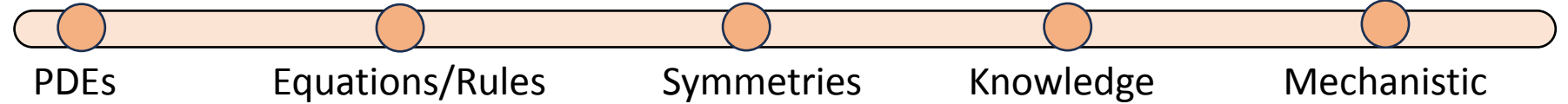


KGML for Aquatic Sciences

Organizing KGML Research: A Multi-Dimensional View

Format Used for Representing Knowledge



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

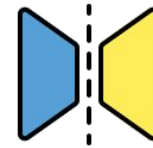
Navier Stokes Equation,
Wave Equation,
Schrodinger Equation, ...

PINNs: Raissi et al. 2019

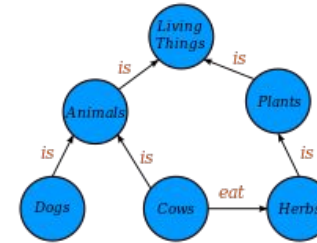
$$\frac{\partial u}{\partial x} \propto \frac{\partial^2 u}{\partial x^2}$$

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

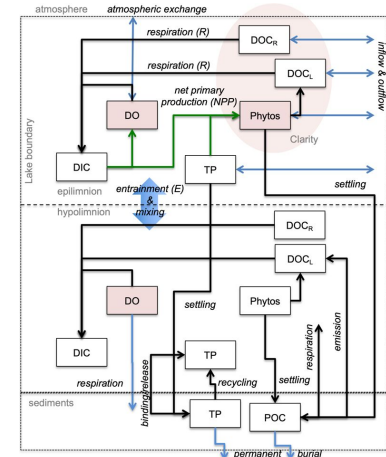
PGNN: Karpatne et al. 2017
PGRNN: Jia et al. 2019
PGA-LSTM: Daw et al. 2020



NequIP: Batzner et al. 2022
Cormorant: Anderson et al. 2019
Equivariant-Net: Wang et al. 2021



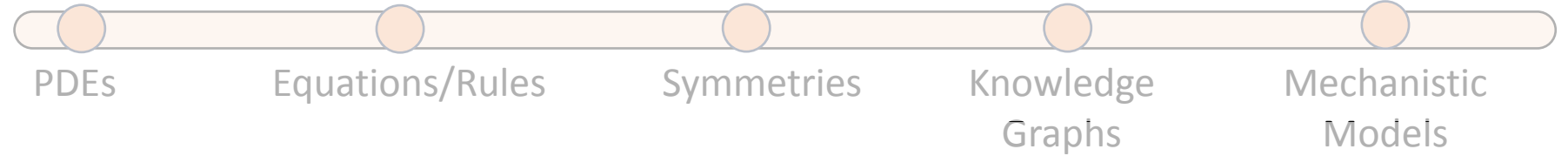
Zareian et al. 2020



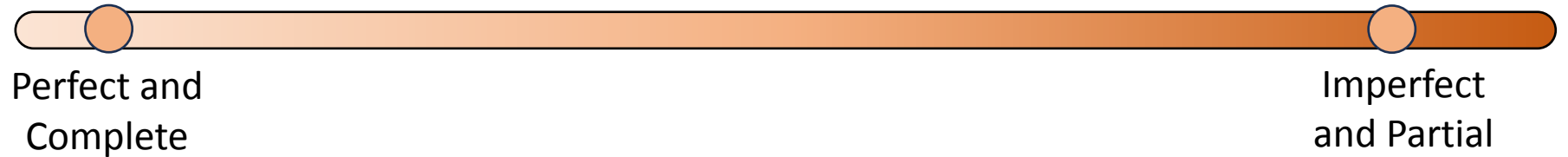
MCL: Ladwig et al. 2024
dPL: Shen et al. 2023

Organizing KGML Research: A Multi-Dimensional View

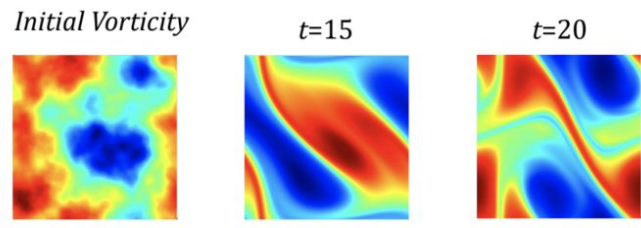
Format Used for Representing Knowledge



Type of Scientific Knowledge



Example: Solving *known* PDEs



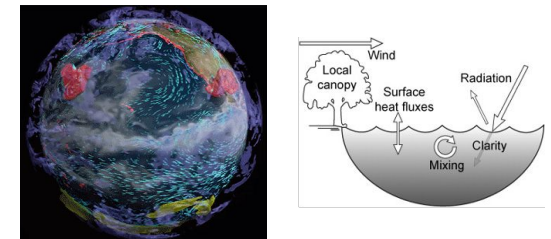
Navier Stokes Eq., Heat Eq., Wave Eq., Schrodinger Eq., ...

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

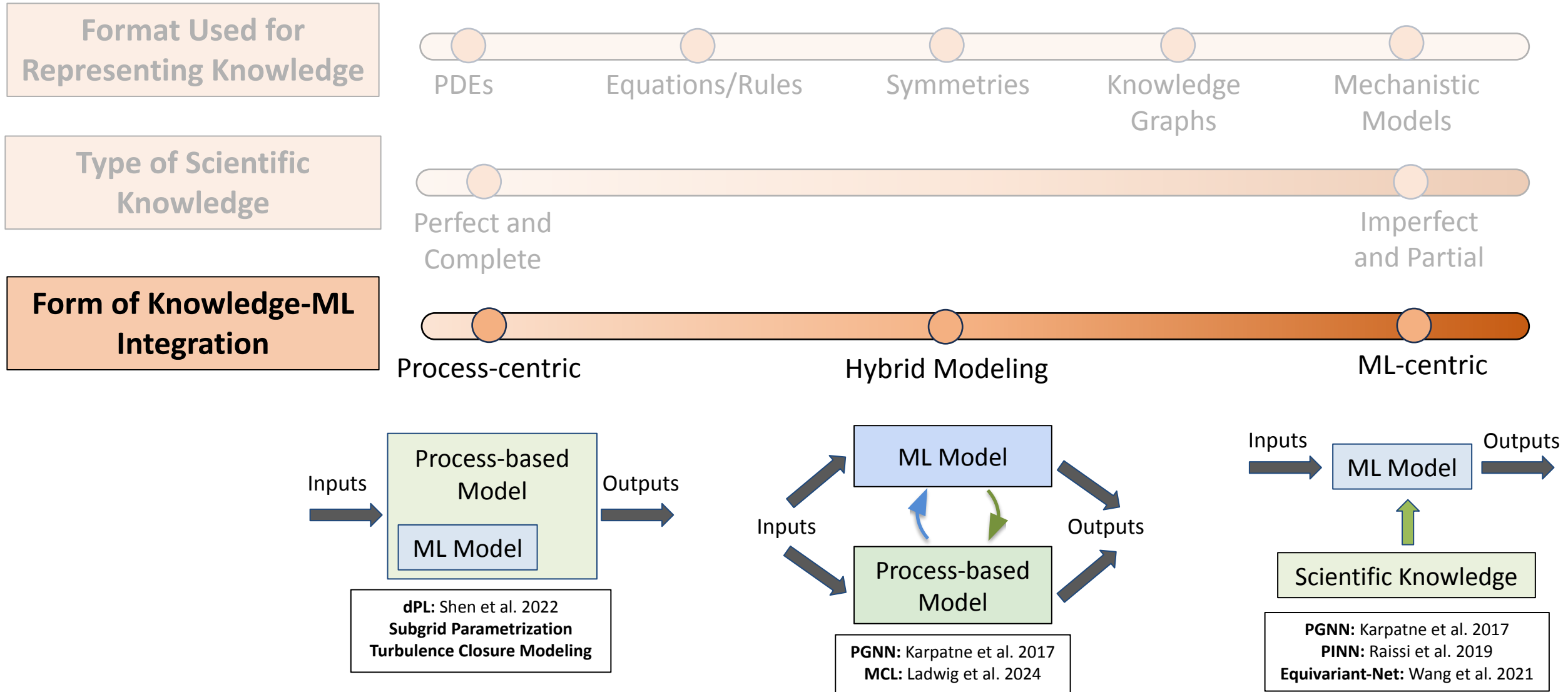
Modeling Turbulence, Multi-phase Flow, Cloud Physics, Aerosols, ...



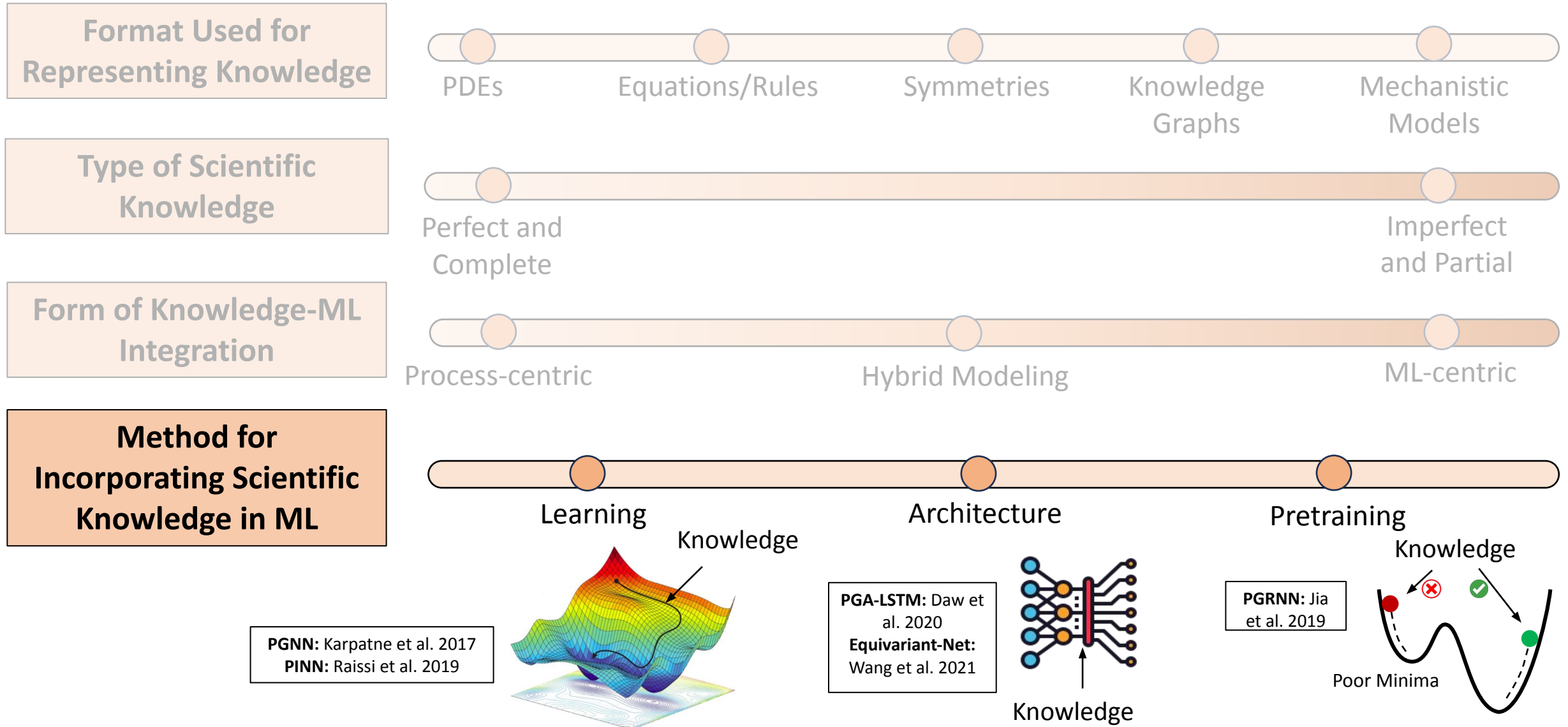
Additional Objective: Improve Modeling Accuracy

