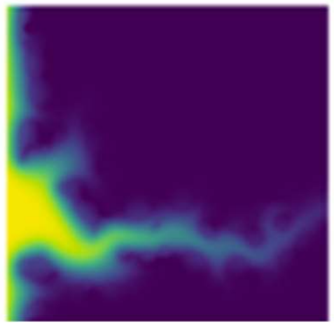
IMPERIAL

Surrogate model for solid-fluid interaction: a grid invariance approach

ECO-AI Workshop



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Summary

1. Application and objectives
2. Compression & Prediction
3. Grid invariance
4. Conclusions & future work

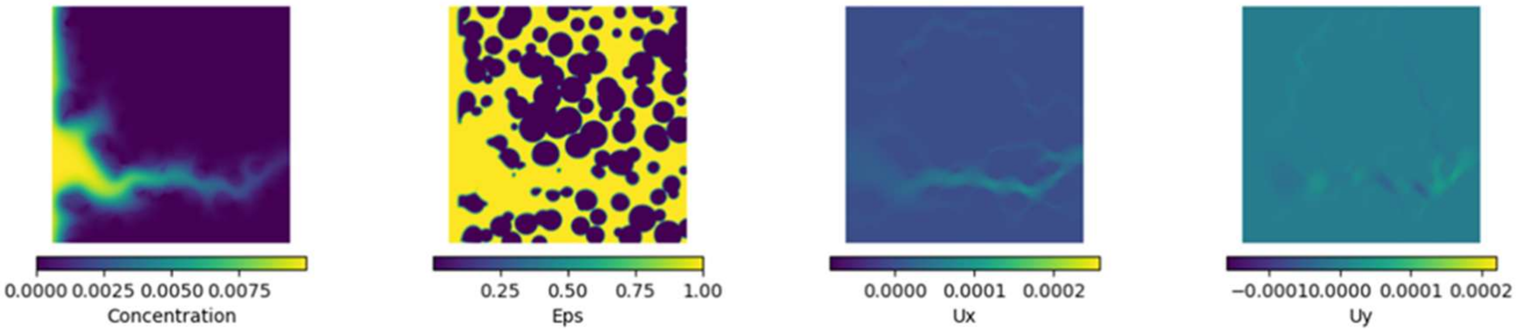
Application & Objectives

Carbon Storage Simulation

This work developed a surrogate model based on a carbon storage in porous media simulation developed in GeoChemFOAM, an equation-based approach to simulate the interaction between the carbon dioxide injected and the rocks. [1]

32 simulations of CO_2 injection in a carbonate to analyse the rock dissolution effect:

- 2D images with 256x256 pixels, each pixel representing 25μm,
- 100 timesteps,
- 4 fields: Concentration Porosity Velocities in x Velocities in y



[1] Julien Maes, Cyprien Soulaine, and Hannah P. Menke. Improved volume-of-solid formulations formicro-continuum simulation of mineral dissolution at the pore-scale. arXiv preprint, 2204.07019,2022.

Application & Objectives

1. Focus on **adaptability to huge datasets** (compression or grid invariance method)

2. **Trade off between** obtaining:

Application for a surrogate model:

Situations that need **fast models**

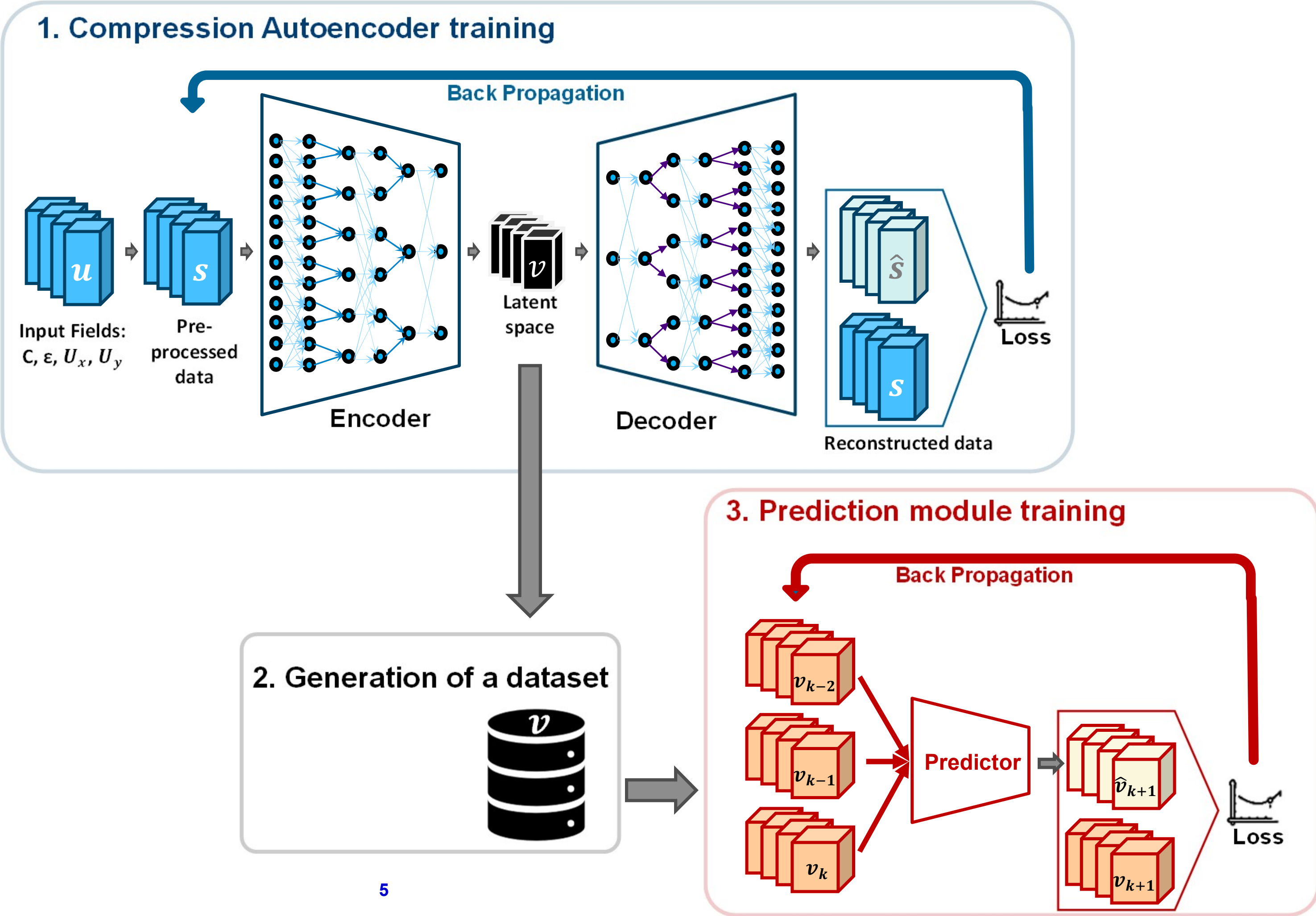
Situations that **don’t need a precise accuracy** (for instance, early phases of a project, when the objective is to compare many scenarios, still with a lot of other uncertainties)

Alternating with a traditional CFD model to **allow faster simulations** (surrogate model used for obtaining the evolution in a number of timesteps)

Compression & Prediction

Surrogate model - Training

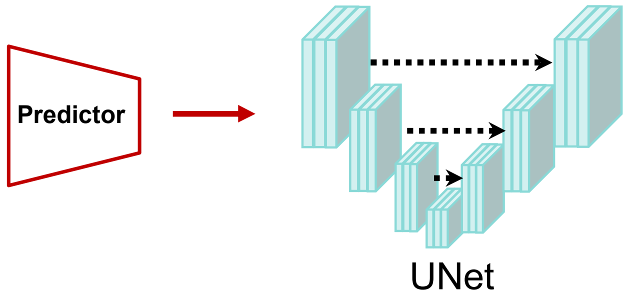
1. Compression autoencoder training
2. Generation of a dataset
3. Predictor training
4. Use model for inference

