A Deep-Learning Recursive Multi-Step Approach for Prediction of Reactive Dissolution in Porous Media

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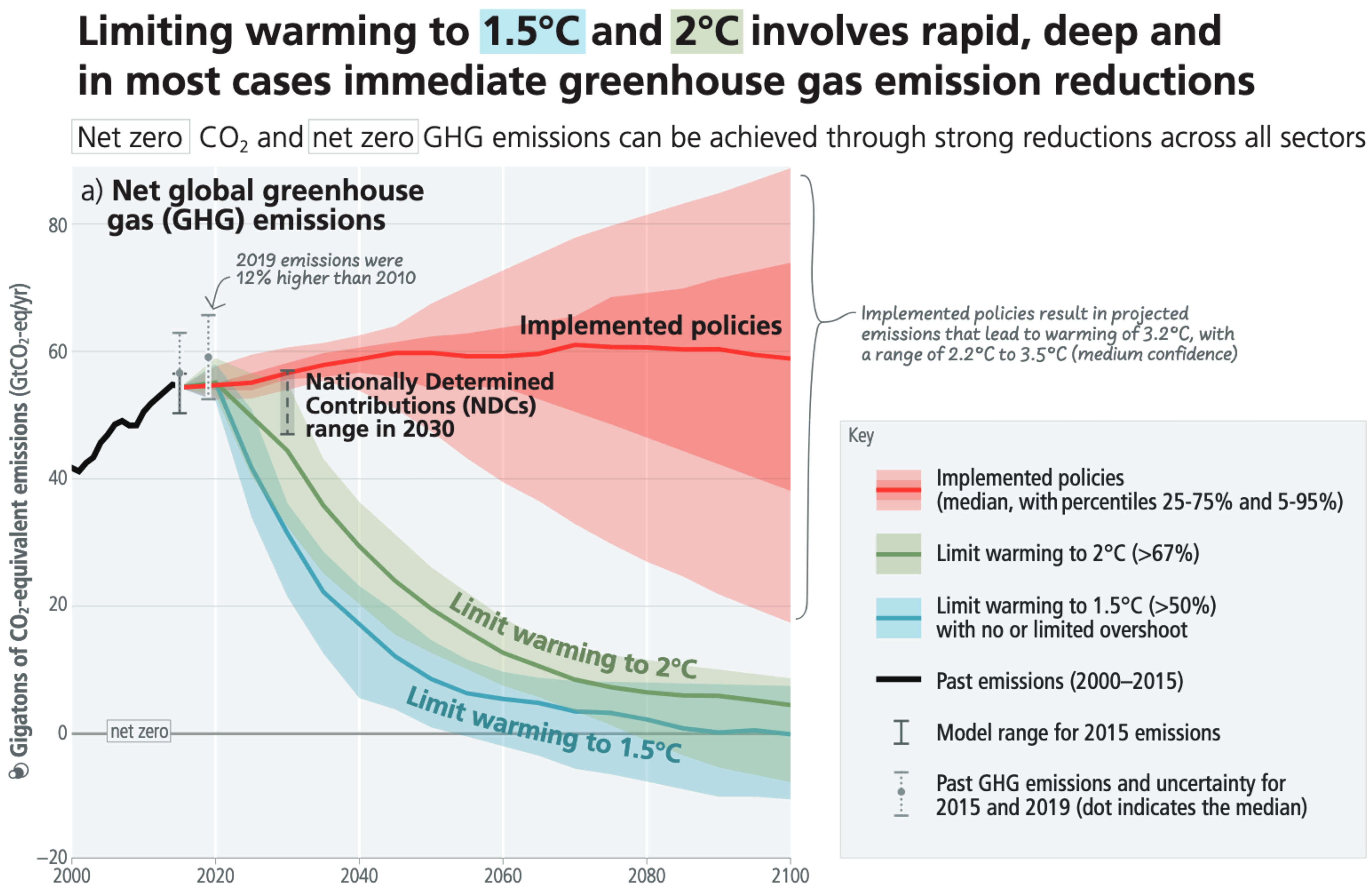
HERIOT WATT UNIVERSITY

