INL/CON-24-77803-Revision-0

Verification, Validation, and Calibration Through a Causal Lens

May 2024

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VVUQ

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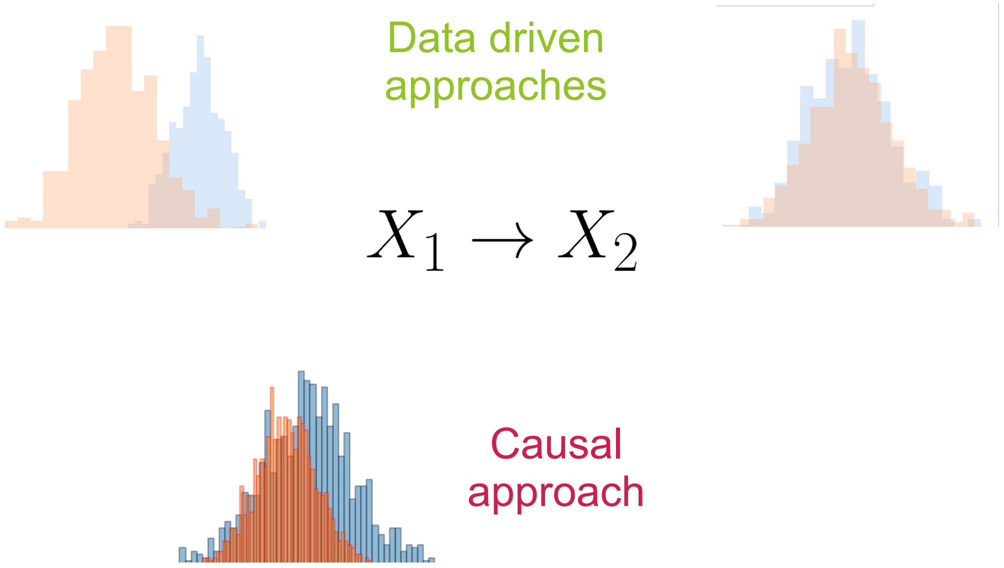
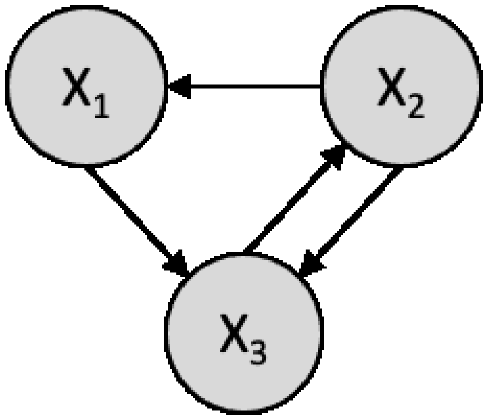
Introduction

- Simulation models are defined by a set of constituent and dynamic mathematical equations (e.g., conservation laws, equations of motion, thermodynamic laws)
  - Encoded cause-effect information
- Current methods for model validation: Data driven
  - Quantitative 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
- This paper: Validation approach based on causal inference
  - Capture the causal relationships between data elements rather than looking at their associations



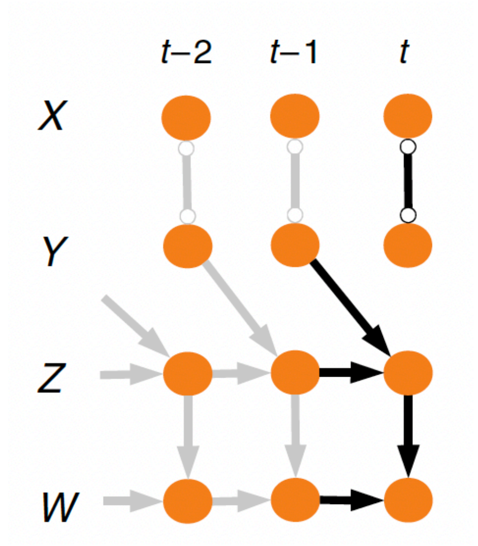
Causal Inference and Discovery

- Probabilistic inference (classical statistics or machine learning methods) is designed to
  - 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 , an SCM consists of a set of structural equations of the form
  - SCM can be visualized in a graphical form: Directed acyclic graph (DAG)
- SCMs and dynamic equations