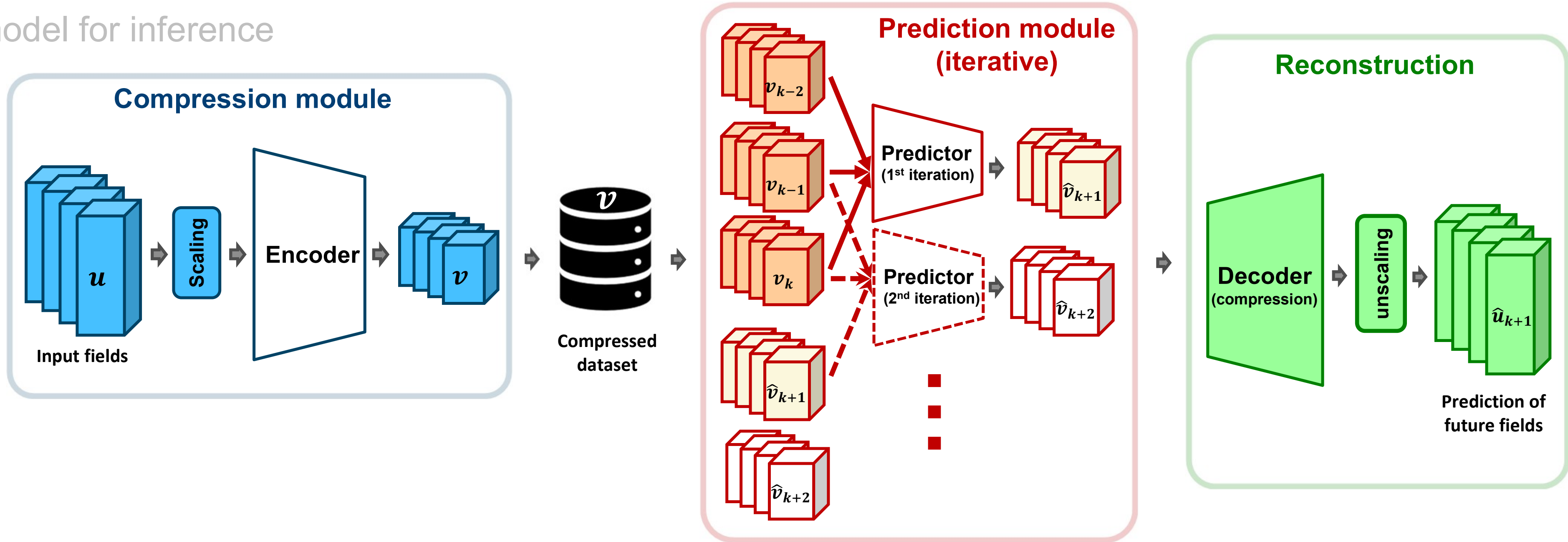


Compression & Prediction

Surrogate model - Inference

1. Compression autoencoder training
2. Generation of a dataset
3. Predictor training
4. Use model for inference





Compression & Prediction

Results - Trained with whole domain