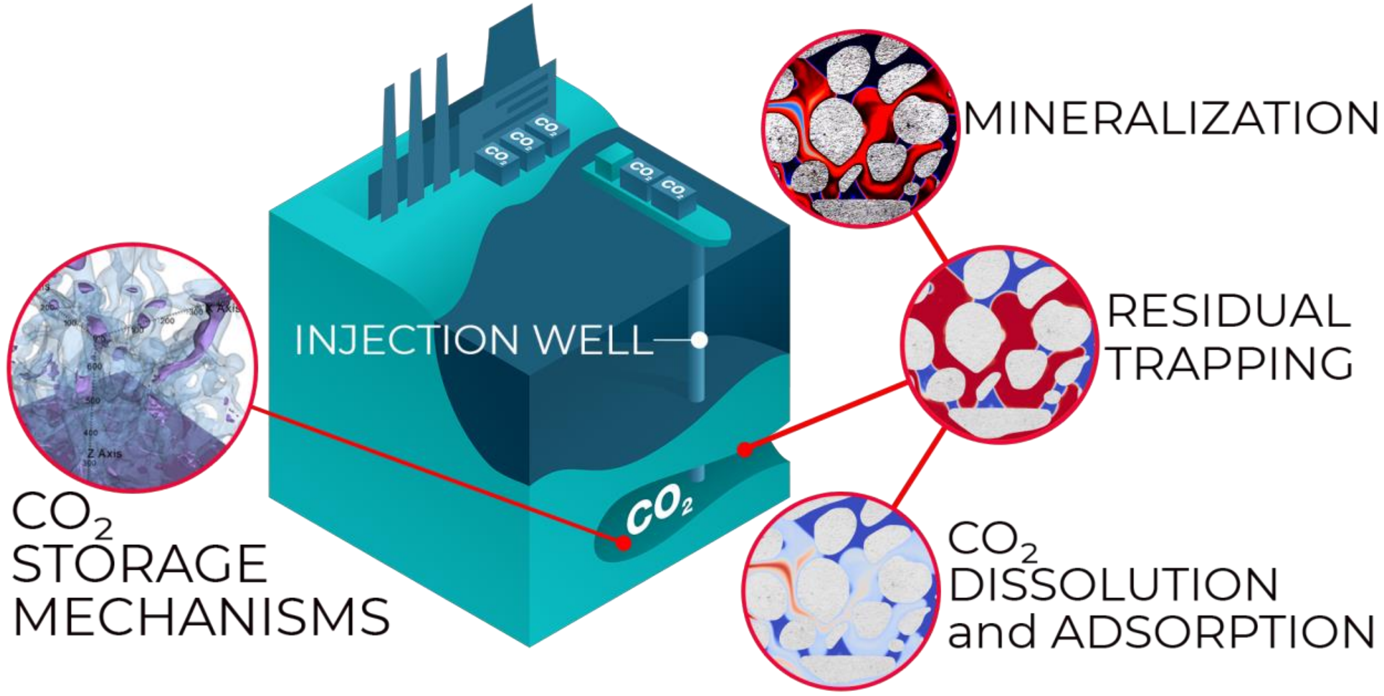
AI FOR NETZERO

Carbon Capture and Storage (CCS) & Global Warming



Source: IPCC Report 2023

Reactive Dissolution for CCS



Source: https://www.ccus.ai

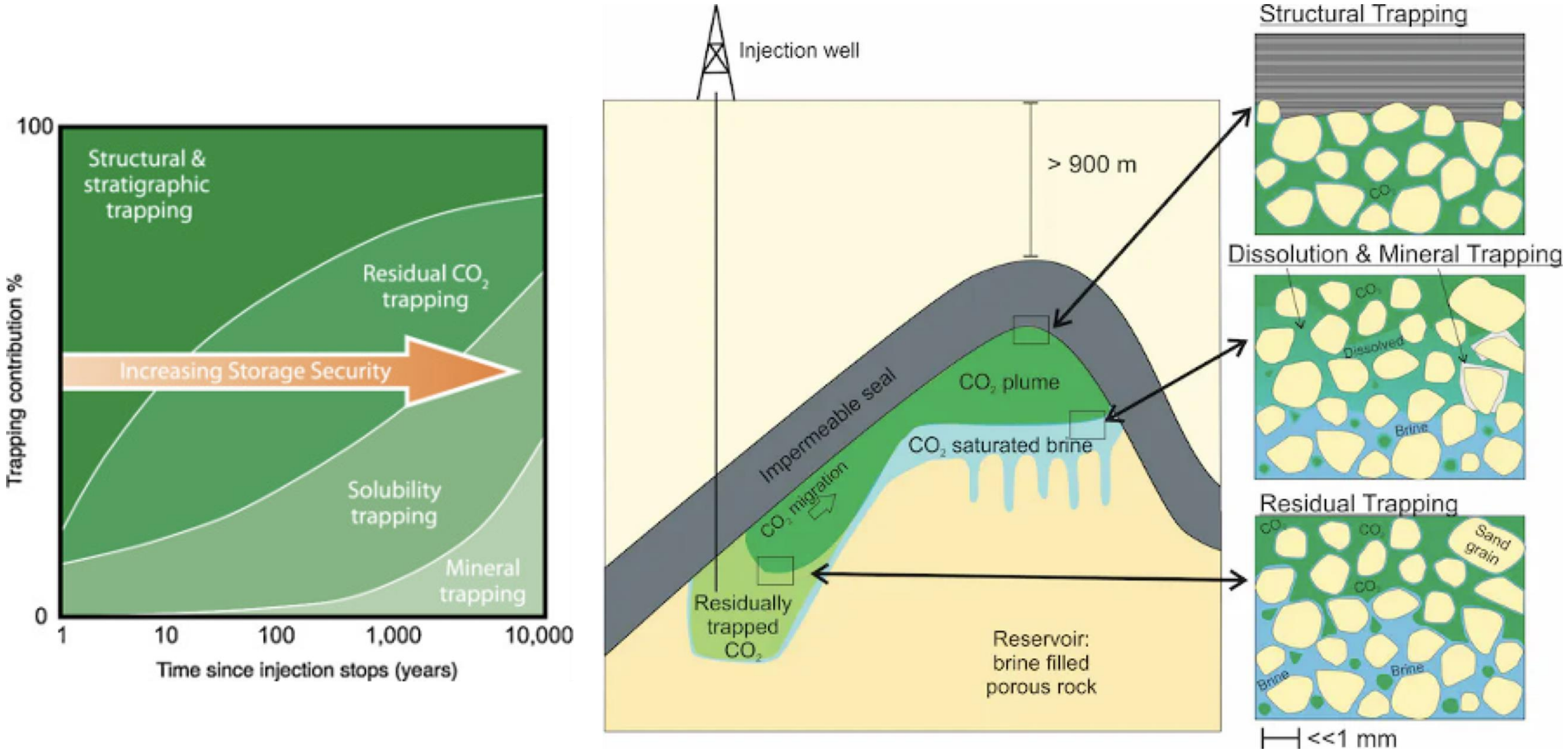
Stability and security of CO_2 storage by injection of acidic solution into subsurface, which leads to mineral and chemical trapping

Enhancing of storage capacity and CO_2 injection rates due to an increasing of pore space and permeability

Long-Term Behavior prediction and understanding of how CO_2 plumes migrate, and potential impacts on rock properties

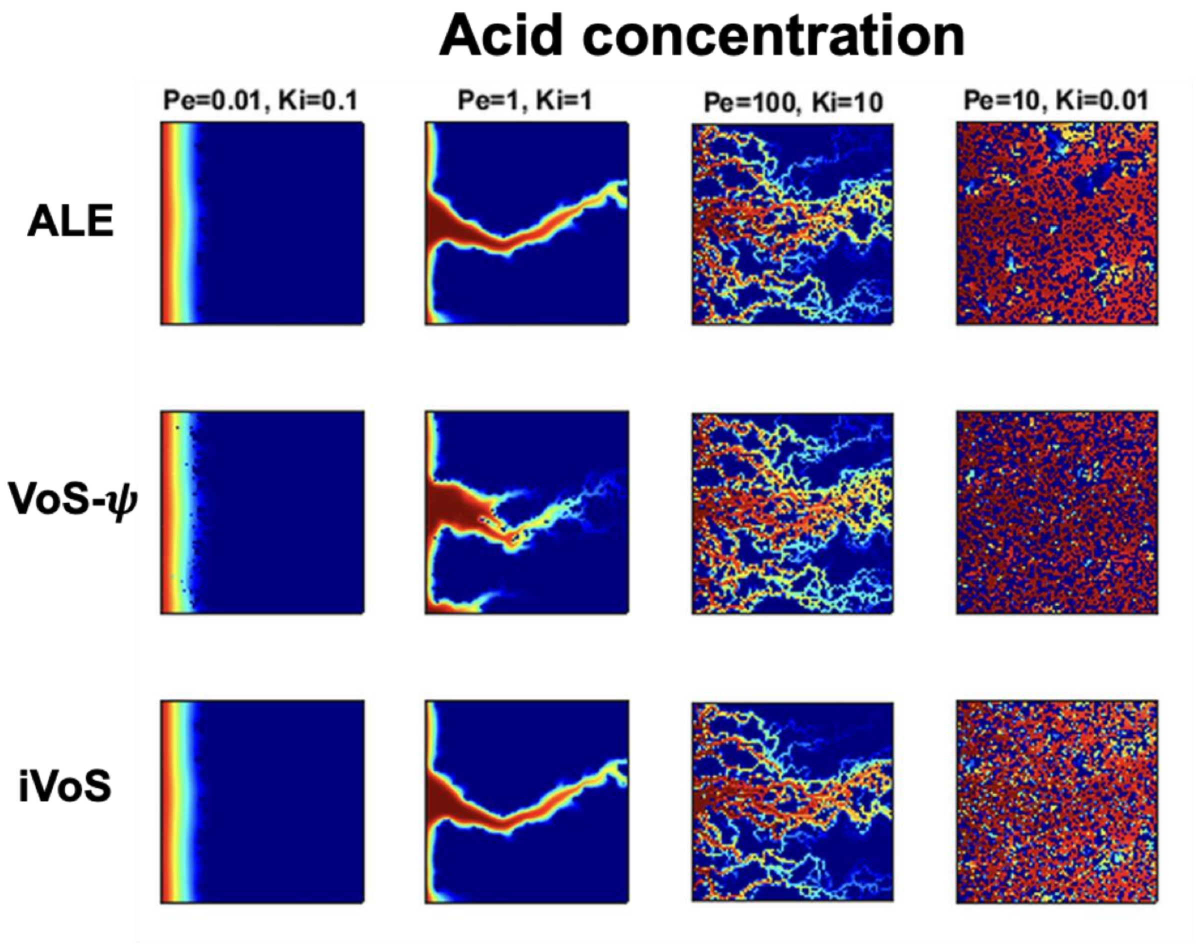
Reactive Dissolution for CCS

Problem: Uncertainty modelling x scaling



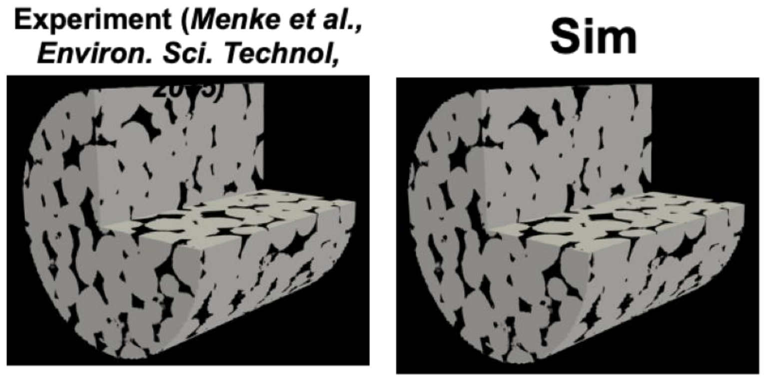
Source: Benson and Cole. **CO2 Sequestration in Deep Sedimentary Formations.** Elements (2008)

