(t)$ vs. $\{X_1(t-1), \dots, X_N(t-1)\}$
 - $X_n(t)$ vs. $\{X_1(t-2), \dots, X_N(t-2)\}$
 - ...



Source: Runge, J., et al. Inferring causation from time series in Earth system sciences. Nature Communications, vol. 10, 2553 (2019).

Causal Discovery From Time Series Data

- **Regression:** Reconstruct approximate form of given temporal profile of $\tilde{X}(t)$ from $X(t) = [X_1(t), \dots, X_N(t)]$

- Vector autoregression (**VAR**):

$$\tilde{X}(t) = \sum_{\tau=0}^k \mathbf{B}_{\tau} \mathbf{X}(t - \tau) + \mathbf{e}(t)$$

- Sparse Identification of Nonlinear Dynamics (**SINDy**)

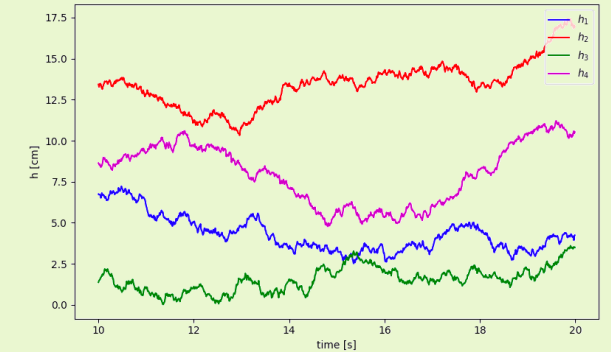
- Determine \tilde{X} in form of differential equations

- **Note:** No classical regression model provides causal information

- “Correlation does not imply causation”

- **Solution:** Couple PC1 with a regression model

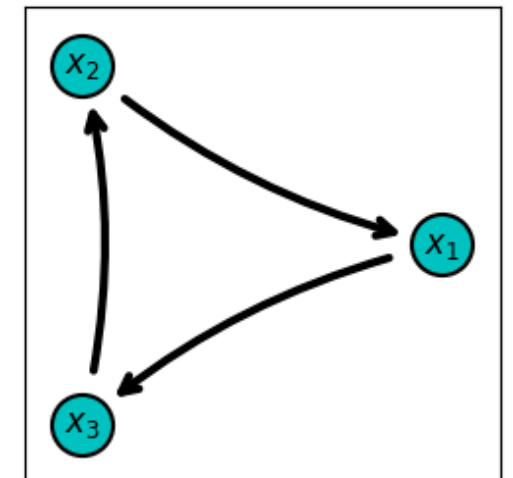
1. Test conditional independence (PC1) from full data set
2. Create regression model
3. Check for conflicts between correlation and causation information
 - Test PC1 on the residual $\tilde{X}(t) - X(t)$
 - Update regression model



$$\begin{cases} \frac{dh_1}{dt} = -\frac{a_1}{A_1} \sqrt{2gh_1} + \frac{a_3}{A_1} \sqrt{2gh_3} + \frac{\gamma_1 k_1}{A_1} u_1 \\ \frac{dh_2}{dt} = -\frac{a_2}{A_2} \sqrt{2gh_2} + \frac{a_4}{A_2} \sqrt{2gh_4} + \frac{\gamma_2 k_2}{A_2} u_2 \\ \frac{dh_3}{dt} = -\frac{a_3}{A_3} \sqrt{2gh_3} + \frac{(1-\gamma_2)k_2}{A_3} u_2 \\ \frac{dh_4}{dt} = -\frac{a_4}{A_4} \sqrt{2gh_4} + \frac{(1-\gamma_1)k_1}{A_4} u_1 \end{cases}$$

Modeling Assumptions and Challenges

- **Causal sufficiency:** Set of variables X_n contains all common causes of any subset of variables
 - Normally guaranteed in a simulation model
 - Experimental data might contain a subset of variables that might have a causal role in the experiment dynamics and are not part of the actual dataset
- **Constant causal structure:** Causal relations between variables X_n do not change with time
 - E.g., sudden activation of a pump during a cooling transient would cause a change in the SCM
 - SCM generation/quantification should be redone after each configuration change
- **Is data enough?** Not really...
 - “Conditional independence testing works well with infinite data”
 - Models that describe system architecture (undirected graph) greatly improve causal discovery performances
- **Cycles in SCMs:** Can be handled if information flow through the loop is “slow”
- **Reliability** of causal inference methods
 - No metrics to assess quality of the obtained results
 - P-values can be misleading