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

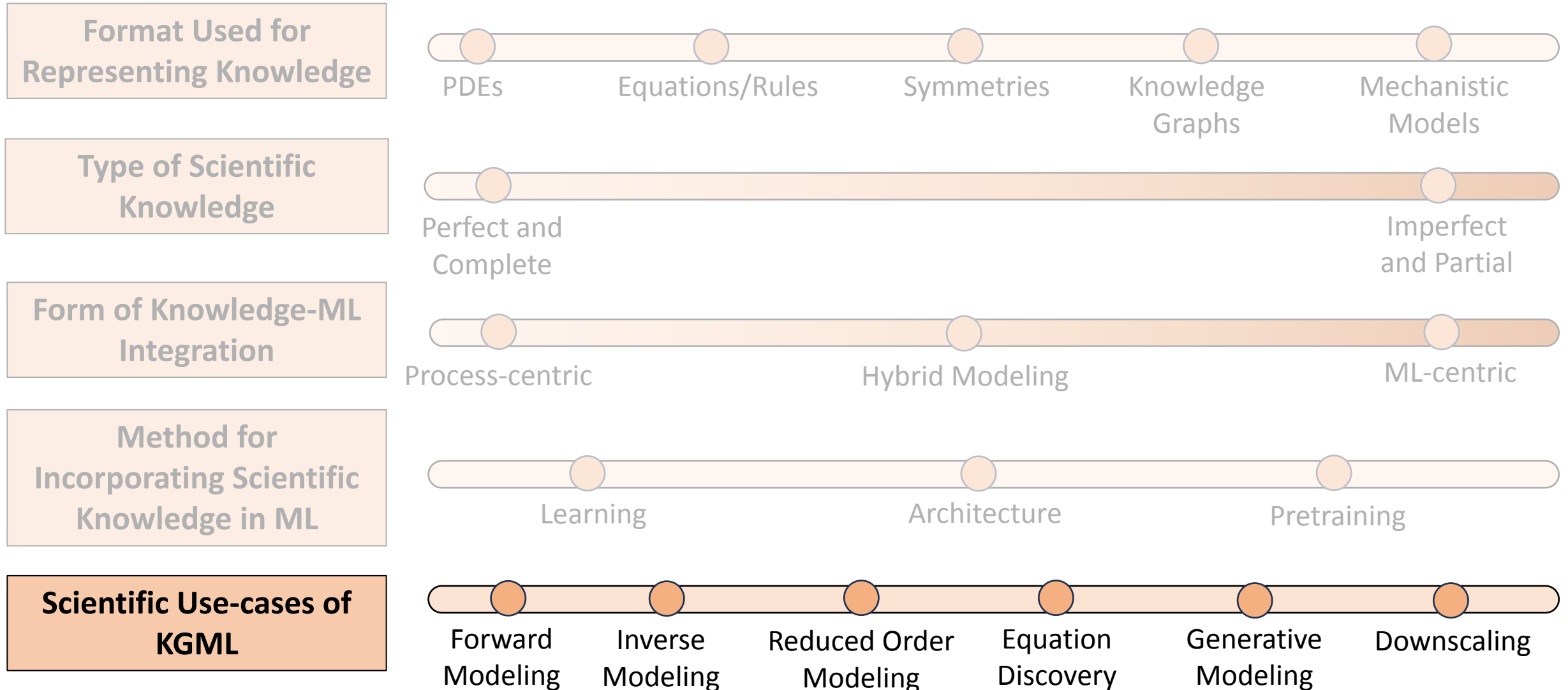


PGNN: Karpatne et al. 2017
PINN: Raissi et al. 2019

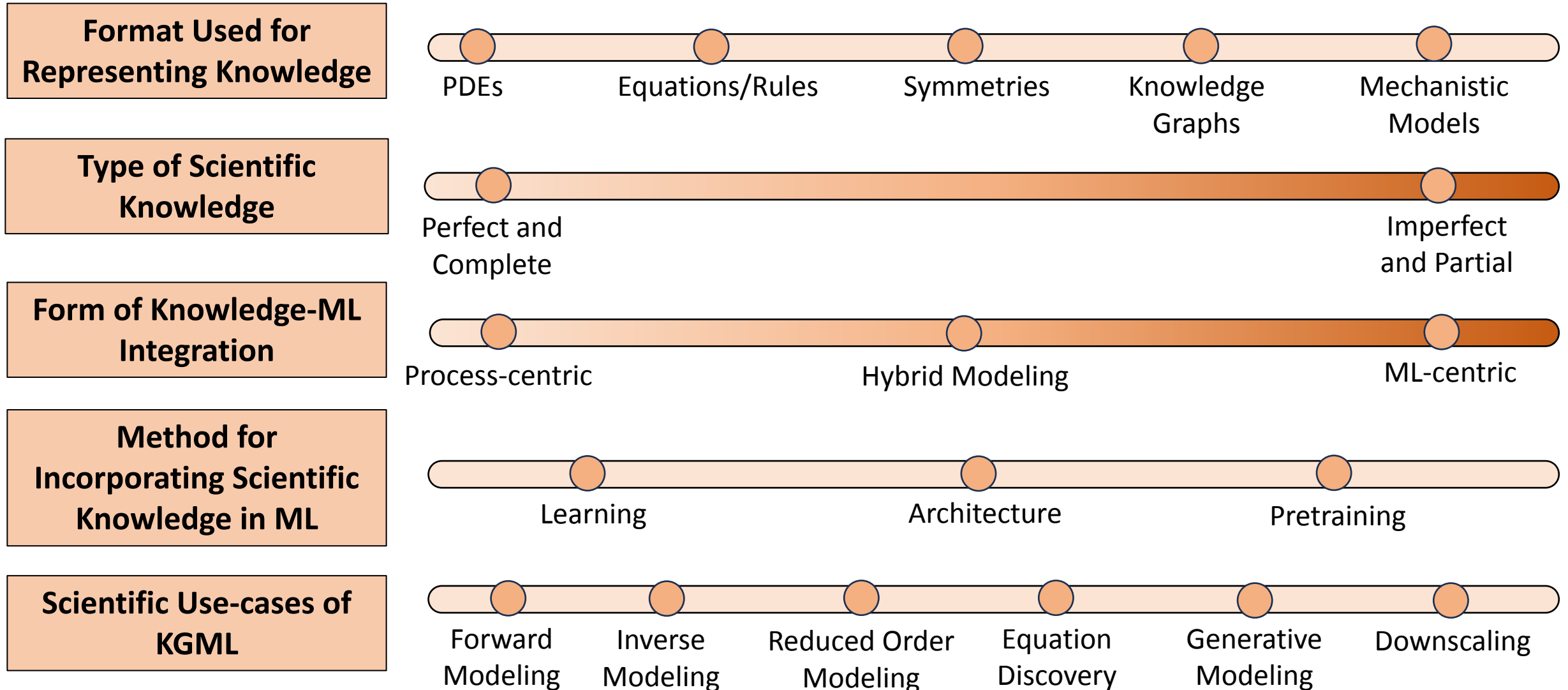
PGA-LSTM: Daw et al. 2020
Equivariant-Net: Wang et al. 2021

PGRNN: Jia et al. 2019

Organizing KGML Research: A Multi-Dimensional View



Organizing KGML Research: A Multi-Dimensional View



KGML Use Cases

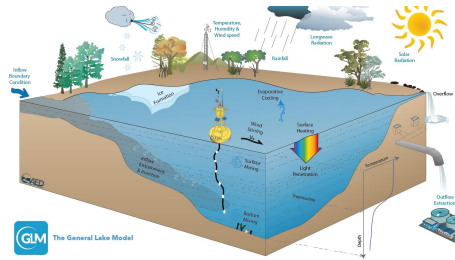
Lake Temperature Modeling

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

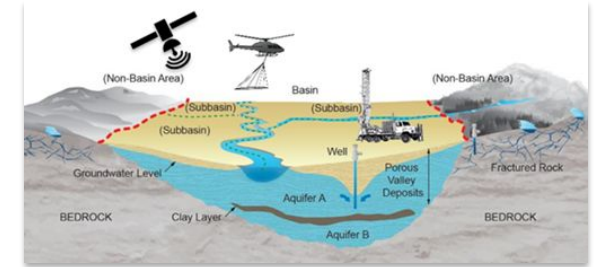
Physics-guided RNNs
(**PGRNNs**): Jia et al. 2019



River-basin Characterization

Goal: Predict basin characteristics of rivers.

- Extract system characteristics from driver and response data.



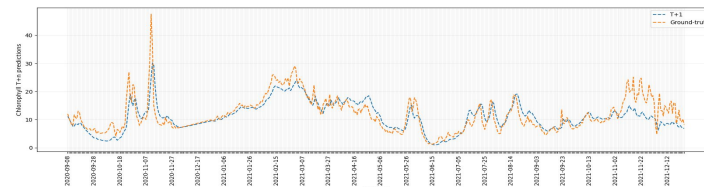
Knowledge-guided Self-supervised
(**KGSSL**): Ghosh et al. 2022

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

Chlorophyll-a Prediction

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

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

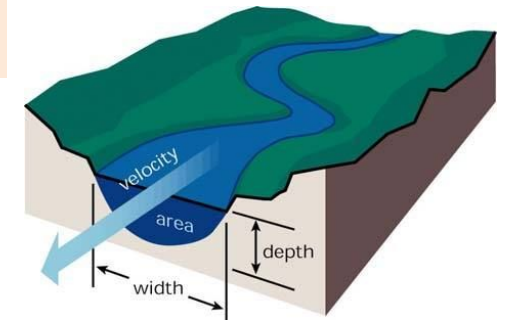


LSTM based Chl-a
Prediction: Cen et al. 2022

Streamflow Forecasting

Goal: Predict the stream flow of rivers.

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

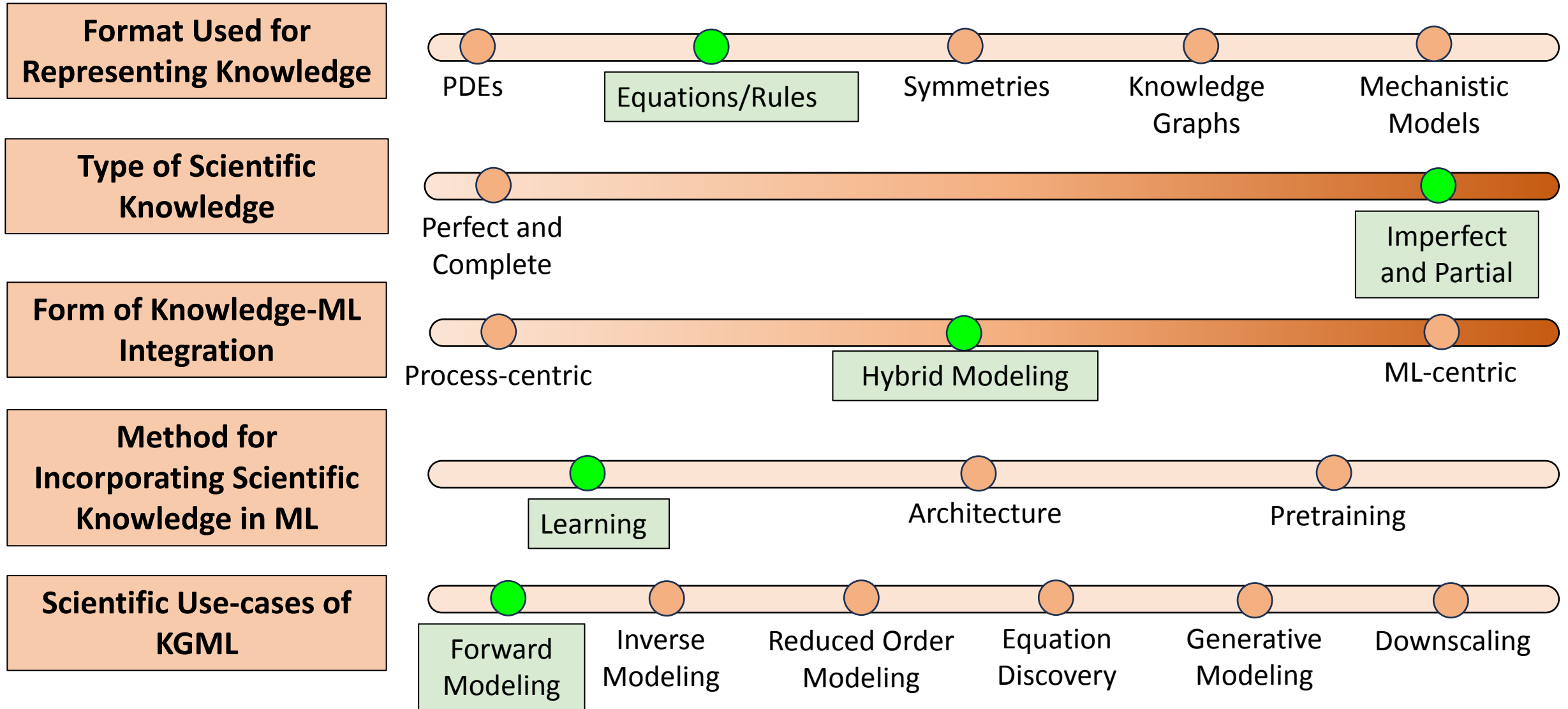


Physics-guided Recurrent Graph
Model (**PGRGnN**): Jia et al. 2020

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

Use Case 1: Lake Temperature Modeling

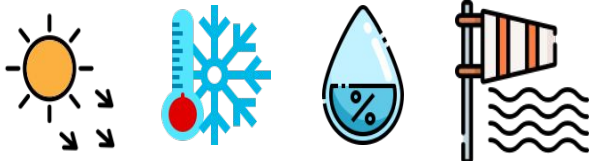
Organizing KGML Research: A Multi-Dimensional View



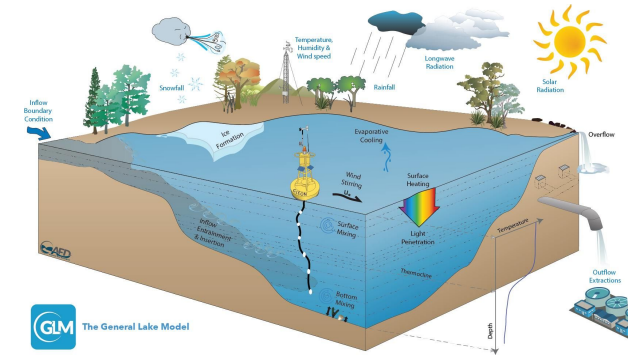
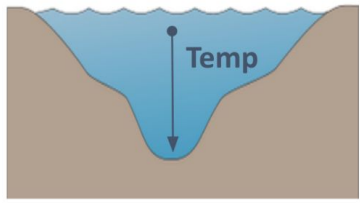
Lake Temperature Modeling

1D Model of Temperature

Meteorological Input Drivers
E.g., longwave/shortwave radiation, air temperature, humidity, wind speed, etc.



Target
Temperature of water at every depth of the lake



Motivation



Growth and survival of fisheries

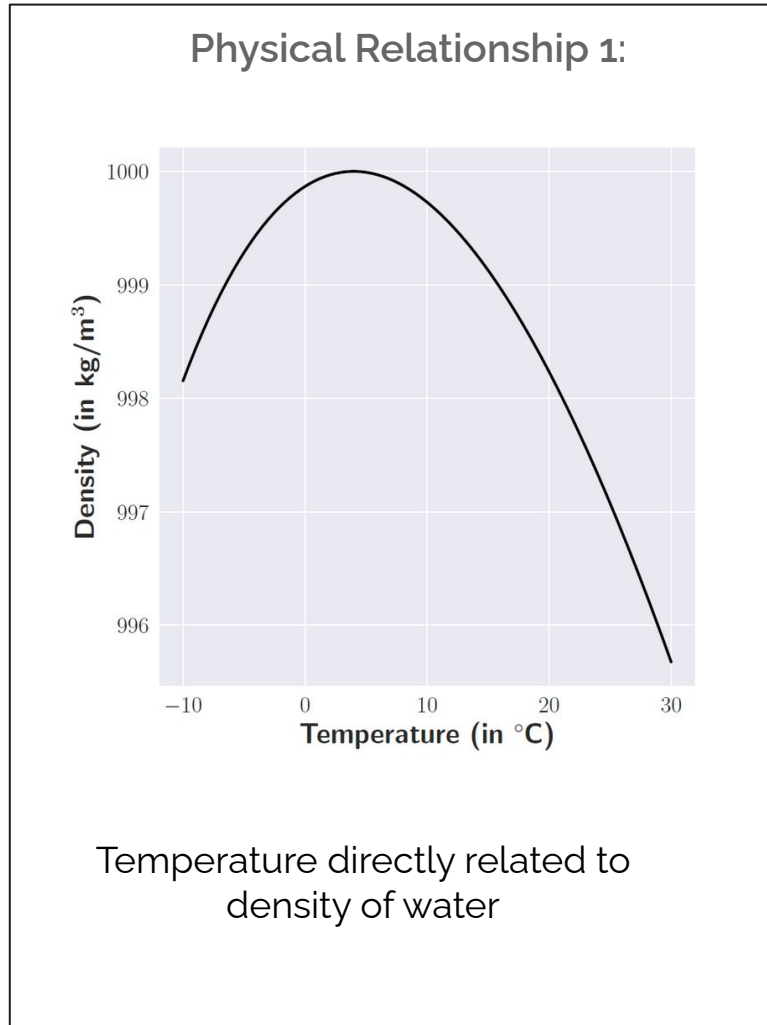


Harmful Algal Blooms



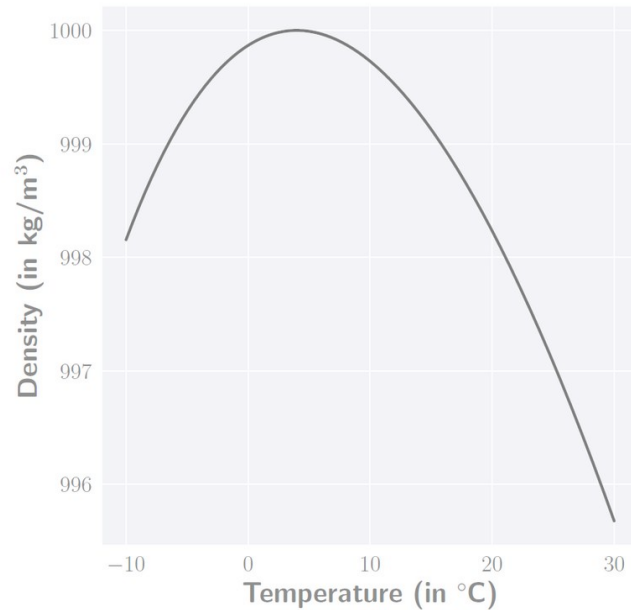
Chemical Constituents:
O₂, C, N

Physical Relationships of Temperature



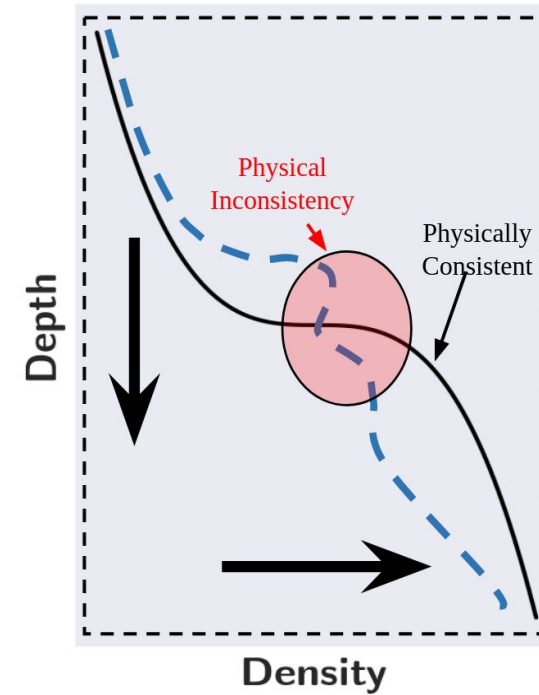
Physical Relationships of Temperature

Physical Relationship 1:



Temperature directly related to density of water

Physical Relationship 2:



Density of water **monotonically increases** with depth

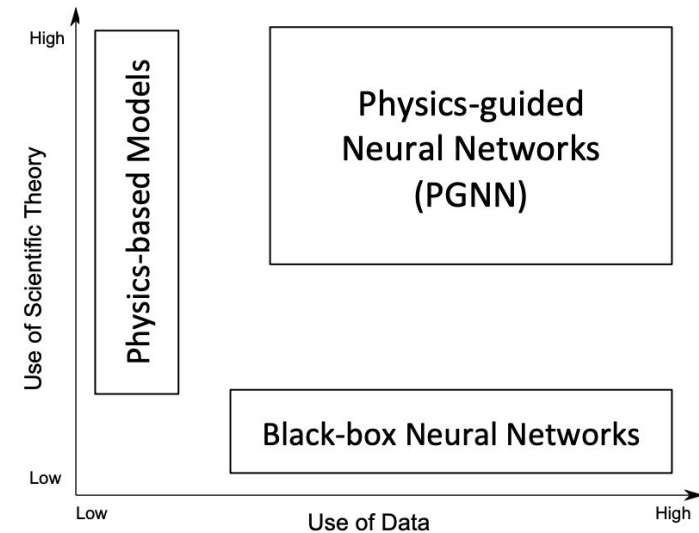
Physics-guided Neural Networks (PGNN)

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

$$\min_{\theta} \underbrace{L(\mathbf{y}, \hat{\mathbf{y}})}_{\text{Empirical Error}} + \underbrace{\lambda_{PHY} L_{PHY}(\hat{\mathbf{y}})}_{\text{Physics-Loss}}$$

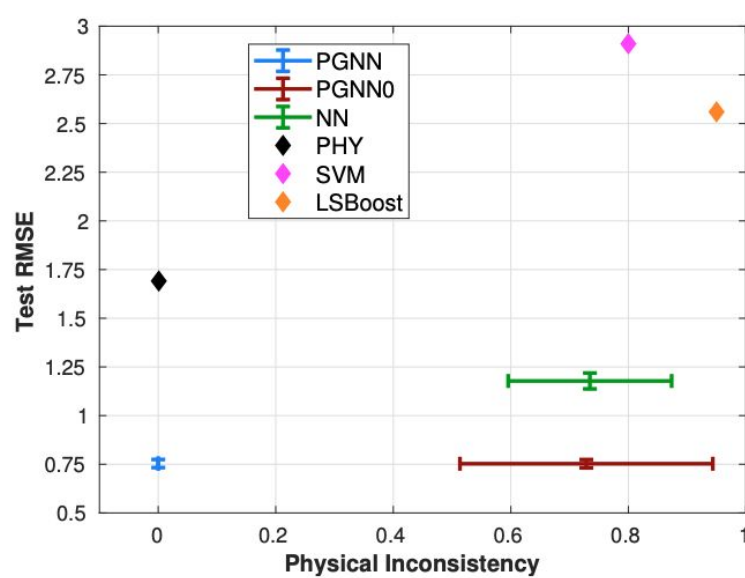


- **Easy to use:** Constraints can be easily incorporated as physics loss functions.
- **Unsupervised:** Physics loss functions can be evaluated on unlabeled data.

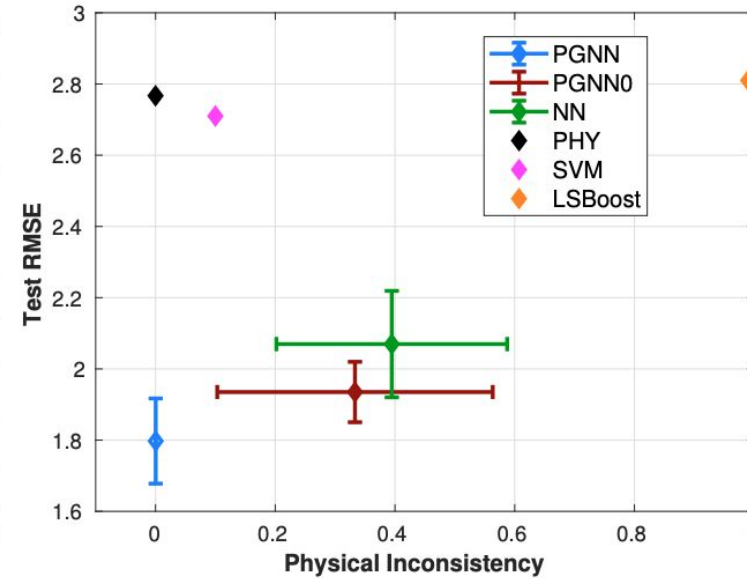


PGNN shows improved generalization

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



(a) Results on Mille Lacs Lake



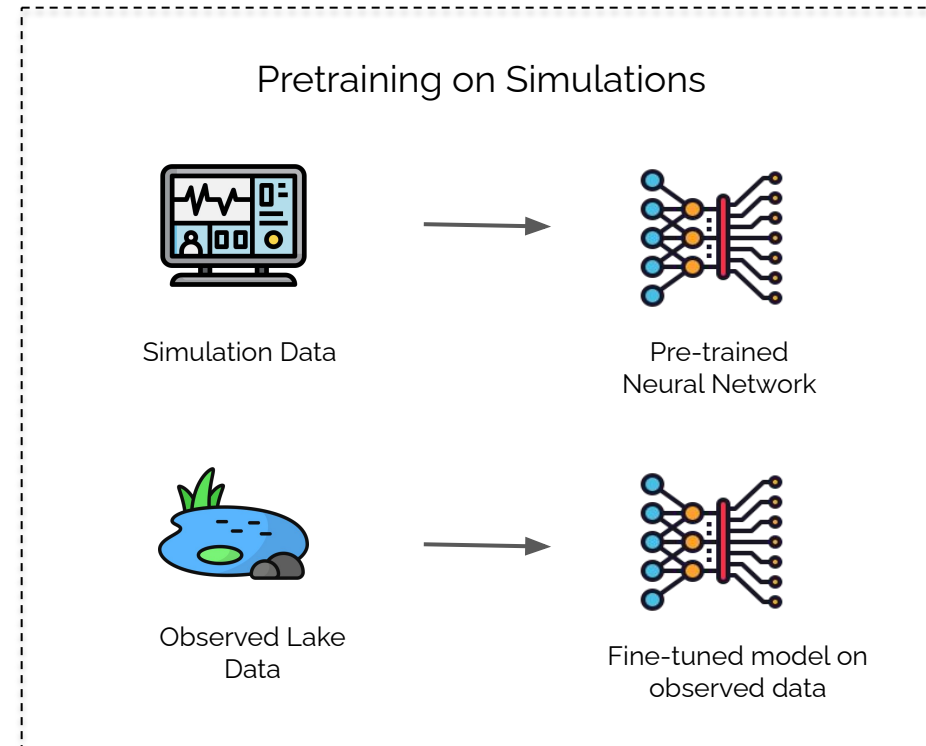
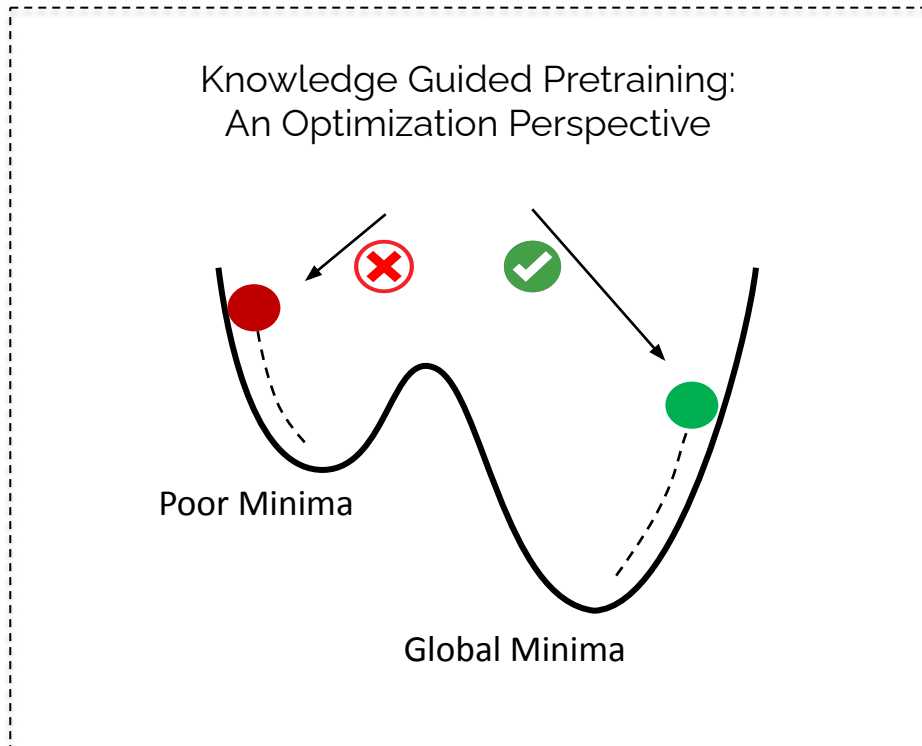
(b) Results on Lake Mendota



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

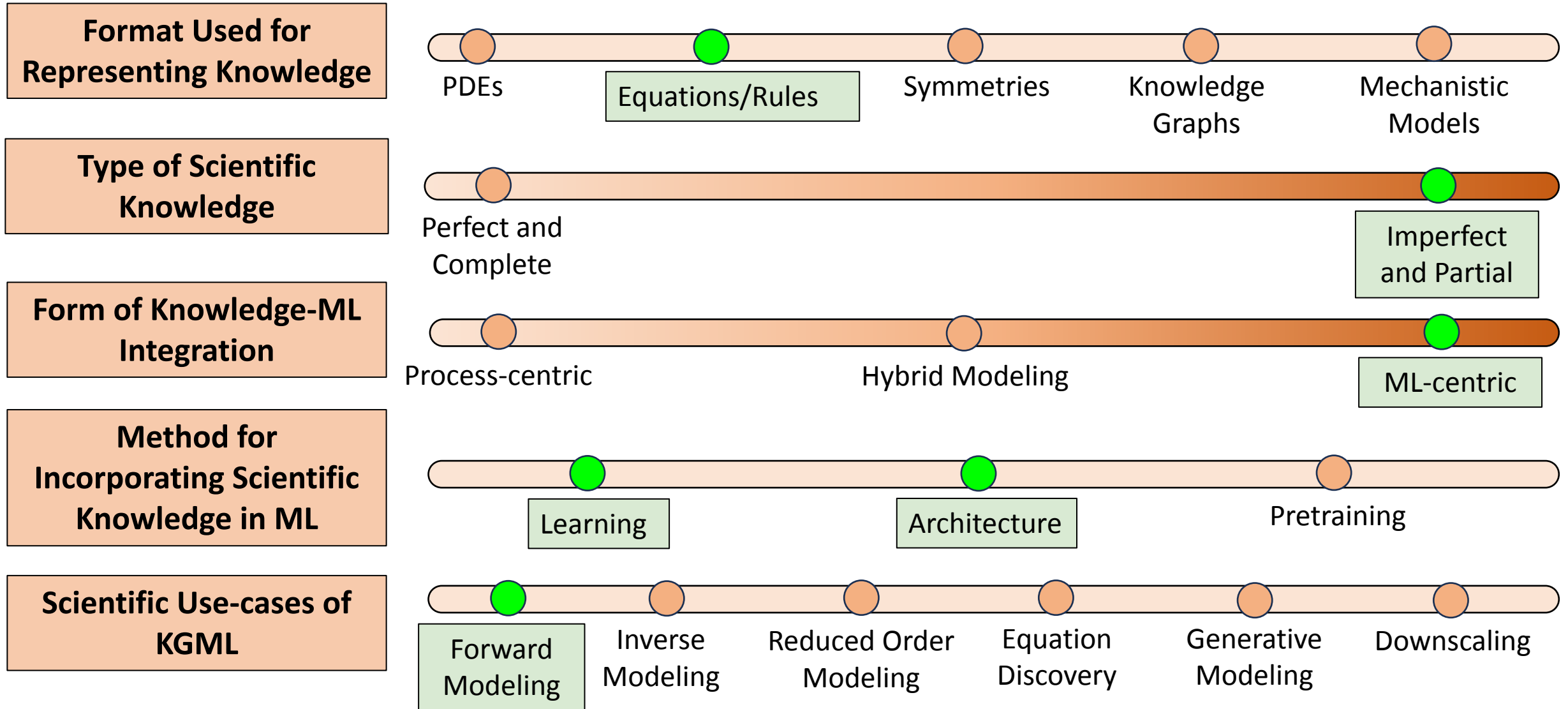
Pretraining on Simulation Lakes

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

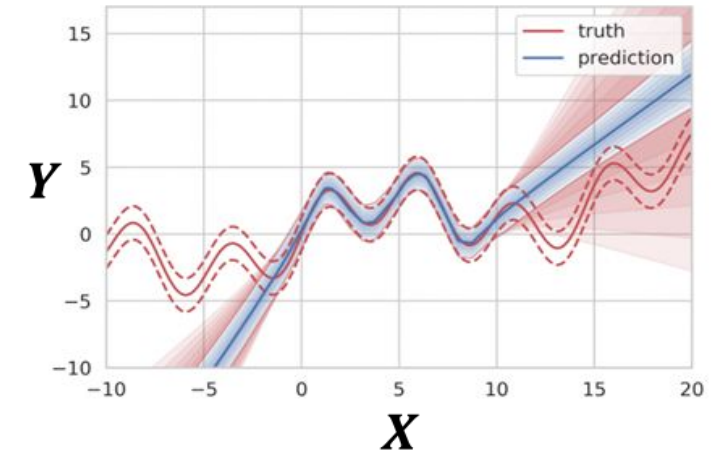


Uncertainty Quantification

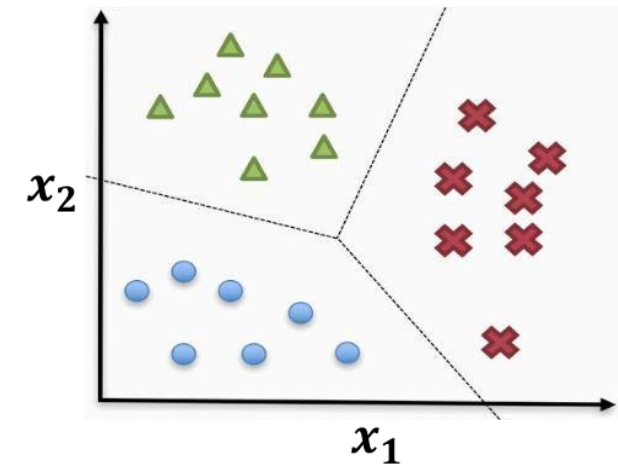


Generate a **distribution** over the predictions rather than point estimates.