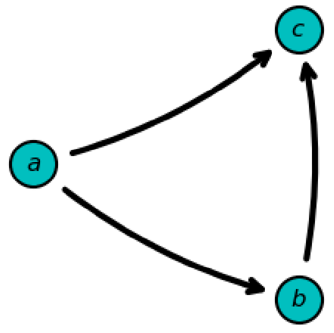


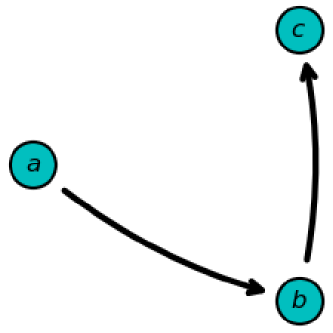
Discovery Methods

- **Input:** Temporal profile of variables
- **PC:** Perform independence tests on all possible connections in the DAG given sufficient conditioning set
  - Classical formulation:
- **PCMCI:** Check for statistical independence
  - Algorithm steps
    1. PC1: (modified PC) Conditional independency testing among variables in a specific timestamp
    2. MCI (Momentary conditional independence): determine causal relationship between variables in different timestamps



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





Discovery Methods

- **SINDy (sparse identification of nonlinear dynamics):** Sparse regression to find a linear combination of basis functions that best capture the dynamic behavior of the physical system. That is, estimating in , where

  Here is the matrix of time series data, is a set of basis functions and is   a presumably sparse coefficient matrix.

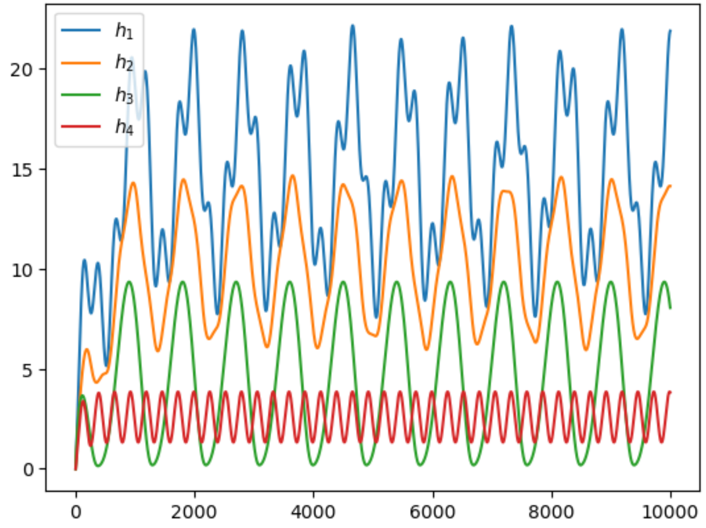
- **MMD:** An intervention-based Maximum Mean Discrepancy (MMD) testing method to automatically identify causal structure of a control system. Tests the physical influence when manipulating the input variables. It is a kernel-based two-sample test method to measure the distance between the kernel mean embeddings of two random variables in the reproducing kernel Hilbert space (RKHS).