Data Pre-Processing

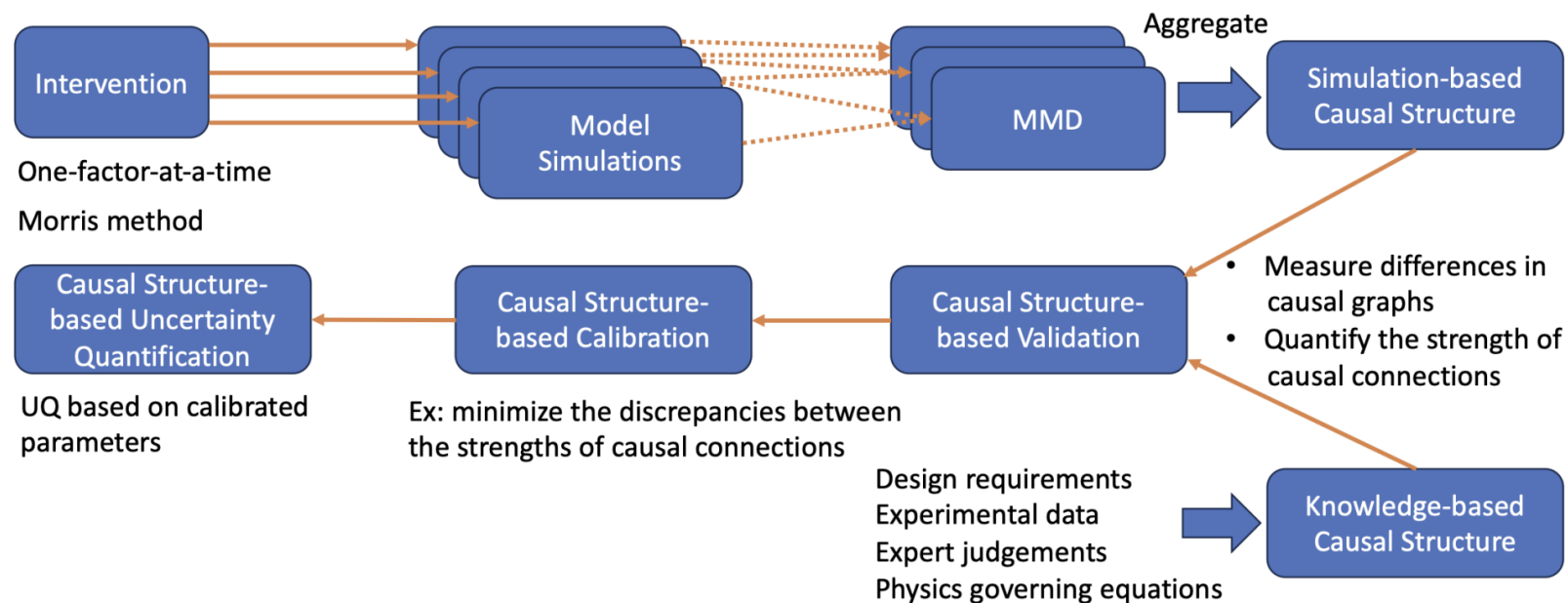
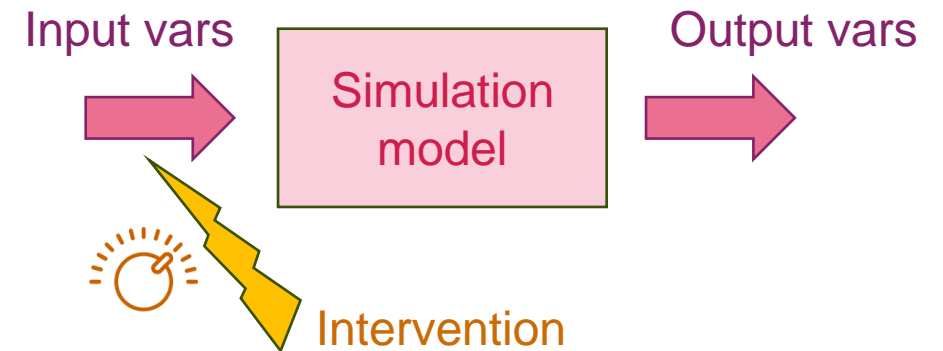
- **Data normalization:** Z-normalization is usually performed

$$\hat{X}_n(t) = \frac{X_n(t) - \text{mean}[X_n(t)]}{\text{std_dev}[X_n(t)]}$$

- **Data synchronicity:** Set of time instants equally spaced in time; they are identical for each variable
 - If needed, data synchronization techniques (e.g., time series resampling, time series interpolation) should be applied
- **Data smoothing:** Should be performed only in few limited cases
 - Data smoothing can alter conditional independence testing results
- **From time domain to frequency domain:** Works have been published, but major improvements have not been observed