Numerical Solvers for Reactive Dissolution



	Case 1 $Pe = 0.01$ $Ki = 0.1$	Case 2 $Pe = 1$ $Ki = 1$	Case 3 $Pe = 100$ $Ki = 10$	Case 4 $Pe = 10$ $Ki = 0.01$
ALE	69	46	19	18
VoS-ψ	3.8	3.3	2.1	2.7
iVoS	5.8	4.6	3.4	4.3

CPU time (hours)

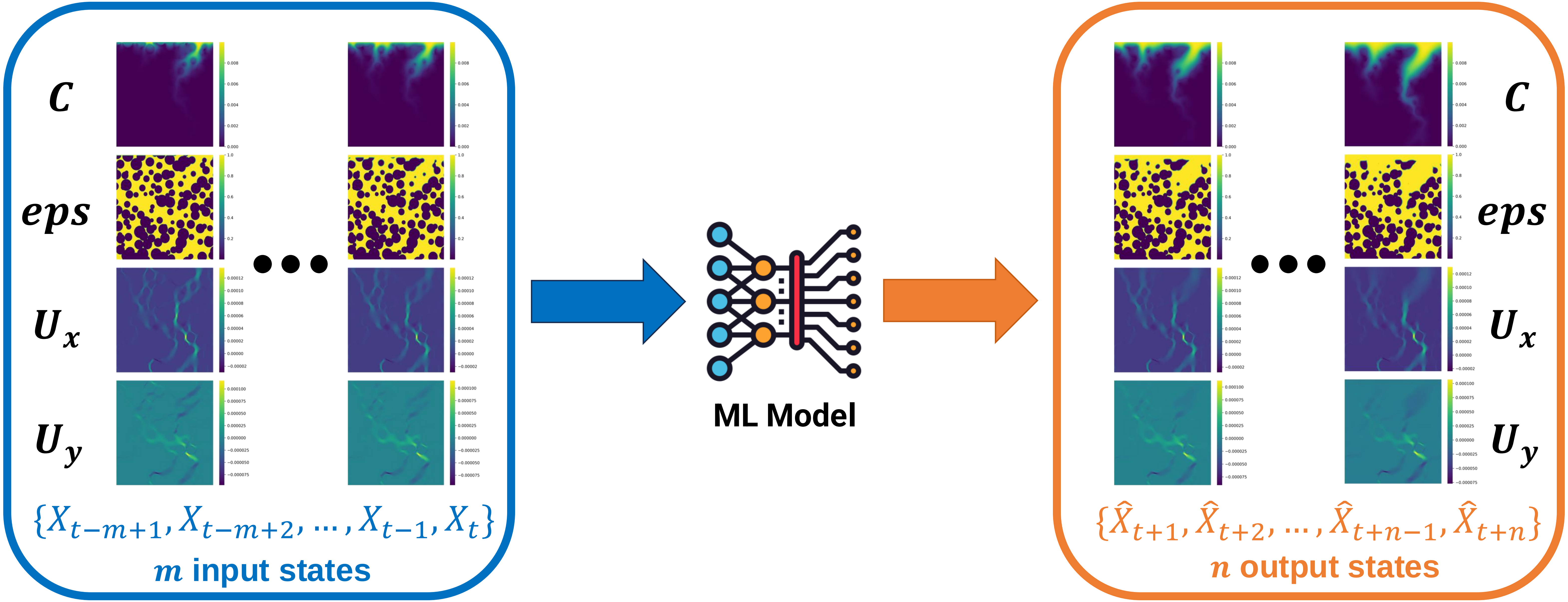


Source: Maes et al. **Improved volume-of-solid formulations for micro-continuum simulation of mineral dissolution at the pore-scale.** Frontiers in Earth Science 10 (2022)

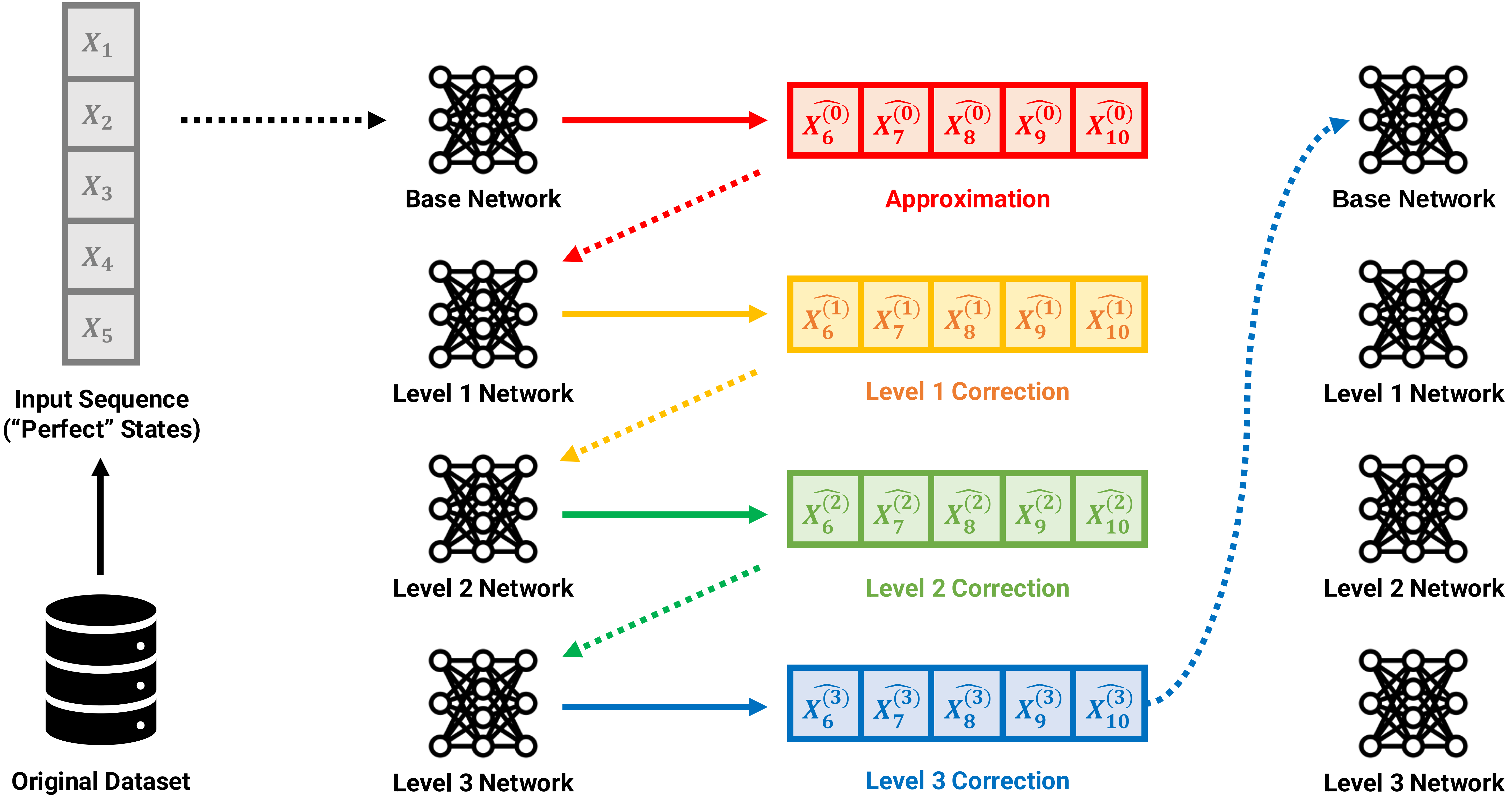
Solvers are typically **very expensive** to produce simulations

Machine Learning / Deep Learning algorithms can be used for **upscaling** and **speeding up** simulations under different conditions