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

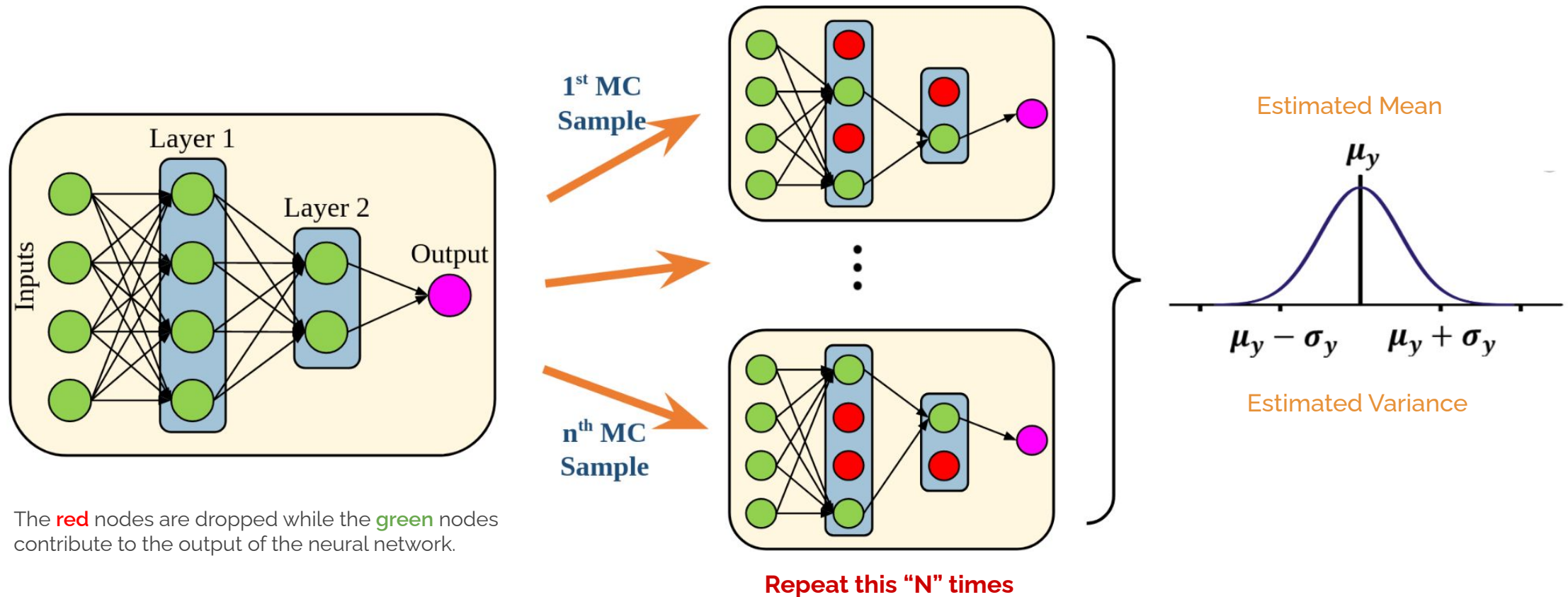


Aims to quantify the **robustness** of the ML models by assessing prediction reliability.

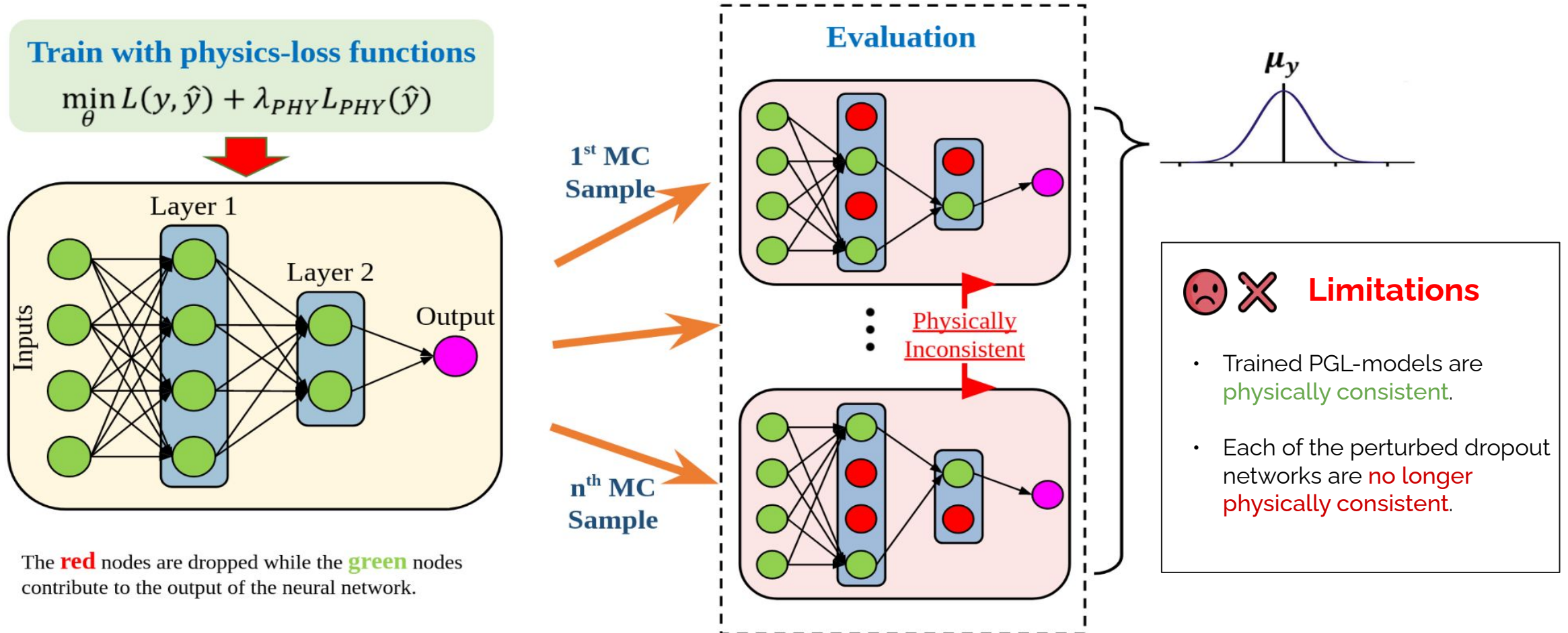


Uncertainty Quantification with MC Dropout

A schematic representation of using Dropouts to estimate uncertainty.

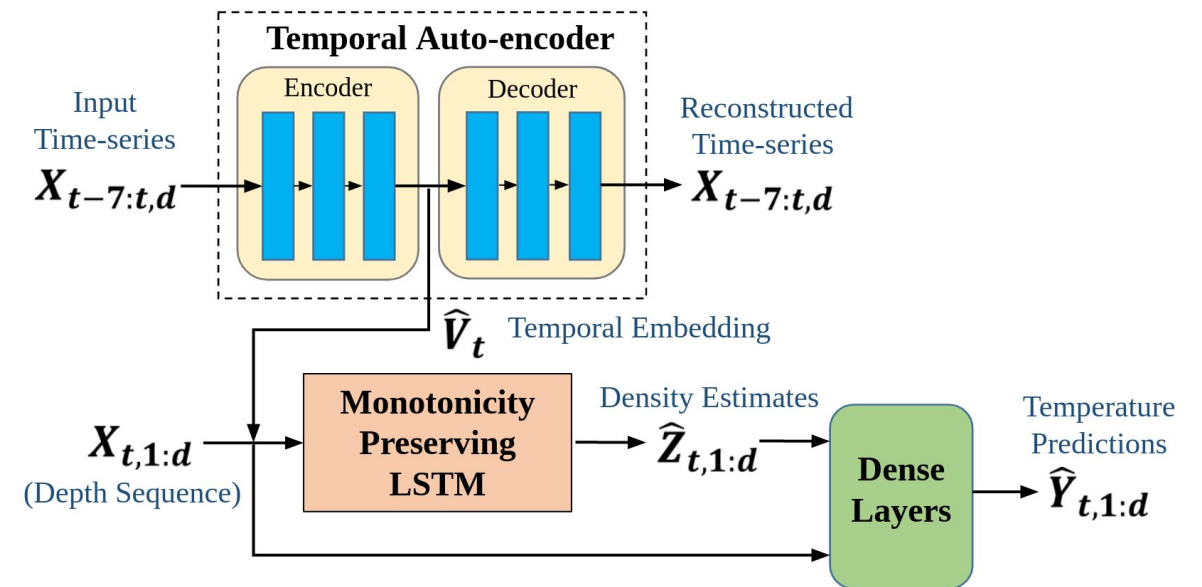


Approach 1: Dropouts with Physics-based Loss

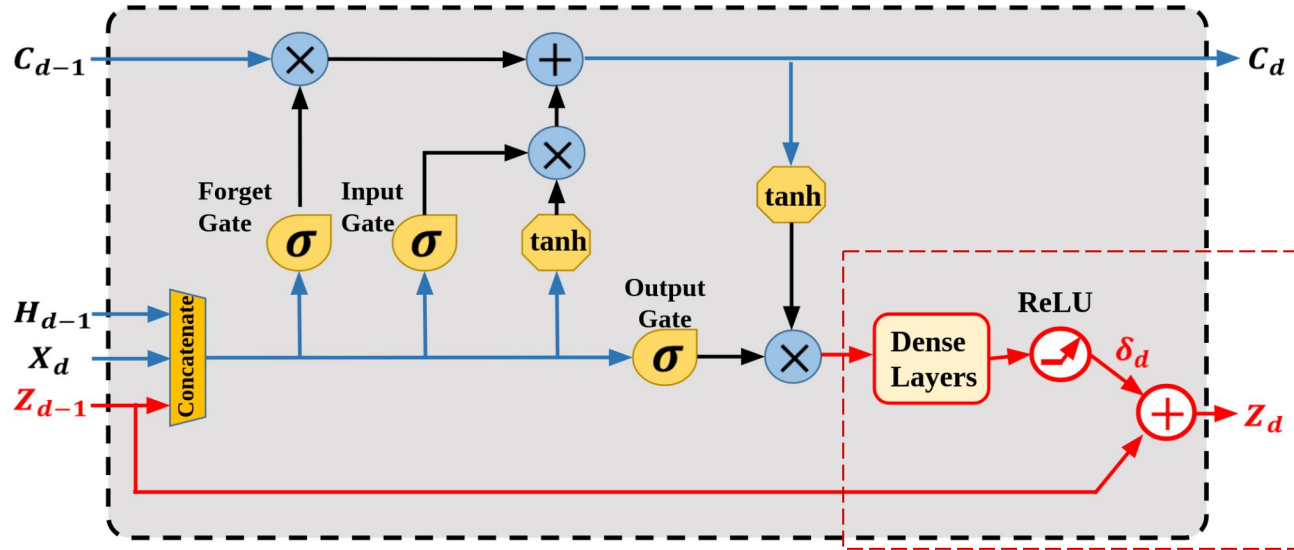


Proposed PGA-LSTM Framework

- **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



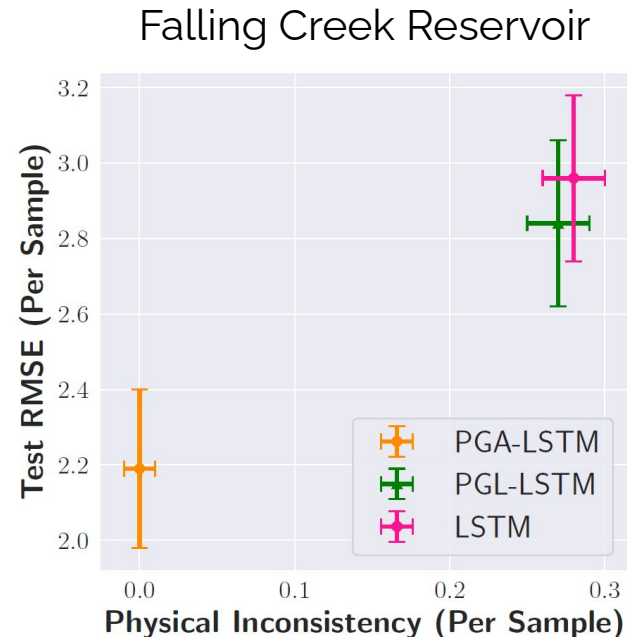
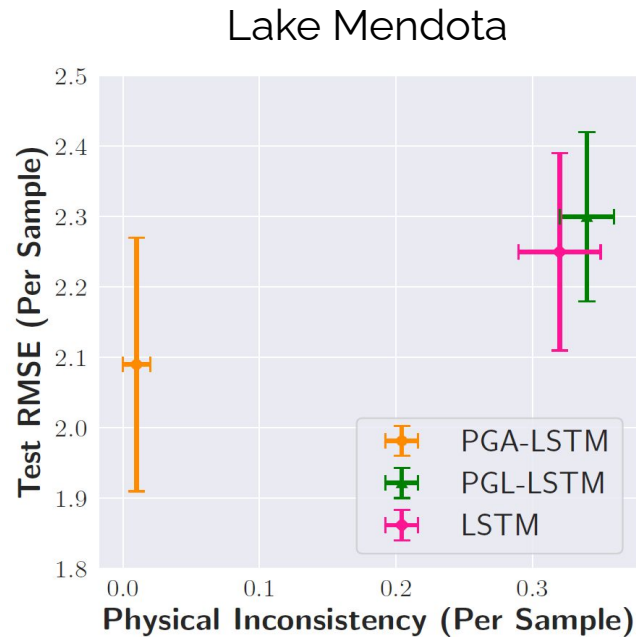
Key Idea


The **ReLU function** ensures that the residual outputs are **non-negative**, thus enforcing the monotonicity constraint.