Modeling Assumptions

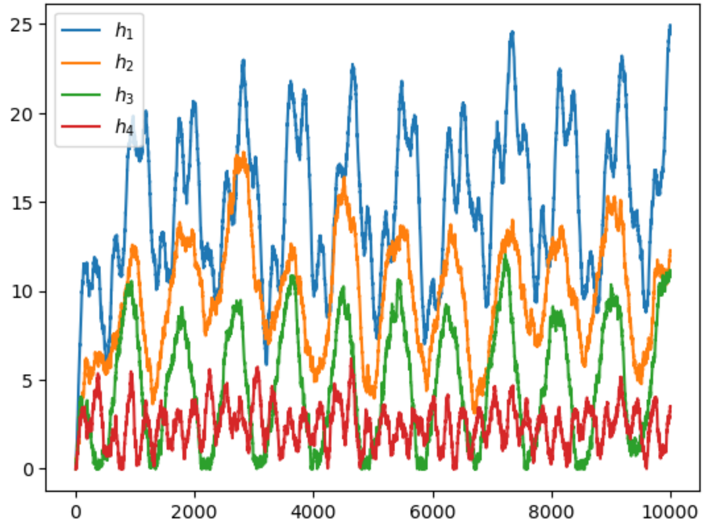
- Causal sufficiency: Assume that the set of variables contains all common causes of any subset of variables
  - Normally guaranteed in a simulation model
  - Experimental data might contain a subset of variables that might have a causal role in the experiment dynamics and are not part of the actual dataset
- Constant causal structure: Causal relations between variables do not change with time
  - E.g., sudden activation of a pump during a cooling transient would cause a change in the SCM
  - If these system configuration changes are recorded, then the SCM generation/quantification should be redone after each configuration change
- Data synchronicity: Set of time instants equally spaced in time they are identical for each variable
  - If these conditions are not satisfied, then proper data synchronization techniques (e.g., time series resampling, time series interpolation) should be applied
- Noisy data: Most methods are able to process the presence of noise as part of the time series
  - Noise terms associated with each variable are assumed to be independent