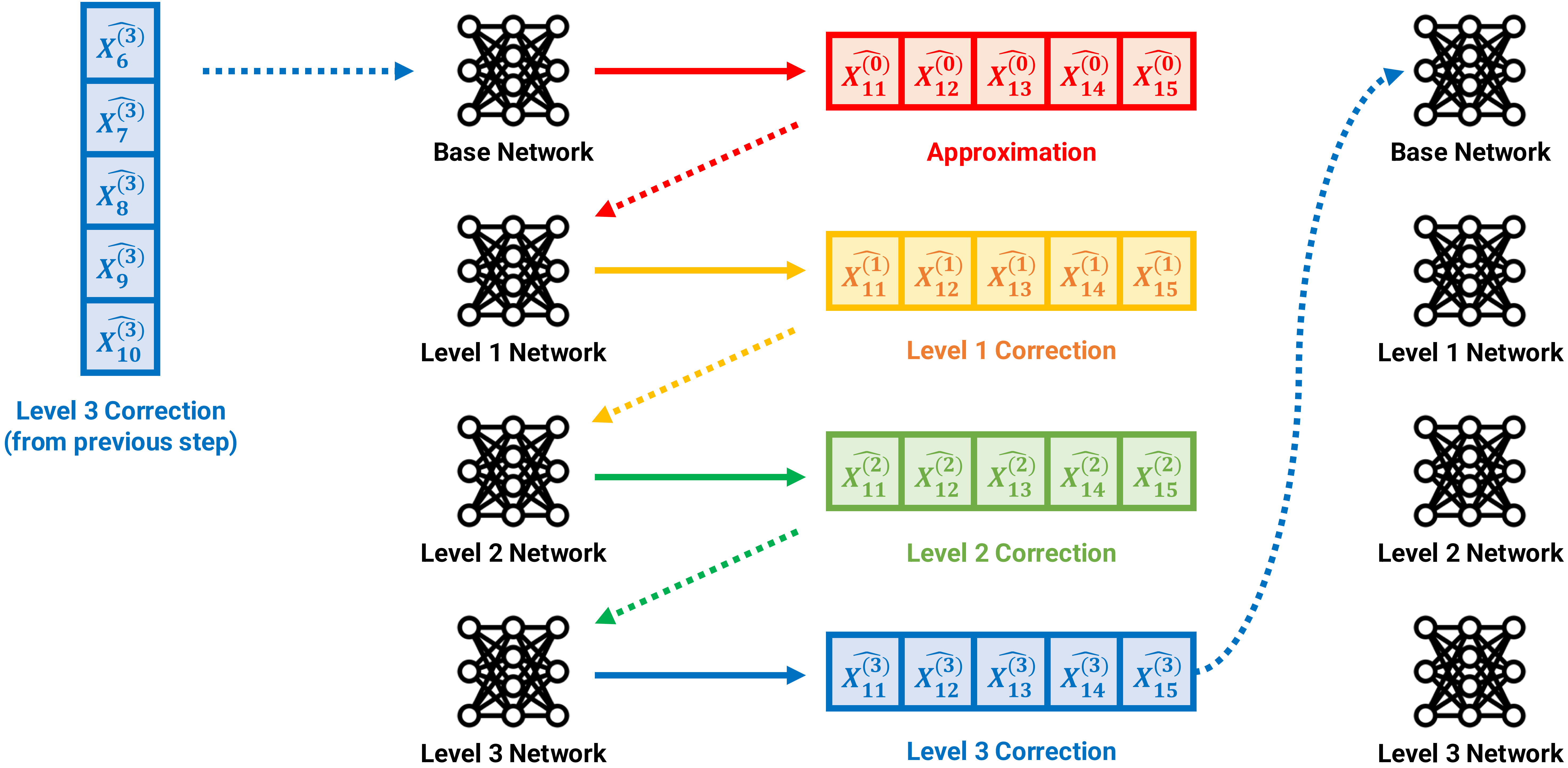
Problem Statement



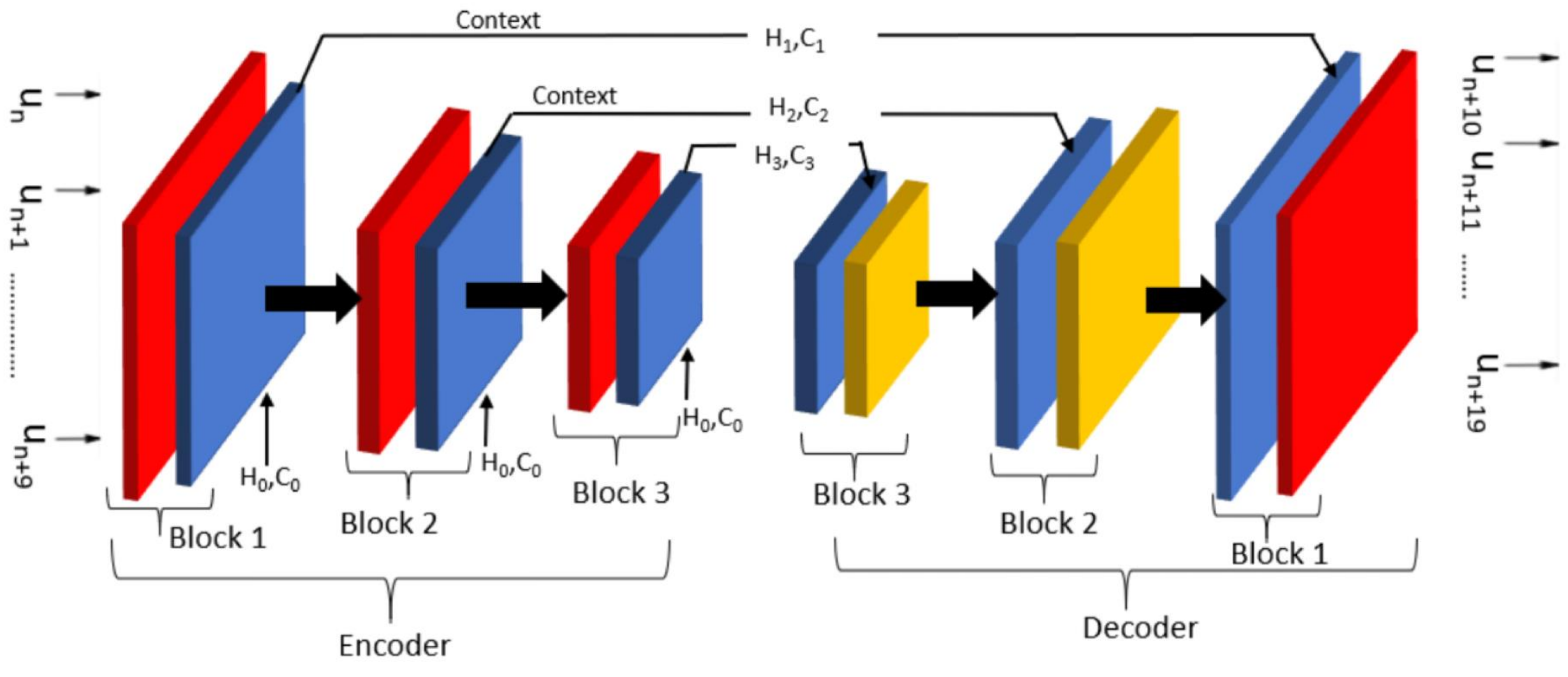
Recursive Multi-Step Prediction with Model Stacking