Compression – AE compressor

$7.47 \cdot 10^{-6}$

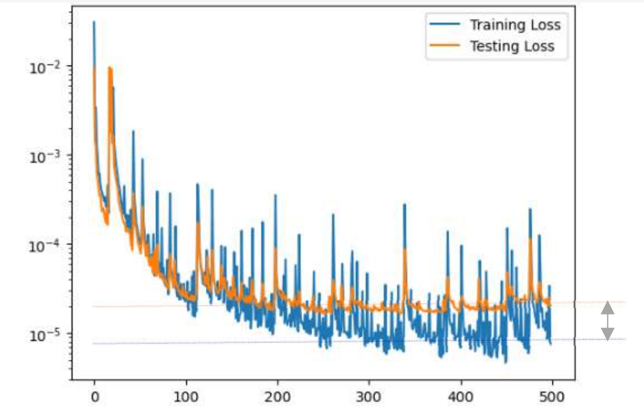
Average MSE for training data

$2.00 \cdot 10^{-5}$

Average MSE for testing data

$16:1$

Memory reduction ratio



Prediction – UNet

0.637

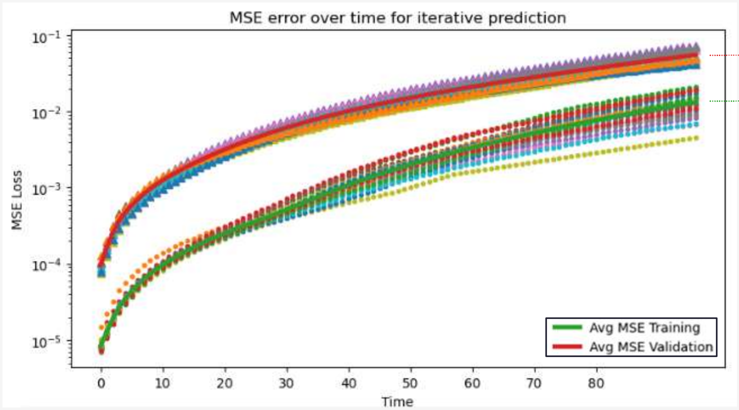
Average Pearson for testing samples