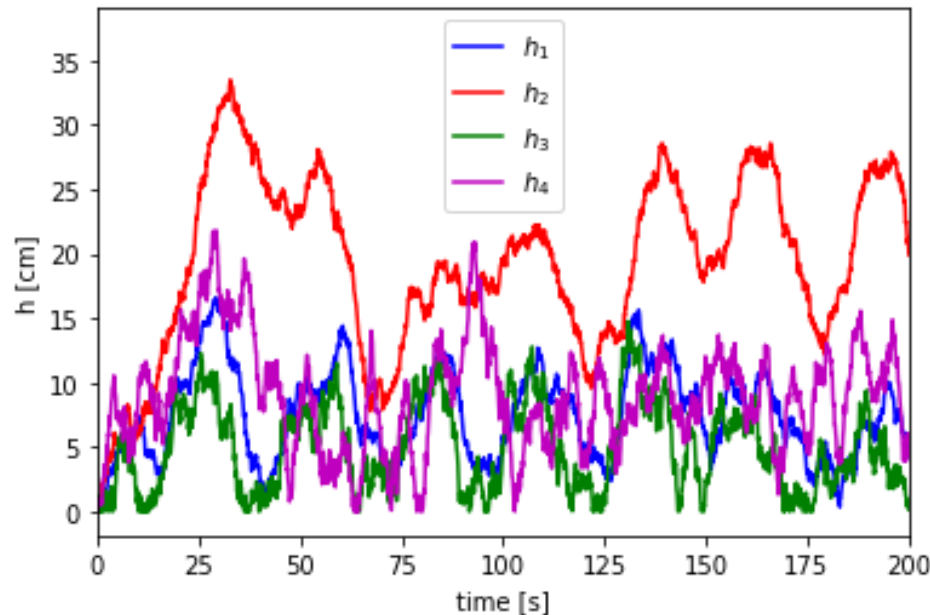
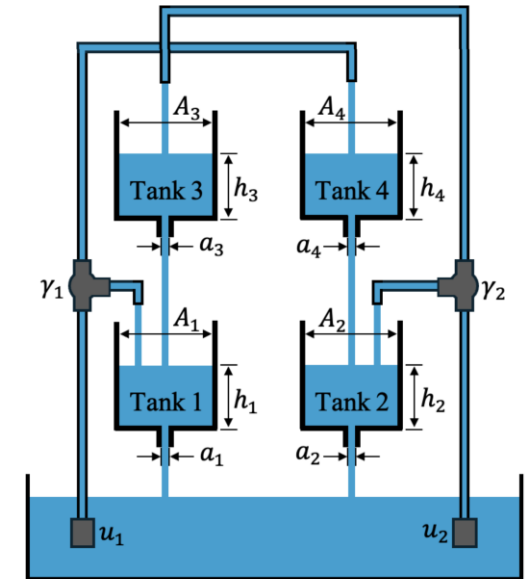
SCMs from Simulation Models

- Two choices
 - Generate SCMs from time series data generated by simulation model
 - Intervention-based approach applied to the model directly
 - Maximum Mean Discrepancy (MMD) approach
 - Still need for post-processing using PC1