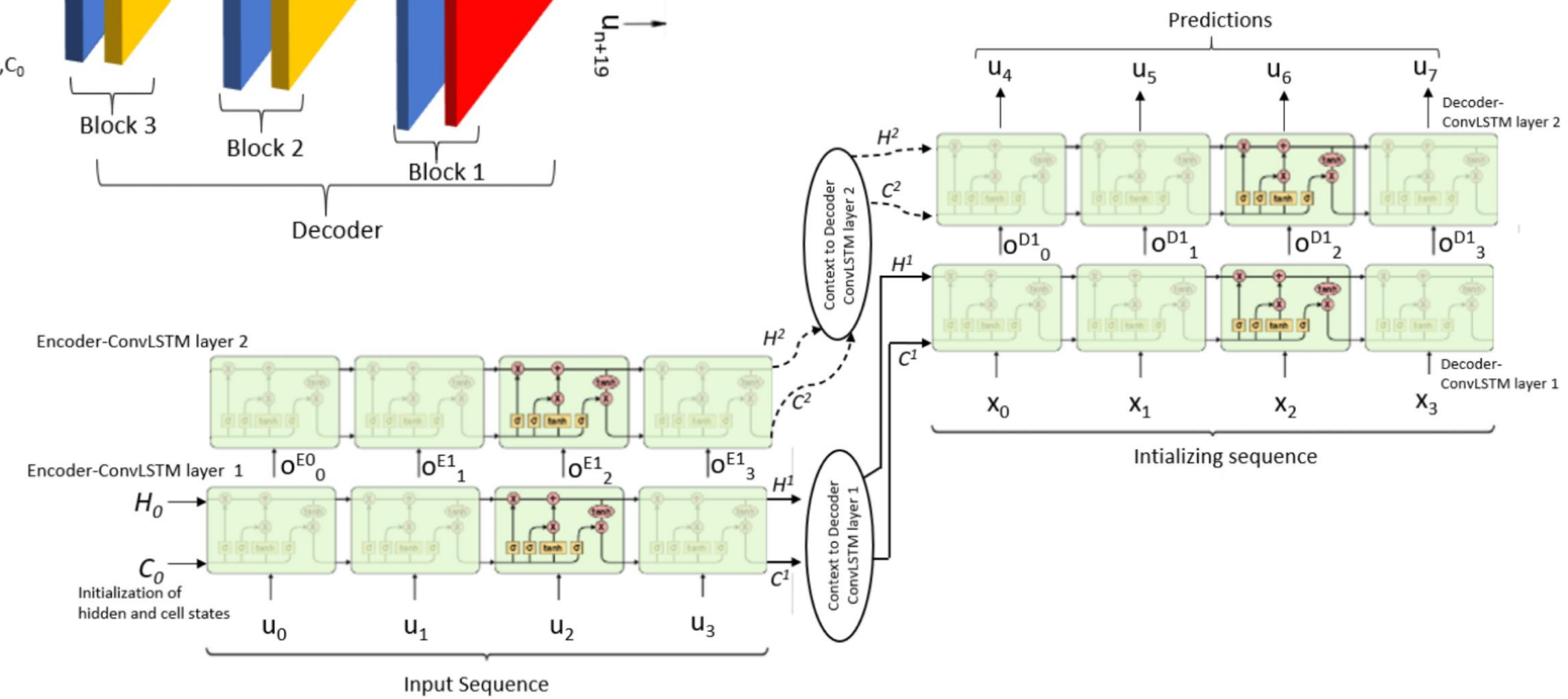


Recursive Multi-Step Prediction with Model Stacking



Encoder-Decoder ConvLSTM





Source: P. Kakka. **Sequence to sequence AE-ConvLSTM network for modelling the dynamics of PDE systems**, arXiv Preprint (2022)

U-Shaped Fourier Neural Operator (U-FNO)

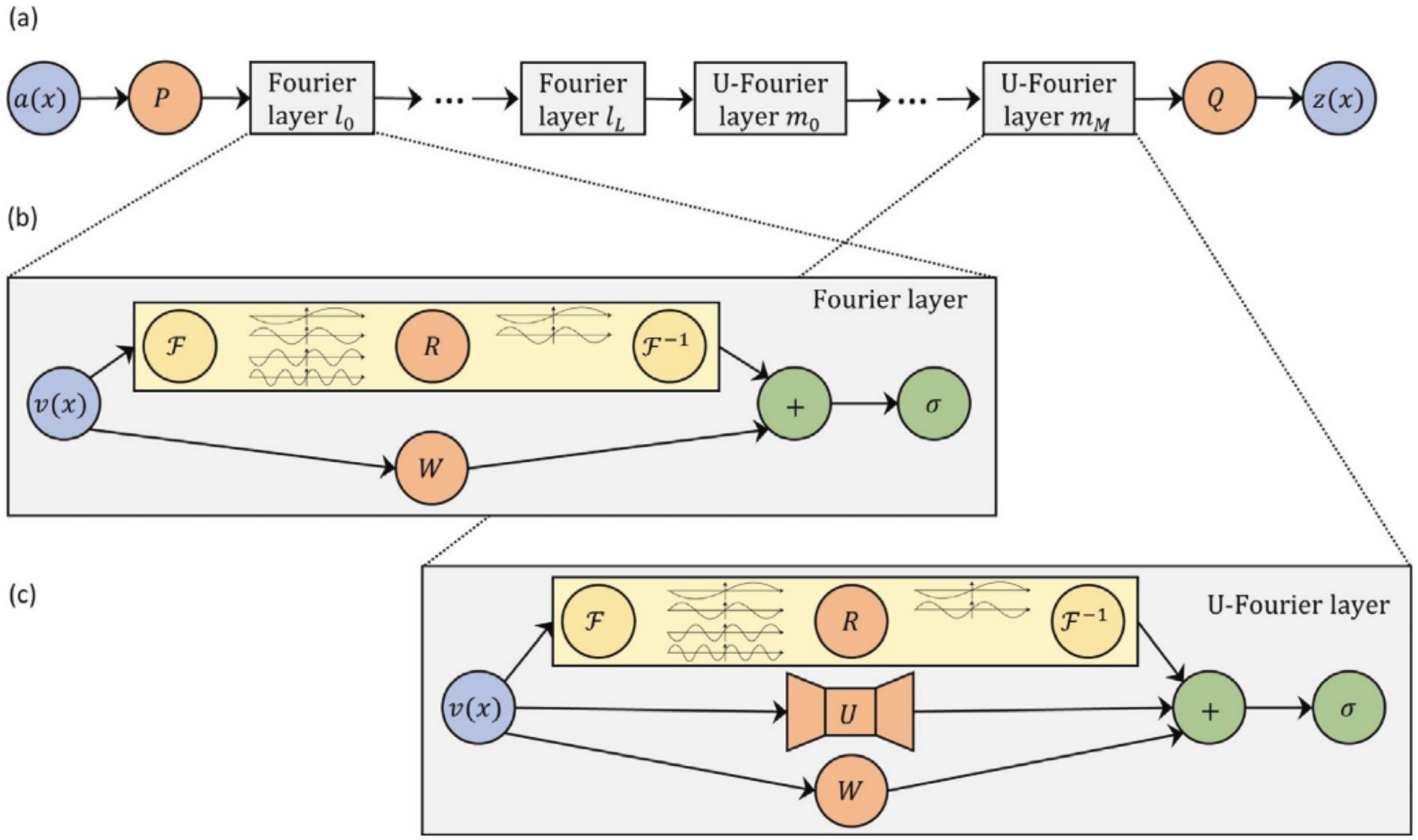


Fig. 2. A. U-FNO model architecture. $a(x)$ is the input, P and Q are fully connected neural networks, and $z(x)$ is the output. B. Inside the Fourier layer, $\mathcal{F}$ denotes the Fourier transform, R is the parameterization in Fourier space, $\mathcal{F}^{-1}$ is the inverse Fourier transform, W is a linear bias term, and σ is the activation function. C. Inside the U-FNO layer, U denotes a two step U-Net, the other notations have identical meaning as in the Fourier layer.