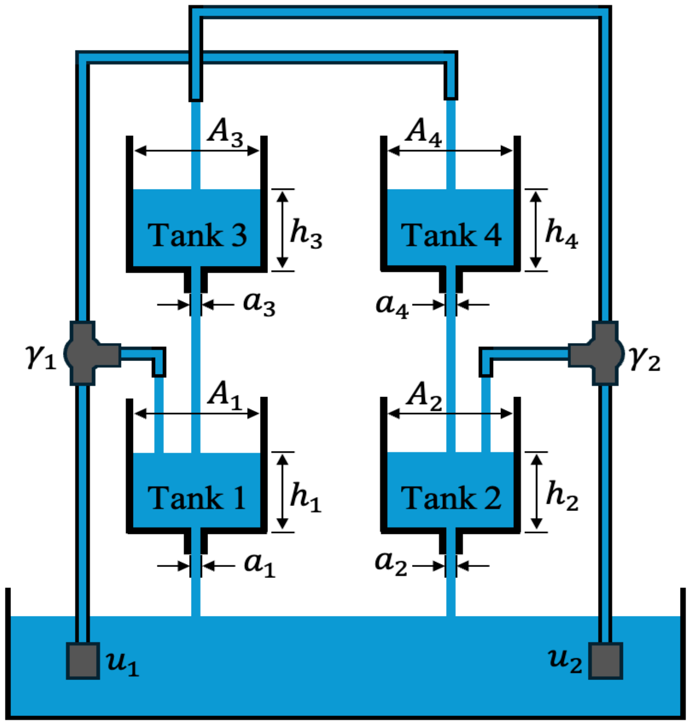
Quadruple Tank Problem

Deterministic

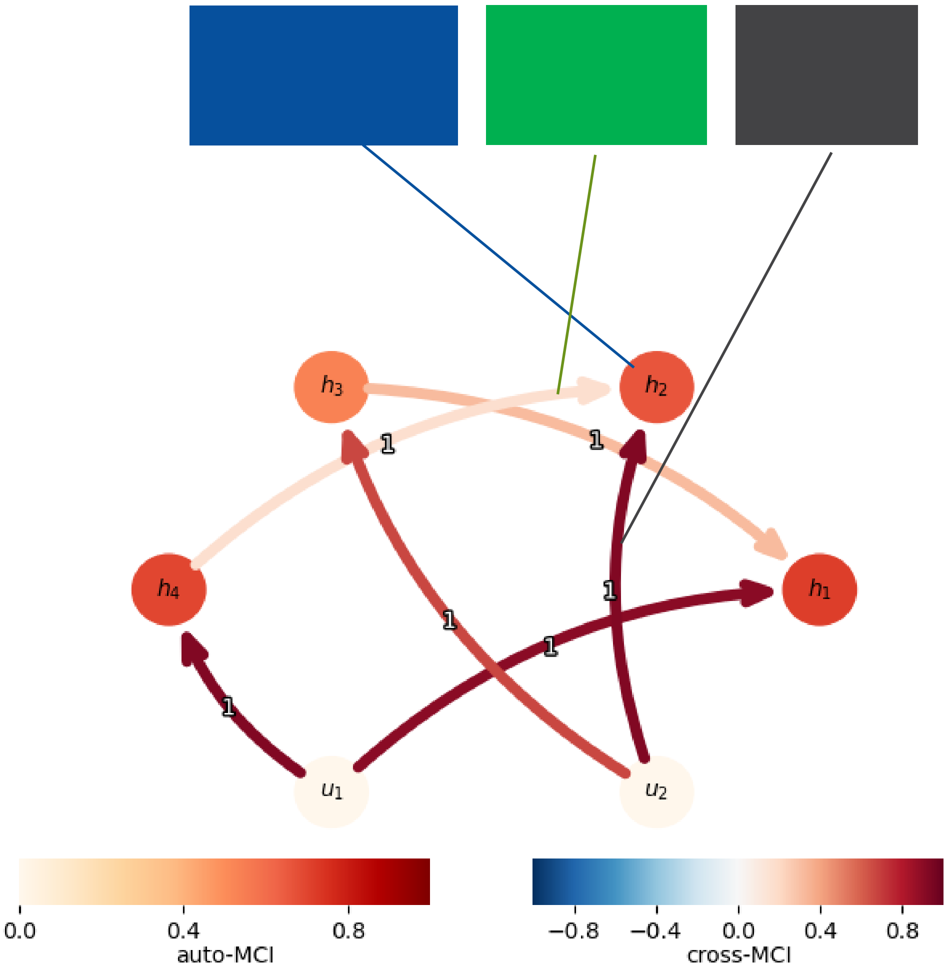


Stochastic



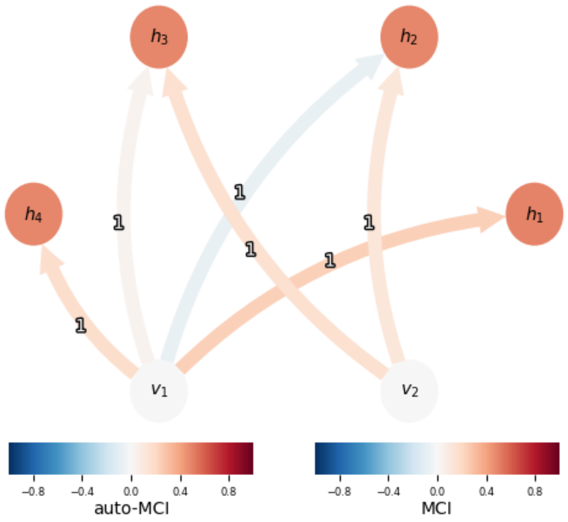


Quadruple Tank Analysis PC/PCMCI

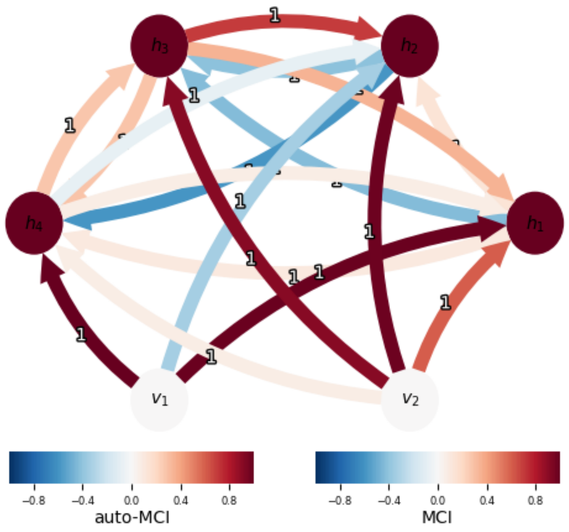


Internal Noise