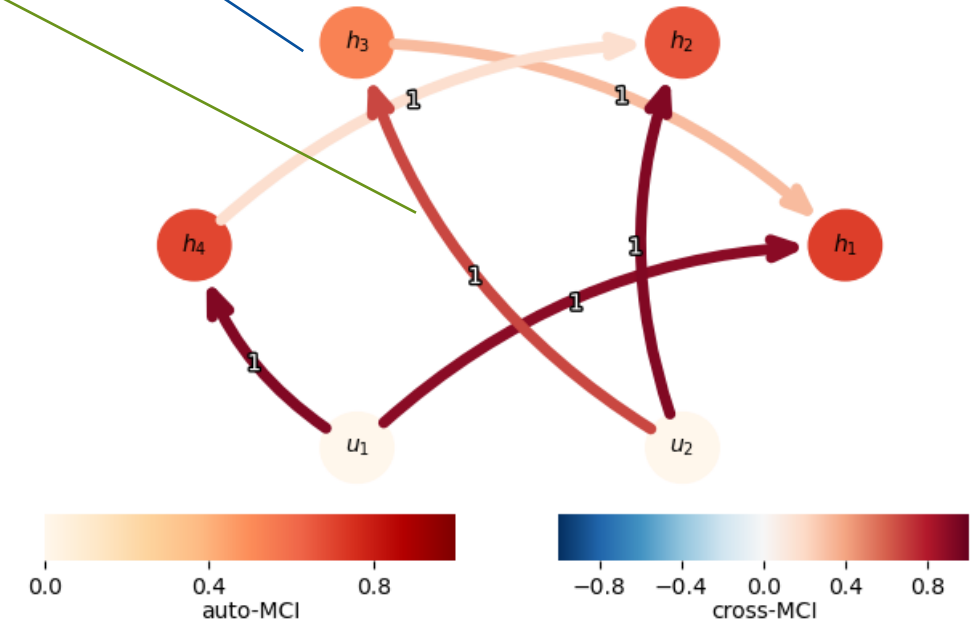


Benchmark: Analysis of Multiple Tank System

- Analytical test case: quadruple tank process*
- System dynamics is solved analytically through a set of 4 ordinary differential equations (ODEs)
 - Mass conservation laws



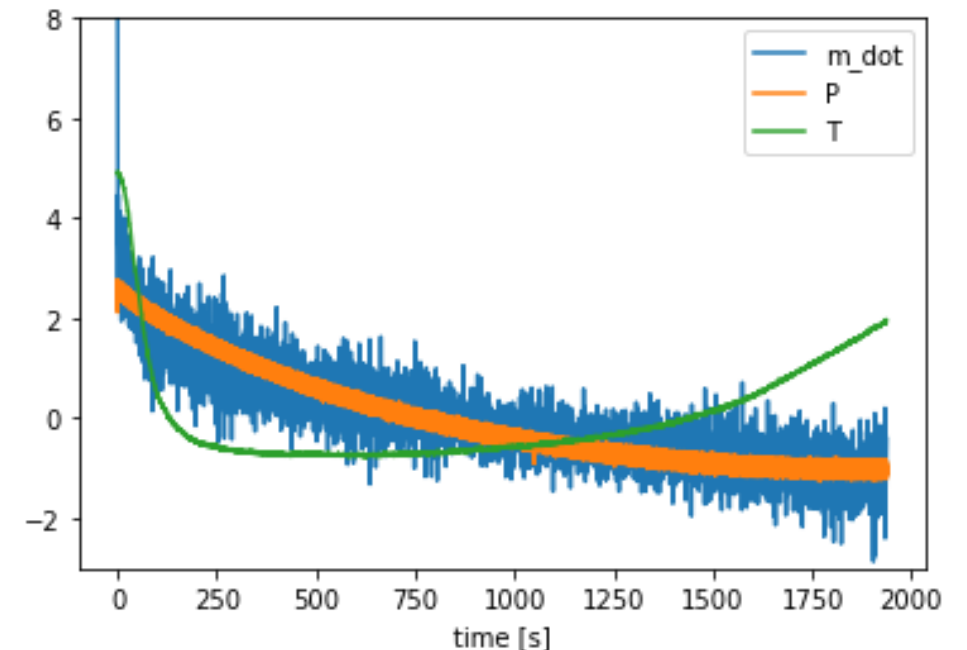
$$\frac{dh_3(t)}{dt} = \frac{(1 - \zeta_2)}{A_3} u_2 - \frac{a_3}{A_3} \sqrt{2gh_3}$$



* Johansson, K. H. 2000. The Quadruple Tank Process: A Multivariable Laboratory Process with an Adjustable Zero. *IEEE Transactions on Control Systems Technology*, 8, no.3.

