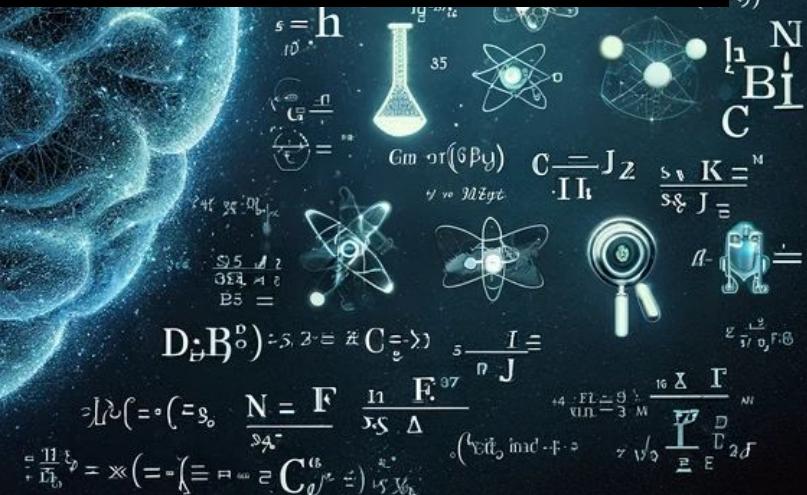
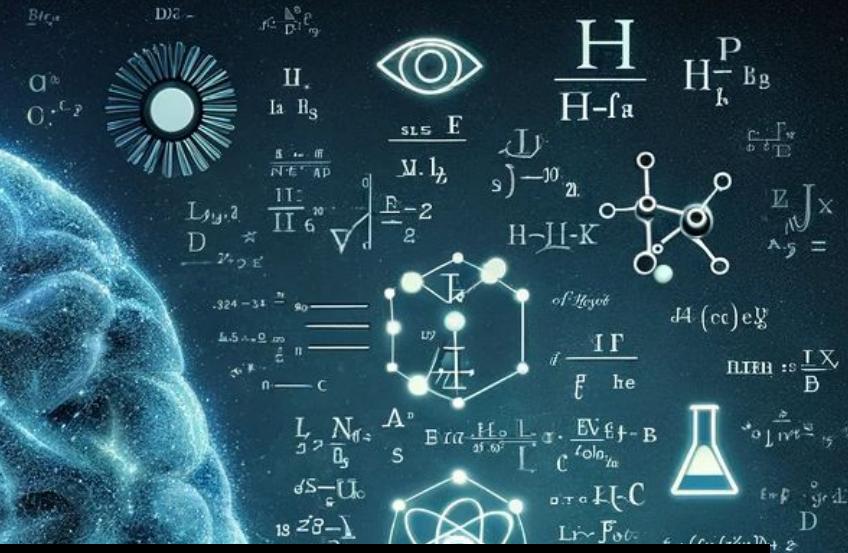
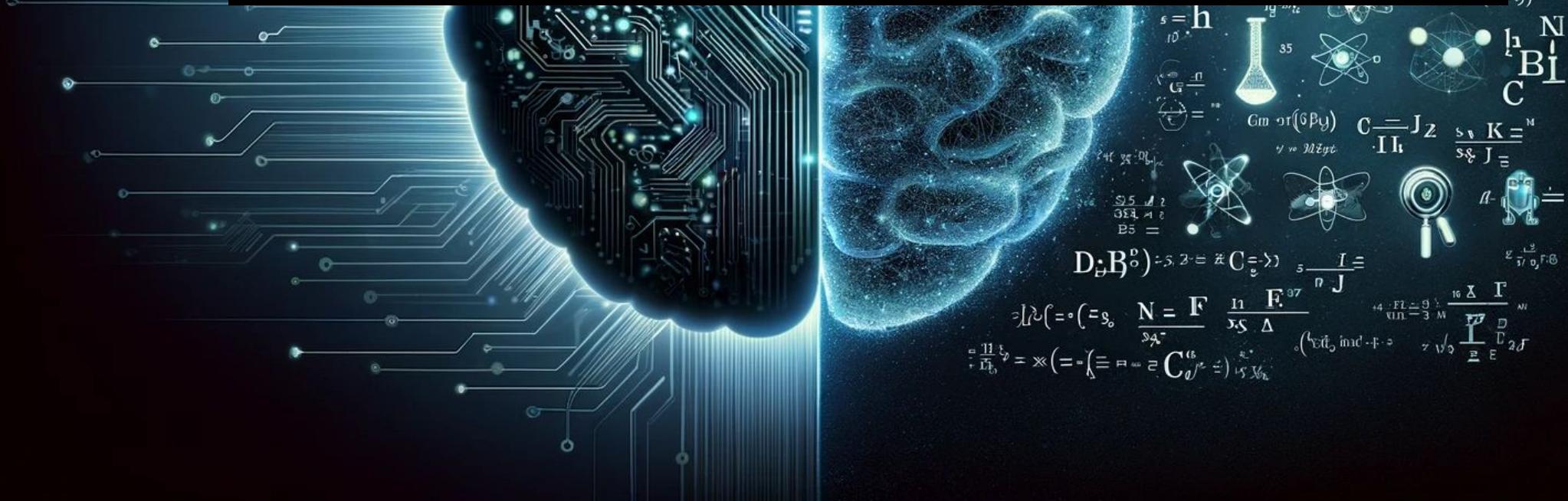


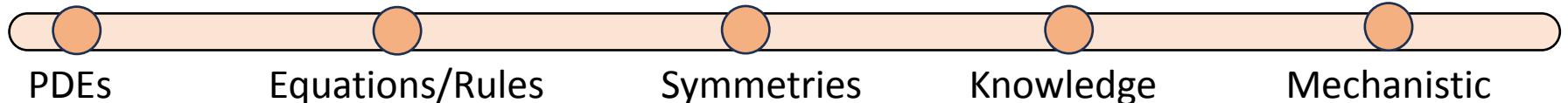


# KGML for Aquatic Sciences



# Organizing KGML Research: A Multi-Dimensional View

## Format Used for Representing Knowledge



$$\frac{\partial u(x, t)}{\partial t} + \mathcal{N}(\lambda, u(x, t)) = 0$$

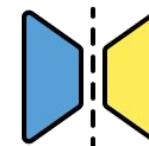
Navier Stokes Equation,  
Wave Equation,  
Schrodinger Equation, ...

PINNs: Raissi et al. 2019

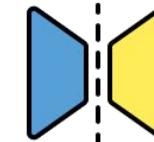
$$\frac{\partial u}{\partial x} \propto \frac{\partial^2 u}{\partial x^2}$$

$$a < \frac{\partial u}{\partial x} < b$$

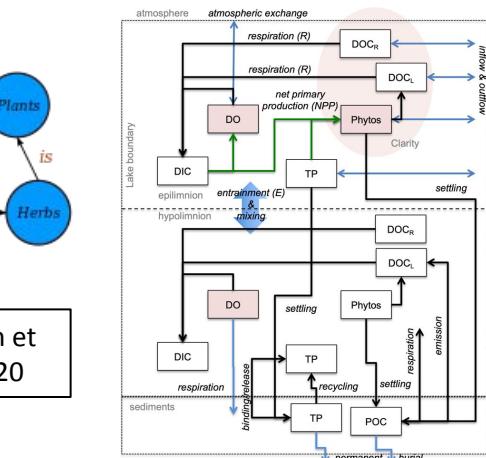
PGNN: Karpatne et al. 2017  
PGRNN: Jia et al. 2019  
PGA-LSTM: Daw et al. 2020



Symmetries



Knowledge Graphs



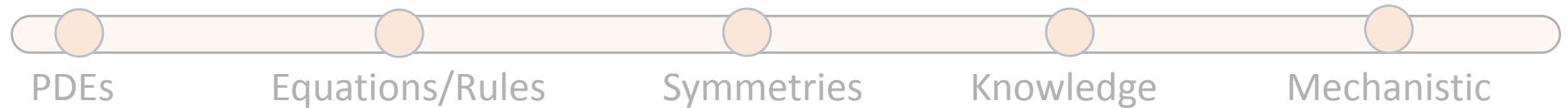
Mechanistic Models

Zareian et al. 2020

MCL: Ladwig et al. 2024  
dPL: Shen et al. 2023

# Organizing KGML Research: A Multi-Dimensional View

Format Used for Representing Knowledge

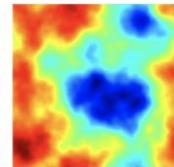


Type of Scientific Knowledge

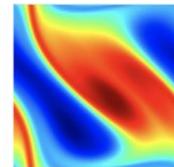


Example: Solving *known* PDEs

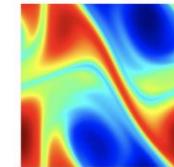
Initial Vorticity



$t=15$



$t=20$



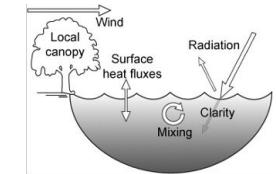
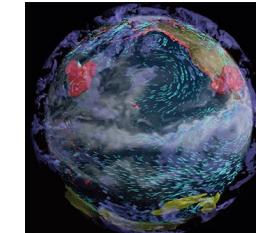
Navier Stokes Eq., Heat Eq., Wave Eq., Schrodinger Eq., ...

Primary Objective: Improve Computational Efficiency

**PINNs:** Raissi et al. 2019, **DeepONets:** Lu et al. 2021, **FNOs:** Li et al. 2021

Example: Modeling complex dynamical systems with missing/imperfect physics

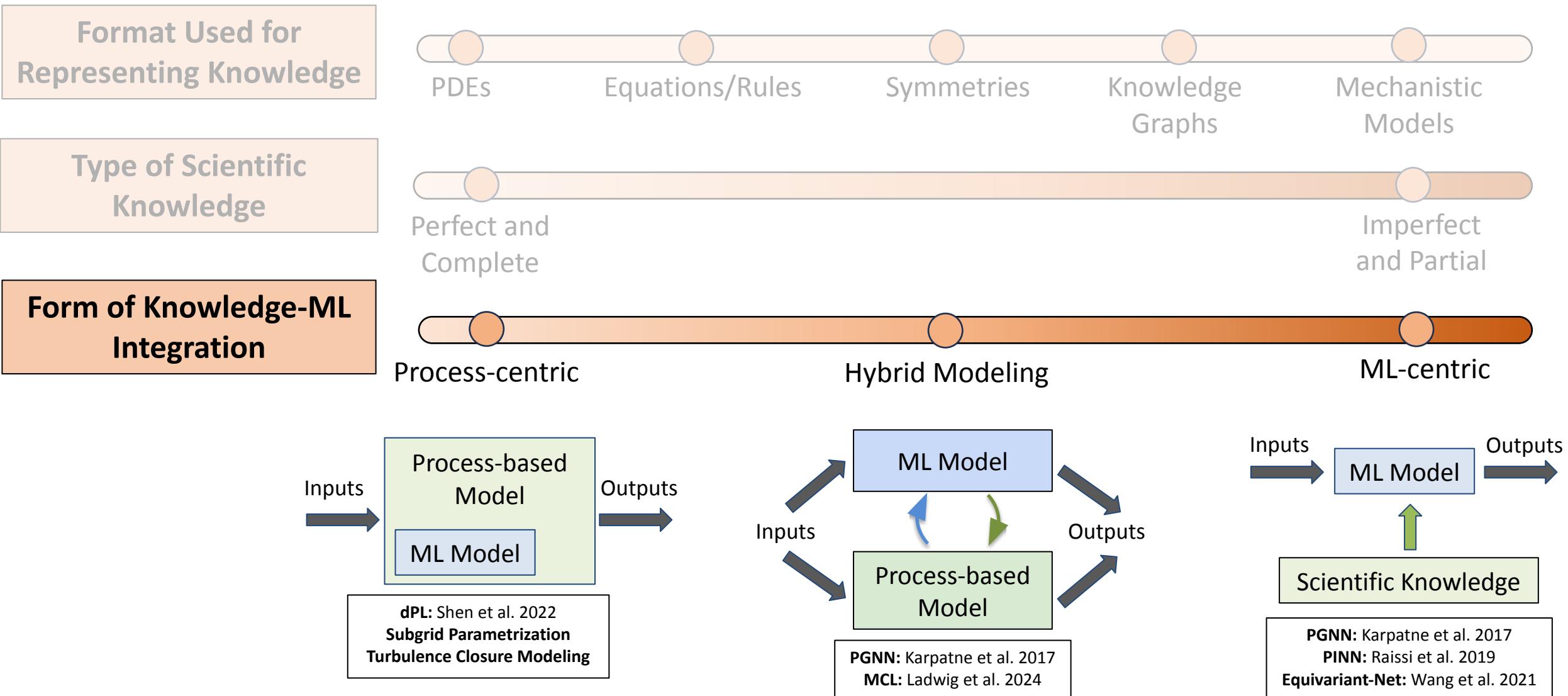
Modeling Turbulence,  
Multi-phase Flow,  
Cloud Physics, Aerosols, ...