$5.51 \cdot 10^{-2}$

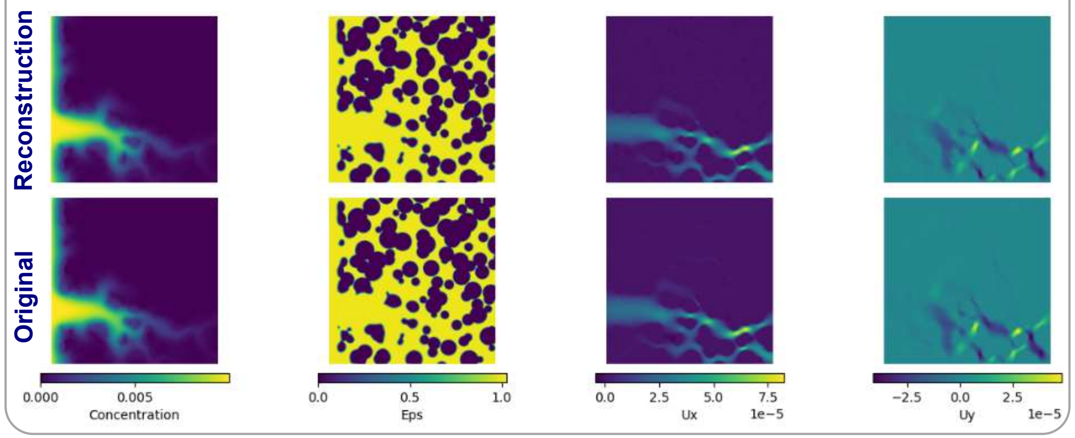
Average MSE for testing data

0.6 sec

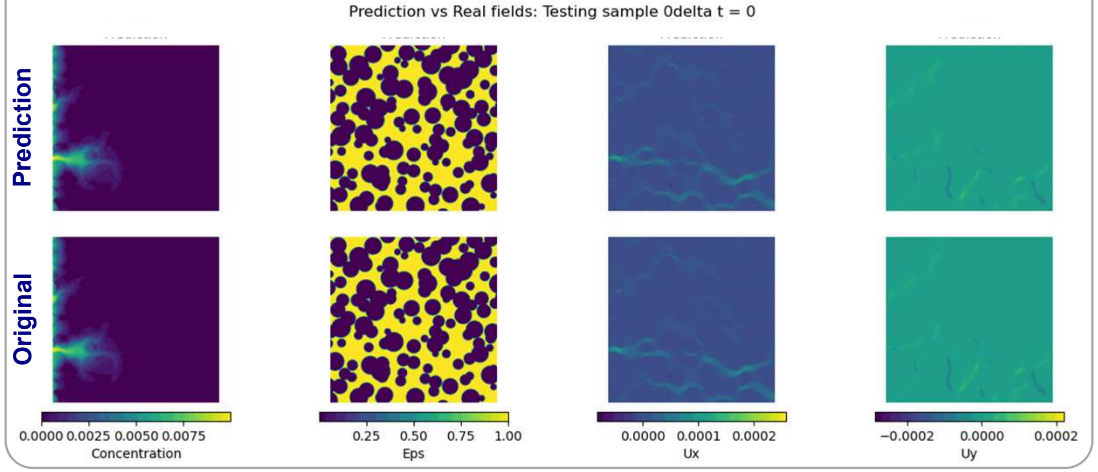
Time for inference



Testing Sample Reconstruction

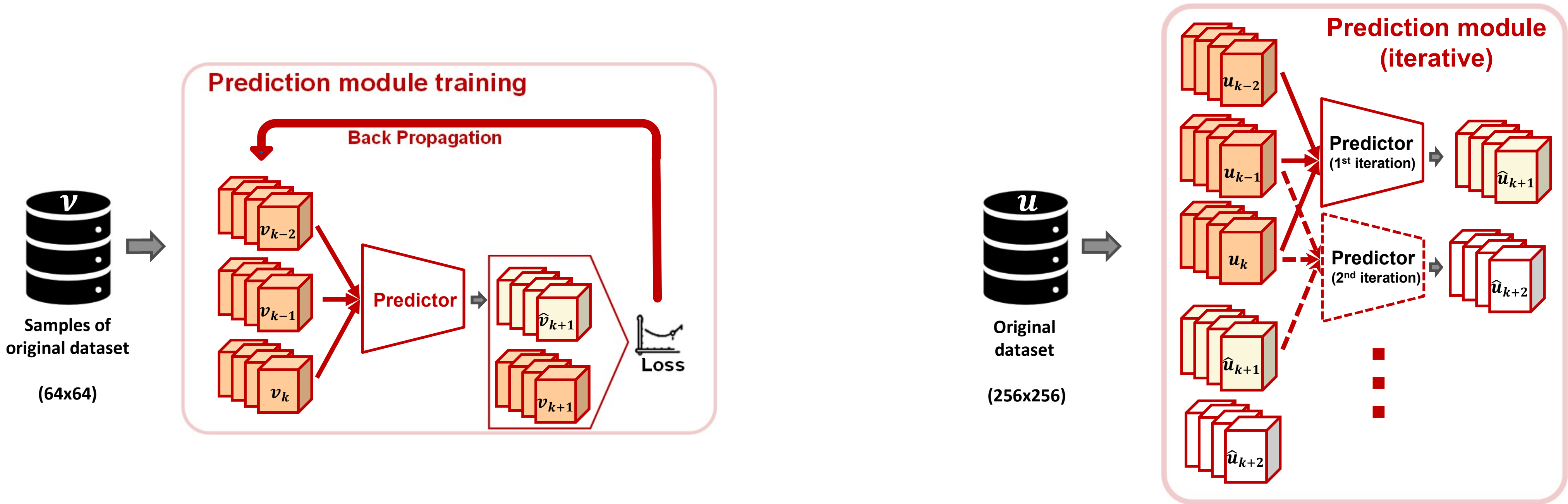


Prediction - UNet



Grid Invariance (GI)