External Noise



Deterministic



Quadruple Tank Analysis SINDy

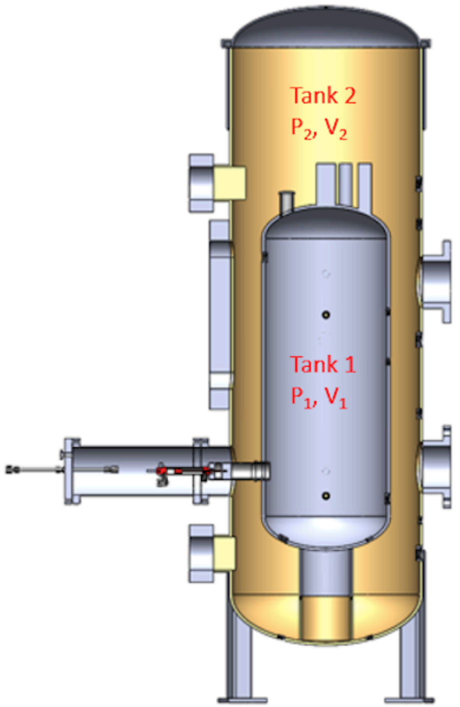
Modeled ODE

External Noise

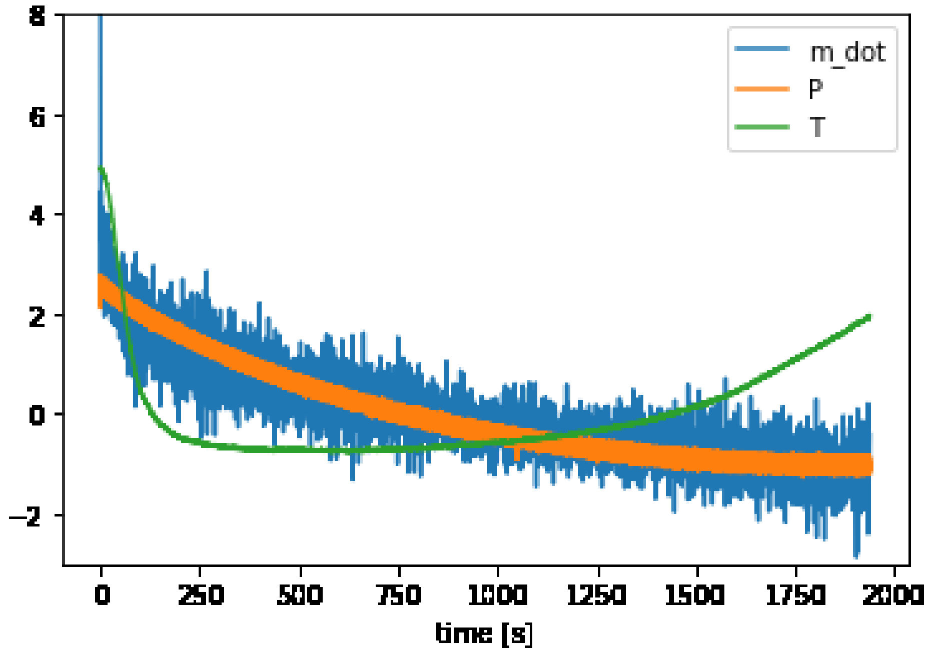
Deterministic

Internal Noise

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: Results