Source: Wen et al. **U-FNO — An enhanced Fourier neural operator-based deep-learning model for multiphase flow**, Advances in Water Resources (2022)

Temporal Attention Unit (TAU)

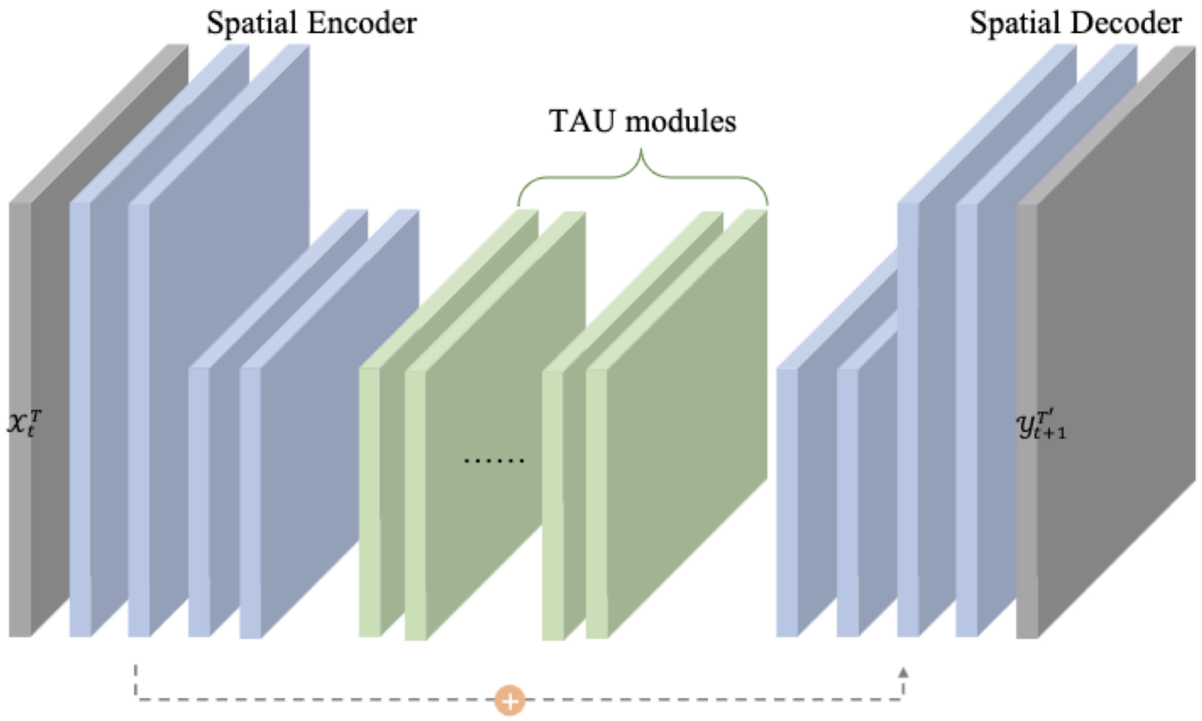


Figure 2. The overview architecture of our proposed model.

$$\mathcal{L}_{reg}(\widehat{\mathcal{Y}}, \mathcal{Y}) = D_{KL}(\sigma(\Delta\widehat{\mathcal{Y}}) \,||\, \sigma(\Delta\mathcal{Y})) = \sum_{i=1}^{T'-1} \sigma(\Delta\widehat{\mathcal{Y}}_i) \log \frac{\sigma(\Delta\widehat{\mathcal{Y}}_i)}{\sigma(\Delta\mathcal{Y}_i)}$$

$$\mathcal{L} = \sum_{i=1}^{T'} \|\widehat{\mathcal{Y}} - \mathcal{Y}\|^2 + \alpha \mathcal{L}_{reg}(\widehat{\mathcal{Y}}, \mathcal{Y})$$

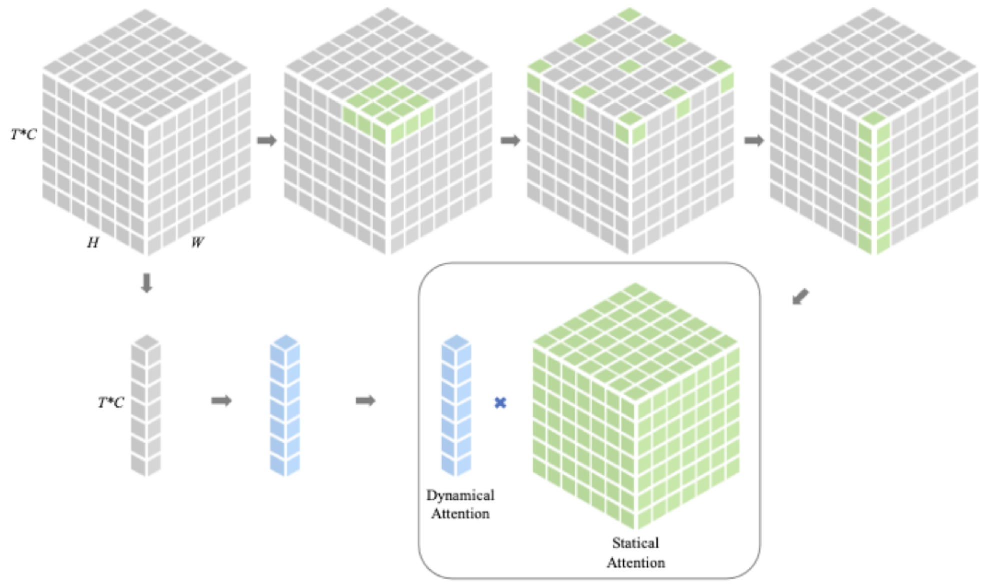


Figure 3. The intra-frame statical attention and the inter-frame dynamical attention.

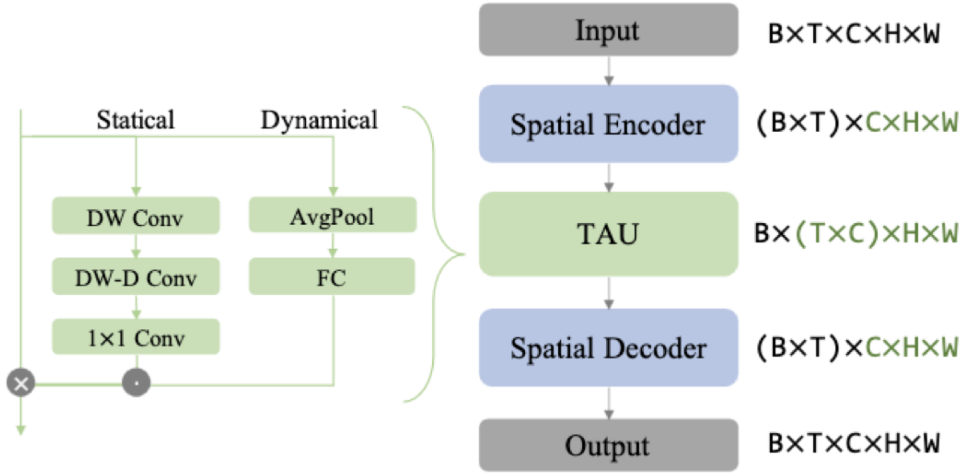


Figure 4. The detailed schema of our model.

Source: Tan et al. **Temporal Attention Unit: Towards Efficient Spatiotemporal Predictive Learning**
IEEE/CVF Conference on Computer Vision and Pattern Recognition (2023)

Training & Evaluation Settings

32 simulation samples of shape 100 x 4 x 256 x 256 (time steps, input properties, width, height)

24 training samples, 8 validation samples

Same dissolution regime for all samples (Peclet Number = Kinetic Number = 1)