Additional Objective: Improve Modeling Accuracy

**PGNN:** Karpatne et al. 2017, **PGRNN:** Jia et al. 2019, **PGA-LSTM:** Daw et al. 2020

# Organizing KGML Research: A Multi-Dimensional View



# Organizing KGML Research: A Multi-Dimensional View

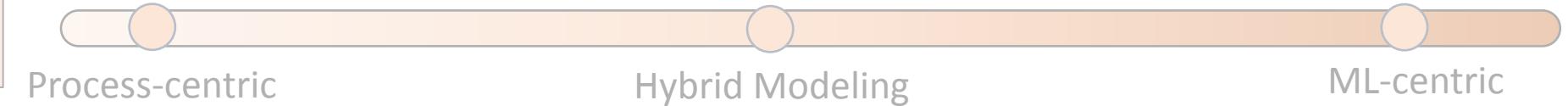
Format Used for Representing Knowledge



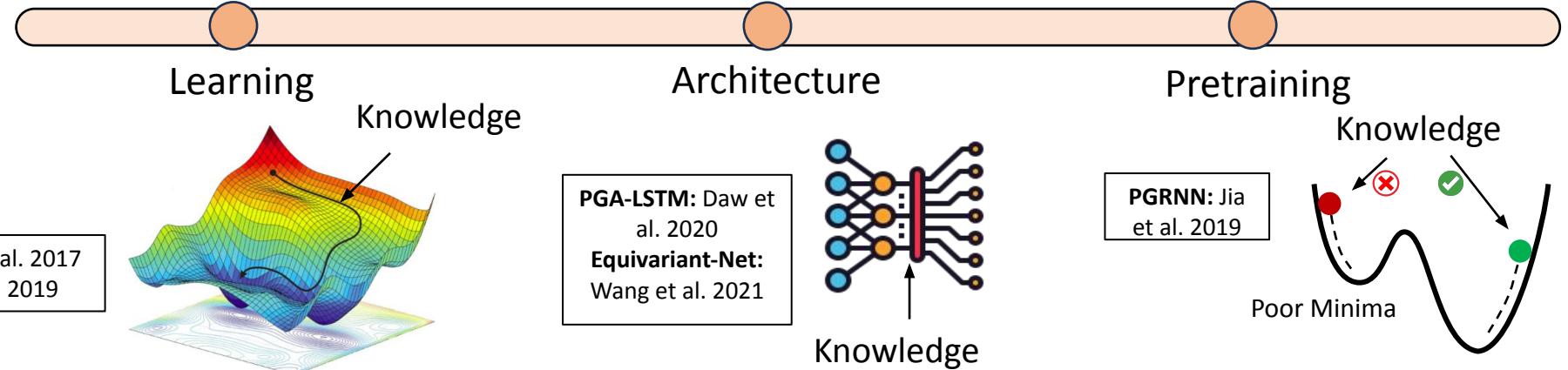
Type of Scientific Knowledge



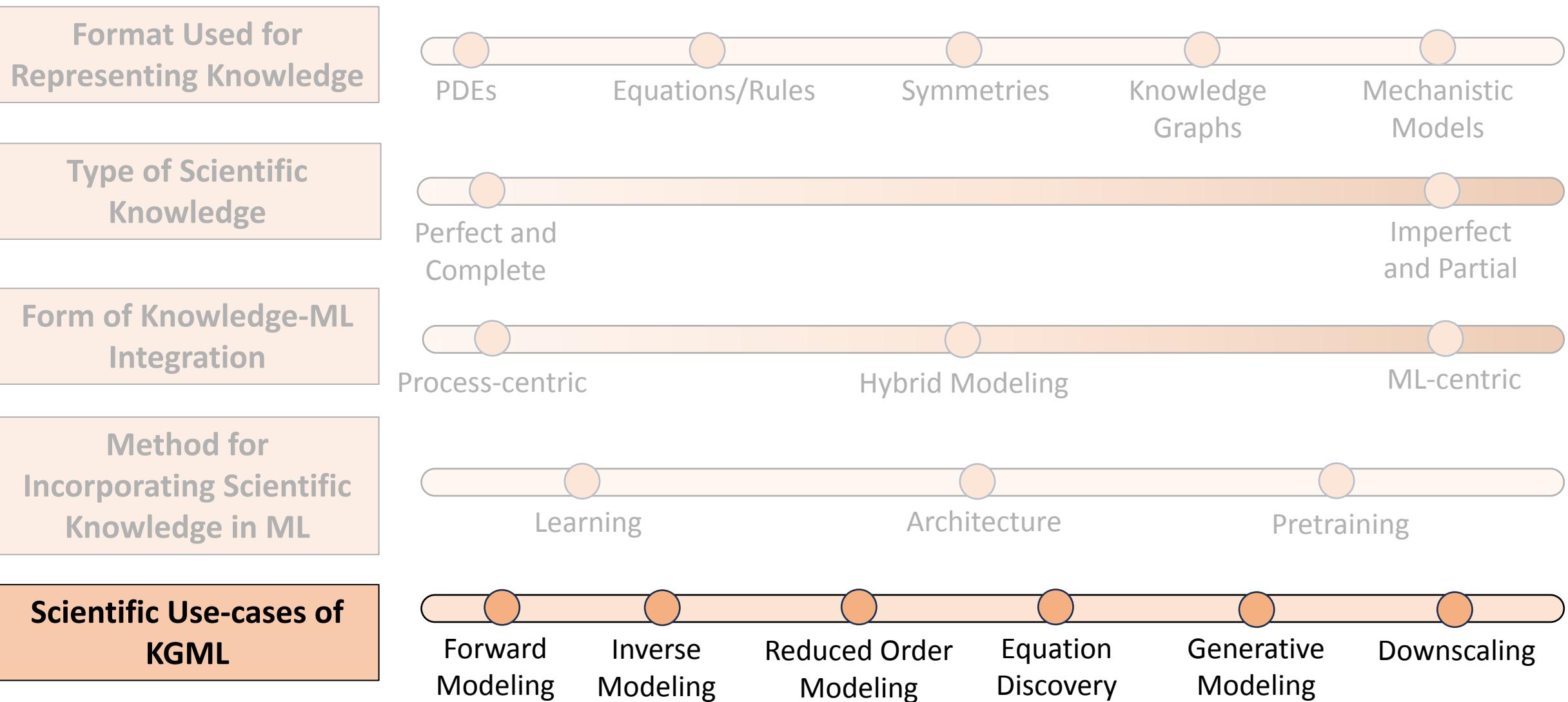
Form of Knowledge-ML Integration



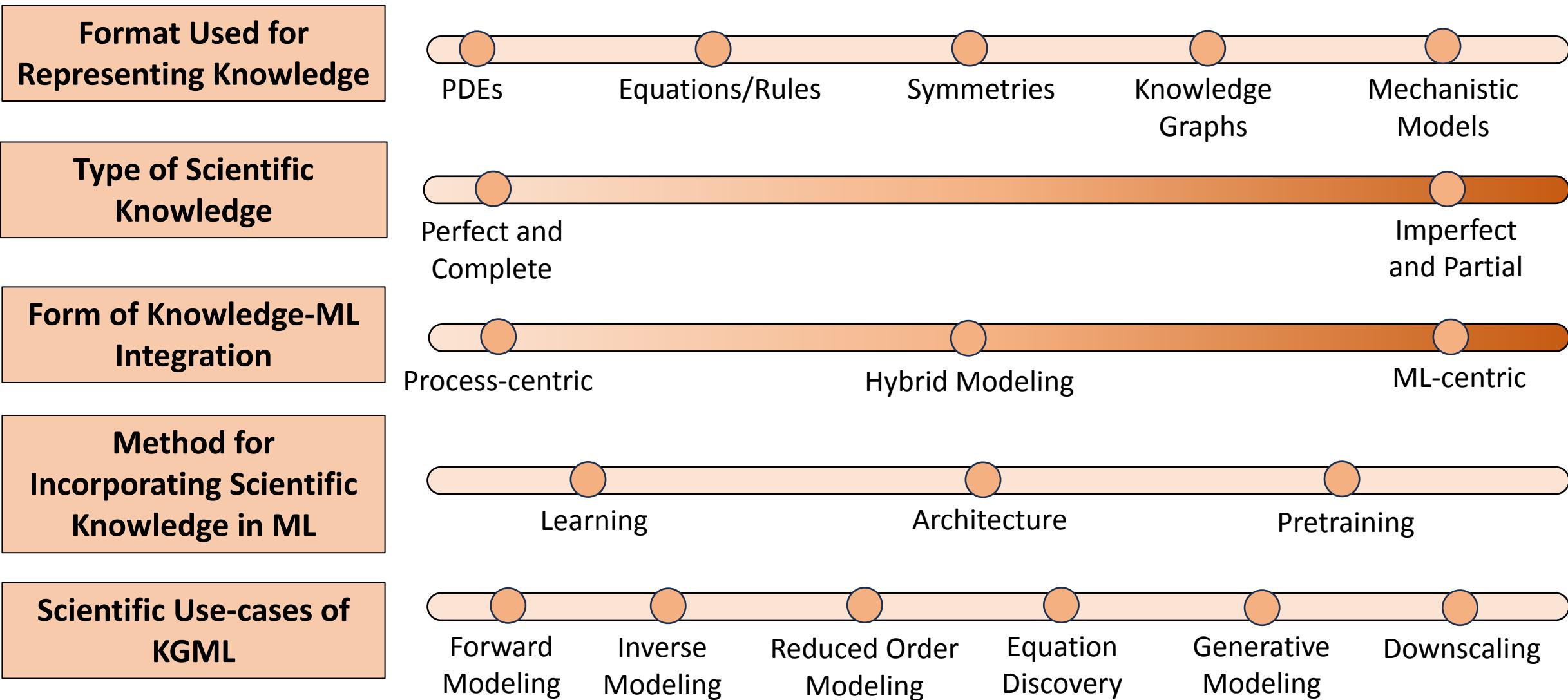
Method for Incorporating Scientific Knowledge in ML



# Organizing KGML Research: A Multi-Dimensional View



# Organizing KGML Research: A Multi-Dimensional View



# KGML Use Cases

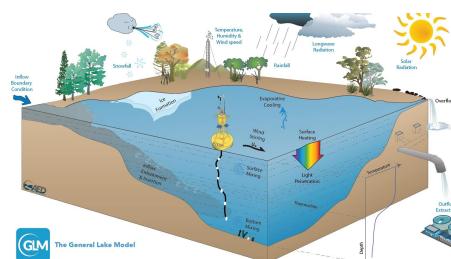
## Lake Temperature Modeling

**Goal:** Predicting the temperature of the lake.

- Use *imperfect* and *partial* knowledge as loss functions
- Use *simulation data* for pre-training and *observational data* for finetuning

Physics-guided NNs  
**(PGNNs):** Daw et al. 2017

Physics-guided RNNs  
**(PGRNNs):** Jia et al. 2019



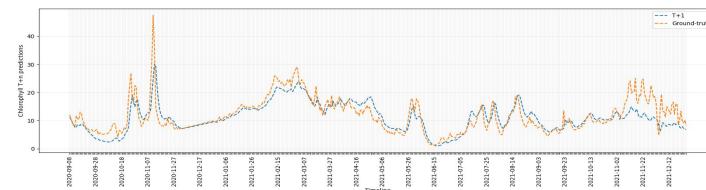
## Chlorophyll-a Prediction

**Goal:** Predicting the chlorophyll-a content of water bodies.

- Sparse observed data for chlorophyll
- Interested in predicting the blooms.



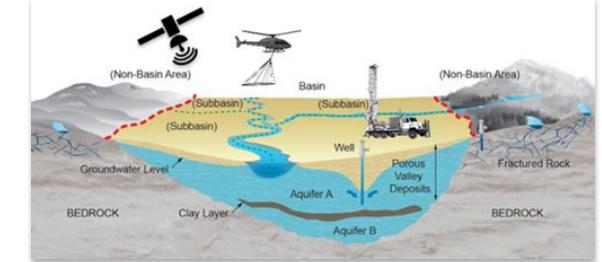
LSTM based Chl-a Prediction: Cen et al. 2022



## River-basin Characterization

**Goal:** Predict basin characteristics of rivers.

- Extract system characteristics from driver and response data.



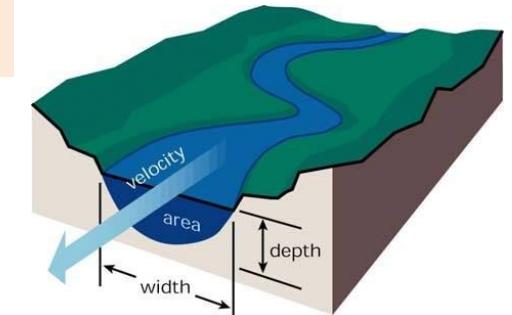
Knowledge-guided Self-supervised  
**(KGSSL):** Ghosh et al. 2022

Uncertainty Quantification  
**(UQ-KGSSL):** Sharma et al. 2022

## Streamflow Forecasting

**Goal:** Predict the stream flow of rivers.

- Use river-network data (graph) and the knowledge of thermodynamics to improve predictions.

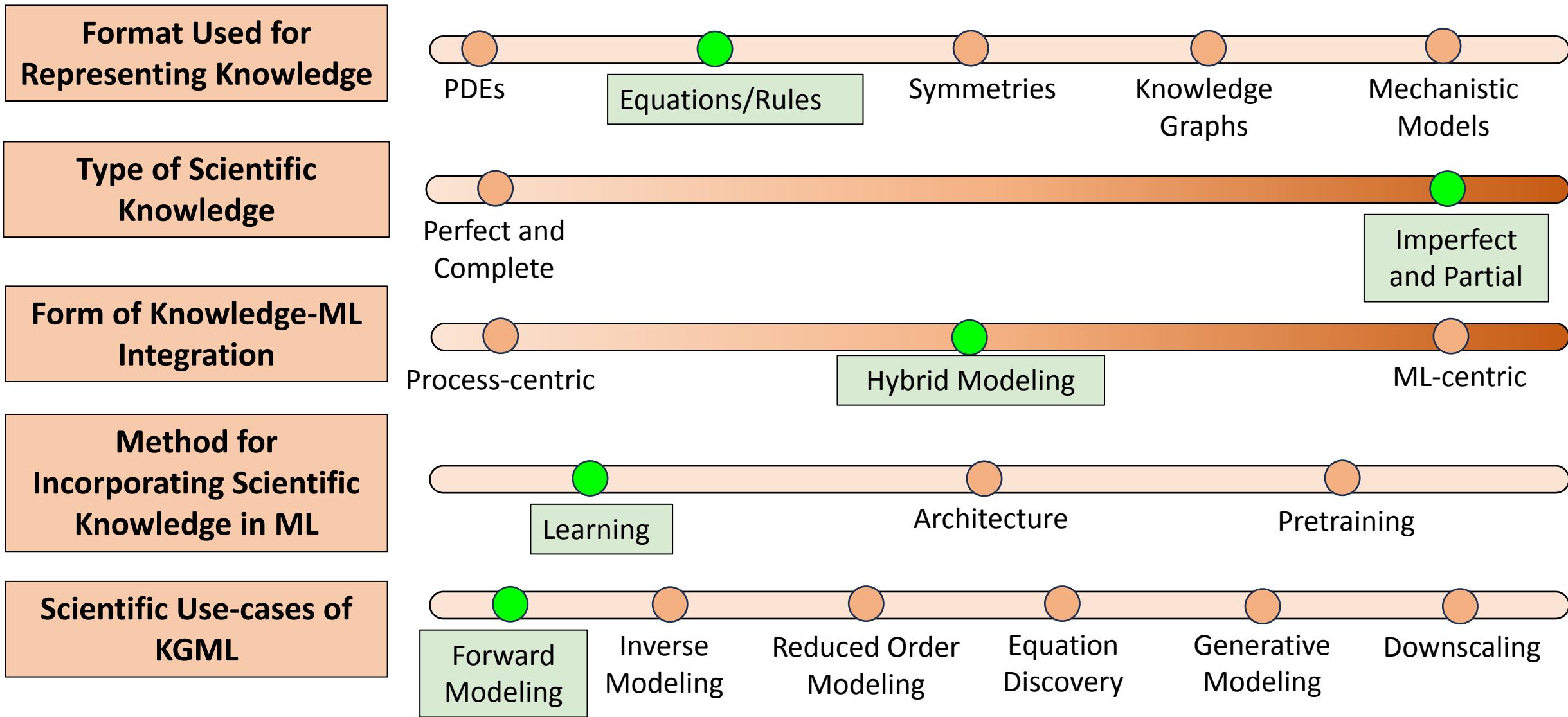


Physics-guided Recurrent Graph Model (PGRGnN): Jia et al. 2020

KGML for Multi-scale Process and Data Assimilation: Kumar et al. 2023

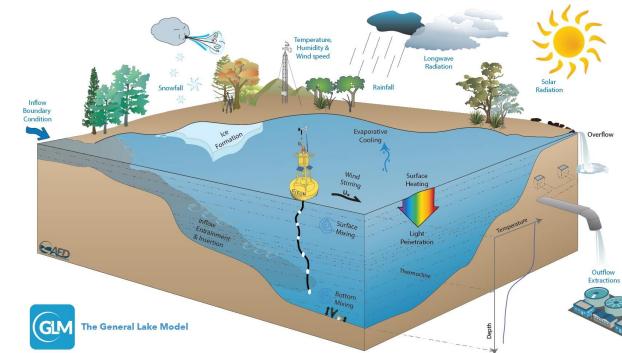
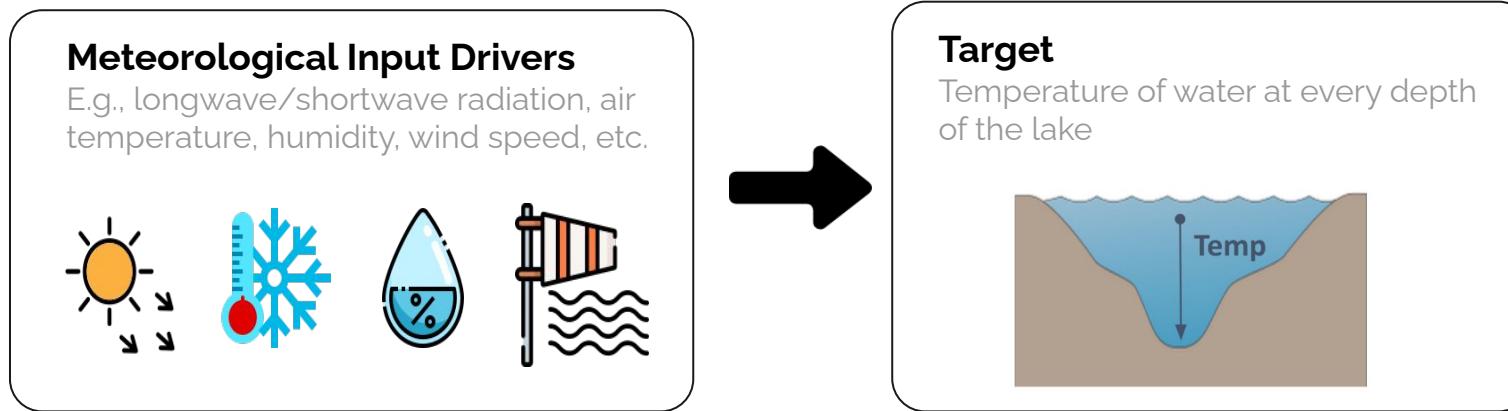
# Use Case 1: Lake Temperature Modeling