Surrogate Model – Training with subsamples and inferencing in the whole domain

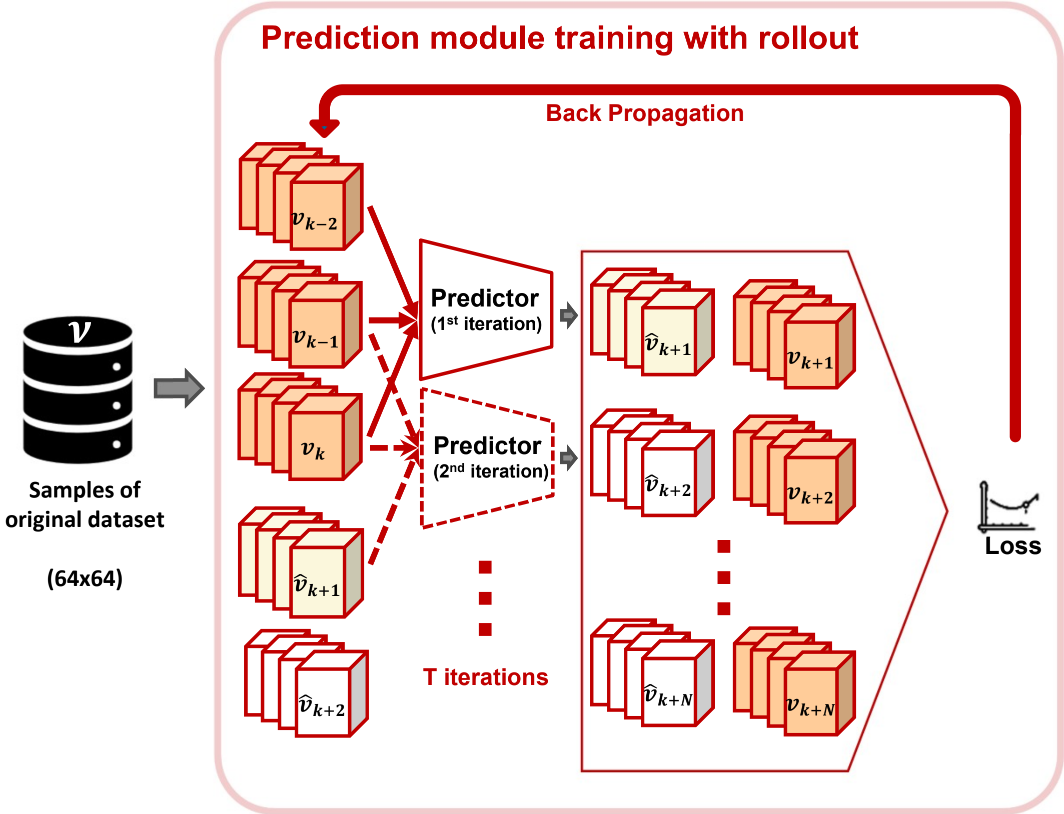


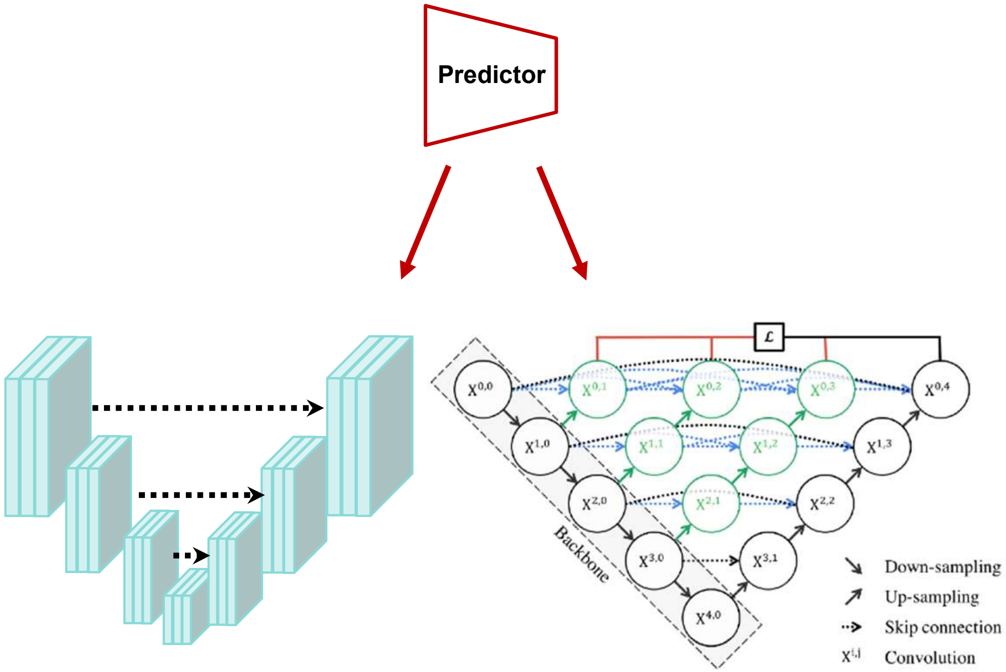
Models with only convolutional networks:

- perform inference across different computational grids;
- ensures the information from neighbouring nodes being collapsed/expanded

