Applications of Machine Learning in Chemical Engineering

Tutorial 4: Hybrid Modeling (Contd.)

Eng/ Samer Hany

Agenda

HYBRID MODELING (CONTD)

- Common architectures of hybrid models:
  - Physics Informed Neural Networks (PINNs)
  - Direct hybrid models (series, parallel, combined)

ARCHITECTURES OF HYBRID MODELS

Architectures of Hybrid Models

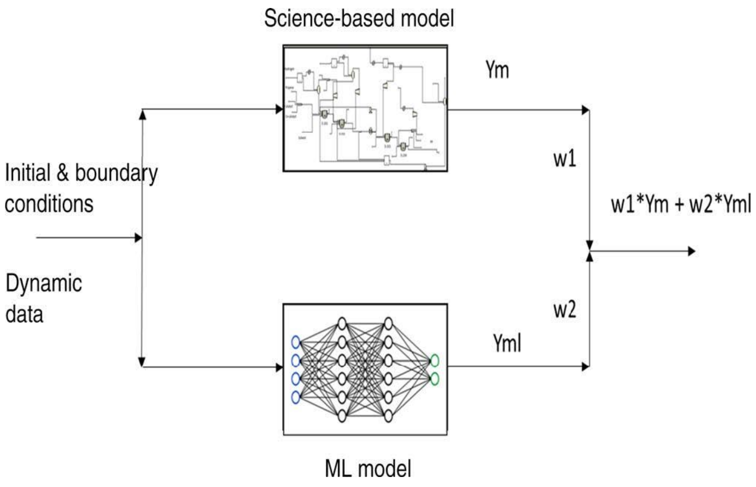
DIRECT HYBRID MODEL

- Combines the output of a first-principles model with the output of a data-based ML model to improve the prediction accuracy.
- These combinations could occur in different configurations:
  - Series
  - Parallel
  - Combined (series–parallel)

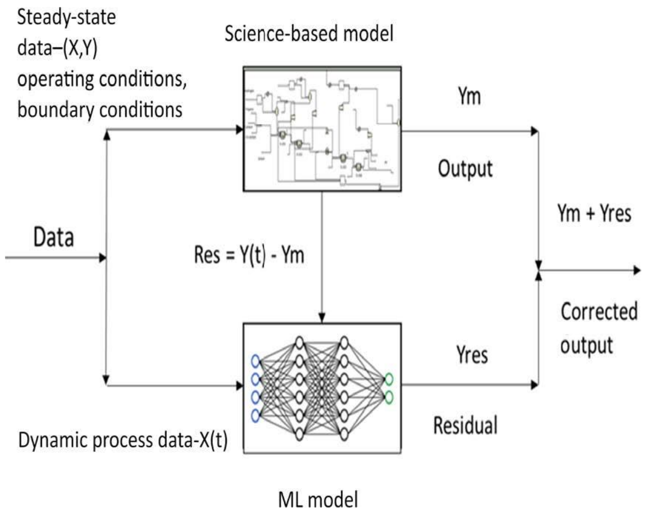
Architectures of Hybrid Models

PARALLEL

Competitive



Cooperative



Architectures of Hybrid Models

PARALLEL

Competitive:

Both models aim for the same prediction, then their outputs are weighted and combined, leveraging each model's strengths for a more robust estimate of the target variable.

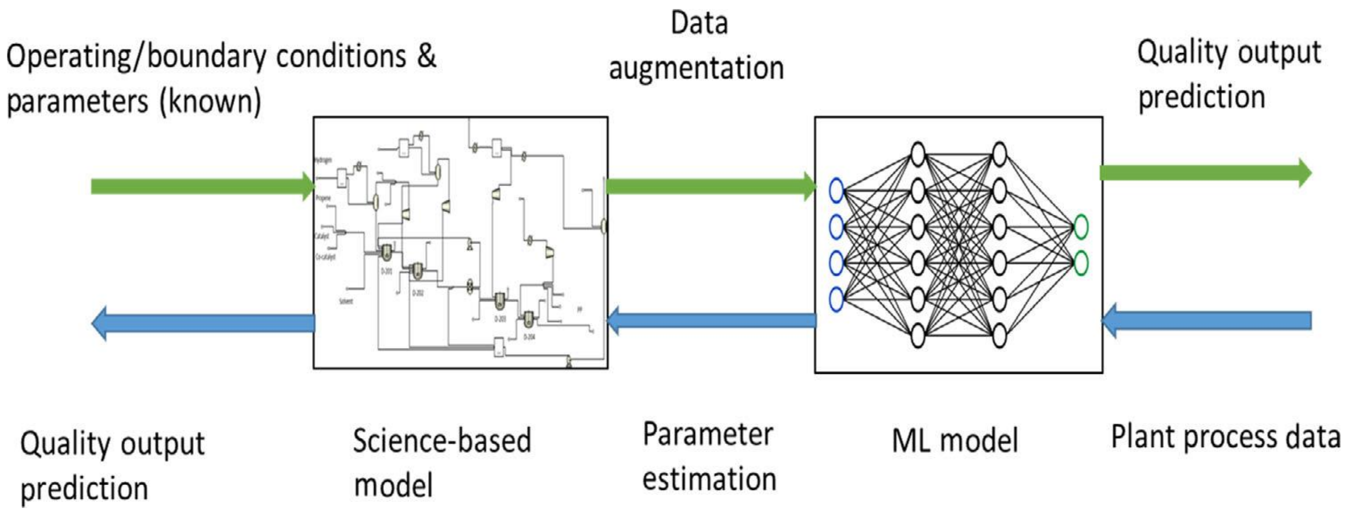
Cooperative:

To improve response accuracy, a data-driven model learns the discrepancies between a mechanistic model's predictions and historical data. This captures real-world effects not explicitly modeled. Predictions from both models are then fused (addition, multiplication, etc.) to create a final, potentially more comprehensive response.

The parallel structure exhibits limitations in extrapolating beyond the training domain. However, its performance improves when the system comprises uncoupled effects, offering advantages in specific contexts.

Architectures of Hybrid Models

SERIAL



Architectures of Hybrid Models

SERIAL: BB→WB

- The **White-Box (WB)** sub-model typically incorporates fundamental conservation laws governing the system. These laws often include mass balance, momentum balance, and energy balance.
- In the context of chemical systems, the **Black-Box (BB)** sub-model often represents empirical relationships that capture various phenomena. These relationships might include:
  - **Reaction kinetics:** Rates of chemical reactions.
  - **Convective and conductive transfer parameters:** Parameters describing the movement of mass and heat within the system (e.g., dispersion and diffusion coefficients).
  - **Thermodynamic parameters:** Properties related to the energy state of the system (e.g., vapor pressure, solubility, physical properties).
  - **Friction factor:** A parameter influencing pressure drop in fluids flowing through pipes or channels.

Architectures of Hybrid Models

SERIAL: WB→BB

- **Simulation Data for BB Training:** In the absence of sufficient real-world data points for training the **black-box (BB)** model, an accurate enough **white-box (WB)** model can be leveraged to generate a training dataset through simulation results.

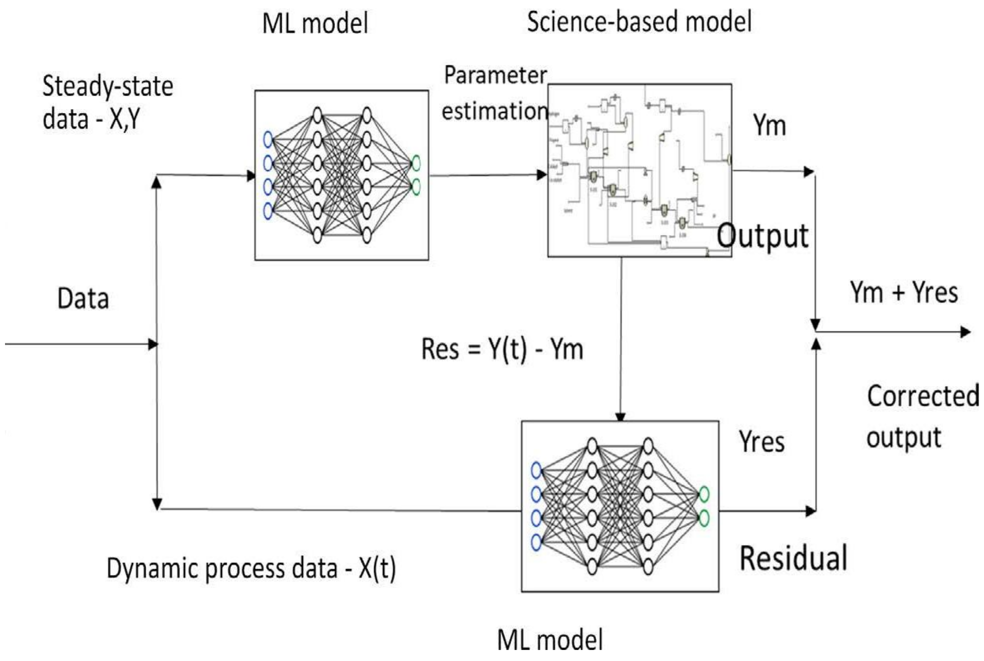
- **Hybridization for Speed:** When computational demands for the **white-box (WB)** model are prohibitive for time-critical applications like adaptive control or optimization, a hybrid approach can be employed by combining the **WB model** with a **black-box (BB)** model, resulting in a computationally more efficient solution.

- **Parallel Estimation Improvement:** estimates from a **white-box (WB)** model and process variables can be used to train a **black-box (BB)** model, similar to a parallel configuration, for improved overall estimation accuracy.

Architectures of Hybrid Models

MIXED STRUCTURE

Based on the system complexity, a mix of series and parallel configurations can be constructed to improve the overall model predictions.



Thank you

- Eng/ Samer Hany
  samer.hany@eng.cu.edu.eg
- Eng/ Nada Ashraf
  bakrynada8@eng.cu.edu.eg