Analysis Of HAIRE Experimental Setup

- **Validation test:** Helium Air Ingress gas Reactor Experimental (HAIRE) facility at University of Michigan
- Available measurements: Pressure P and temperature T
 - Mass flow rate is calculated from perfect gas state equation
- Depressurization experiments
 - Reactor vessel is vacuumed and pressurized with the gas of interest
 - The initiation mechanism is released which allows the depressurization to start
 - The gaseous depressurization continues until an equilibrium pressure is reached between atmosphere and the pressure vessel
- Experiments were performed with a variety of initial pressures, gases, and crack diameters



Analysis Of HAIRE Experimental Setup

- **Simulation model:** Temporal evolution of tank pressure and mass flow rate (iso-thermal conditions)
 - Mass flow rate formulation changes when critical pressure is reached
 - SCMs are generated separately before and after critical pressure is reached

Experimental

	P	\dot{m}	T
P	1	-3.4E-7	3.6E-8
\dot{m}	8.7E-6	1	9.5E-7
T	-1.7E-5	1.9E-5	1

	P	\dot{m}	T
P	1	-2.9E-7	4.2E-7
\dot{m}	9.5E-8	1	2.7E-7
T	-2.5E-7	9.92E-9	1

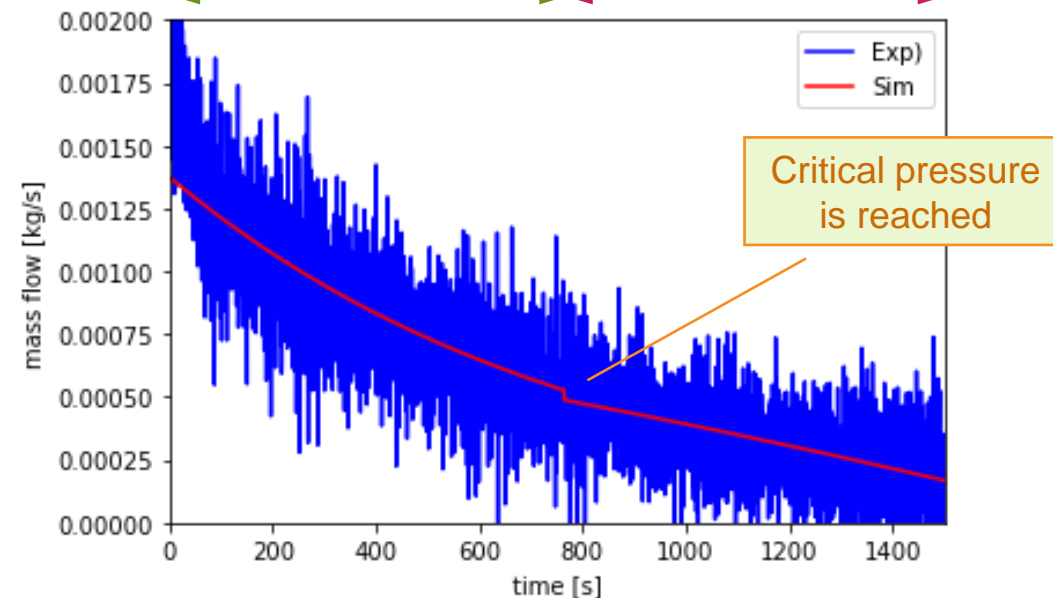
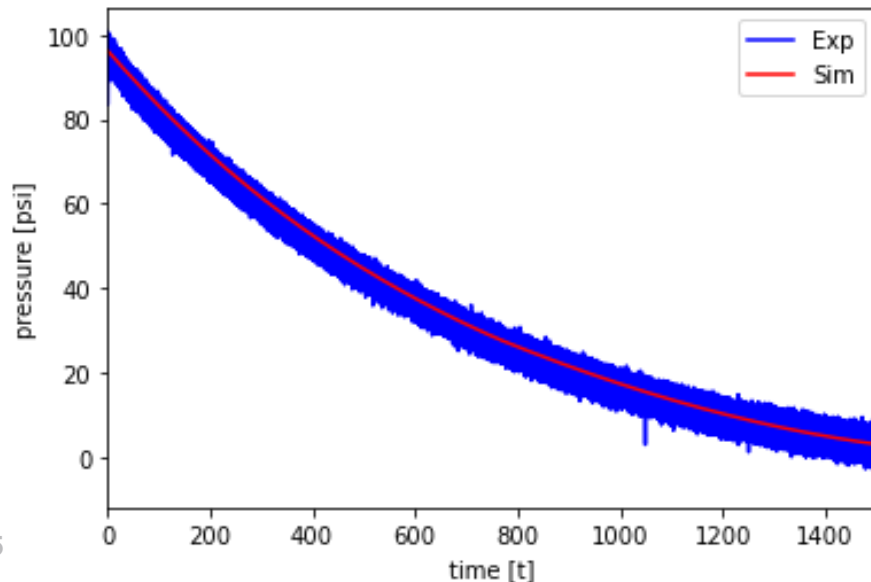
	P	\dot{m}	T
P	1	-2.5E-7	4.4E-7
\dot{m}	2.6E-7	1	3.2E-7
T	-6.4E-7	4.7E-7	1