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



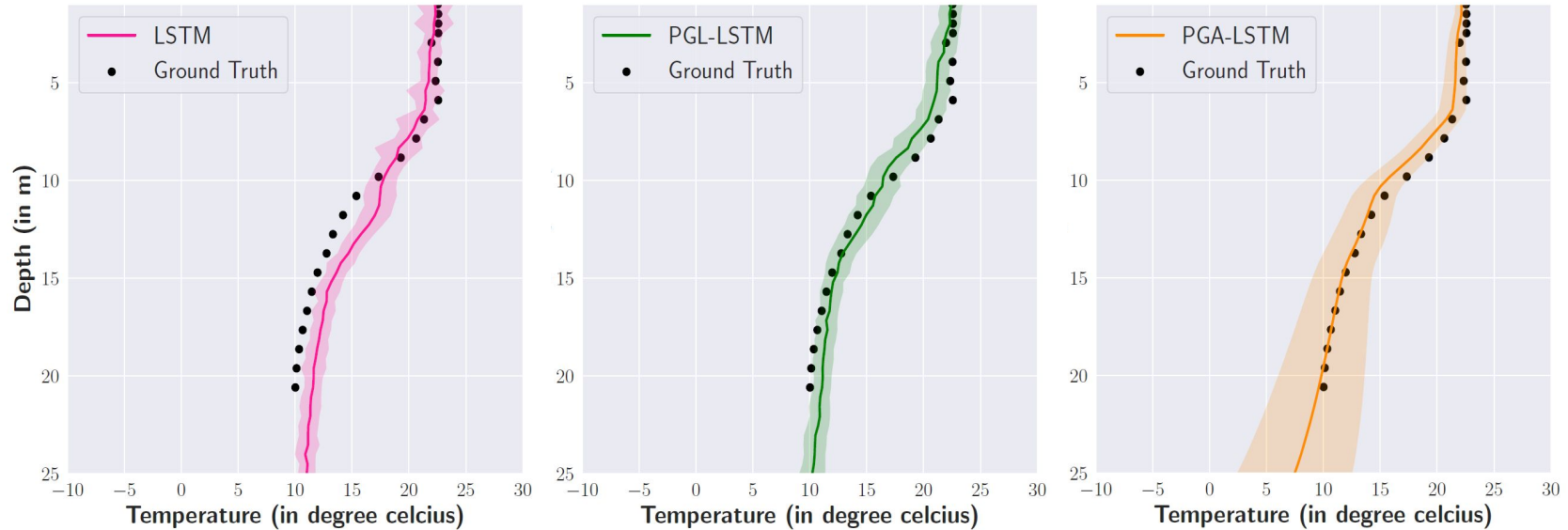
 **Evaluation Metrics**

- Test RMSE \Downarrow
- Physical Inconsistency \Downarrow



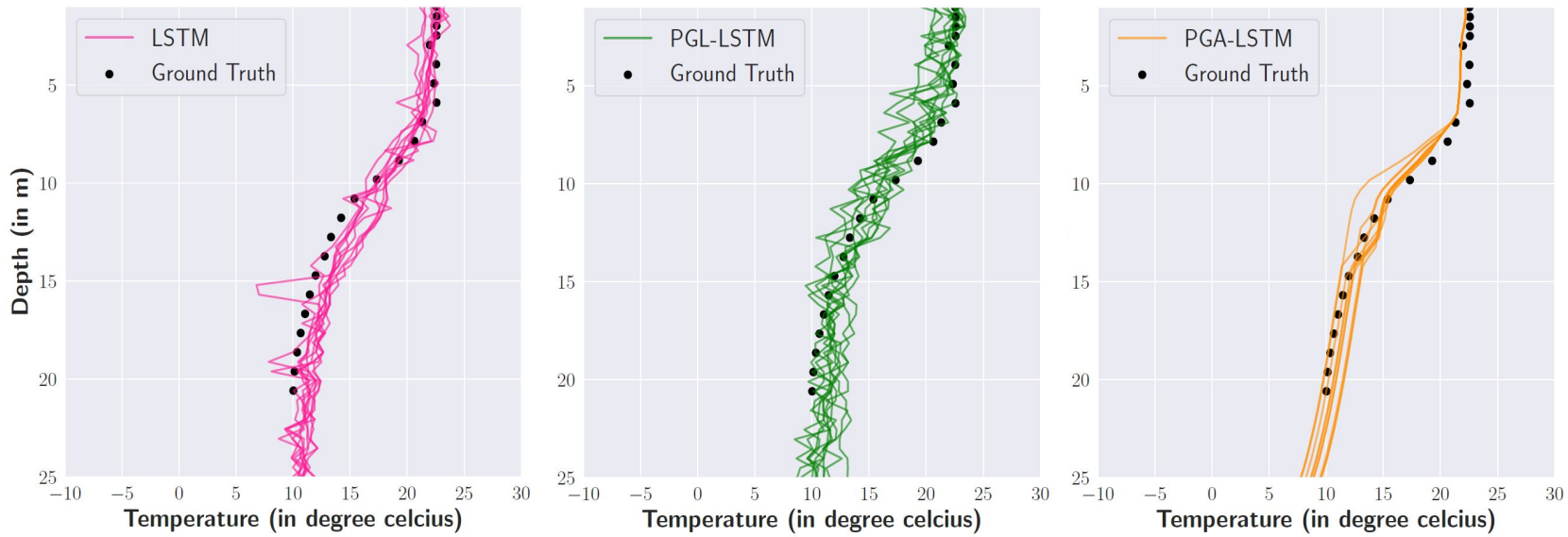
PGA-LSTM improves the Test RMSE while always being physically consistent across both lakes.

Monotonicity Preserving LSTM



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

Monotonicity Preserving LSTM



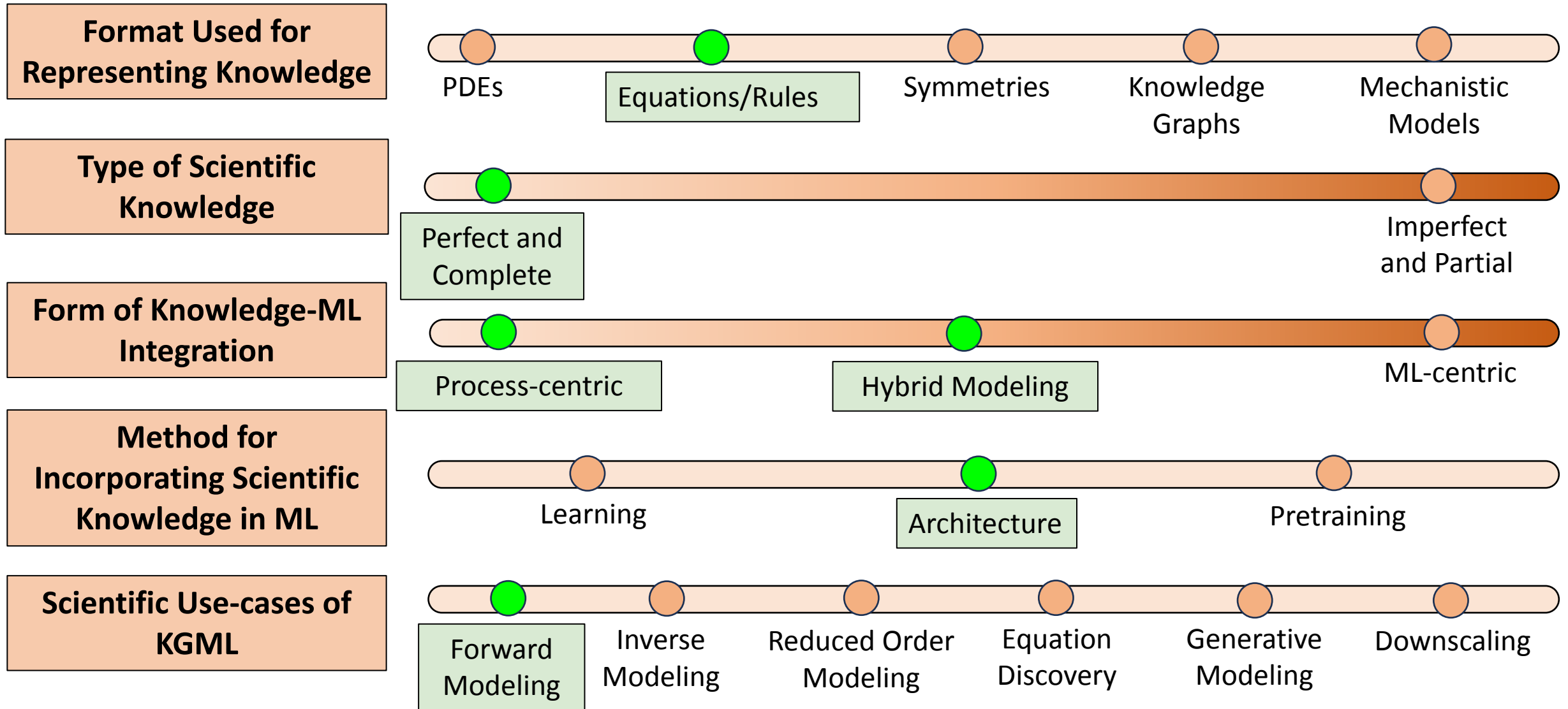
The PGA-LSTM samples are always physically consistent while PGL-LSTM and LSTM samples are very much physically inconsistent.



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

Use Case 3: Hybrid Modeling

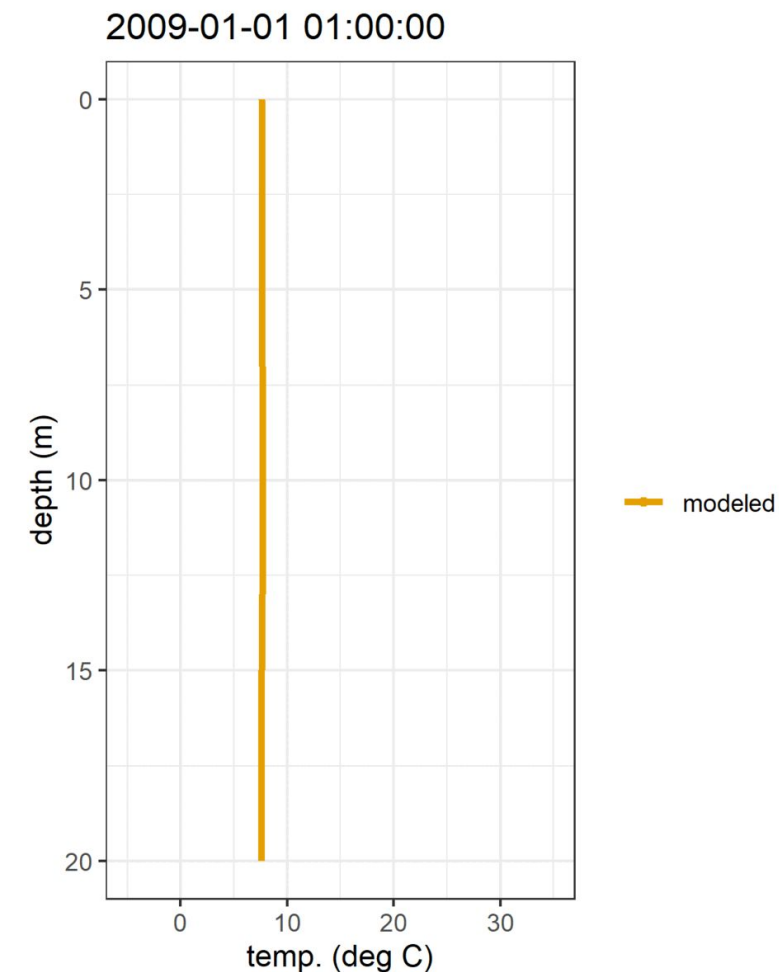
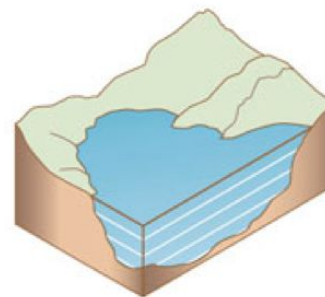
Organizing KGML Research: A Multi-Dimensional View



Process-based Modeling

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

1D: One-dimensional



Process-based Modeling

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

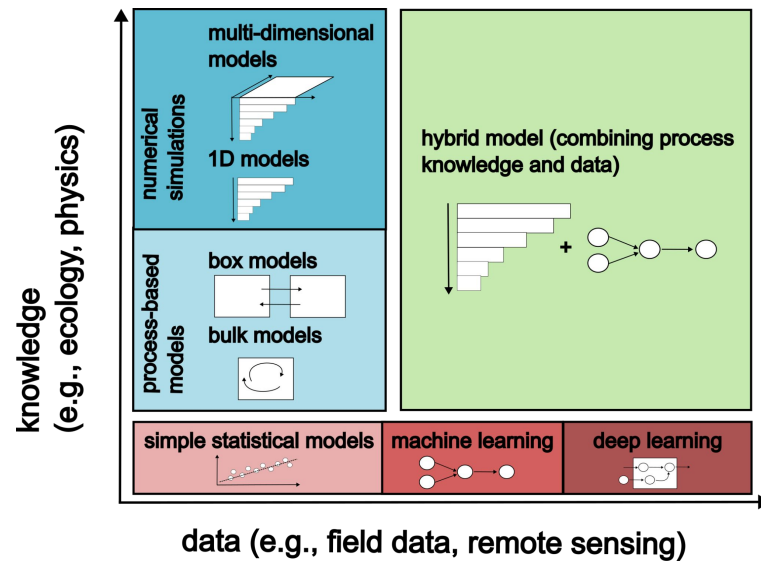
1D: One-dimensional



2009-01-01 01:00:00



Can we combine these process models with data?