# Organizing KGML Research: A Multi-Dimensional View

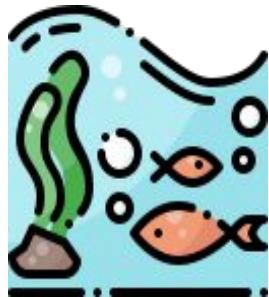


# Lake Temperature Modeling

## 1D Model of Temperature



## Motivation



Growth and survival of fisheries

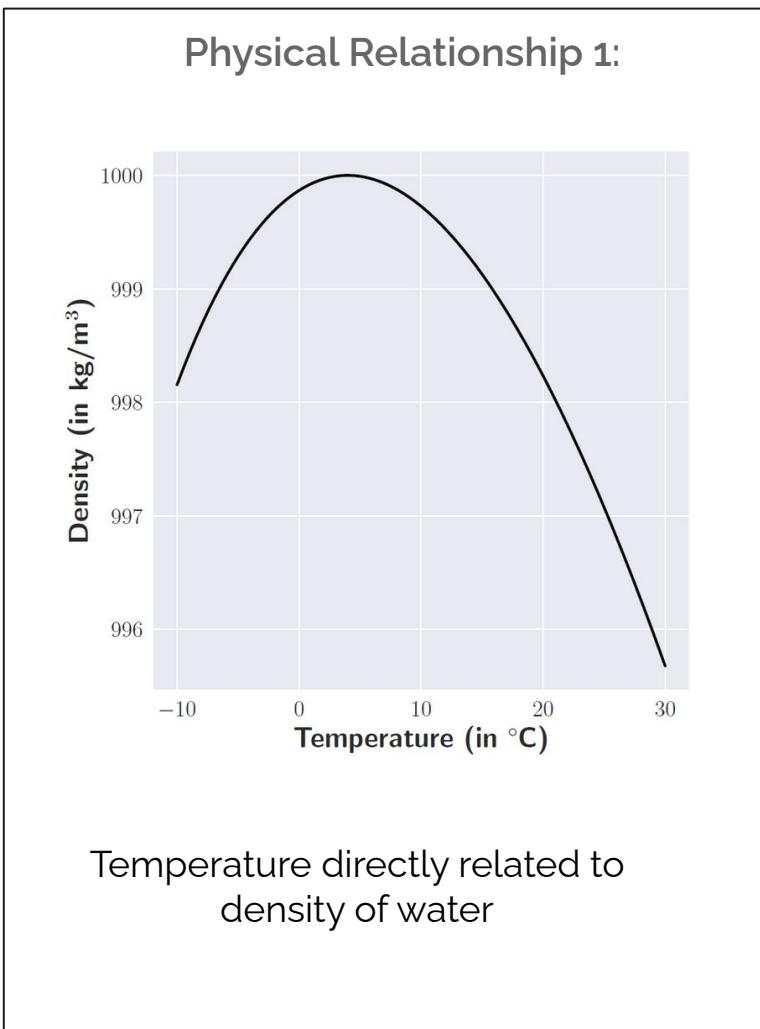


Harmful Algal Blooms

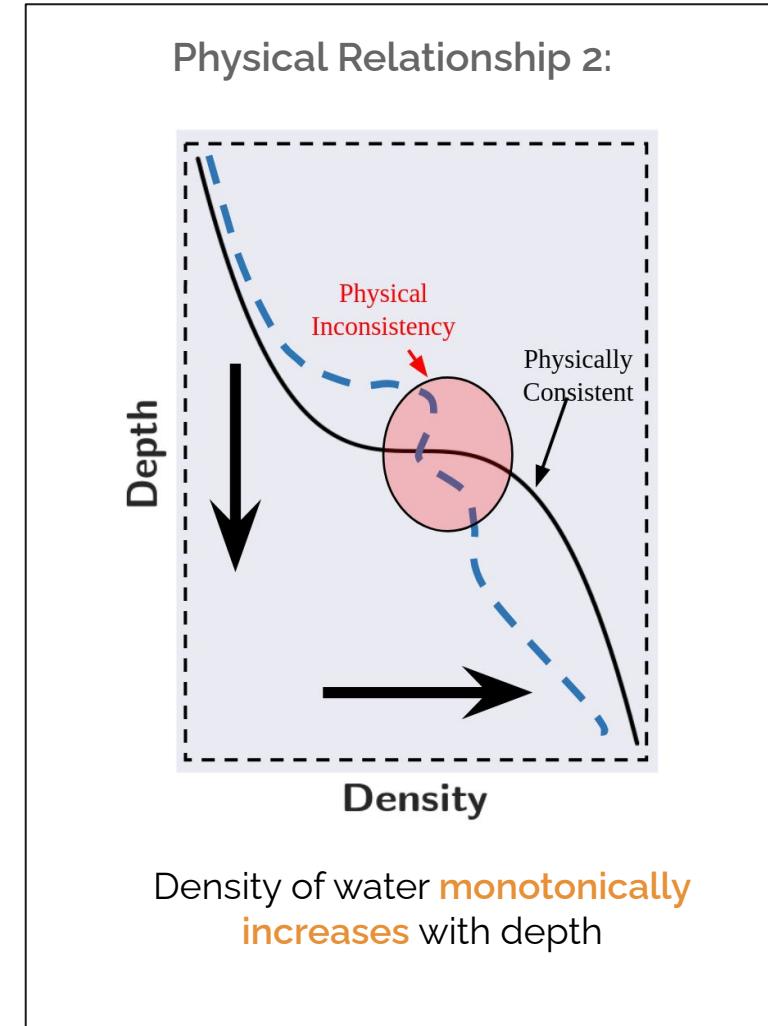
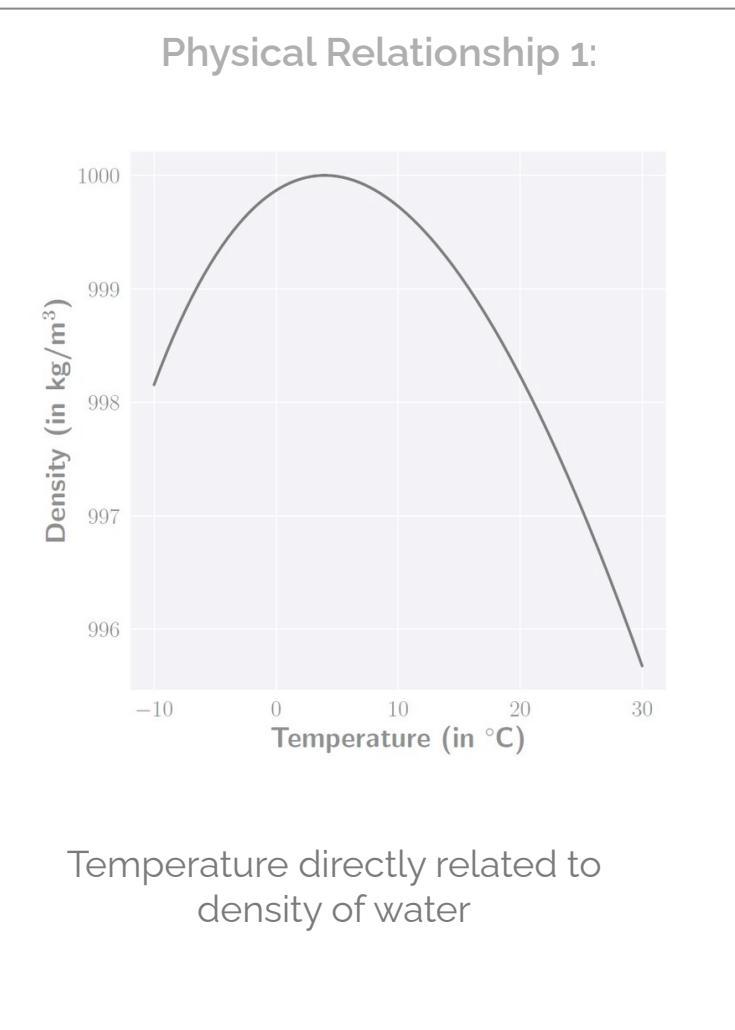


Chemical Constituents:  
O<sub>2</sub>, C, N

# Physical Relationships of Temperature



# Physical Relationships of Temperature

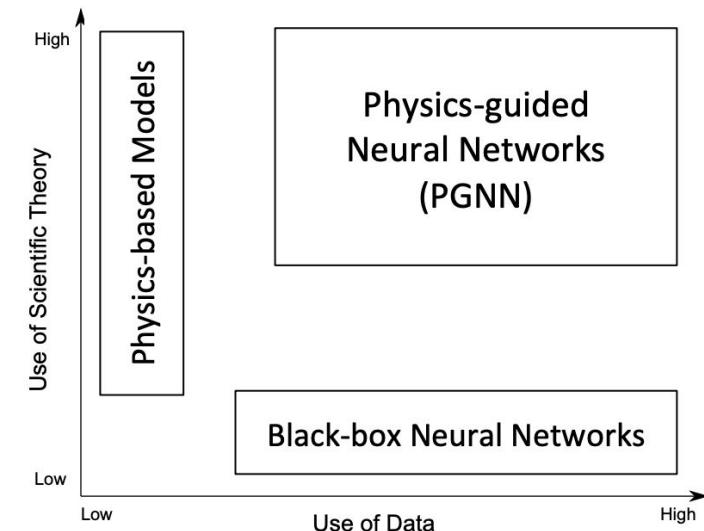


# Physics-guided Neural Networks (PGNN)

The physics supervision is enforced as a soft constraint where the model is penalized when the predictions of the model violate the physics constraint.

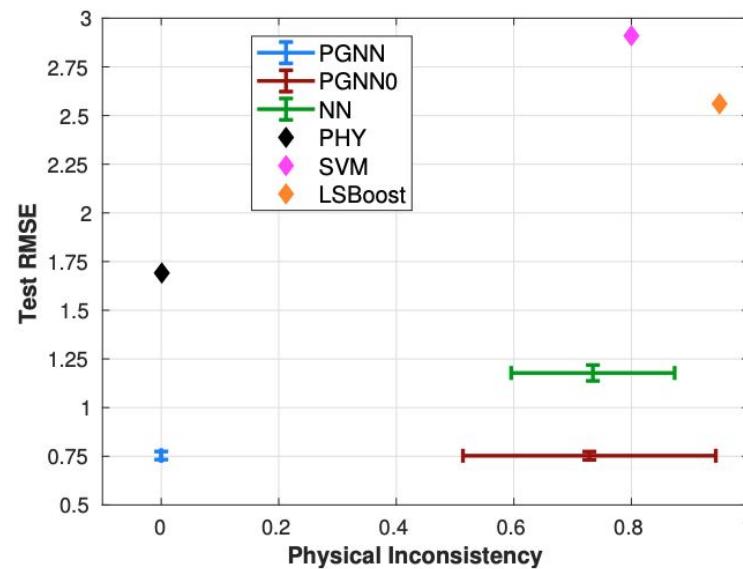


- **Easy to use:** Constraints can be easily incorporated as physics loss functions.
  - **Unsupervised:** Physics loss functions can be evaluated on unlabeled data.

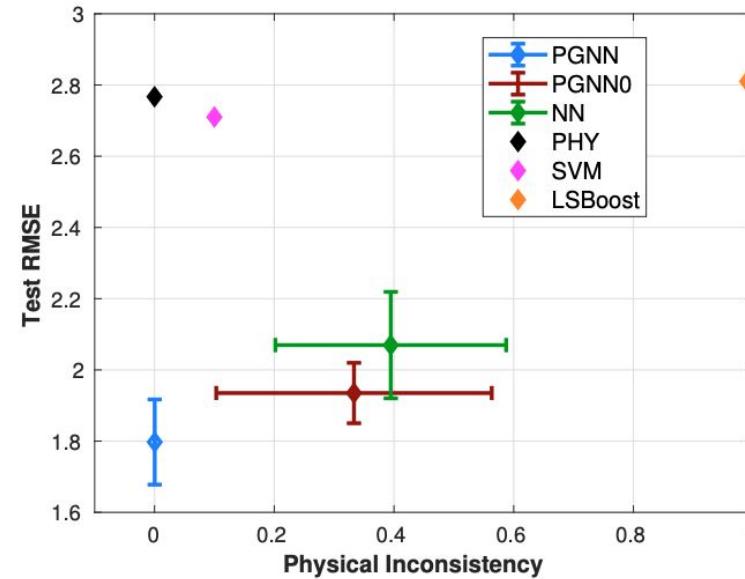


# PGNN shows improved generalization

Results on two different lakes: Lake Mille Lacs and Lake Mendota



(a) Results on Mille Lacs Lake



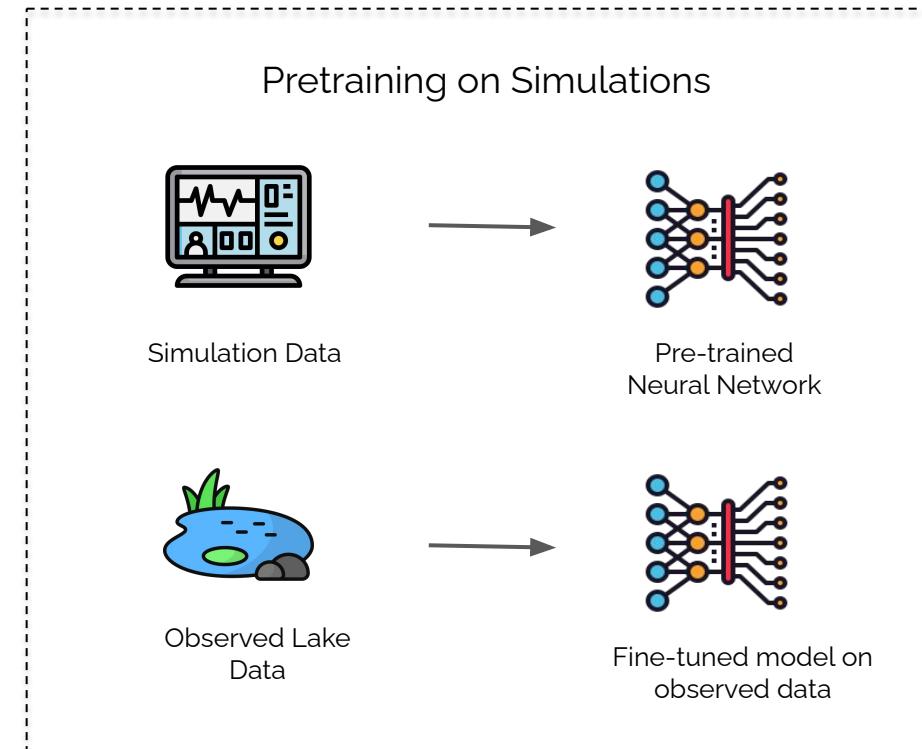
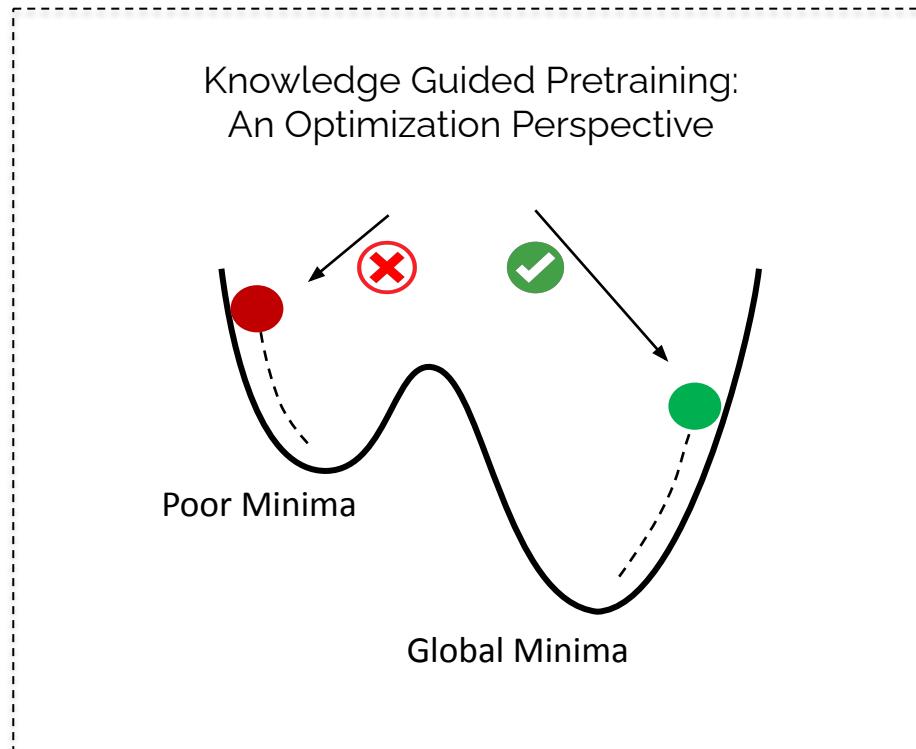
(b) Results on Lake Mendota



PGNN consistently outperforms the other baselines for both lakes showing better Test RMSE and Physics Consistency.