	P	\dot{m}	T
P	1	-2.8E-7	6.1E-8
\dot{m}	3.7E-7	1	5.1E-8
T	4.1E-8	-6.1E-7	1

Simulated

	P	\dot{m}
P	1	-2E-7
\dot{m}	7.6E-8	1

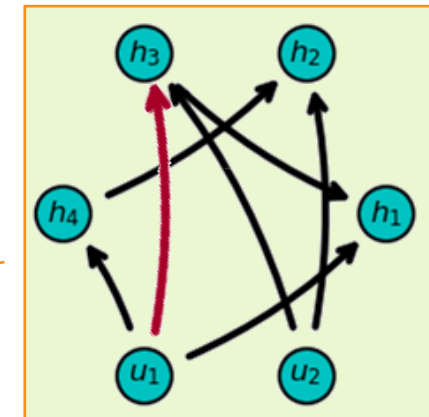
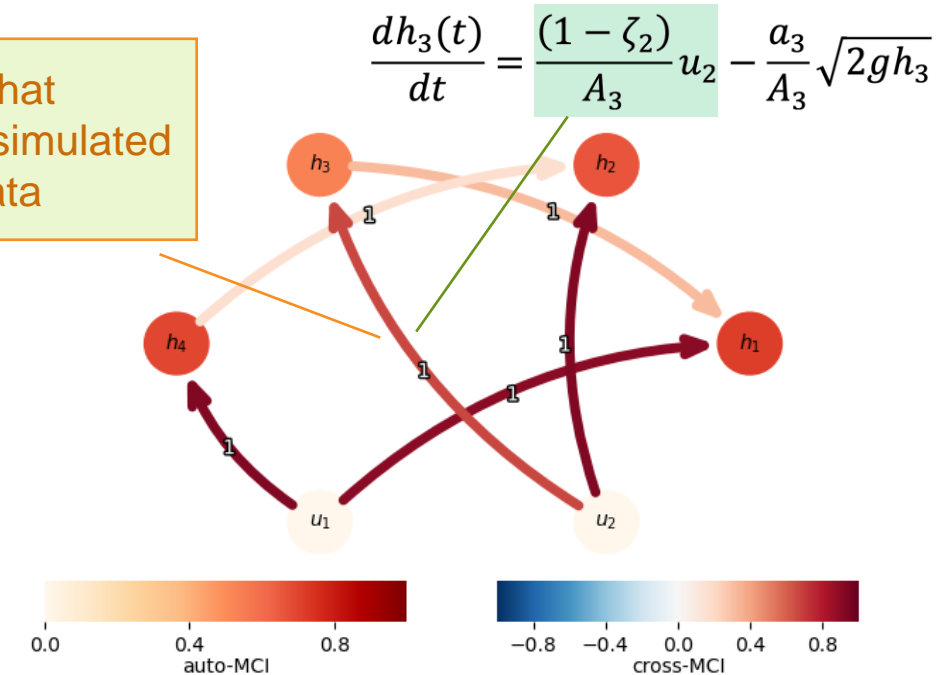
	P	\dot{m}
P	1	-3E-7
\dot{m}	4.3E-8	1



Impact on Model Calibration and System Control

- **Model calibration:** Process of refining model parameters that impact the identified causal relationships
- Relations between model equations and SCM provide indication on the parameter(s) to be changed
- **System control**
 - **Anomaly detection**
 1. Perform causal discovery in time windows
 2. Detect changes between SCMs obtained in consecutive time windows
 3. Identify causes of such changes
 - **Formulate control profiles**
 - Determine temporal profile of controlled variables that satisfy control requirements
 - **Test hypotheses**
 - Test SCM structure (e.g., new edge)

Causal relation that differs between simulated and observed data



Final Remarks

- **This talk:** An initial evaluation of methods based on causal inference to analyze data in an engineering operational context
 - Deviation from classical statistical and machine learning algorithms
 - An SCM is generated from time series data
- Main application: Validation (and calibration) of simulation codes
 - Performed by comparing SCMs obtained from simulation model and observed experimental data
- Causal inference can enhance current machine learning models
 - Bring back the physics mindset into the data analysis process