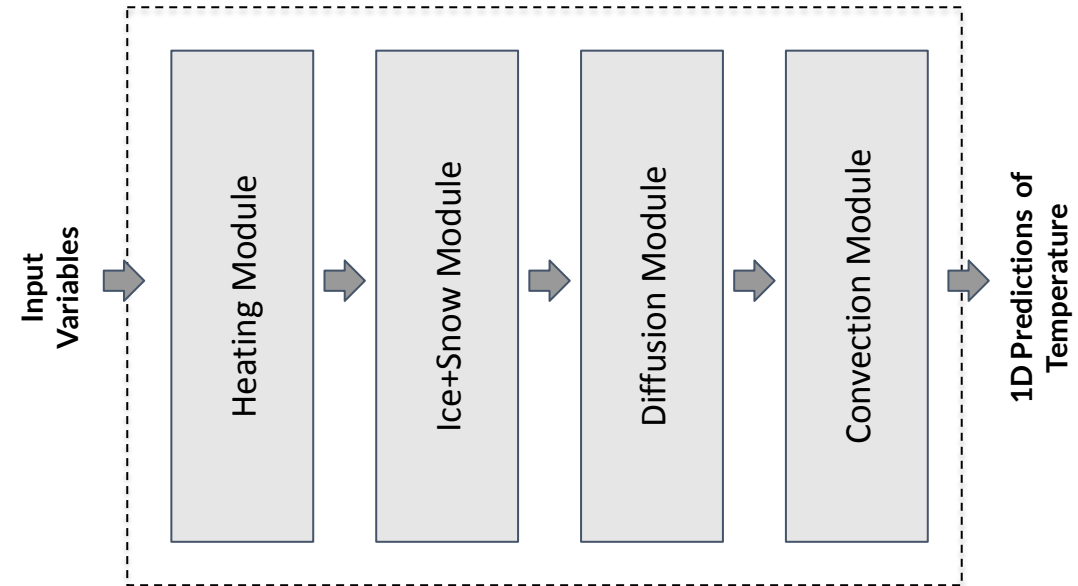
Modularized 1D Model

Modularized Process Models:

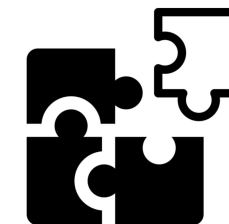
- a) heating (atmosphere and geothermal)
- b) ice, snow and snow-ice formation
- c) vertical diffusion
- d) convective overturn

☹️ ❌ **CONS**

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



Modular Compositional Learning (MCL)

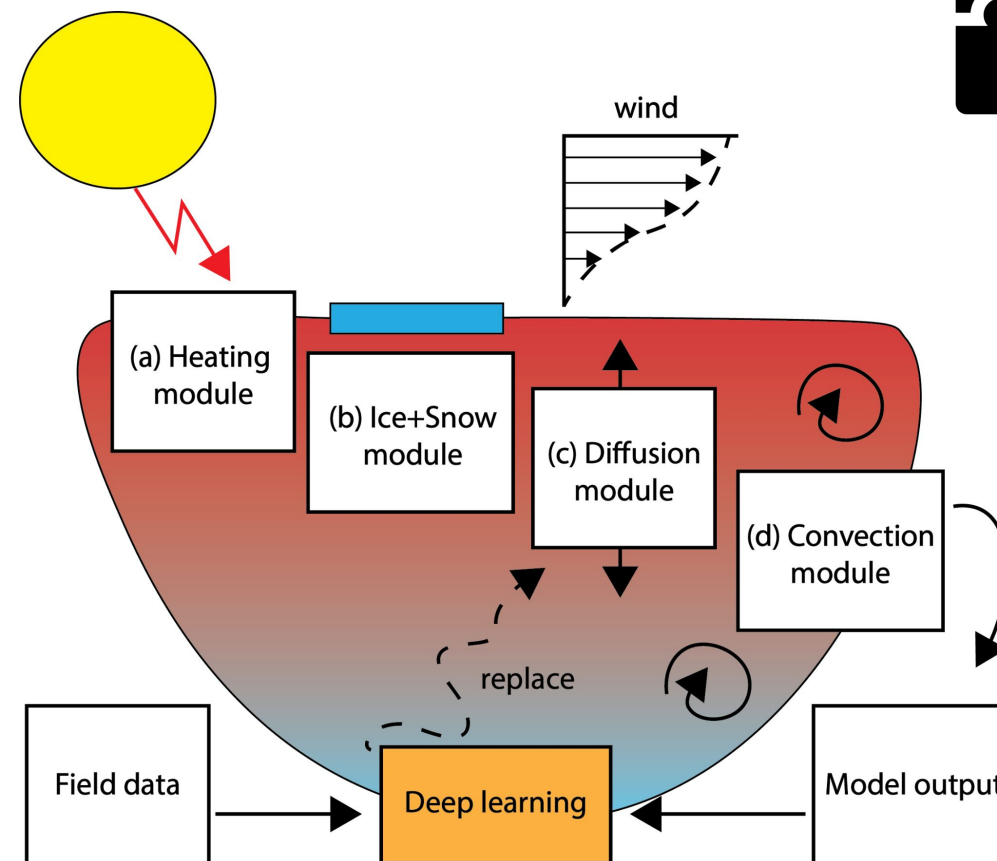


Imperfect Modules: Diffusion Module

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

😊 ✓ PROS

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



Modular Compositional Learning (MCL)

Process-based framework



Process-based, pretrained deep learning, finetuned deep learning

Robert Ladwig

Modular Compositional Learning (MCL)

Process-based framework



Pretraining



Process-based, pretrained deep learning, finetuned deep learning

Robert Ladwig

Modular Compositional Learning (MCL)

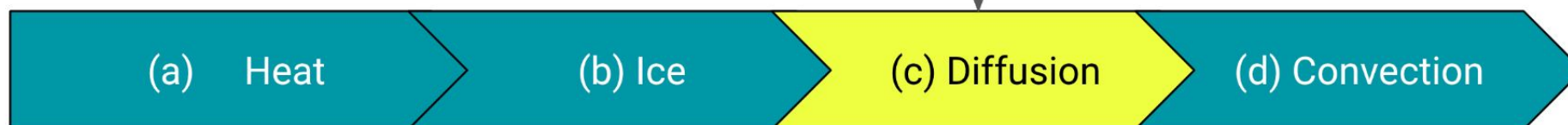
Process-based framework



Pretraining



Finetuning



Observed data

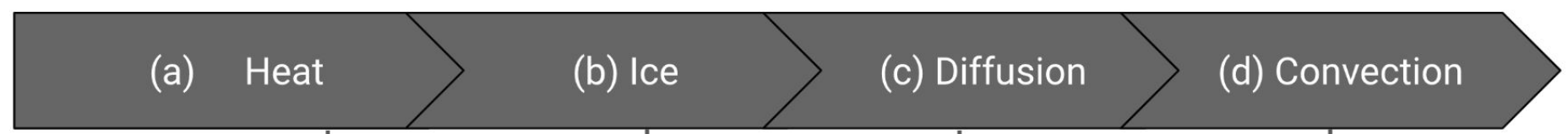


Process-based, pretrained deep learning, finetuned deep learning

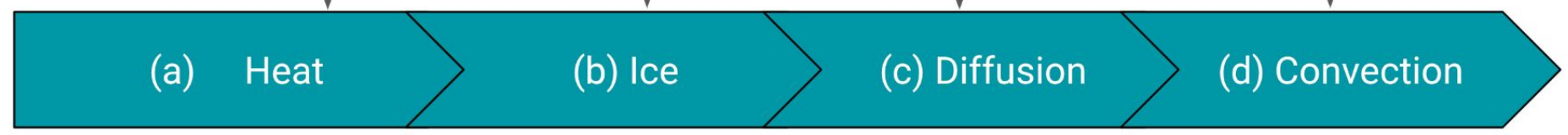
Robert Ladwig

Modular Compositional Learning (MCL)

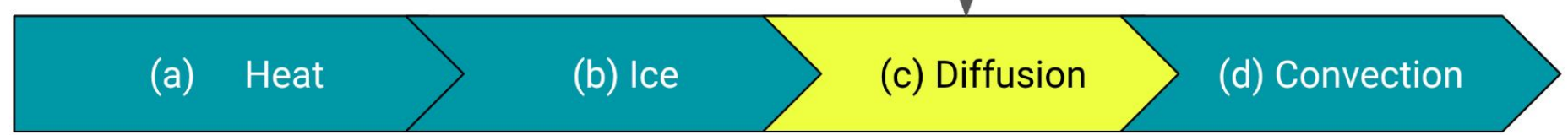
Process-based framework



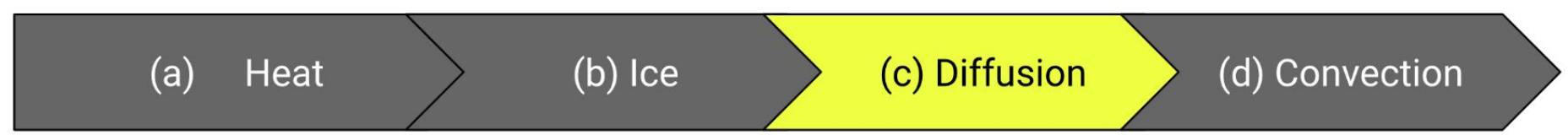
Pretraining



Finetuning



Hybrid framework



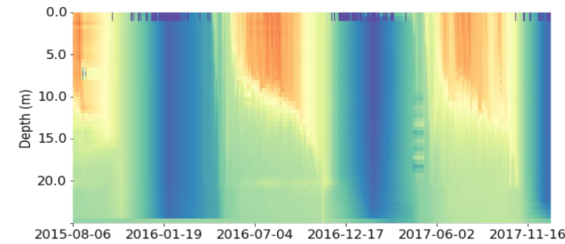
Process-based, pretrained deep learning, finetuned deep learning

Robert Ladwig

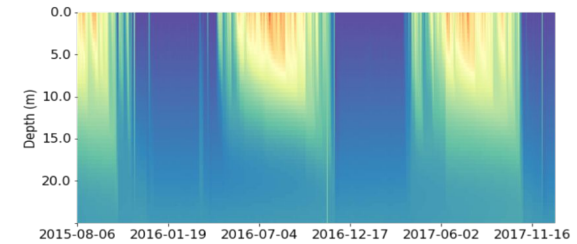
Empirical Evaluation (Test Period 2015-17)

Comparing Observed Data and Processed-based model

A Observed data

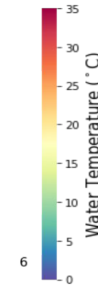
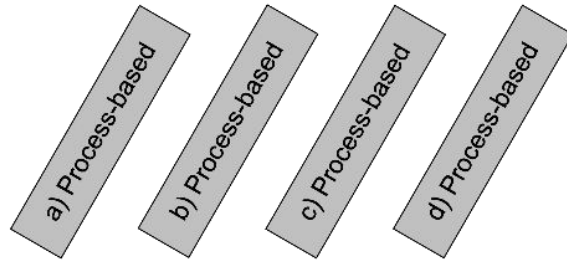


D Process-based framework



Test RMSE: 4.46

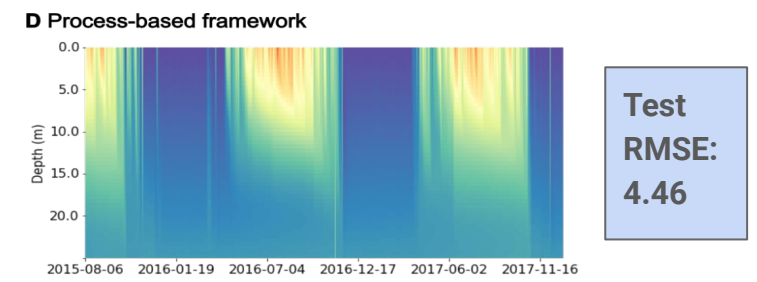
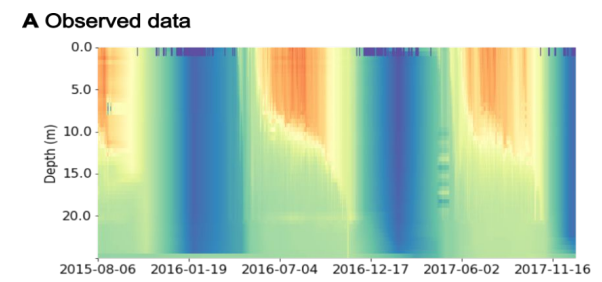
1 Process-based model framework



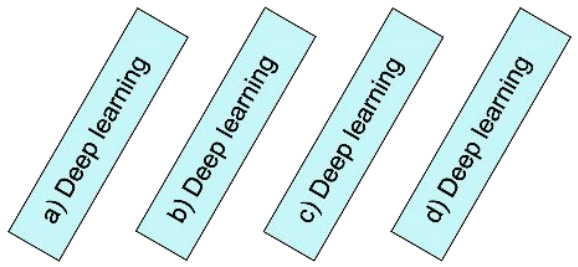
Empirical Evaluation (Test Period 2015-17)

Comparing the models:

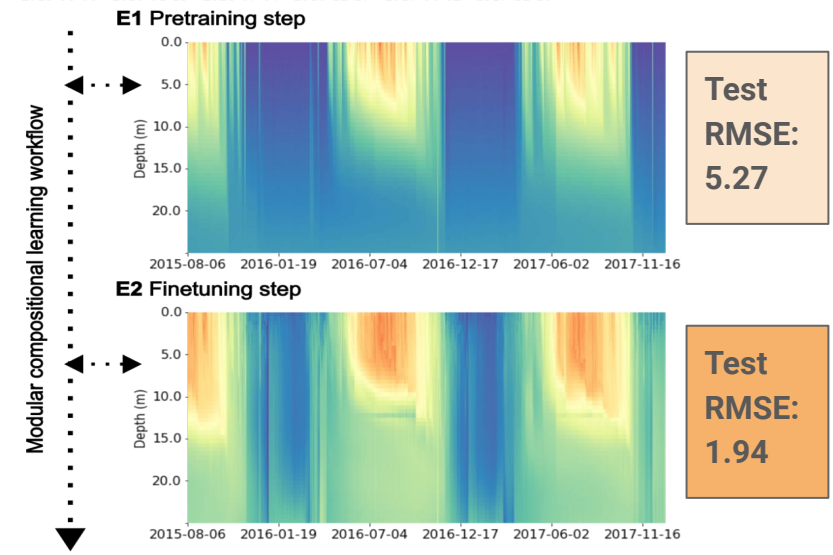
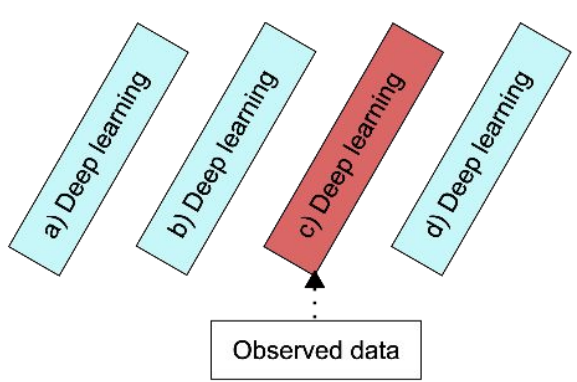
1. After pretraining each of the deep learning models on simulation data.
2. Finetuning the entire deep learning pipeline on observed data.