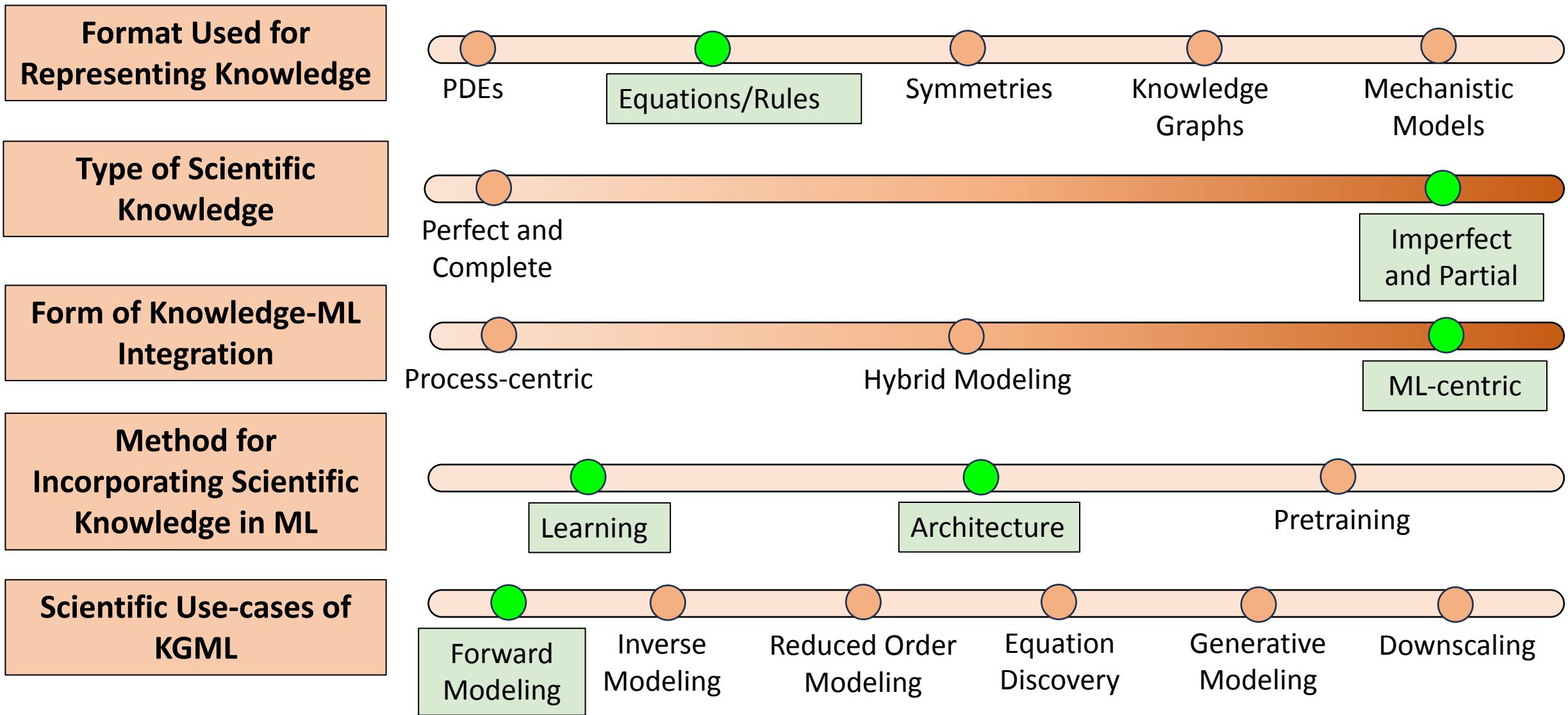
# Pretraining on Simulation Lakes

Simulation Data from the different lakes can be used to pretrain the RNN model. This will serve as a “better” initialization.



# Use Case 2: KGML with Uncertainty Quantification

# Organizing KGML Research: A Multi-Dimensional View

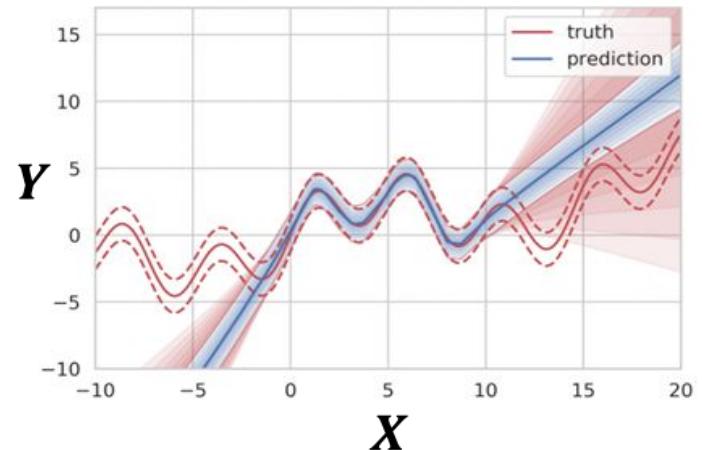


# Uncertainty Quantification

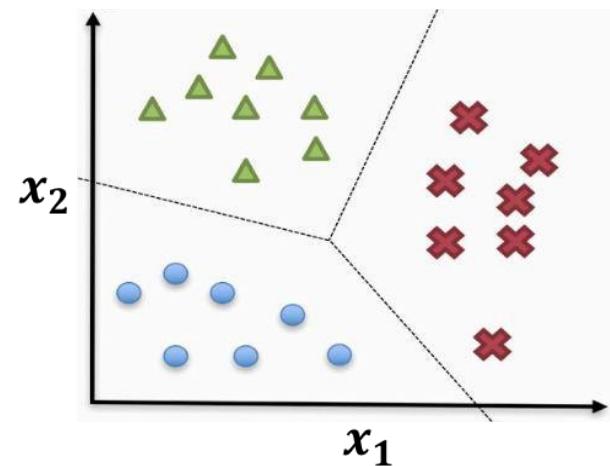


Generate a **distribution** over the predictions rather than point estimates.

- **Regression:** Predict the variance along with the output mean.
- **Classification:** Predict the confidence along with the output labels.

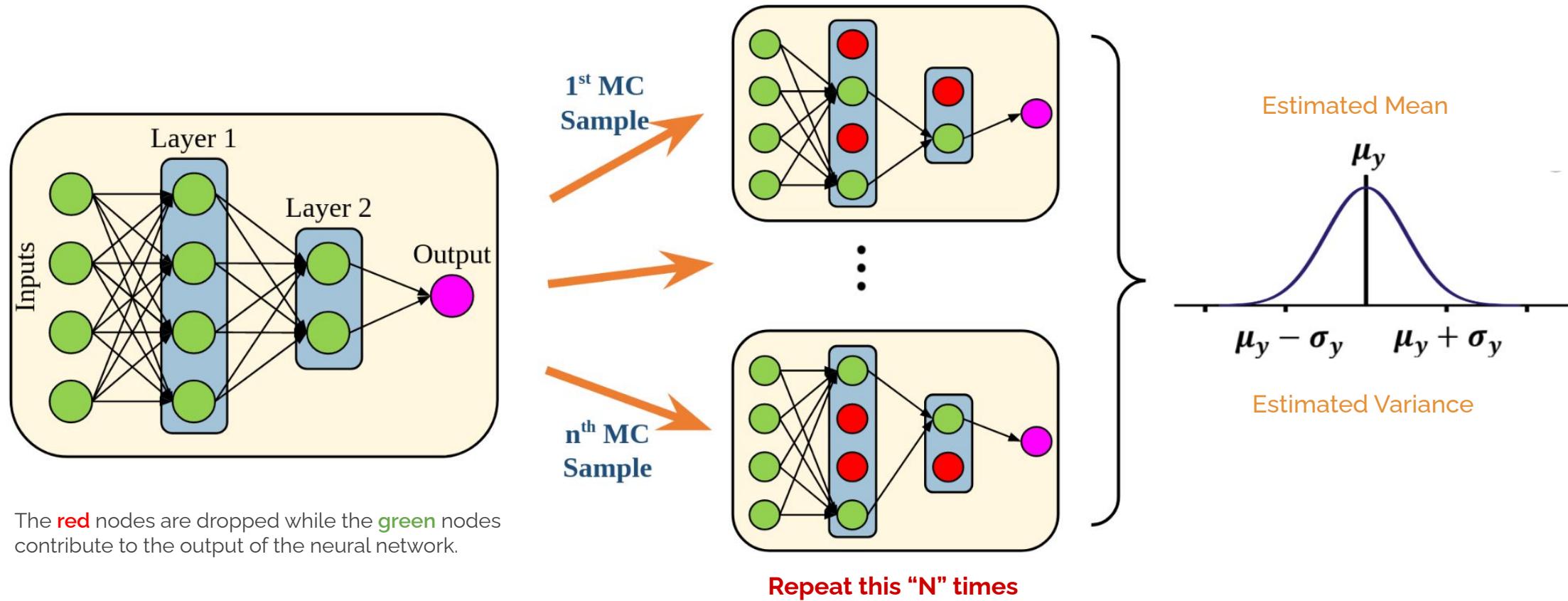


Aims to quantify the **robustness** of the ML models by assessing prediction reliability.

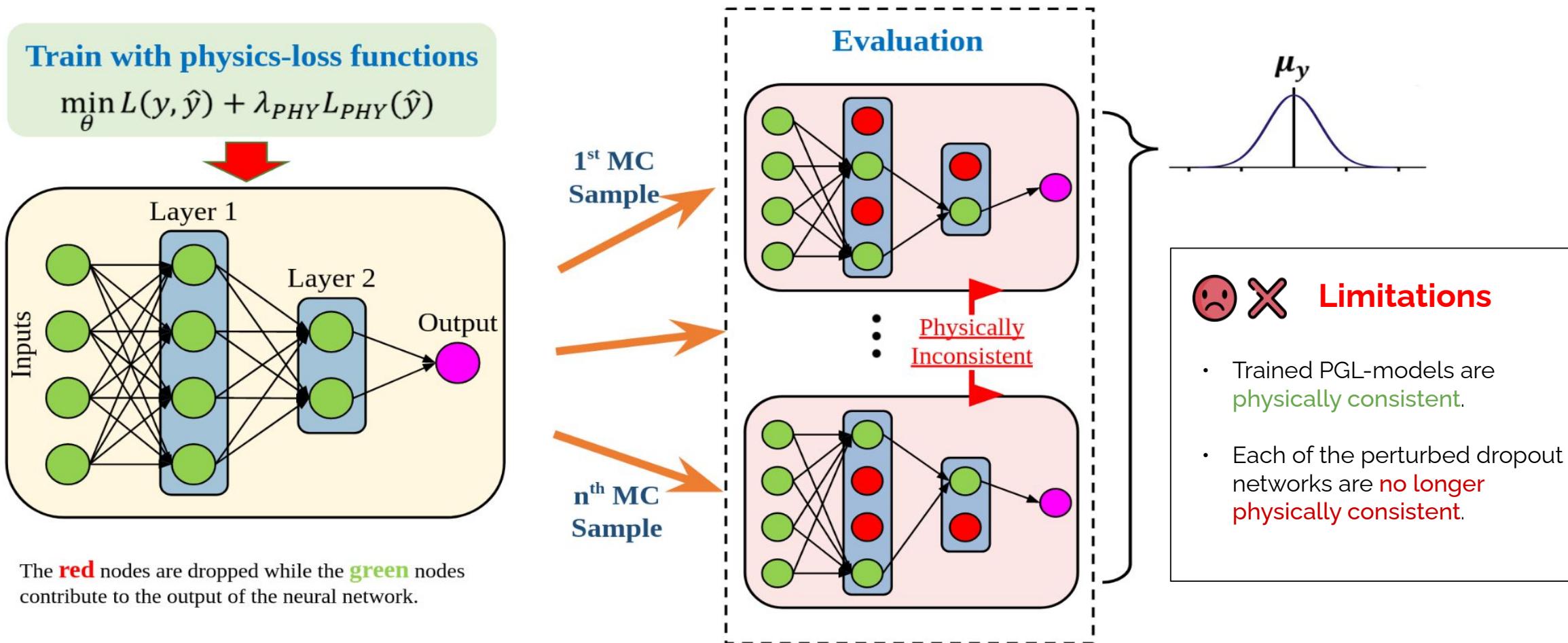


# Uncertainty Quantification with MC Dropout

A schematic representation of using Dropouts to estimate uncertainty.

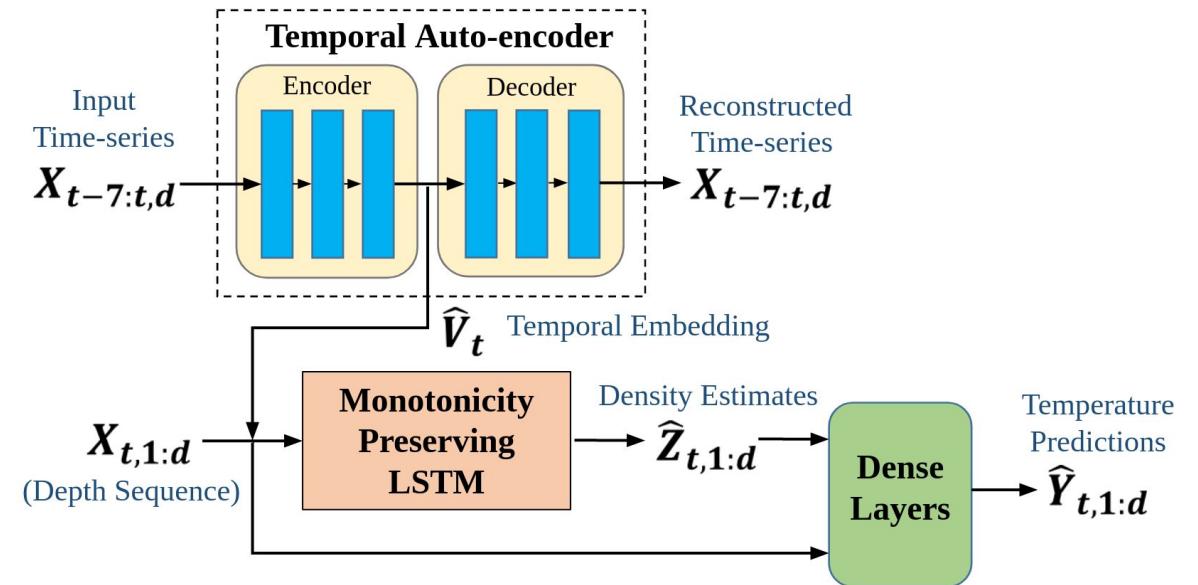


# Approach 1: Dropouts with Physics-based Loss

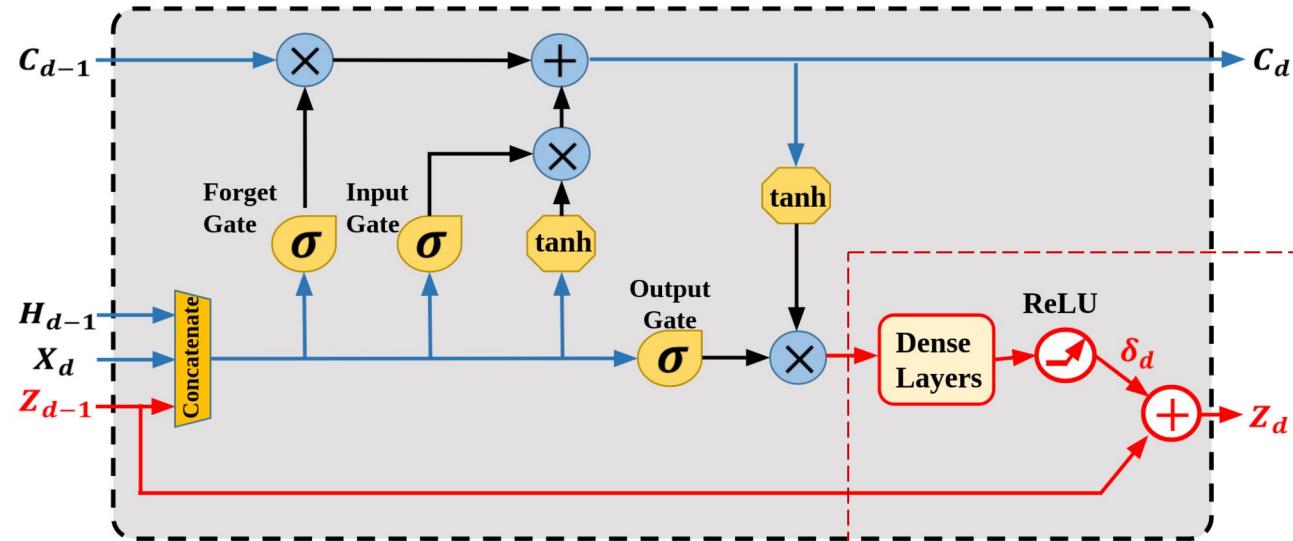


# Proposed PGA-LSTM Framework

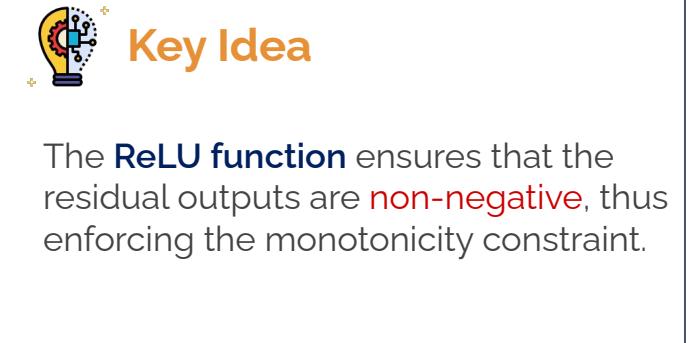
- **Temporal Autoencoder:** Encodes the input time series to obtain a temporal embedding.
- **Monotonicity Preserving LSTM:** Enforces the monotonicity constraint on the density predictions.
- **Dense Layers:** Takes the density estimates and the input drivers to predict temperature.