- 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

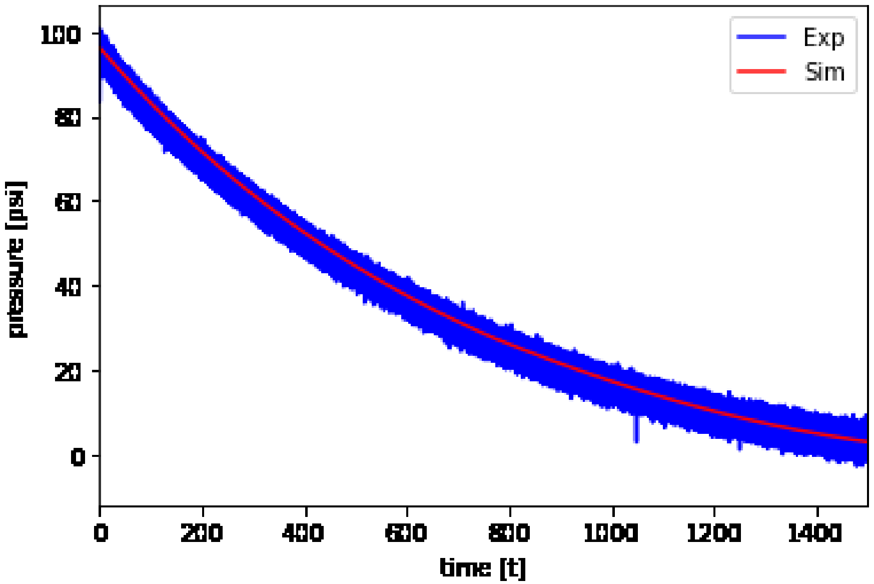
	P	$\dot{m}$	T
P	1	-2.5E-7	4.4E-7
$\dot{m}$	2.6E-7	1	3.2E-7
T	-6.4E-7	4.7E-7	1

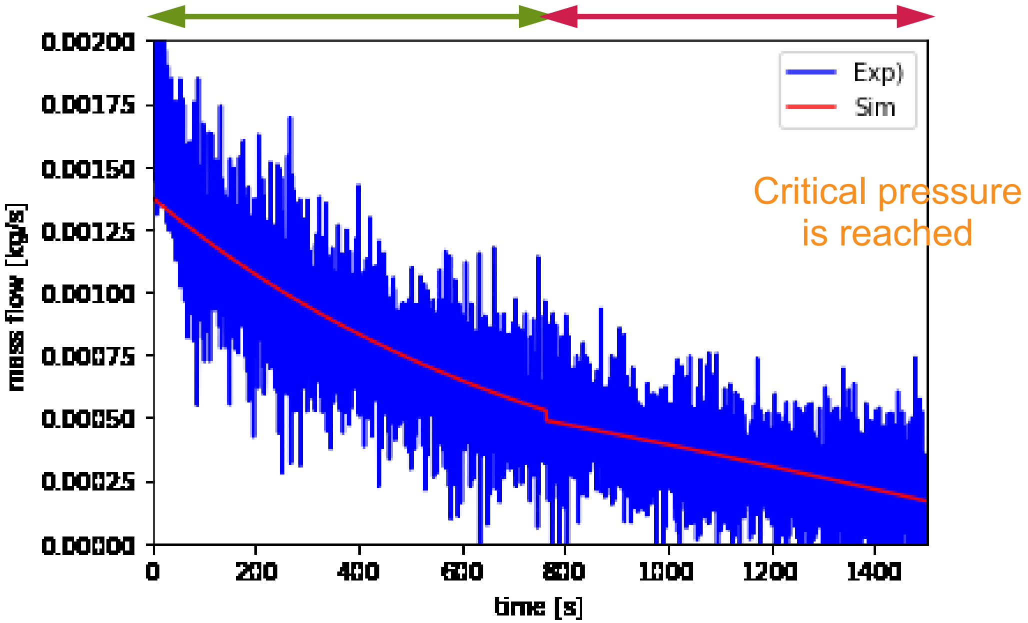
	P	$\dot{m}$	T
P	1	-2.8E-7	6.1E-8
$\dot{m}$	3.7E-7	1	5.1E-8
T	4.1E-8	-6.1E-7	1