2 Pretrained deep learning framework



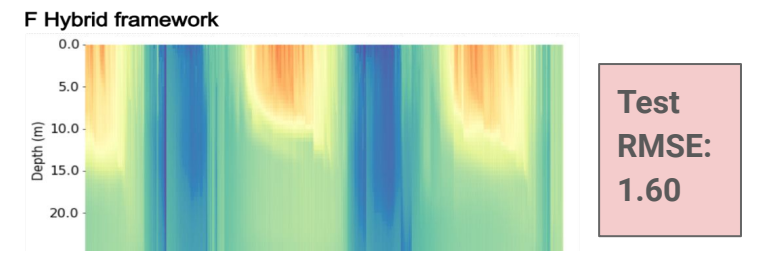
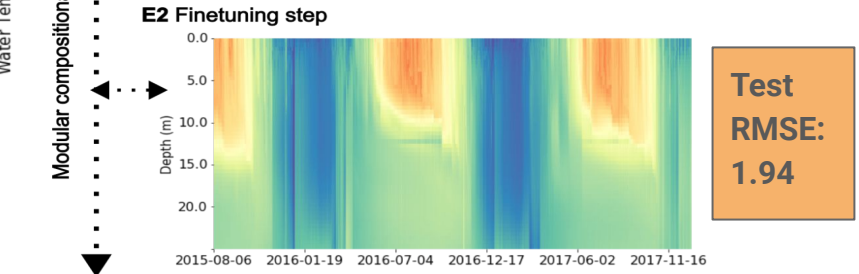
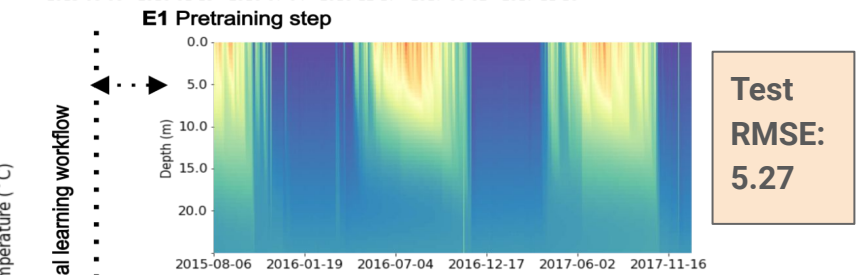
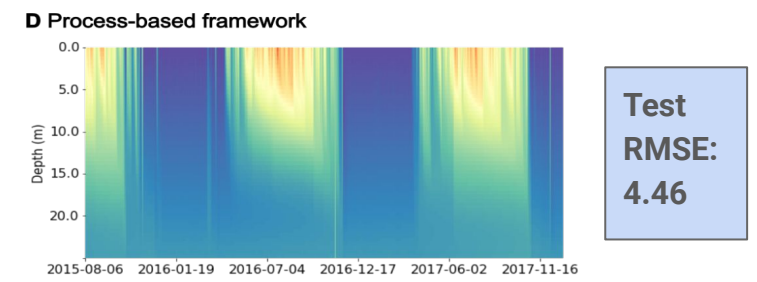
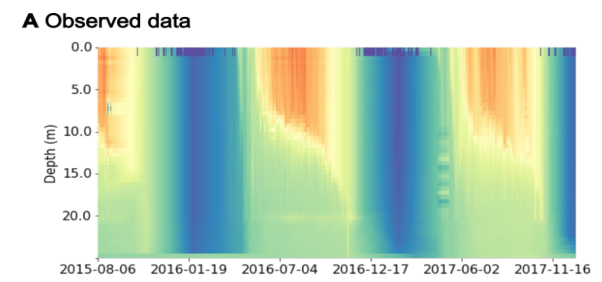
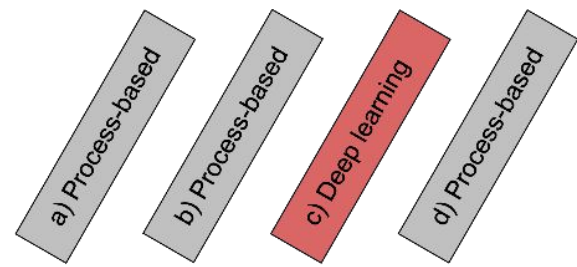
3 Finetuned deep learning framework



Empirical Evaluation (Test Period 2015-17)

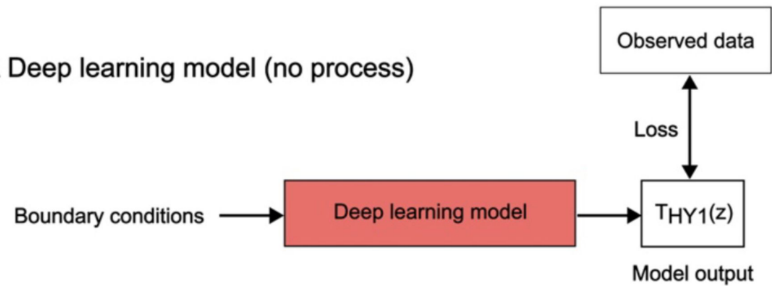
Plugging the deep-learning module into the process-based module pipeline.

4 Hybrid model framework



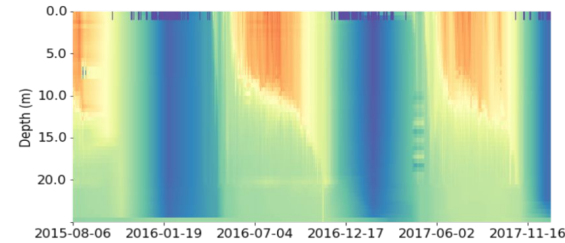
Empirical Evaluation (Test Period 2015-17)

A Deep learning model (no process)

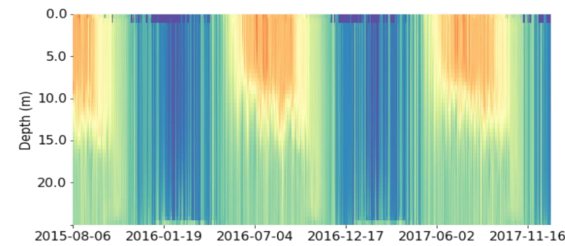


Test RMSE: 2.10

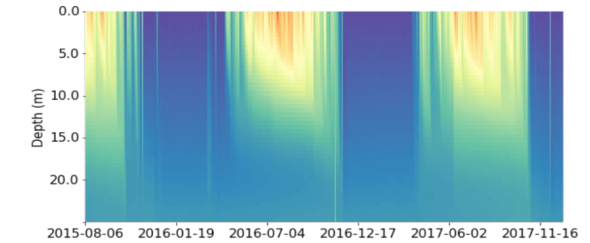
A Observed data



B Deep learning model (no process)

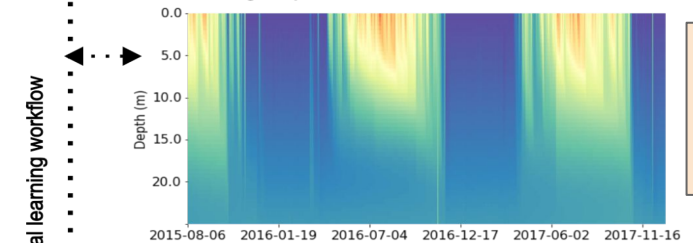


D Process-based framework



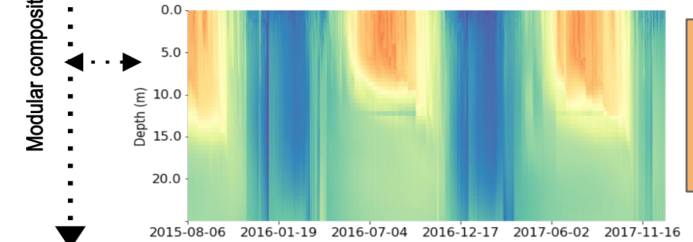
Test RMSE: 4.46

E1 Pretraining step



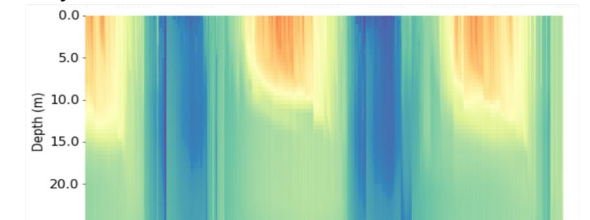
Test RMSE: 5.27

E2 Finetuning step



Test RMSE: 1.94

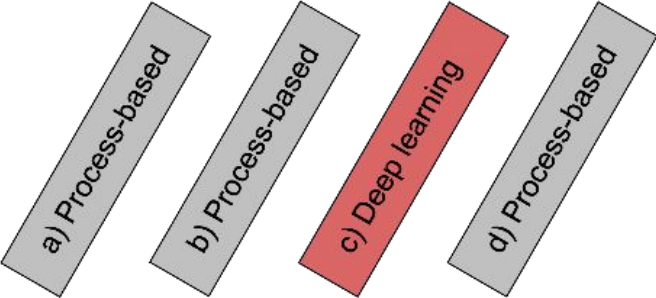
F Hybrid framework



Test RMSE: 1.60

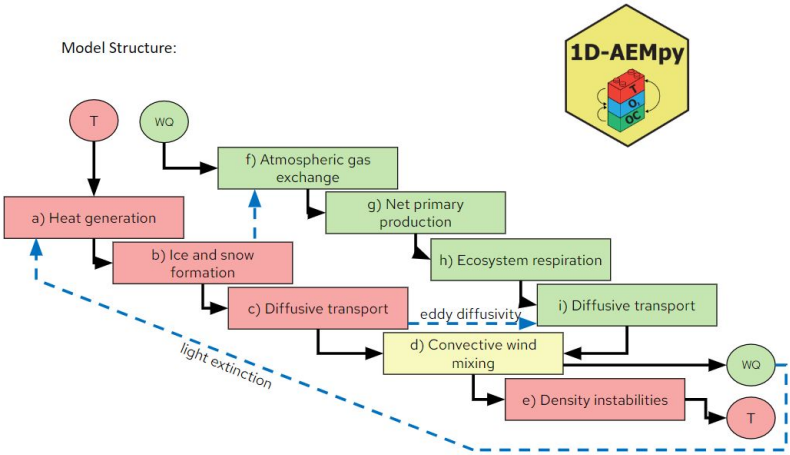
Current Work in MCL

4 Hybrid model framework



1D Lake Physics with MCL

1D Water Quality with MCL

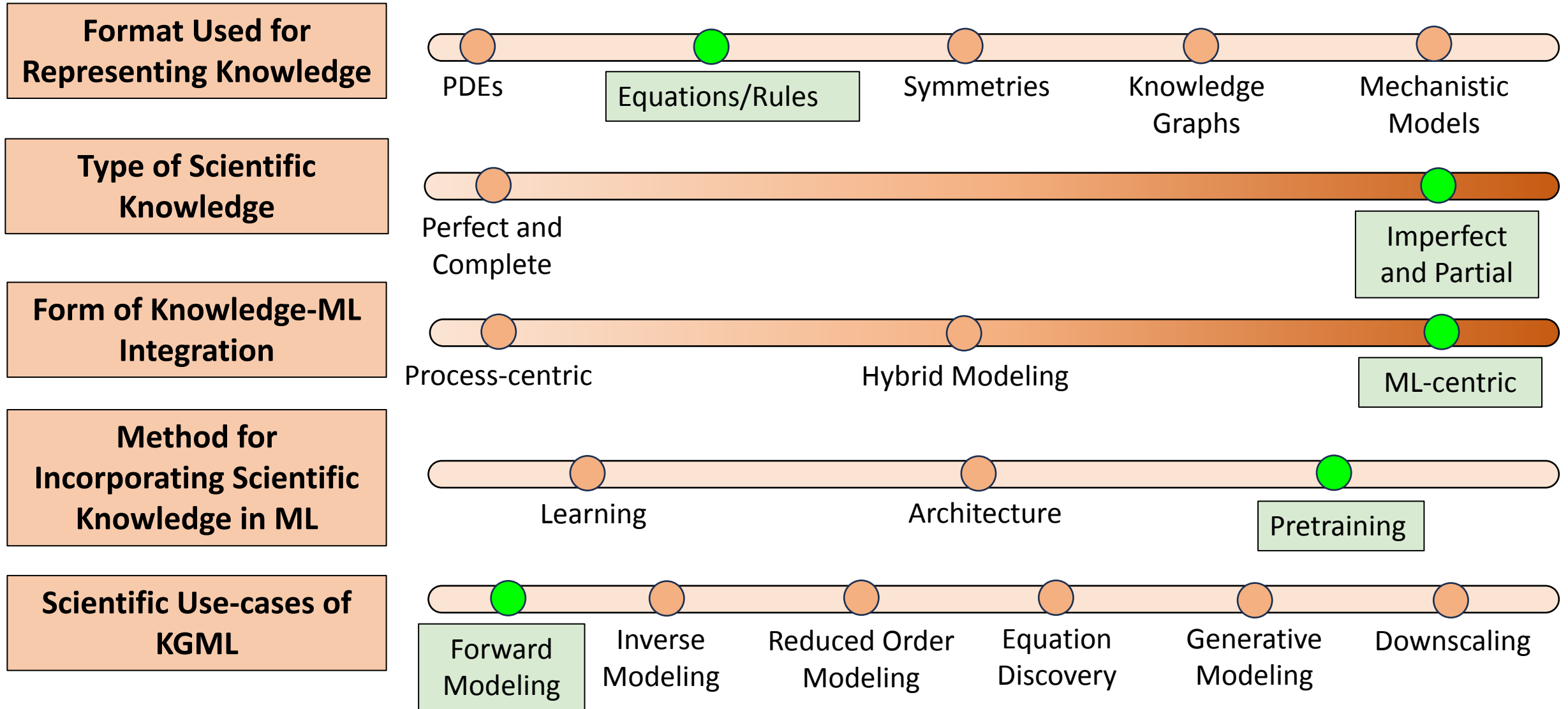


1D Lake Physics with MCL: memory for multiple lakes



Use Case 5: Lake Chlorophyll-a Prediction

Organizing KGML Research: A Multi-Dimensional View



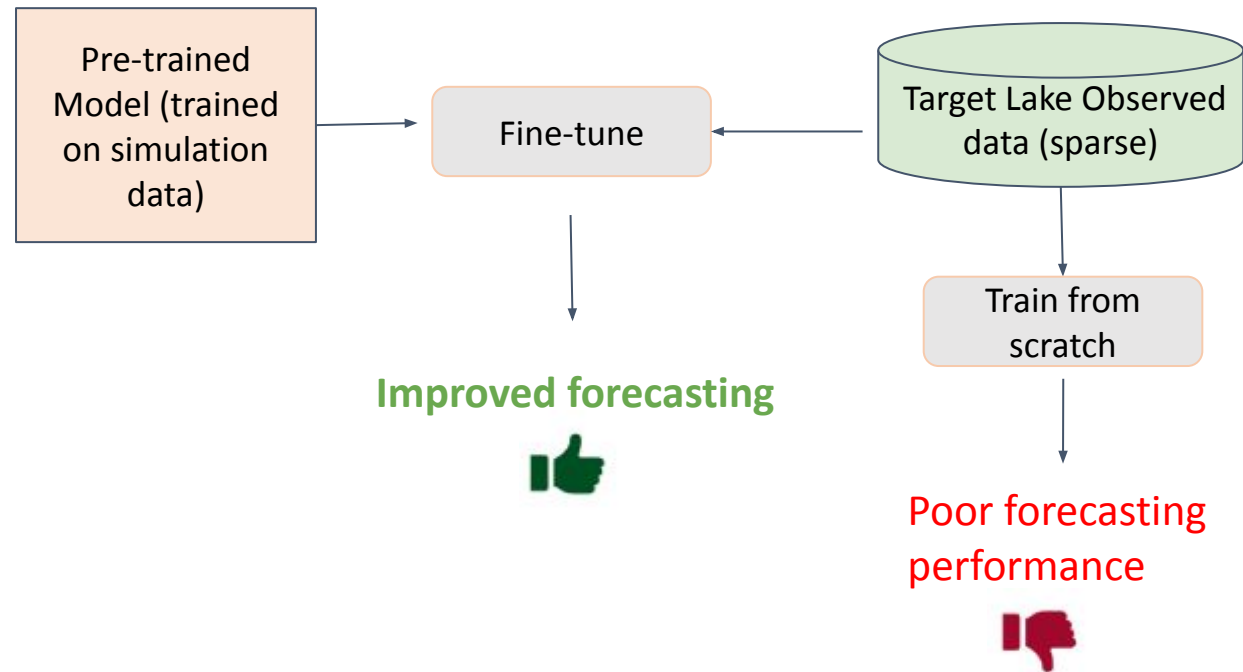
Transfer Learning for Chlorophyll-a Prediction