# Monotonicity Preserving LSTM



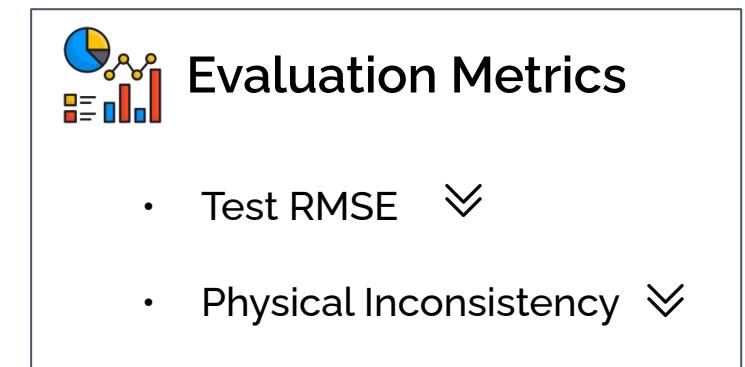
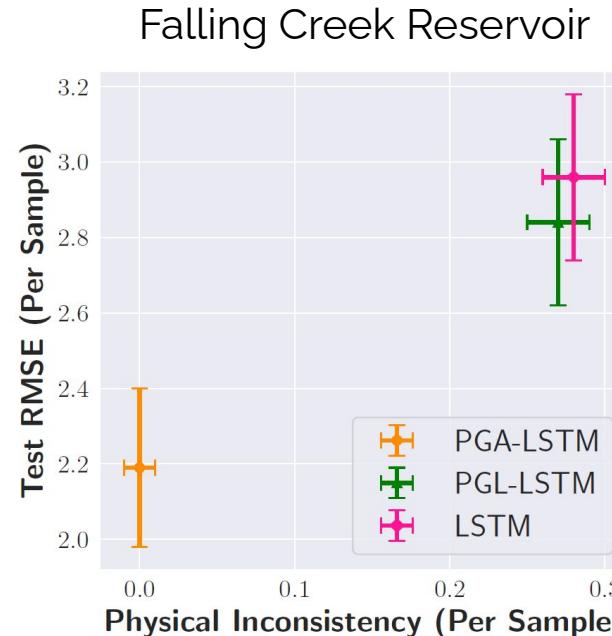
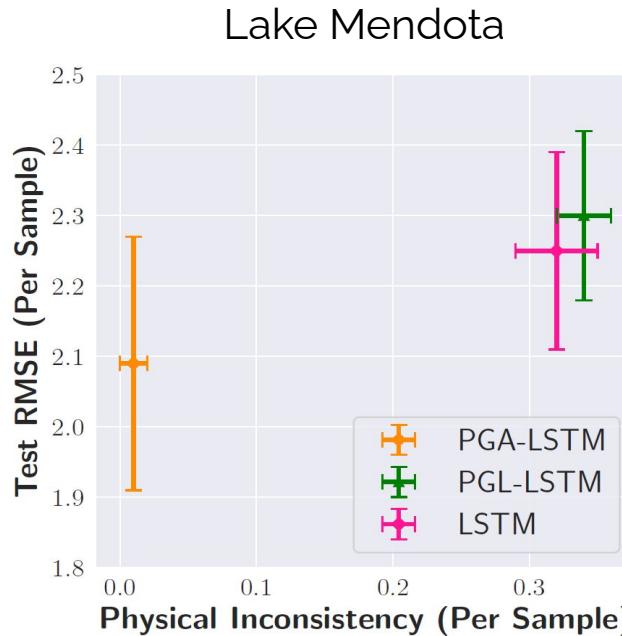
Components in red represent the novel physics-informed innovations in LSTM



The monotonicity preserving LSTM:

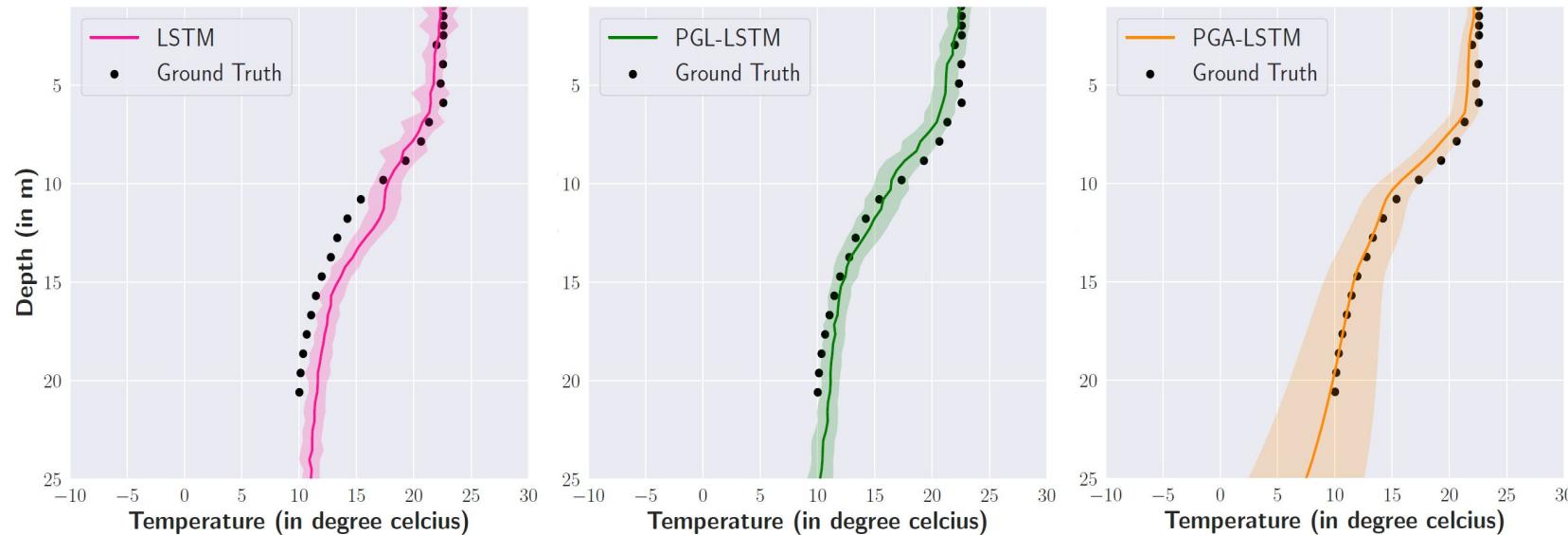
1. Adds a layer of **interpretability** into the model outputs,
2. Makes it more **robust** to small perturbations in the model weights
3. Ensures physics-**generalization** on unseen test set.

# Impact on predictive performance and physical consistency



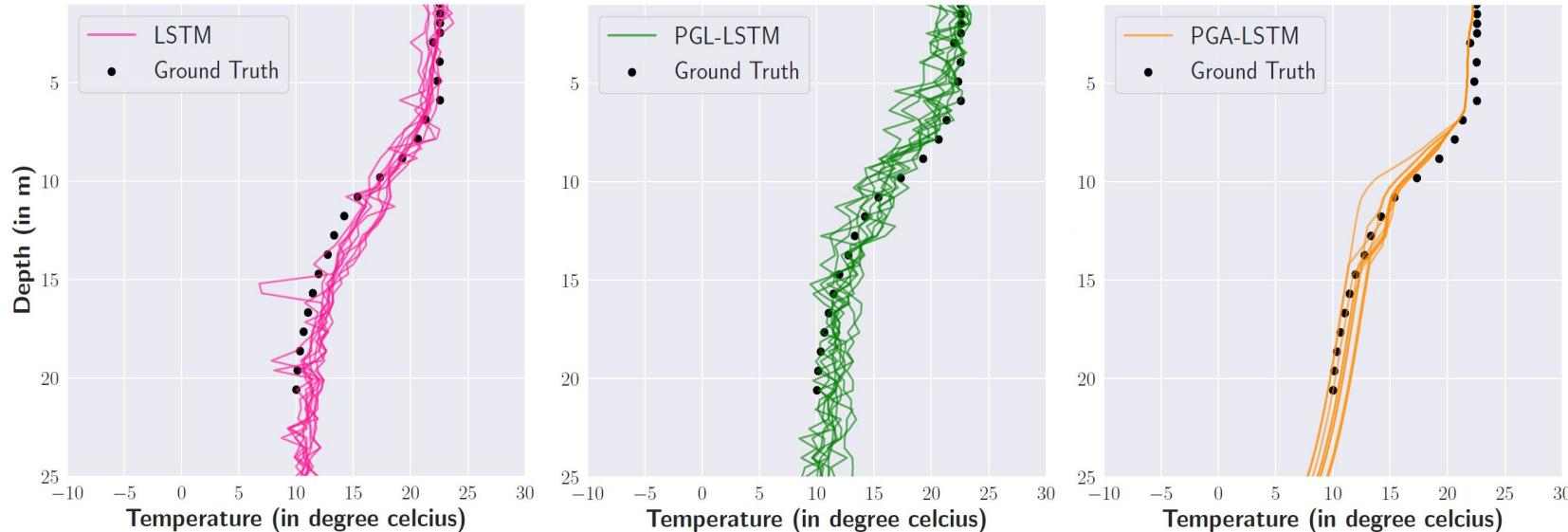
PGA-LSTM improves the Test RMSE while always being physically consistent across both lakes.

# Monotonicity Preserving LSTM



The mean and the variance of the three models are computed from **100 MC-Samples**.

# Monotonicity Preserving LSTM



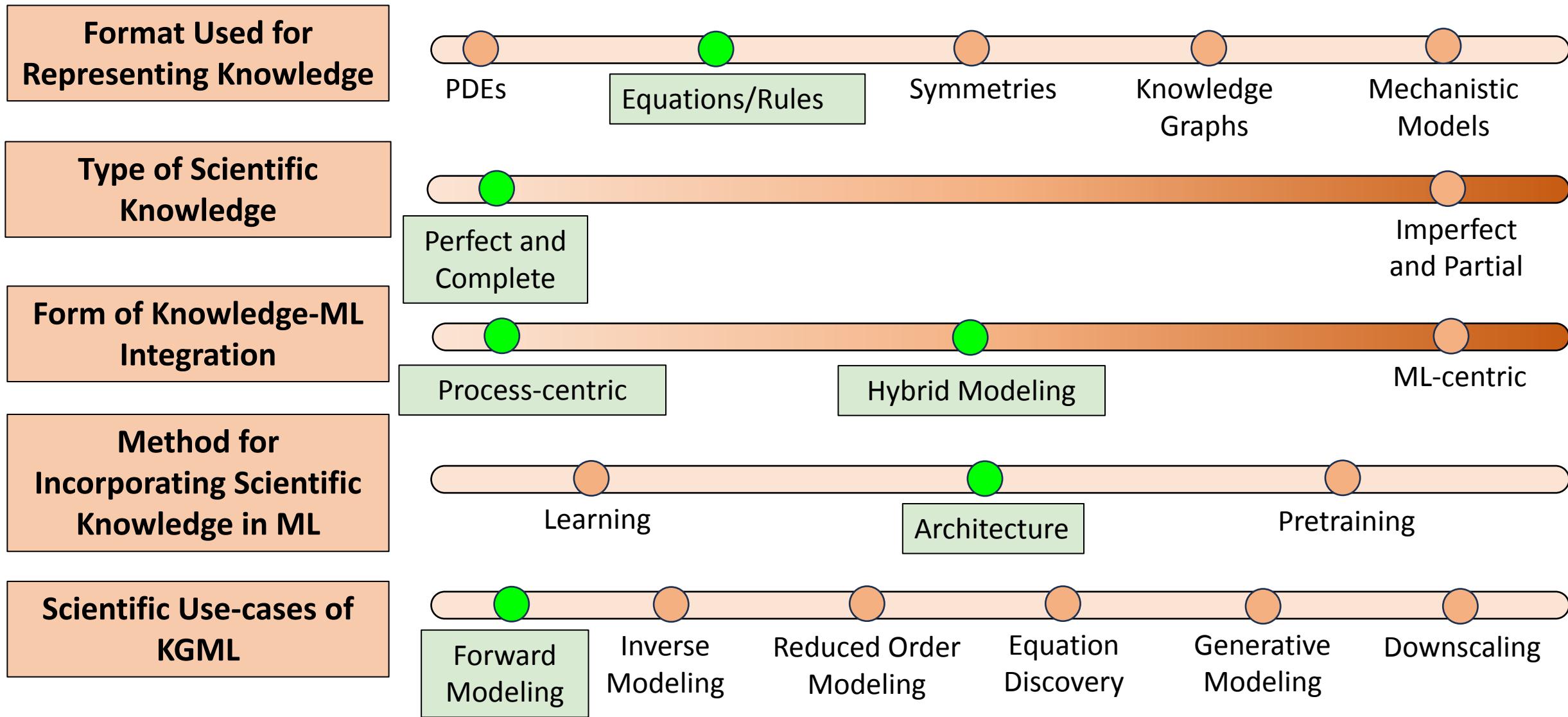
The PGA-LSTM samples are always physically consistent while PGL-LSTM and LSTM samples are very much physically inconsistent.



Predictions are **more robust to minor perturbations** in model weights!

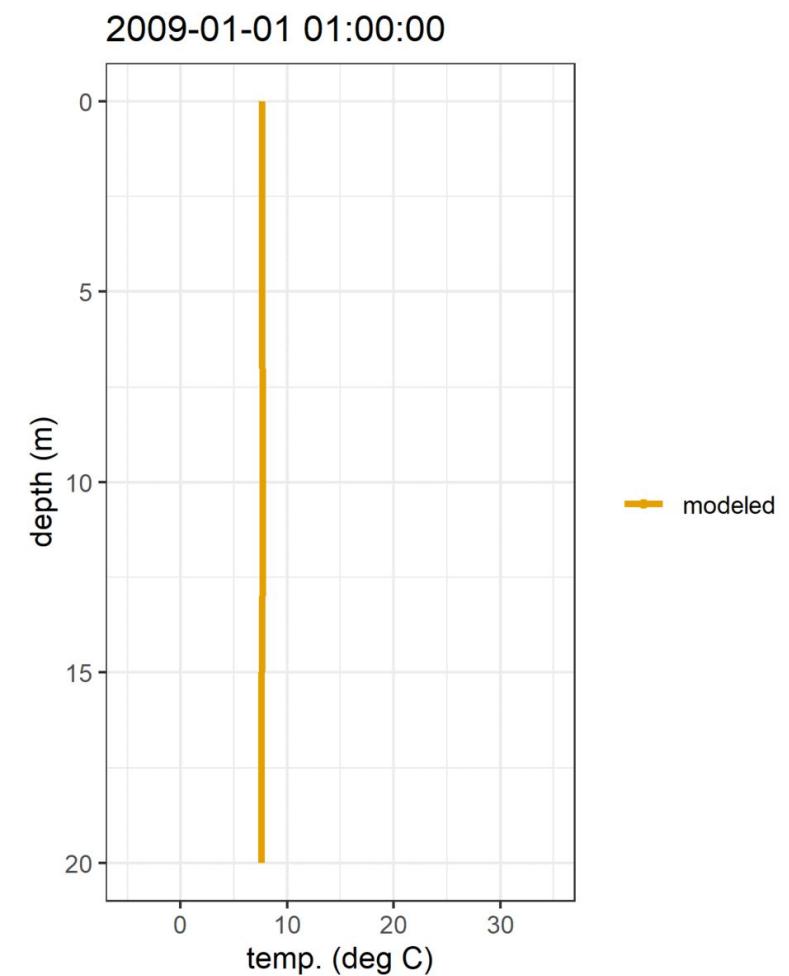
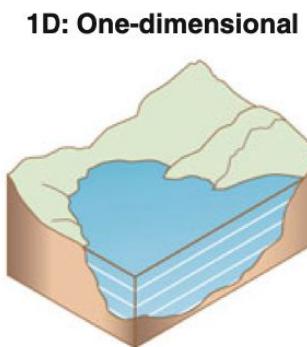
# Use Case 3: Hybrid Modeling

# Organizing KGML Research: A Multi-Dimensional View



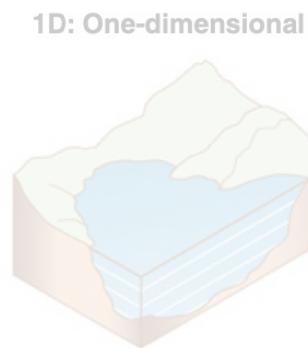
# Process-based Modeling

- plethora of model approaches:
  - **energy-balance** models: mixing depth by external energy
  - **turbulence-based** models: advanced turbulence-closure