Grid Invariance

Training strategies and predictors





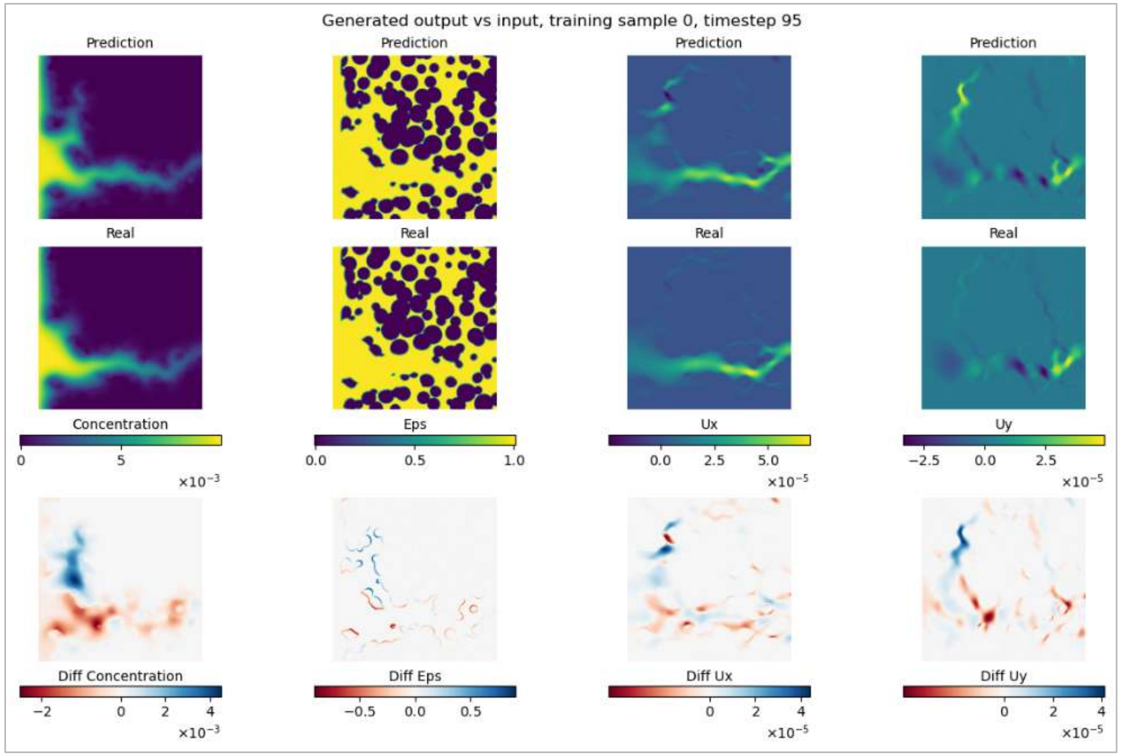
UNet
7,762,788 parameters

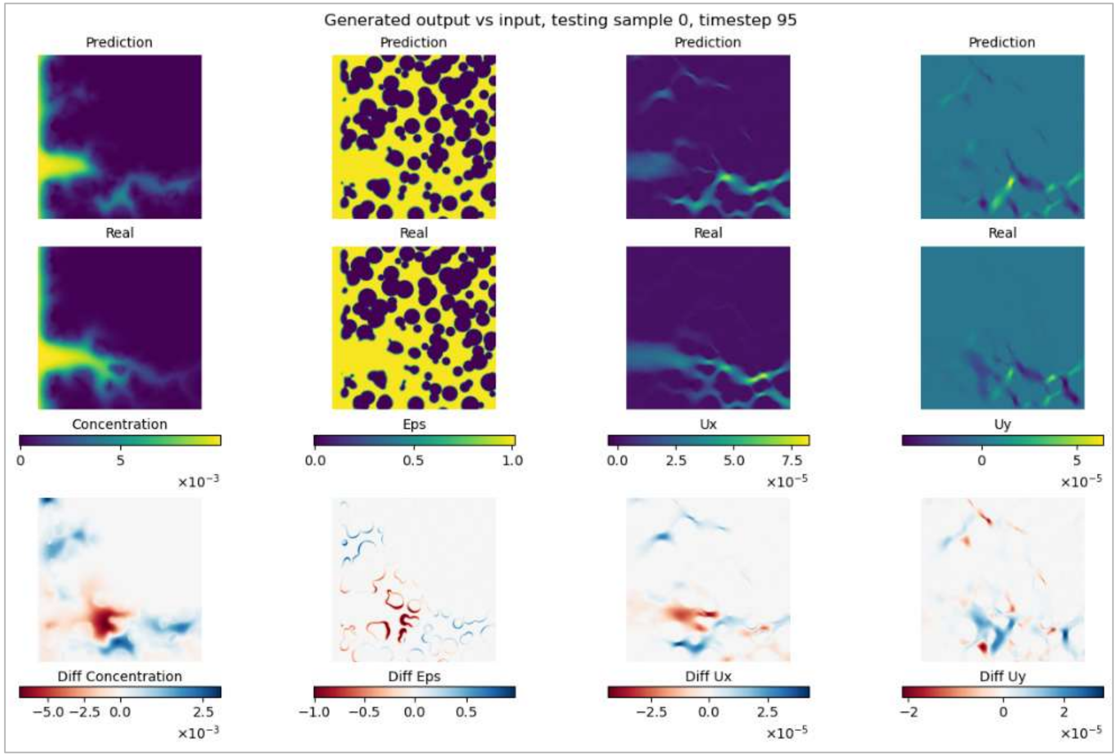
Unet++ [1]
9,045,264 parameters

[1] Zongwei Zhou, Md Mahfuzur Rahman Siddiquee, Nima Tajbakhsh, and Jianming Liang. Unet++:A nested u-net architecture for medical image segmentation, 2018.