Problem Context:

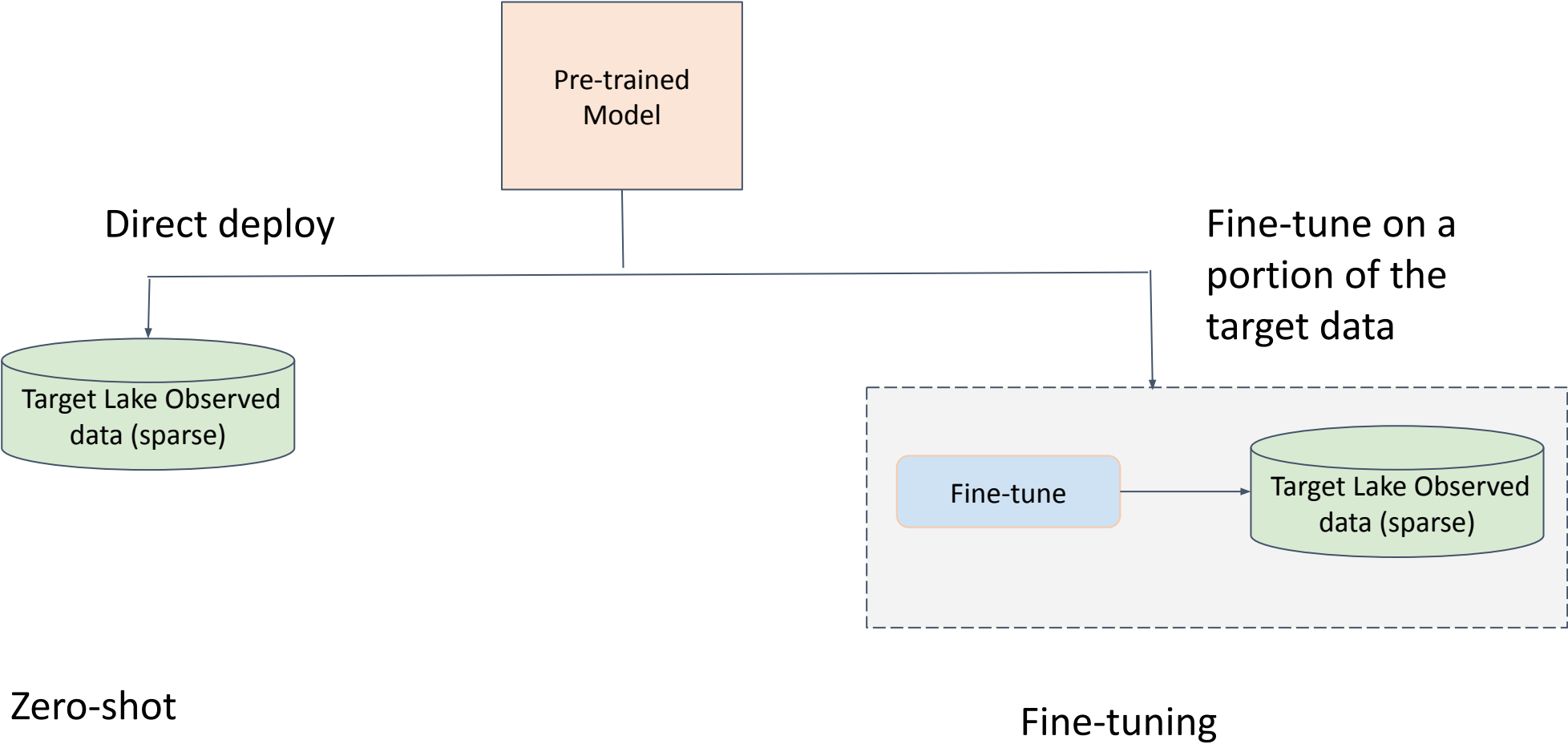
- Observations of chlorophyll-a vary across lakes, some being well-observed, others less-observed.
- Deep learning models are data-hungry, show poor forecasting performance on target lakes with sparse data.

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

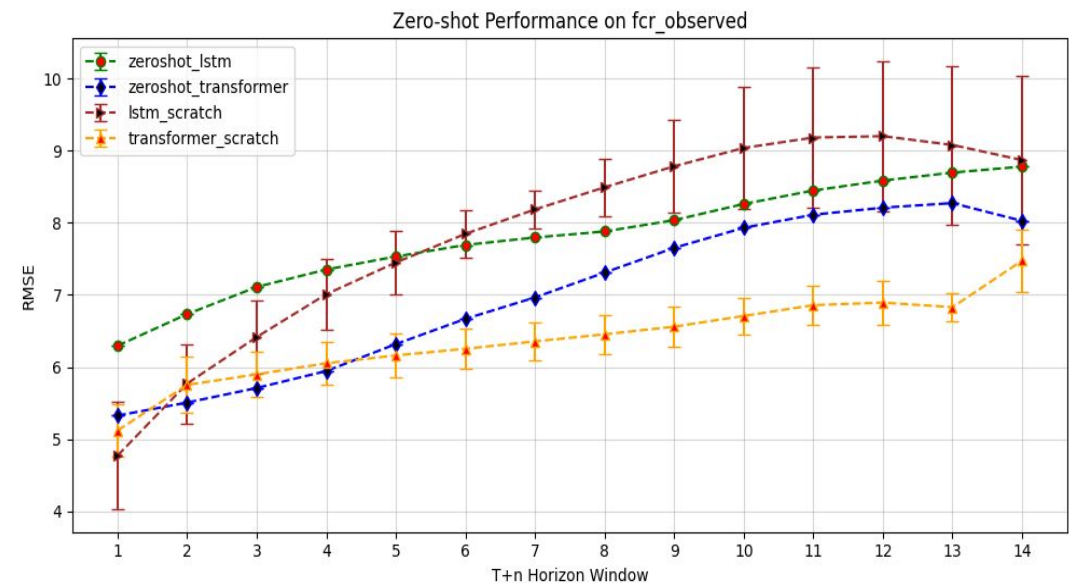
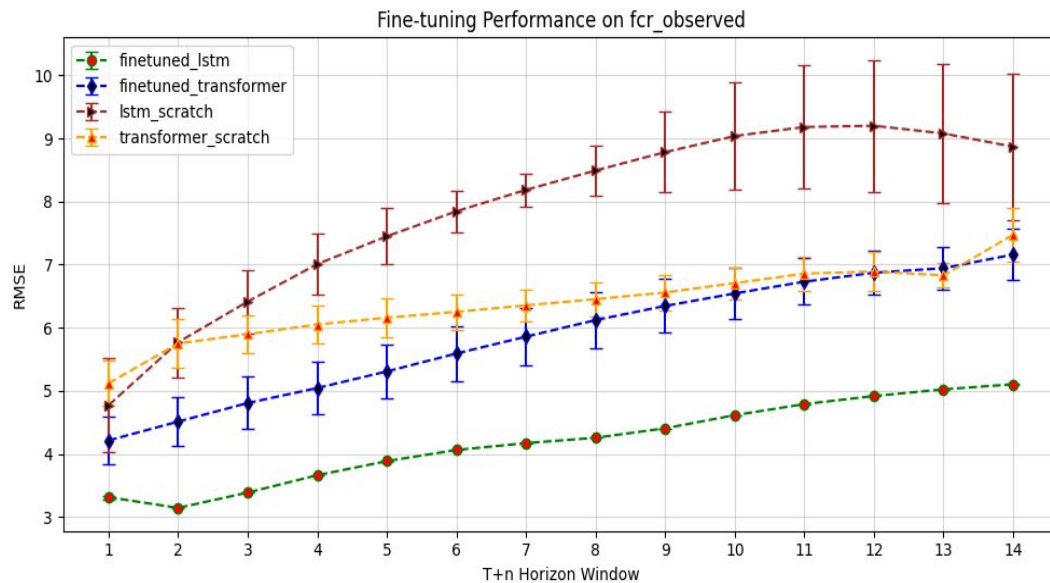
Problem Setup

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. (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

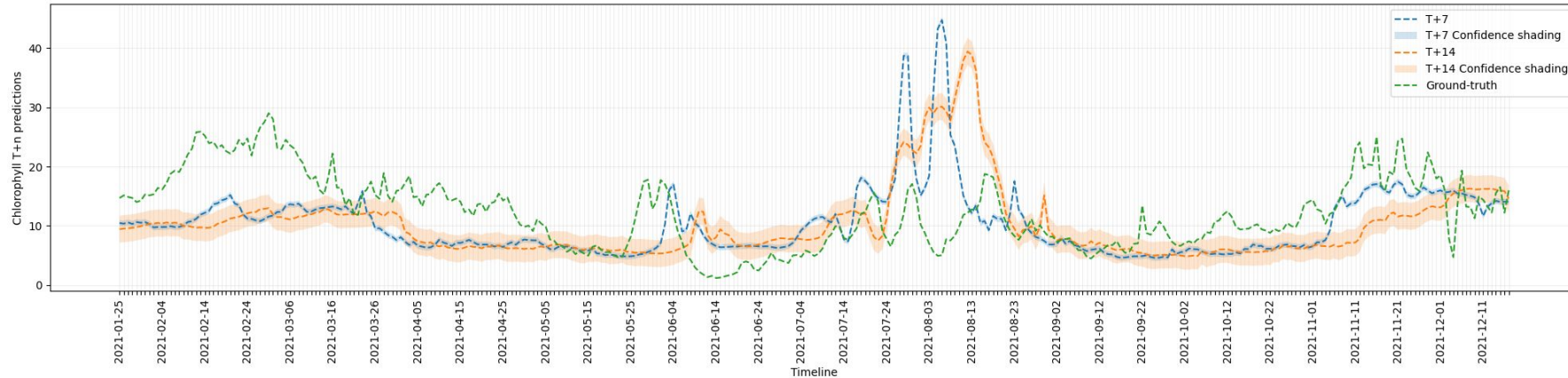
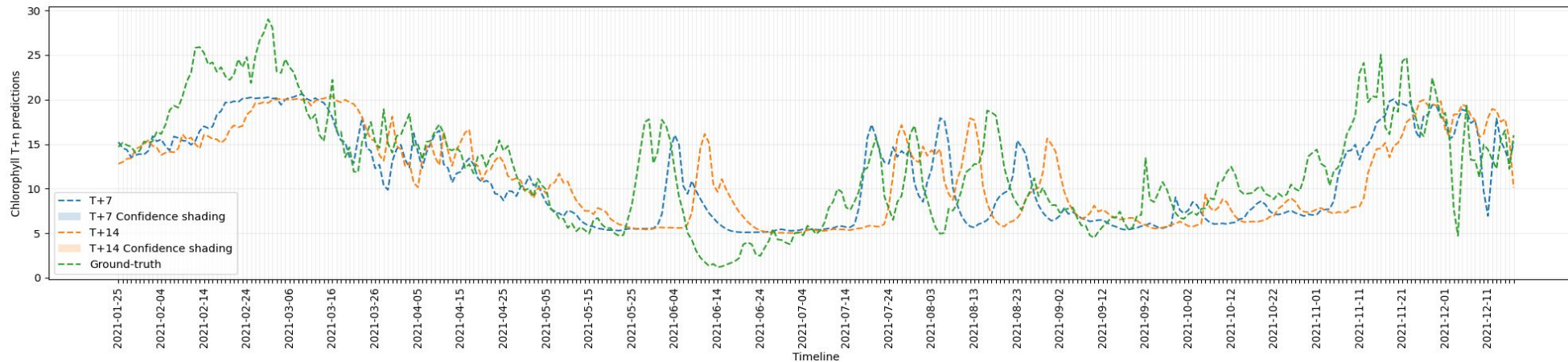


Fig. 1 Predictions on FCR observed Test portion - Model trained from scratch

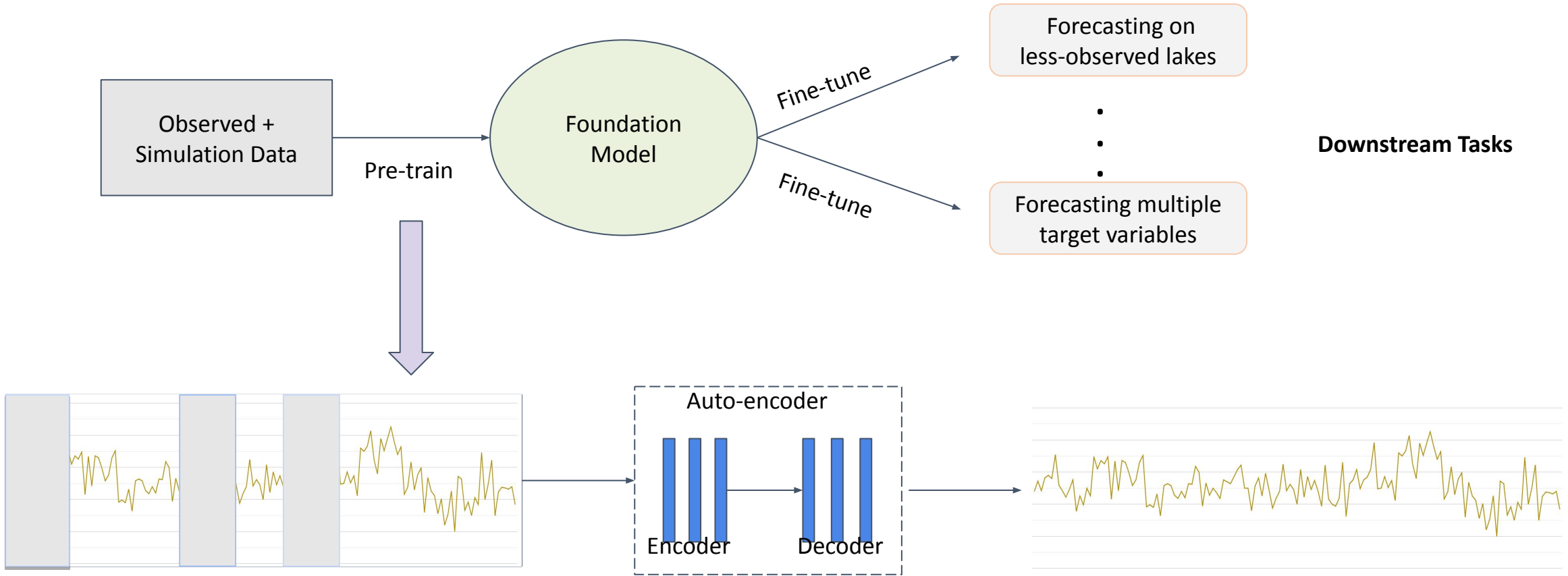
- Fine-tuned model aligns with the ground-truth scale of chlorophyll data
- Fine-tuned model shows relatively more confident predictions



LSTM model

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

Towards a Foundation Model



Learning Time-series representation