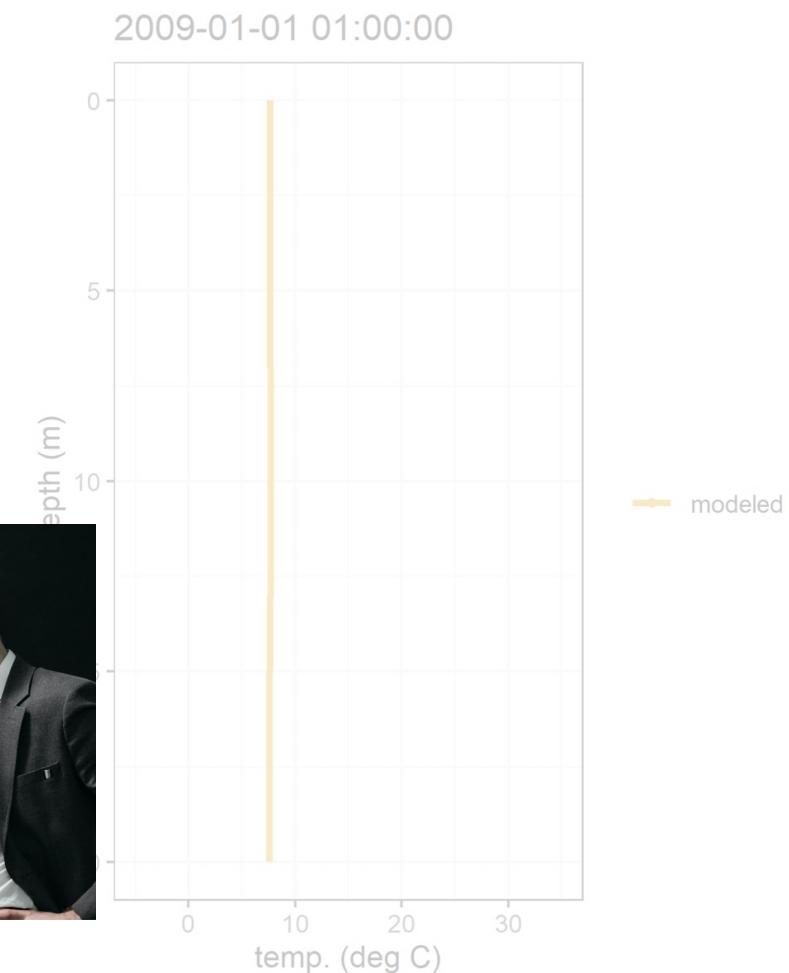
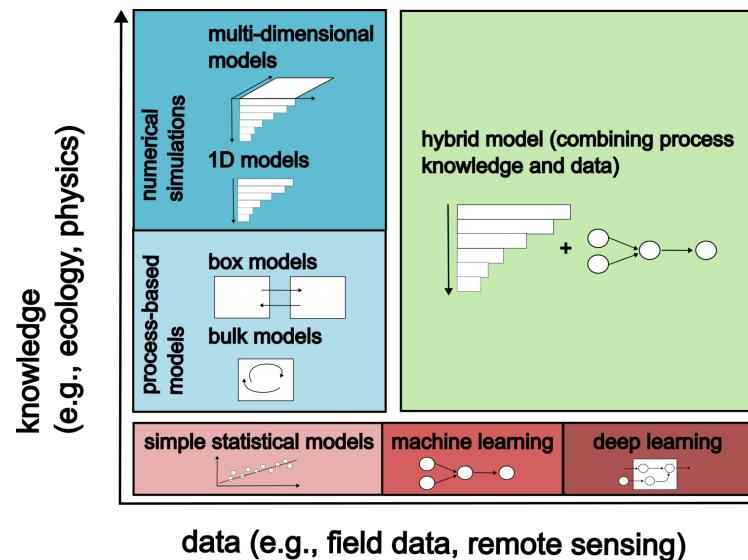


# Process-based Modeling

- plethora of model approaches:
  - **energy-balance** models: mixing depth by external energy
  - **turbulence-based** models: advanced turbulence-closure



**Can we combine these process models with data?**



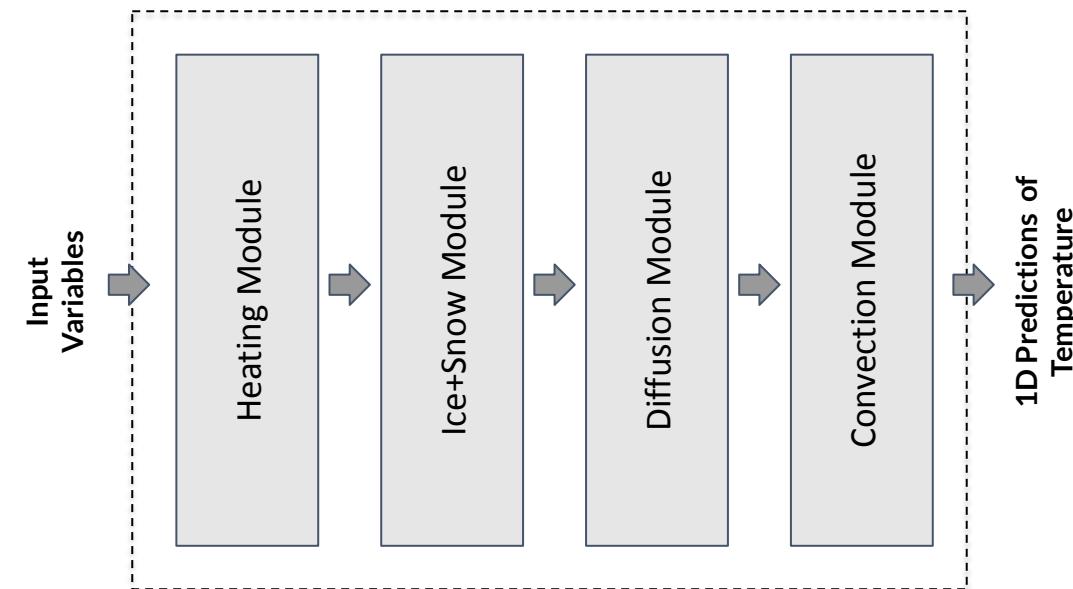
# Modularized 1D Model

## Modularized Process Models:

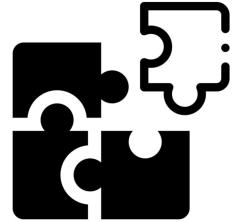
- a) heating (atmosphere and geothermal)
- b) ice, snow and snow-ice formation
- c) vertical diffusion
- d) convective overturn



- **Imperfect Module:** All of the physics modules are not perfect, i.e., some of the physical phenomena are more complex.



# Modular Compositional Learning (MCL)

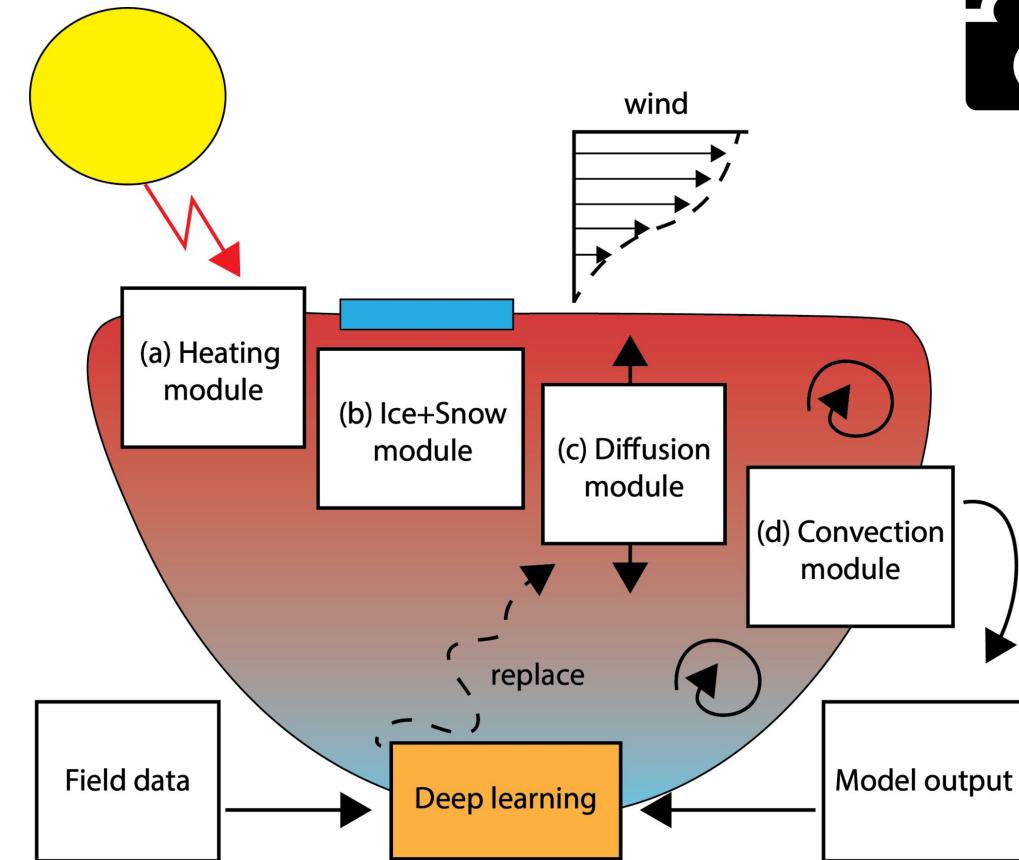


## Imperfect Modules: Diffusion Module

Idea: Replace the imperfect modules with deep learning based models.



- **Richer Physics knowledge:** We retain the interpretability and knowledge of the modular process based modules.
- **Hybrid modeling:** Deep learning modules learns to dynamics of the necessary "missing" module (in this case diffusion module) to learn a more accurate model.



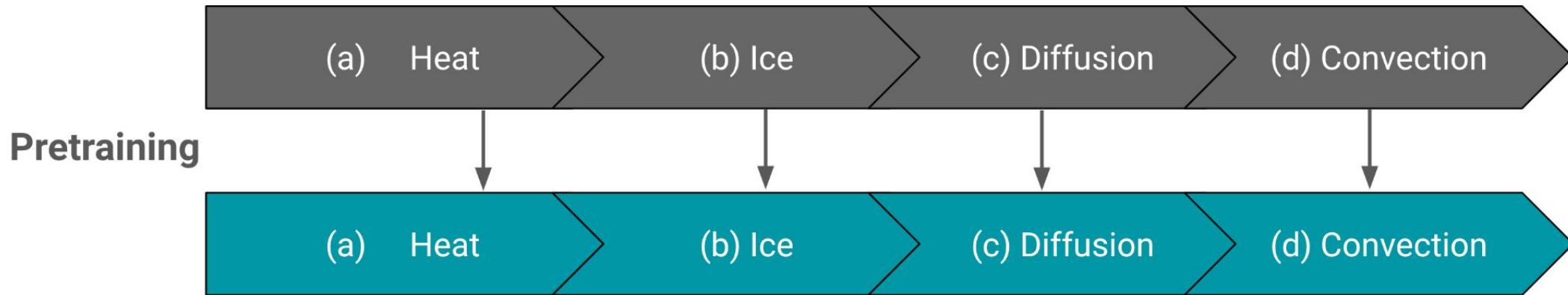
# Modular Compositional Learning (MCL)

## Process-based framework



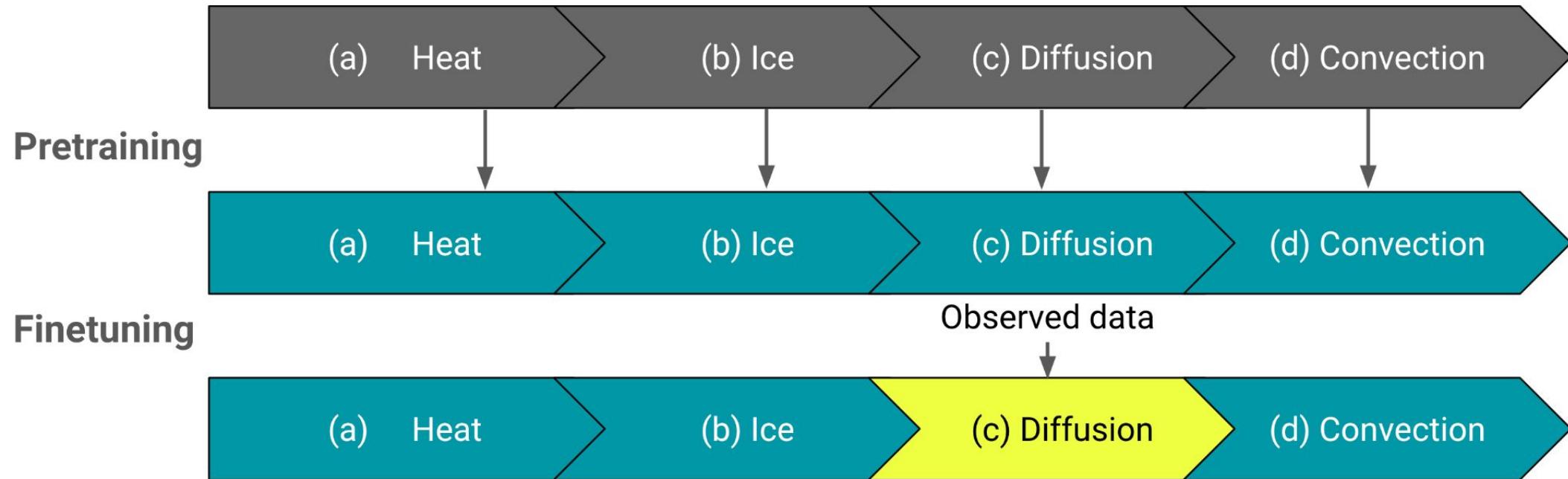
# Modular Compositional Learning (MCL)

## Process-based framework



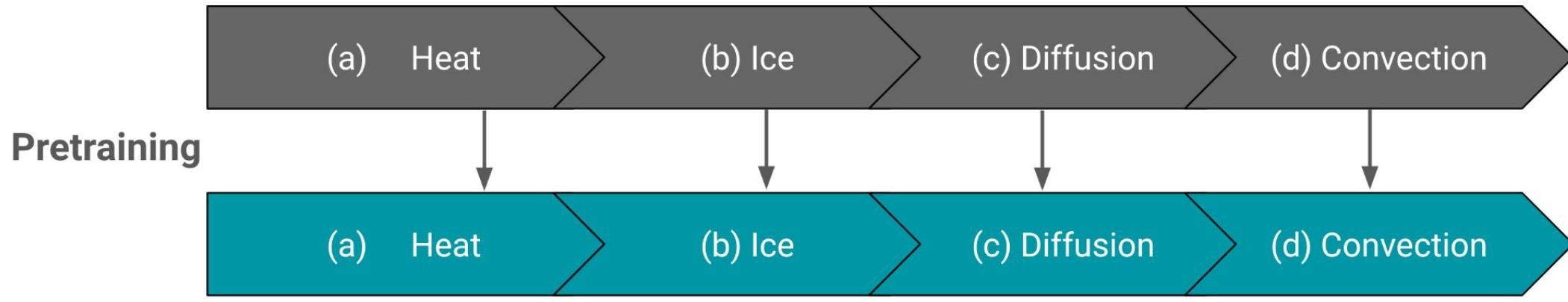
# Modular Compositional Learning (MCL)

## Process-based framework



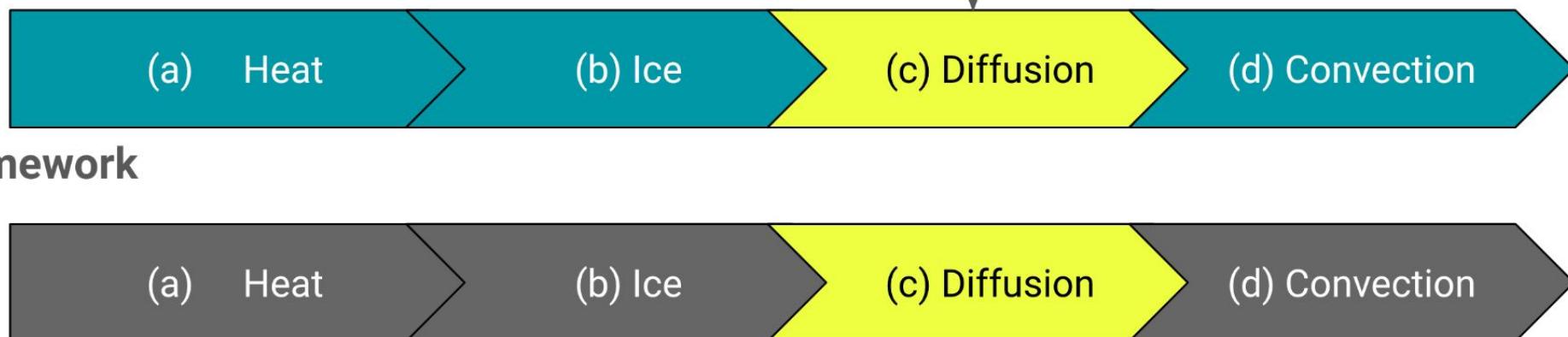
# Modular Compositional Learning (MCL)

## Process-based framework



## Finetuning

## Hybrid framework

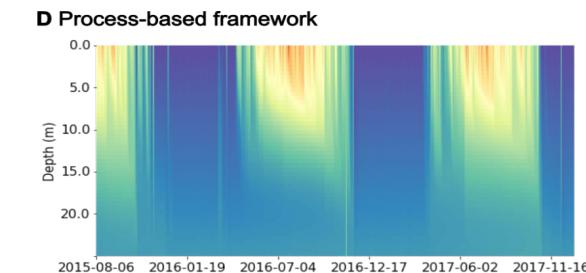
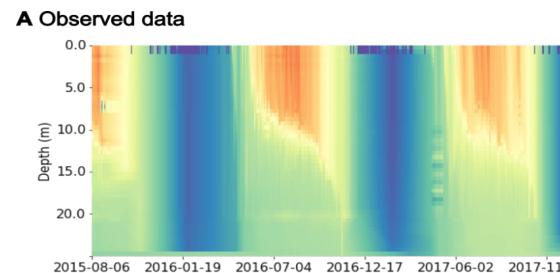


Process-based, pretrained deep learning, finetuned deep learning

Robert Ladwig

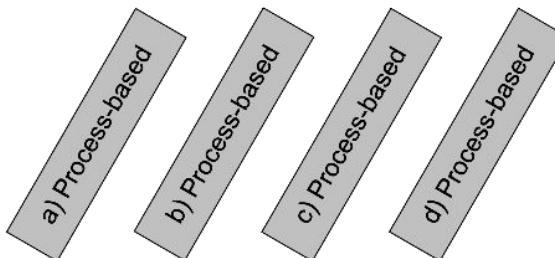
# Empirical Evaluation (Test Period 2015-17)

Comparing Observed Data and Processed-based model



Test  
RMSE:  
4.46

1 Process-based model framework

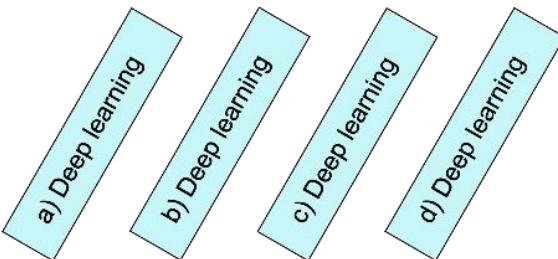


# Empirical Evaluation (Test Period 2015-17)

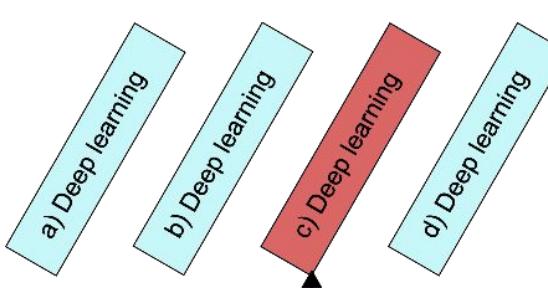
## Comparing the models:

1. After pretraining each of the deep learning models on simulation data.
2. Finetuning the entire deep learning pipeline on observed data.