Trained algorithms: ConvLSTM, U-FNO and TAU

Model stacking up to Level 3 Correction

Input Steps = Output Steps = 5

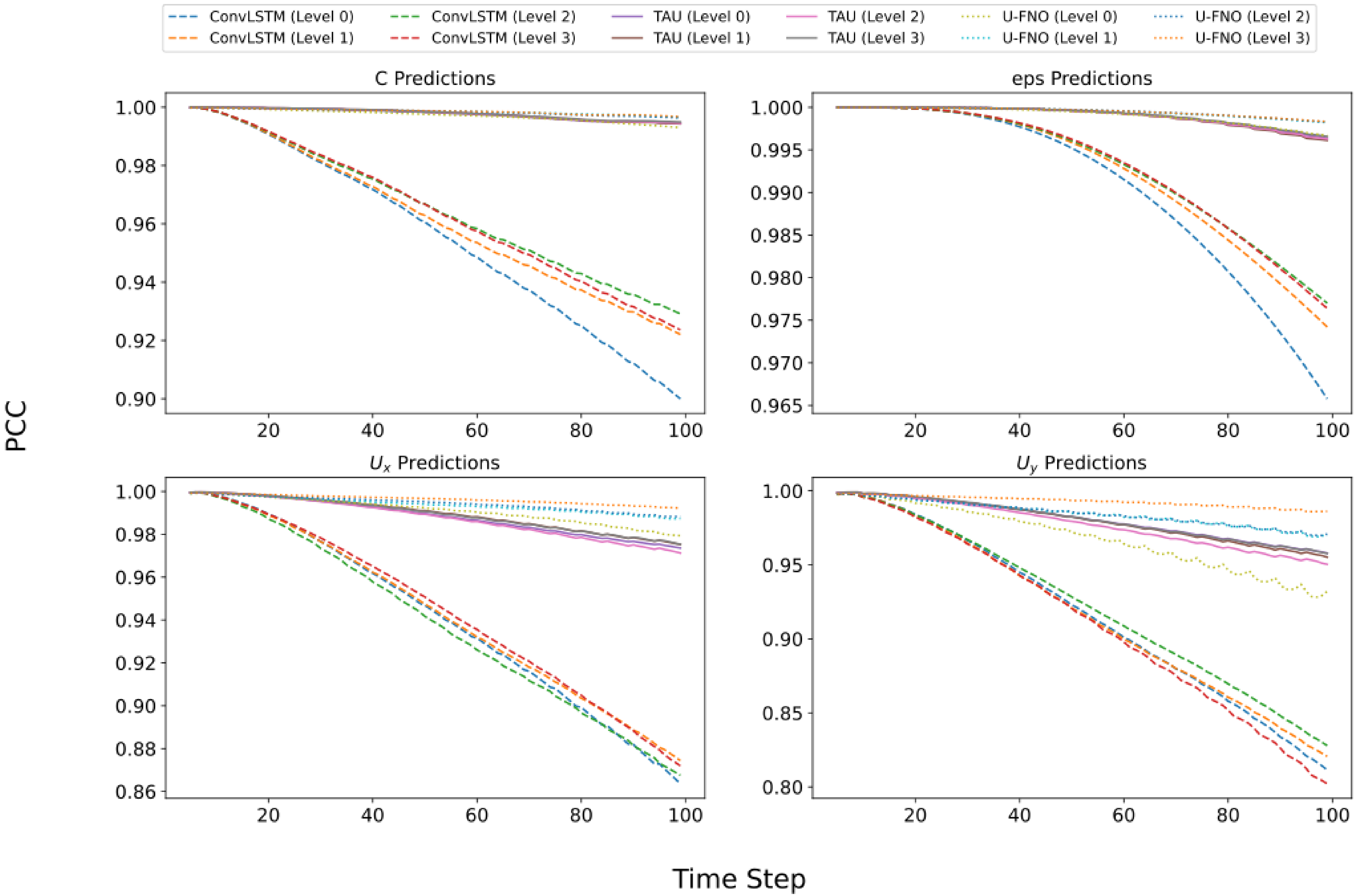
Training Epochs = 100

Evaluation Metric: Pearson Correlation Coefficient (PCC)

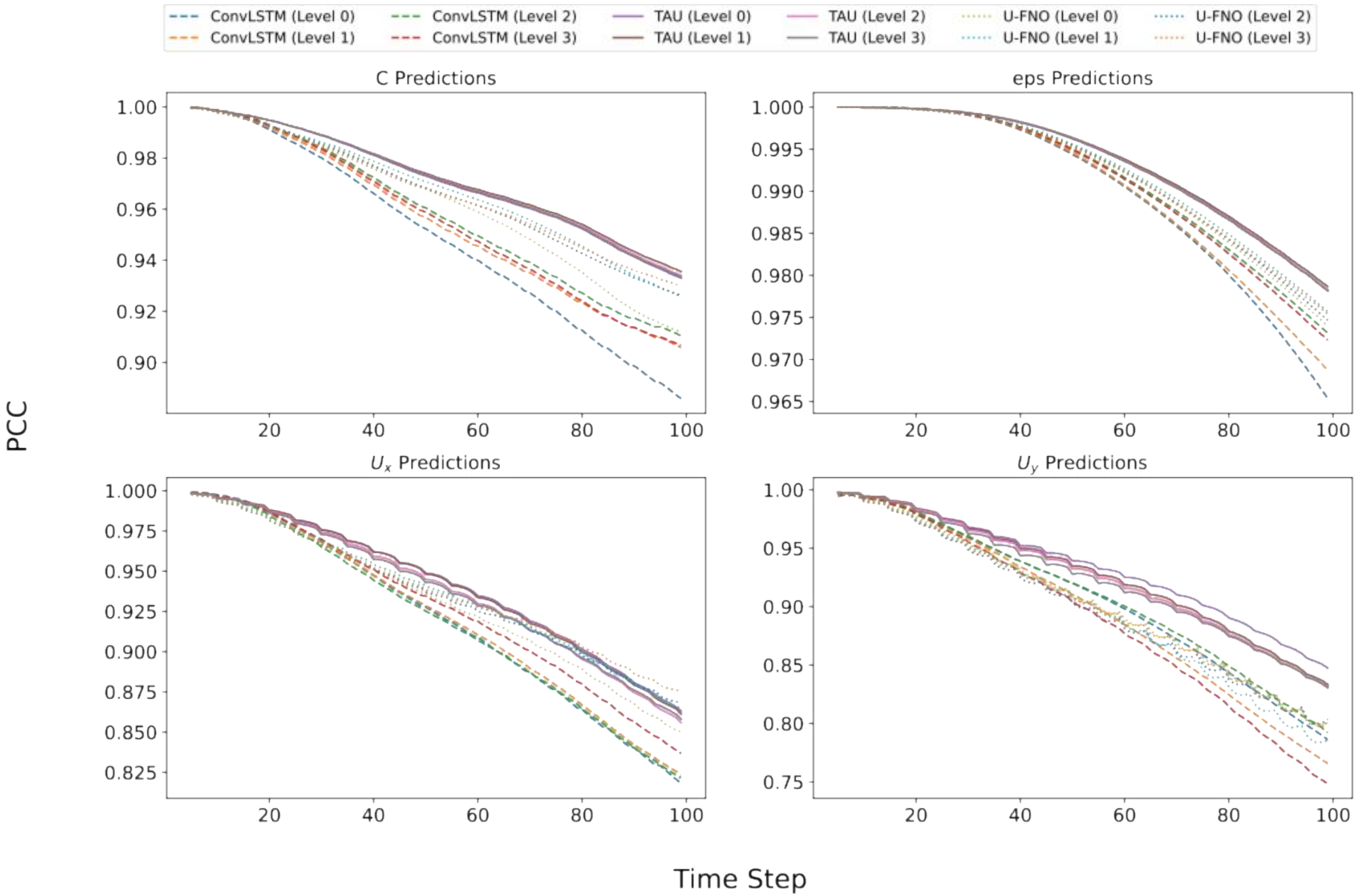
(for each predicted property and time step)

$$PCC(X,Y) = \frac{\sum_{i=1}^{n}(x_i - \bar{X})(y_i - \bar{Y})}{\sqrt{\sum_{i=1}^{n}(X_i - \bar{X})^2 \sum_{i=1}^{n}(Y_i - \bar{Y})^2}} = \frac{\mathrm{cov}(X,Y)}{\sigma(X)\cdot\sigma(Y)}$$