Gridinvariance: Training with subsamples, evaluating in whole domain

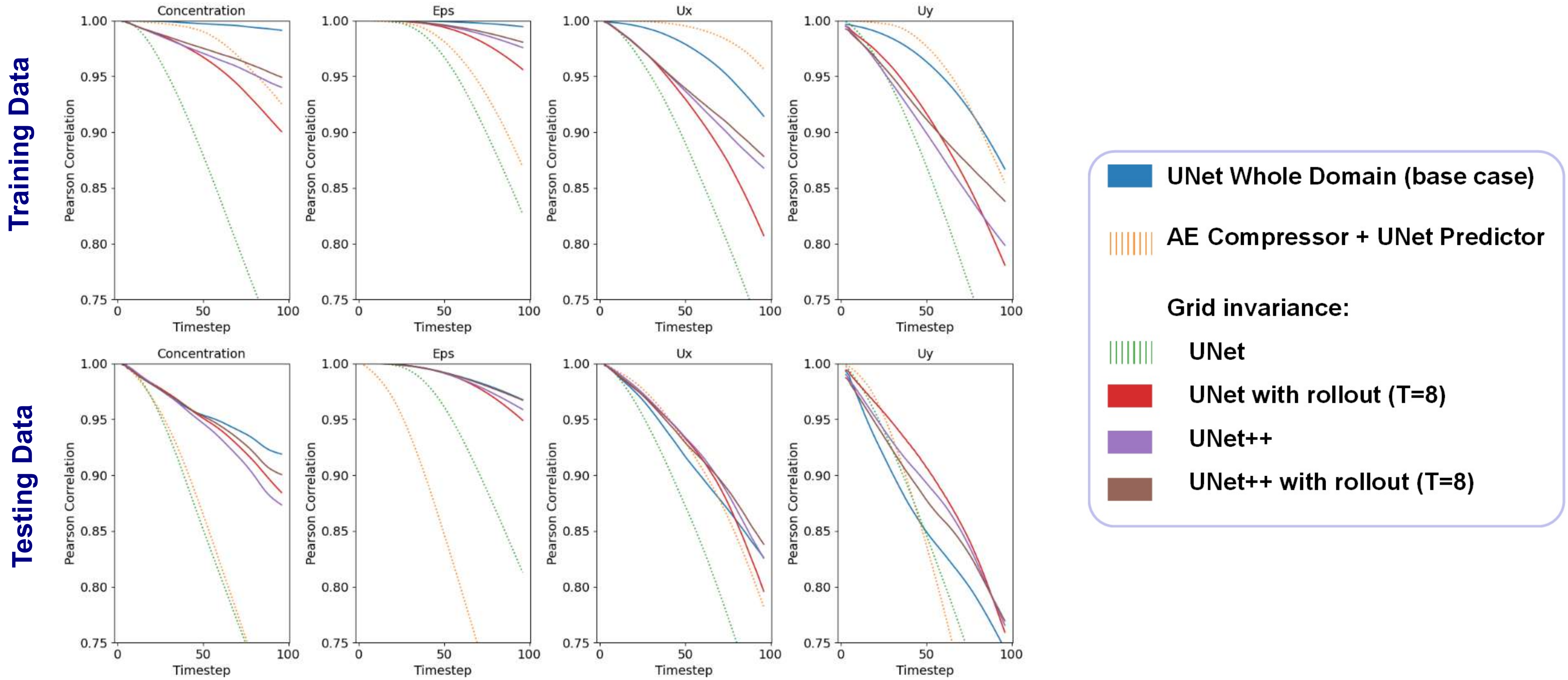
UNet++ prediction model, 4 fields, 3 timesteps input → 1 timestep output , rollout training with T=8





Conclusions & future work

Comparisons – Pearson correlations



Conclusion and future work

Compression *vs* Grid invariance

Compression on a ratio 16:1

Useful **for a window** of iterative timesteps

Compression mixes fields:

Degrading porosity field

Grid invariance:

Increased Reliability

Memory & Time consumption

Model Inference:

Up to 5000x faster than original PDE-based model

Grid Invariance on **training**:

Memory **reduction**

Grid Invariance on **inference**:

Memory reduction **when combined** with a subdomain approach

Future Work

Apply to **3D dataset**

Alternating between surrogate and **PDE-based solver** (GeoChemFOAM or AI4PDEs)

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Thank you

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