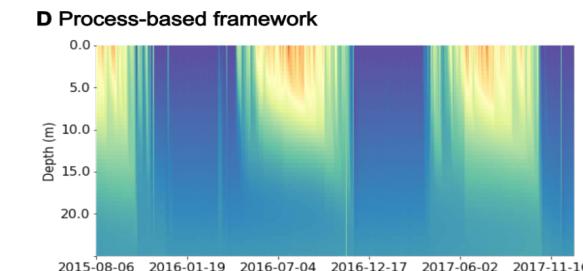
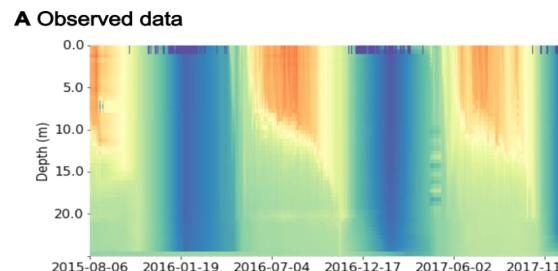
## 2 Pretrained deep learning framework



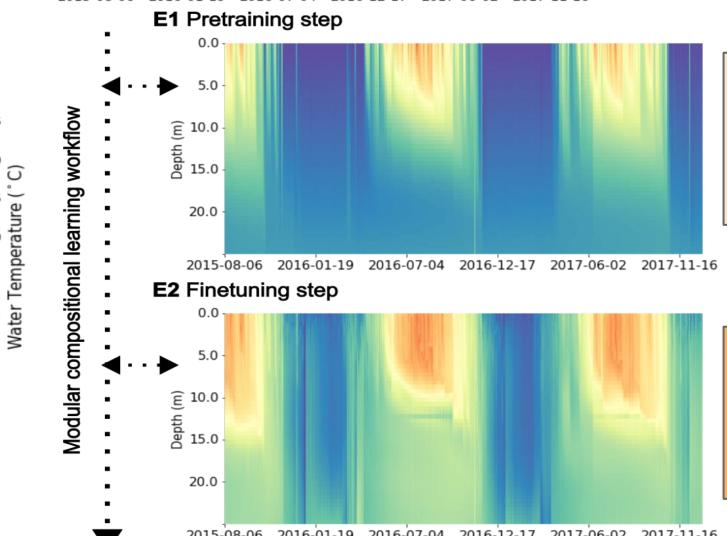
## 3 Finetuned deep learning framework



Observed data



Test  
RMSE:  
**4.46**



Test  
RMSE:  
**5.27**

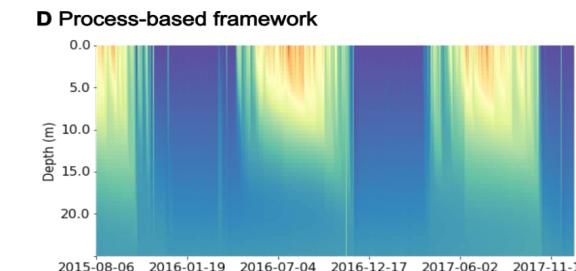
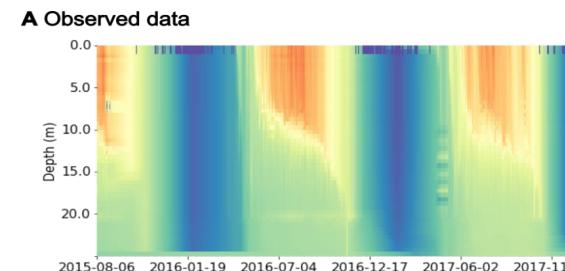
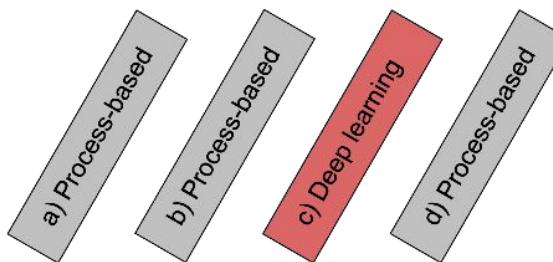
Test  
RMSE:  
**1.94**

Modular compositional learning workflow

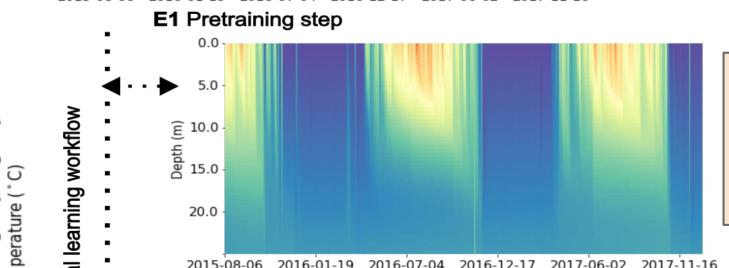
# Empirical Evaluation (Test Period 2015-17)

Plugging the deep-learning module into the process-based module pipeline.

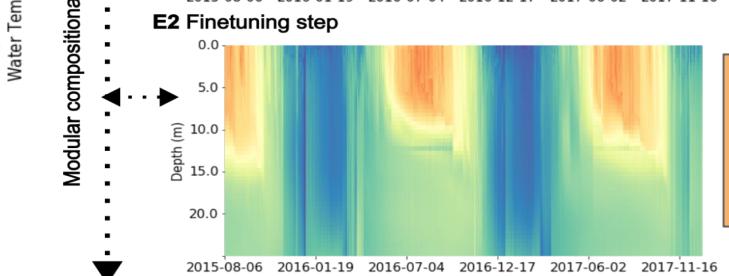
## 4 Hybrid model framework



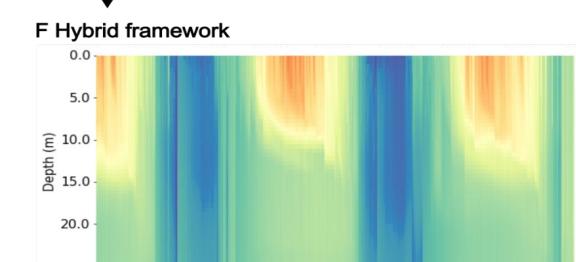
**Test RMSE: 4.46**



**Test RMSE: 5.27**

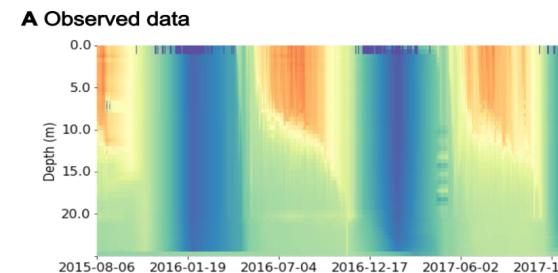
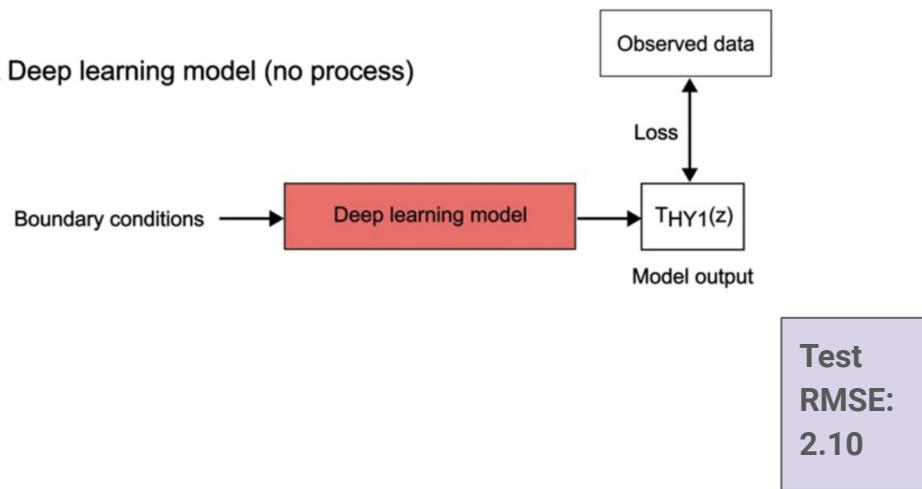
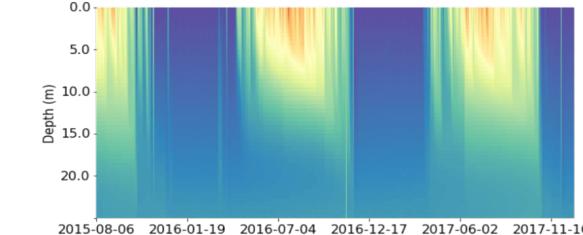
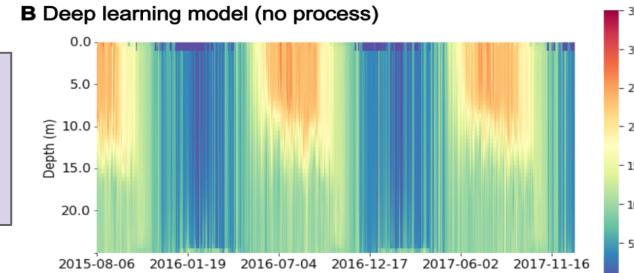
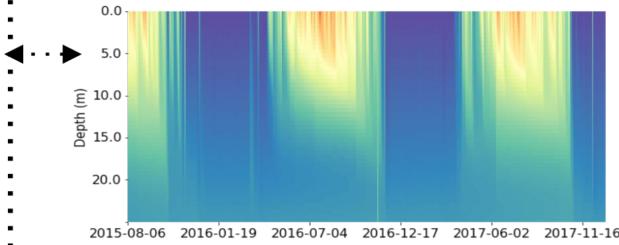
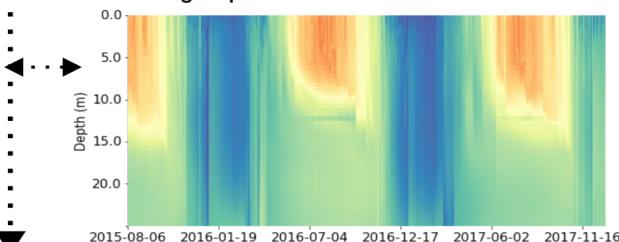
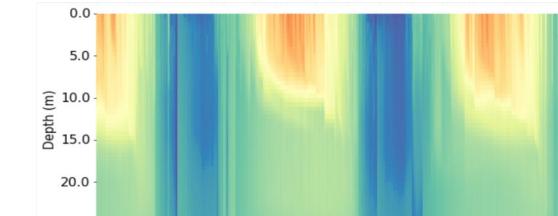


**Test RMSE: 1.94**



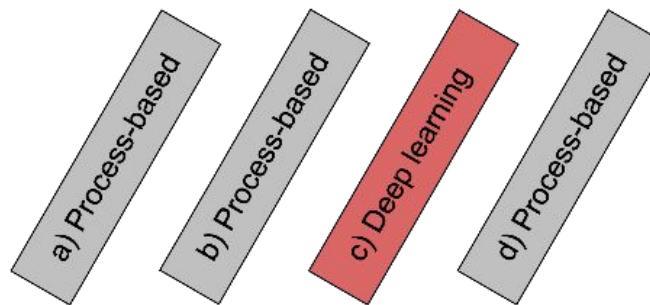
**Test RMSE: 1.60**

# Empirical Evaluation (Test Period 2015-17)

**A Deep learning model (no process)****Test RMSE: 2.10****D Process-based framework****Test RMSE: 4.46****B Deep learning model (no process)****Test RMSE: 5.27****E1 Pretraining step****Test RMSE: 1.94****E2 Finetuning step****F Hybrid framework****Test RMSE: 1.60**