Simulated

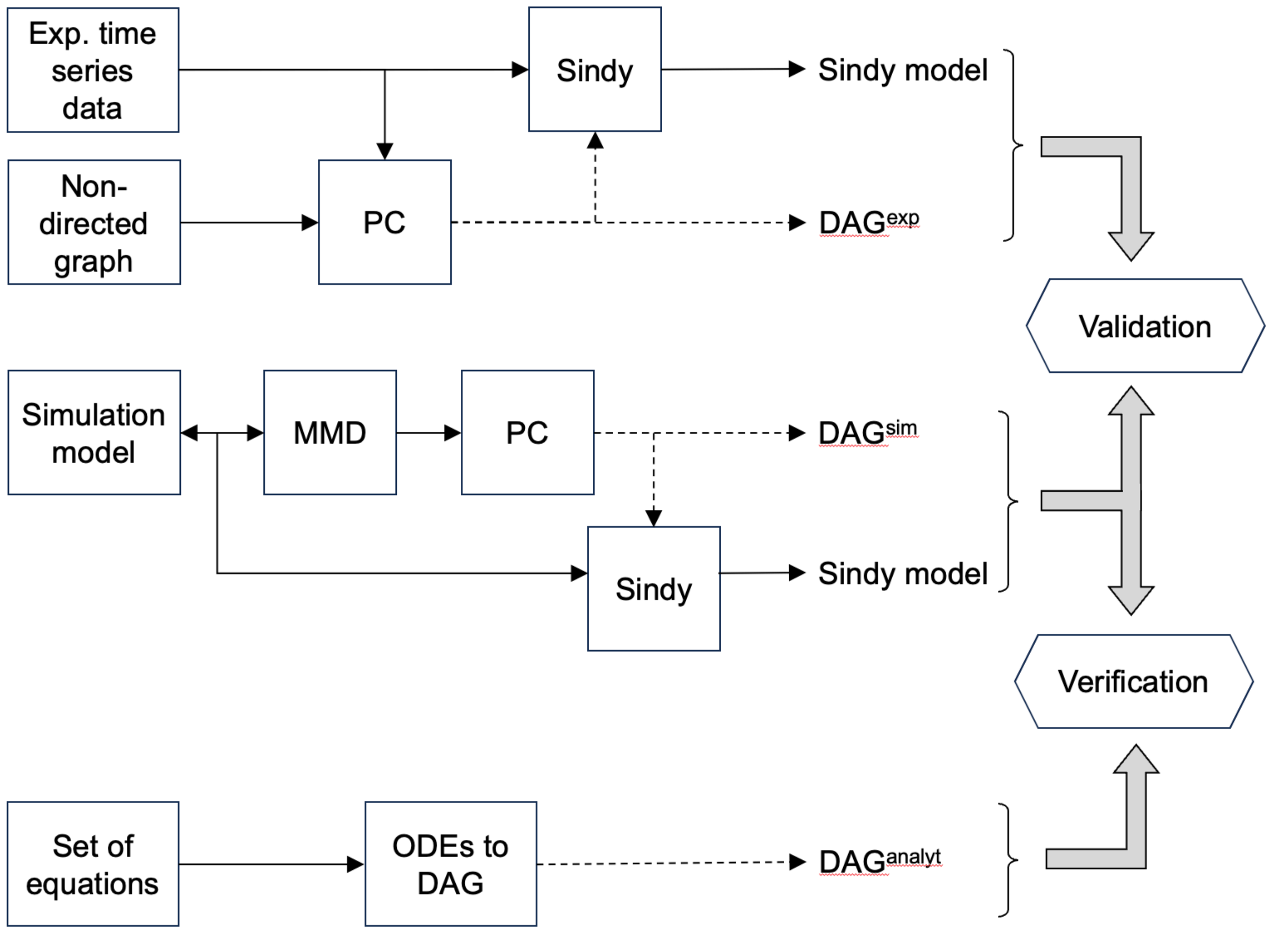
	P	$\dot{m}$
P	1	-2E-7
$\dot{m}$	7.6E-8	1

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





Current direction



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