Correlation Results on Training Set



Correlation Results on Validation Set



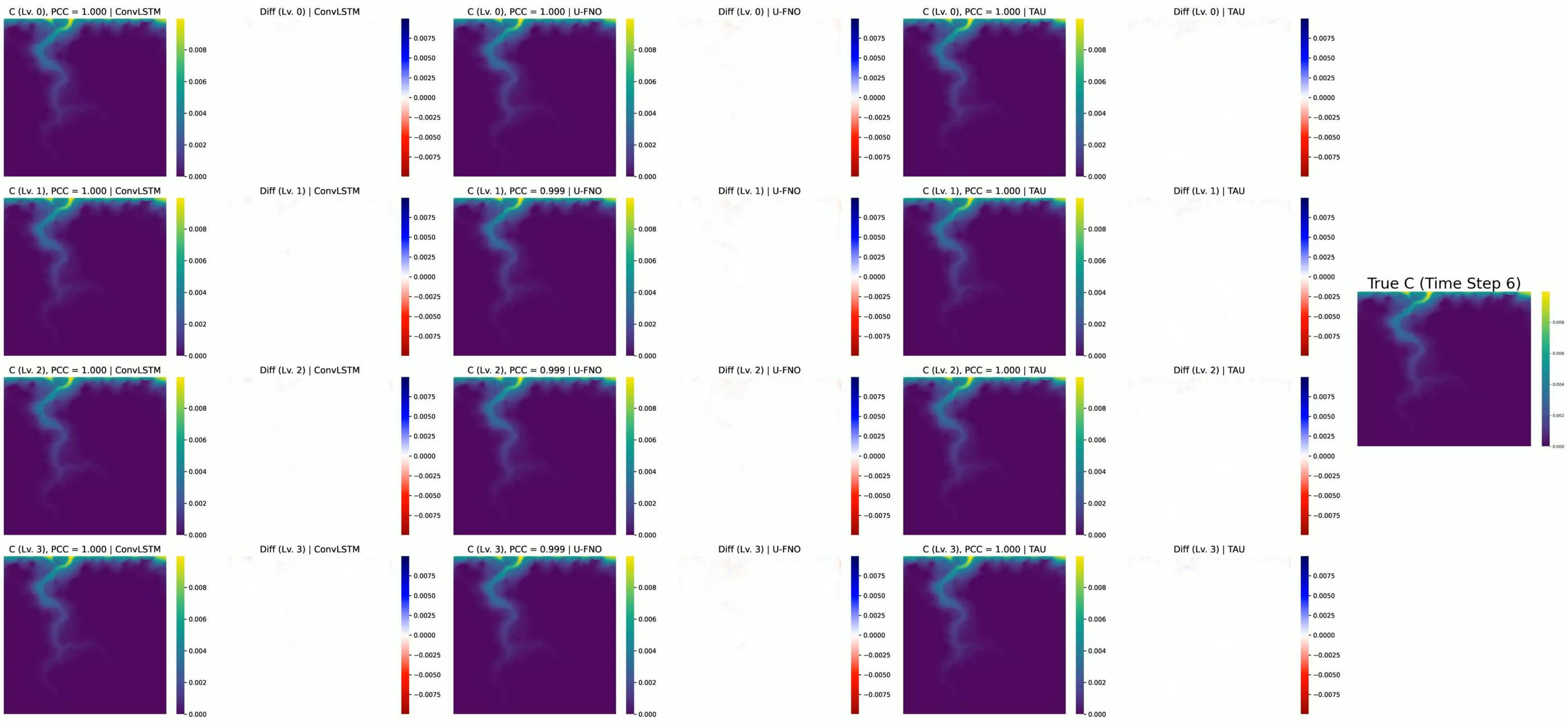
Test Case Analysis: Prediction of C

Lv. 0

Lv. 1

Lv. 2

Lv. 3

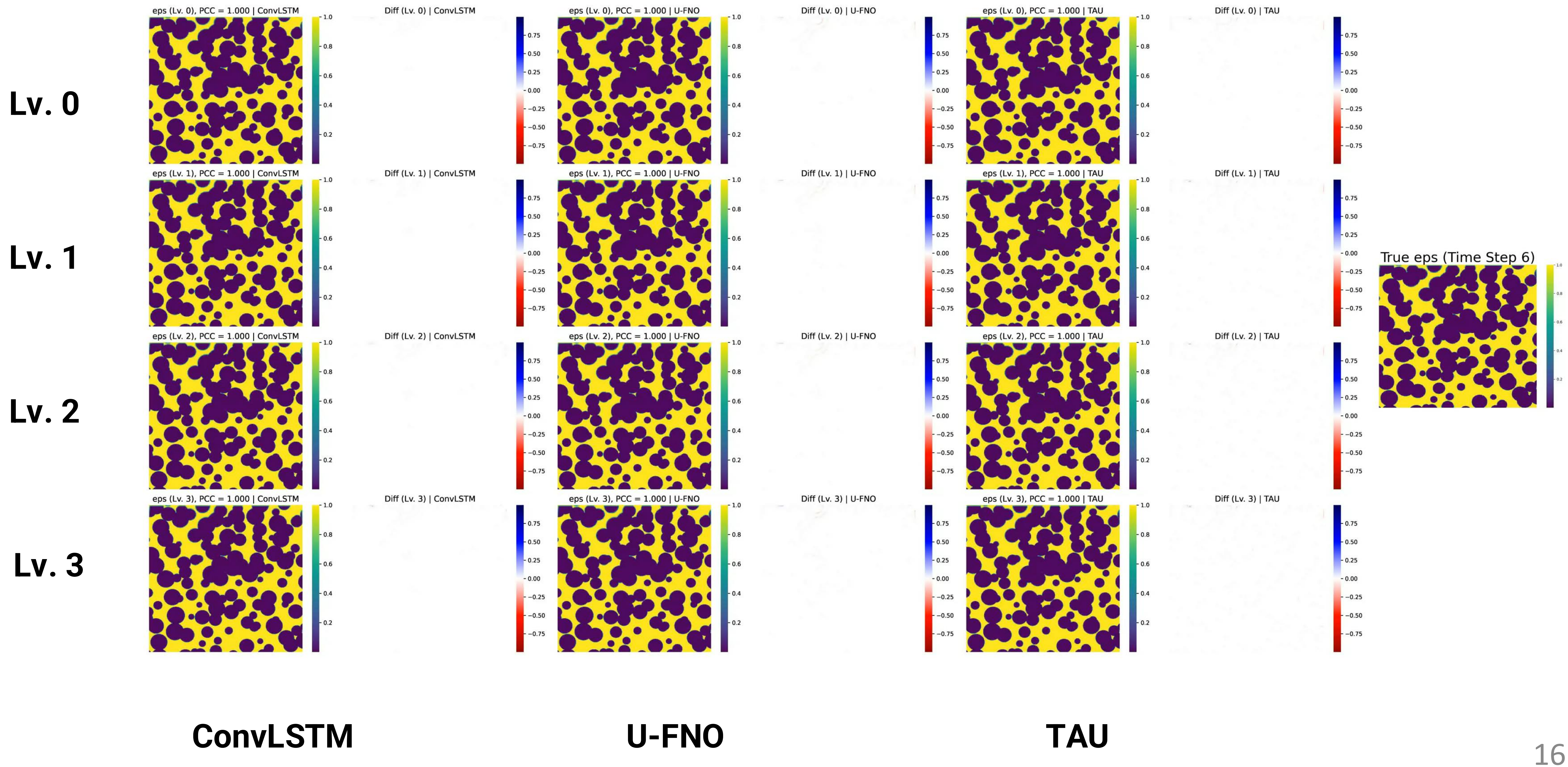


ConvLSTM

U-FNO

TAU

Test Case Analysis: Prediction of eps



Conclusions

Prediction Effectiveness

Data-driven deep-learning methods can be used effectively in predicting the dynamics of reactive dissolution

Error Accumulation Issues

Error accumulation from recursive strategies can be mitigated by extracting relevant spatiotemporal features

Coupling with Numerical Solvers

High correlation predictions make it possible to couple with (or replace) traditional numerical solvers with ML/DL solutions

Acknowledgements

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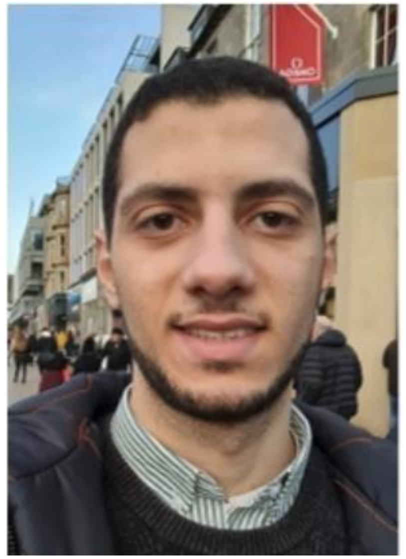
Prof. Dr. Hannah Menke



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THANK YOU!

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