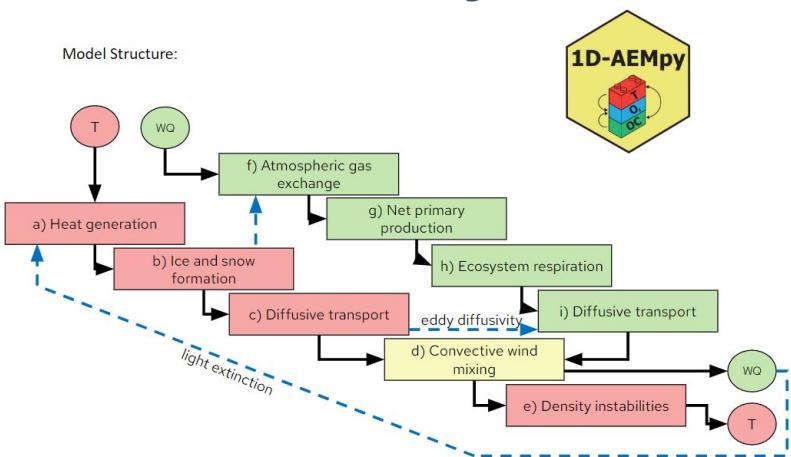
# Current Work in MCL

4 Hybrid model framework



## 1D Lake Physics with MCL

### 1D Water Quality with MCL

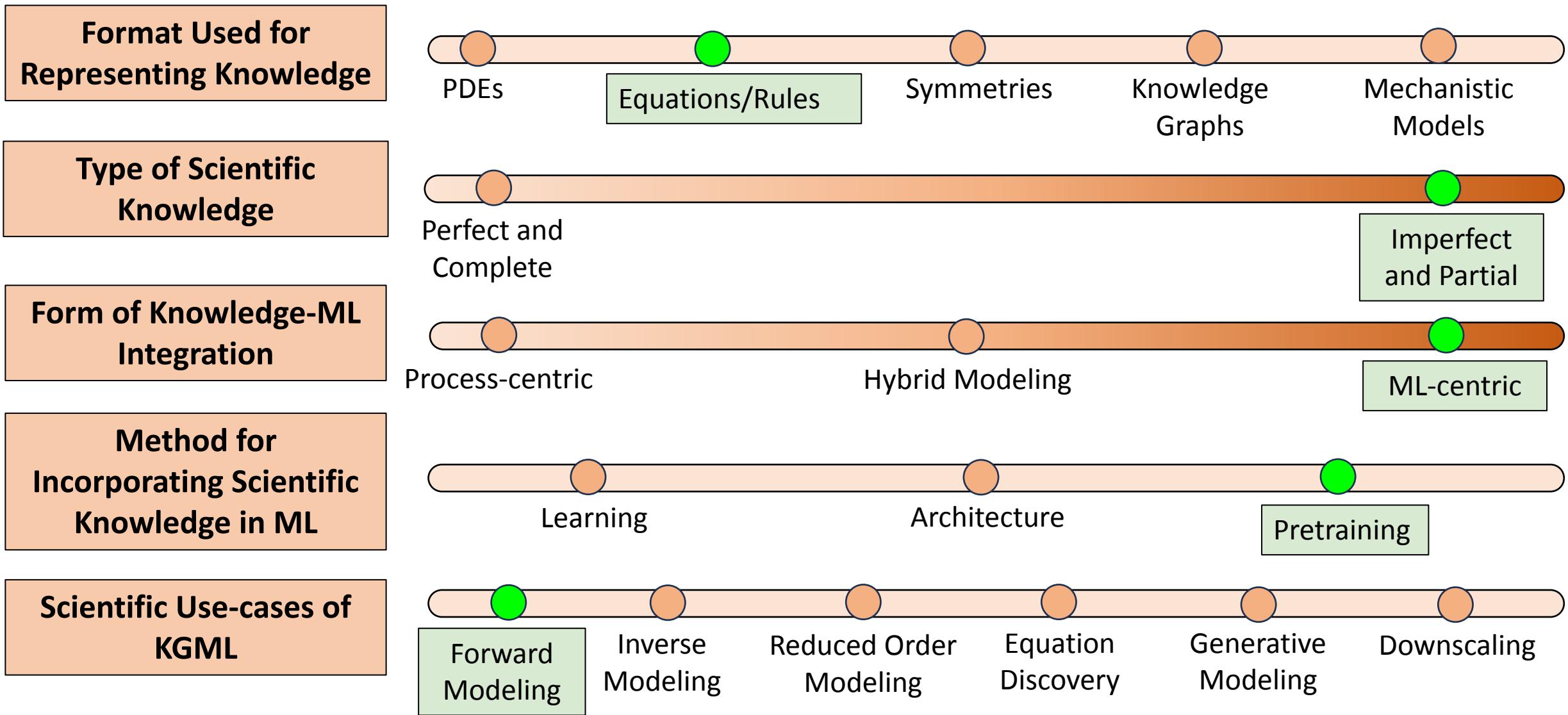


### 1D Lake Physics with MCL: memory for multiple lakes



# Use Case 5: Lake Chlorophyll-a Prediction

# Organizing KGML Research: A Multi-Dimensional View



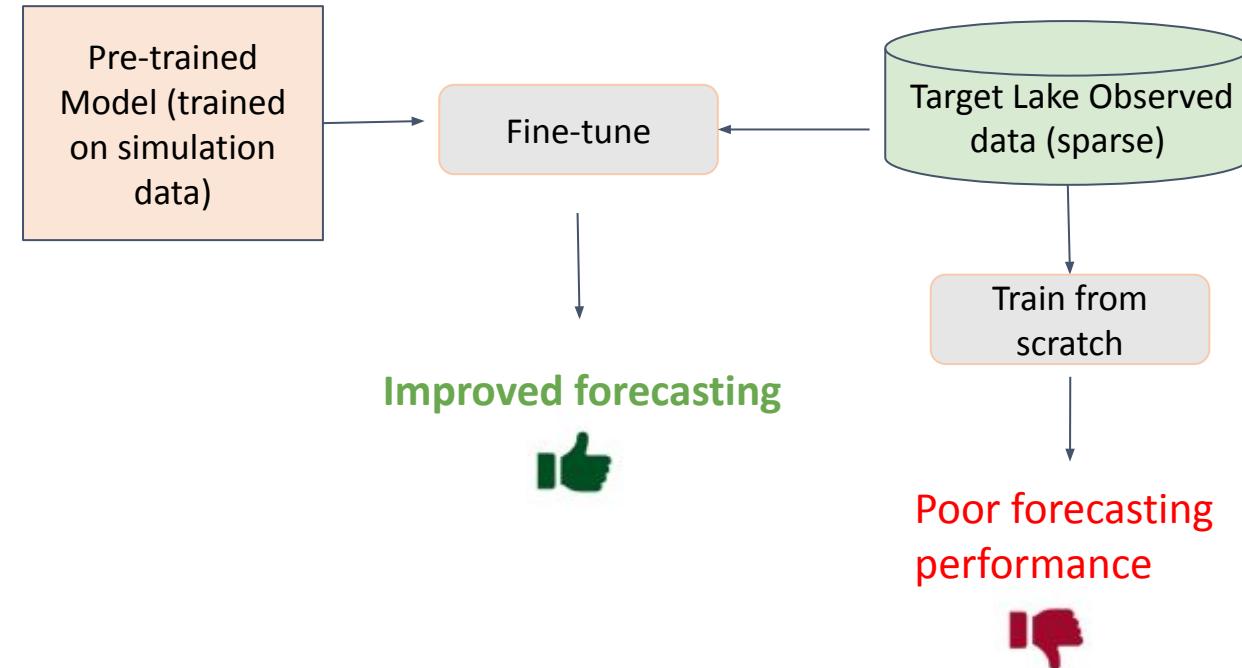
# Transfer Learning for Chlorophyll-a Prediction

## Problem Context:

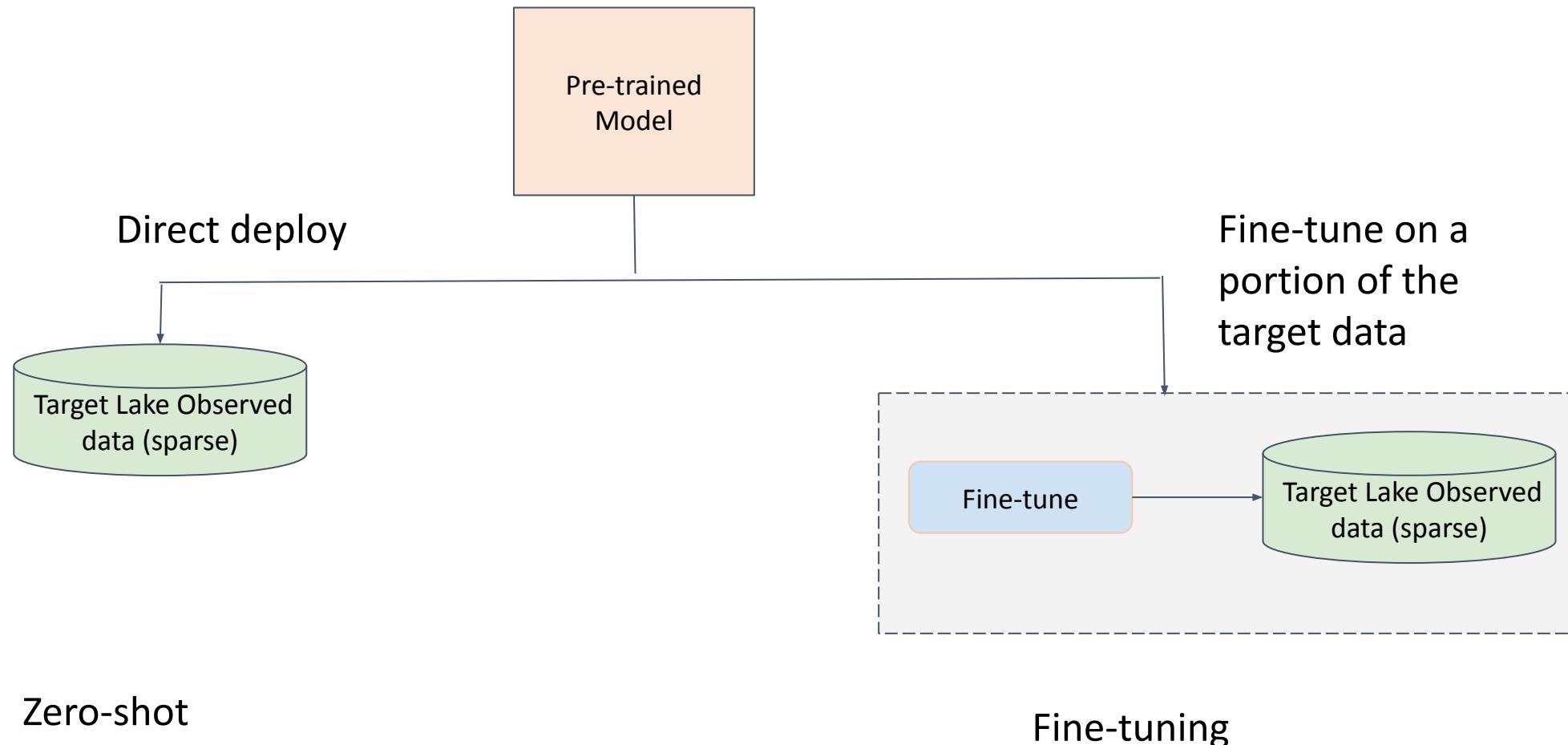
- Observations of chlorophyll-a vary across lakes, some being well-observed, others less-observed.
- Deep learning models are data-hungry, show poor forecasting performance on target lakes with sparse data.

**Research Question:** *How can we improve forecasting performance of chlorophyll-a on lakes with few observations?*

**Approach:** Instead of “training from scratch” *transfer Learning* enables us to transfer knowledge learned from data-rich source lakes (in the form of pre-trained models) to target lakes.



# Types of Transfer Learning methods



# Transfer Learning for Chlorophyll-a Prediction

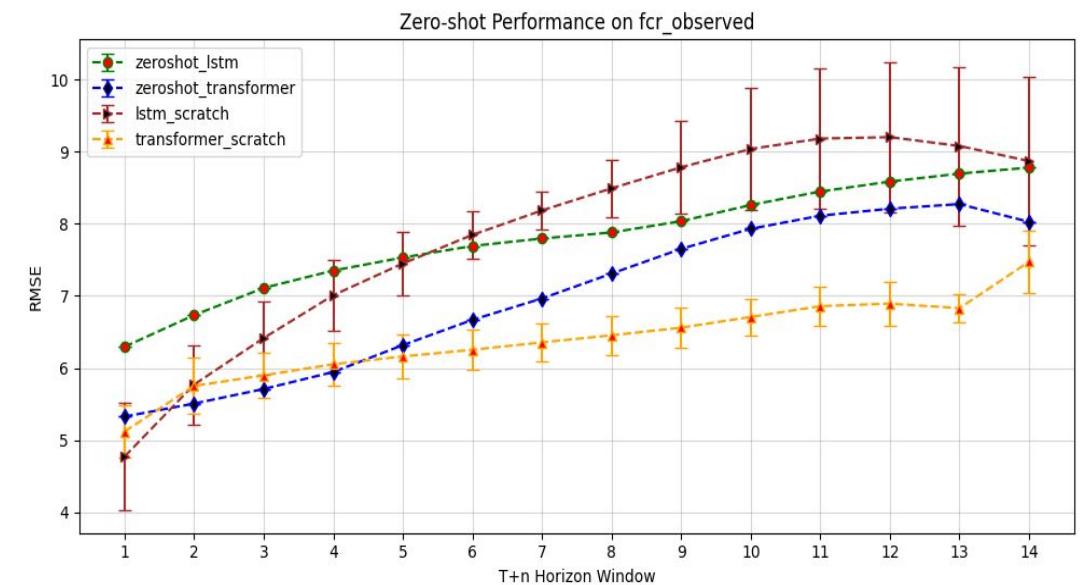
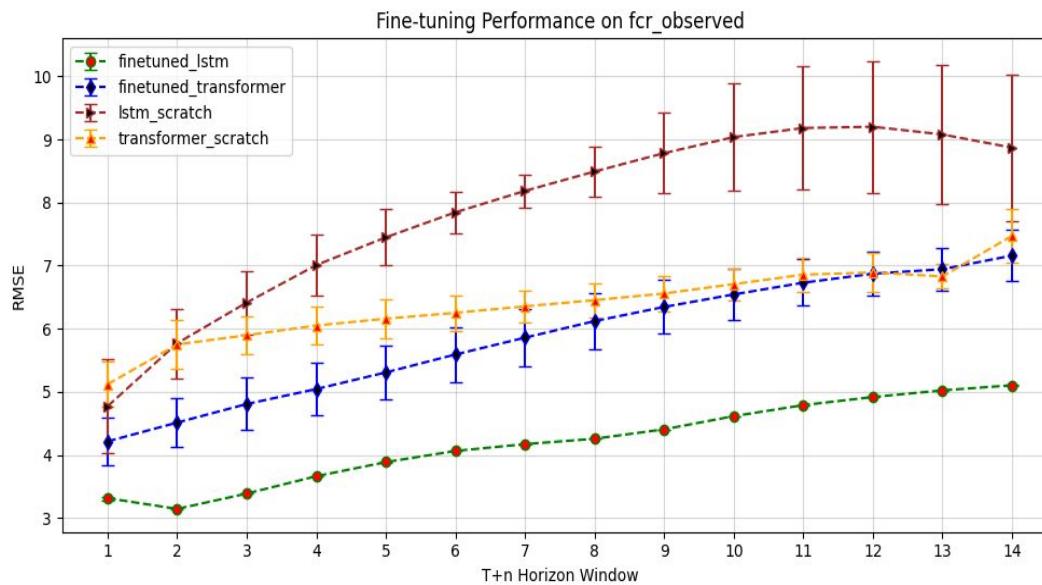
## Problem Setup

Pre-training: Model pre-trained on simulation data of lakes Mendota, Sunapee, FCR.

Models: LSTM [1], Transformer [2]

Data split in target lake = 70:30  
Model trained/fine-tuned on the 70% and tested on the 30% data.

>Following results are on the test set (i.e. 30% of data)



1. Hochreiter, S., & Schmidhuber, J"urgen. (1997). Long short-term memory. *Neural Computation*, 9(8), 1735–1780.
2. Vaswani, Ashish, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Łukasz Kaiser, and Illia Polosukhin. "Attention is all you need." *Advances in neural information processing systems* 30 (2017).

# Transfer Learning for Chlorophyll-a Prediction

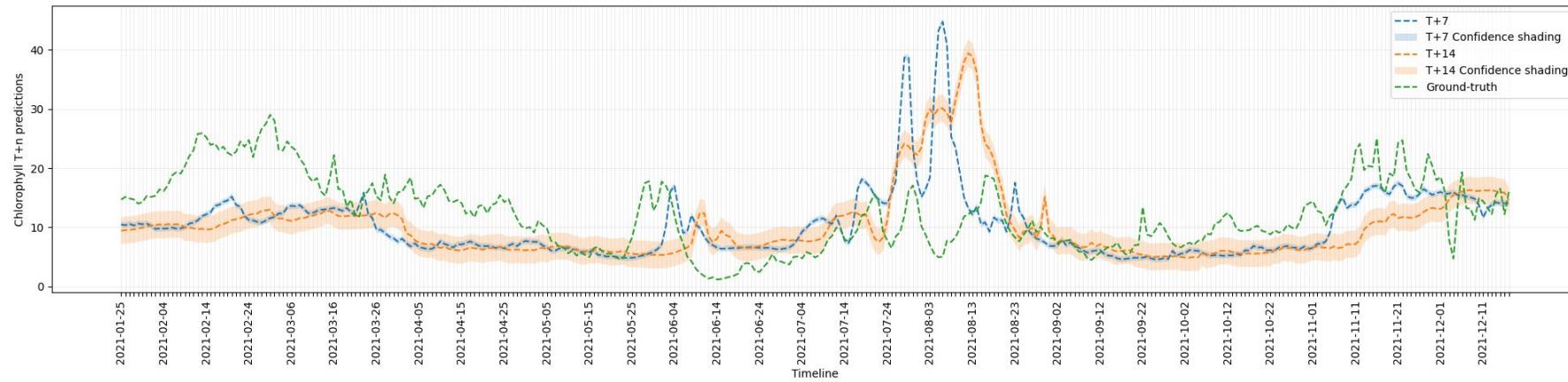
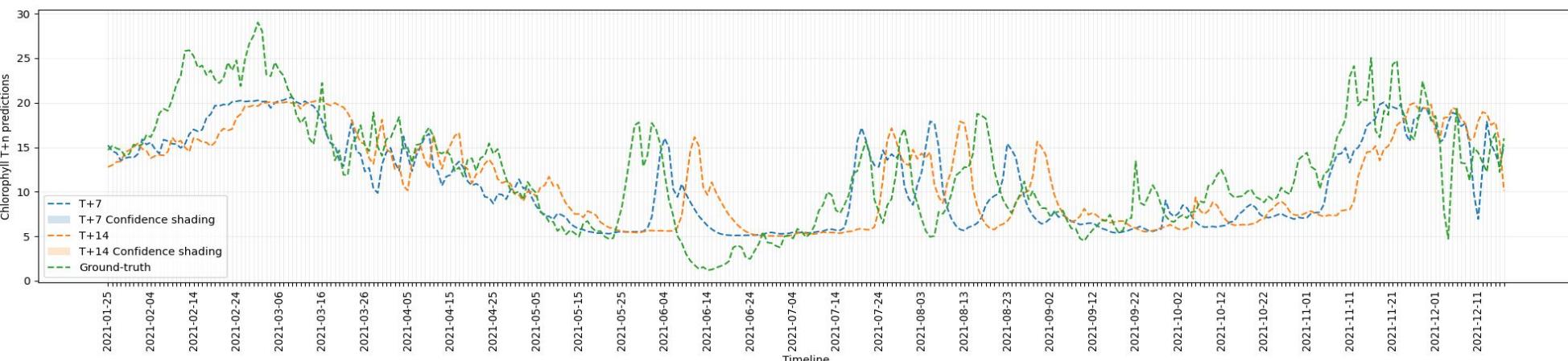


Fig. 1 Predictions on FCR observed Test portion - Model trained from scratch

- Fine-tuned model aligns with the ground-truth scale of chlorophyll data
- Fine-tuned model shows relatively more confident predictions



LSTM model

Fig. 2 Predictions on FCR observed Test portion - Model fine-tuned on FCR observed

# Towards a Foundation Model

