Physics-Informed Surrogate Modeling for Supporting Climate Resilience at Groundwater Contamination Sites

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BERKELEY LAB

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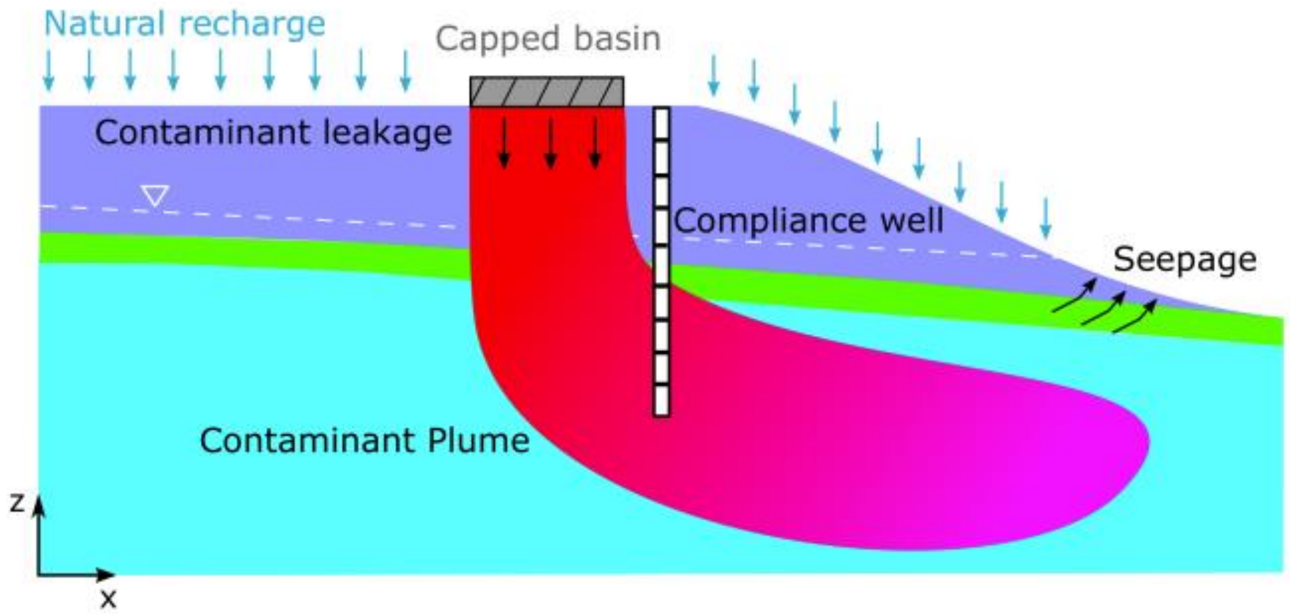
EARTH & ENVIRONMENTAL SCIENCES

Changing climate on groundwater contamination sites

Extreme precipitation and increased recharge

Savannah River Site (SRS) with wastewater

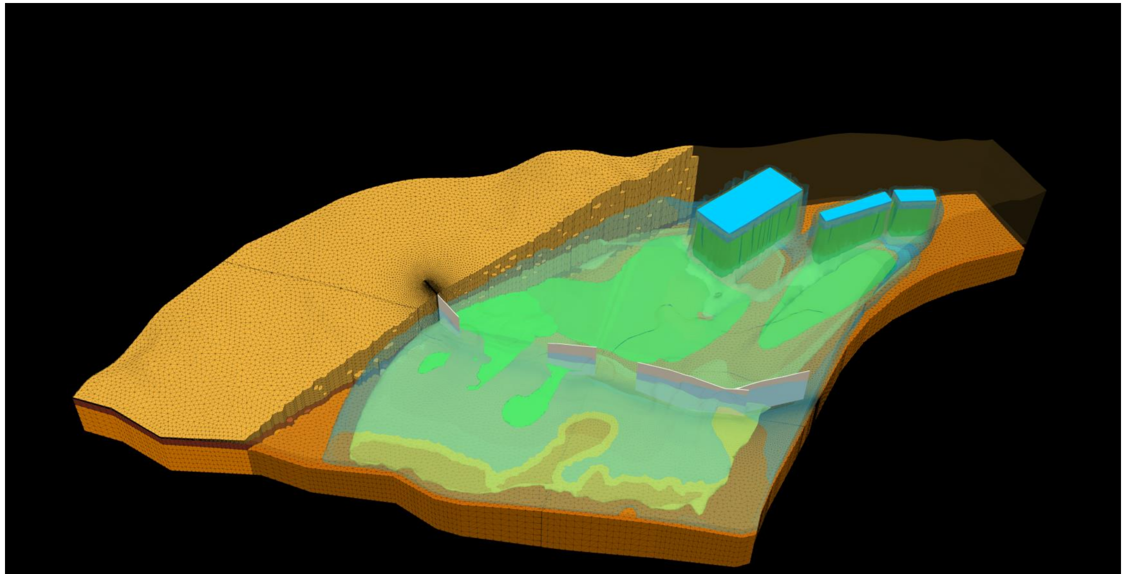
2D cross section of SRS



Dilution vs remobilization

Bridging the gap between science and decision with machine learning (ML)

Where and when to make remediations? Put monitoring wells?



Amanzi-ATS model

An SRNS subcontractor technician takes radiological readings of soil near Lower Three Runs, part of a major project to complete the cleanup of a contaminated 25-mile-long stream corridor at SRS. (Photo: DOE)

Slow and uncertain: Flow and transport simulations with climate models

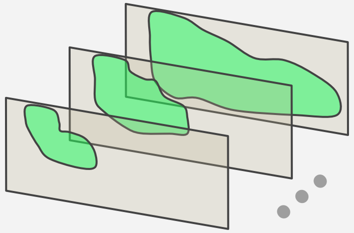
Fast and high risk: Design attenuation strategies under climate disturbances

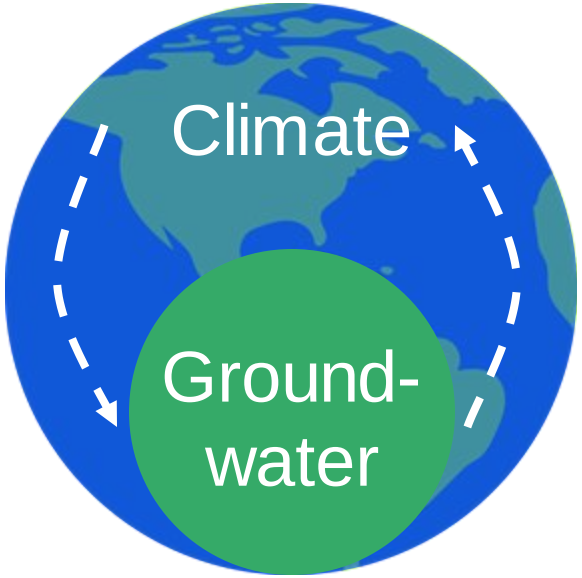
Physics-informed surrogate modeling

Physics-informed surrogate modeling

Uncertain climate, surface and subsurface properties

Physical simulations with Amanzi-ATS





Fast predictions

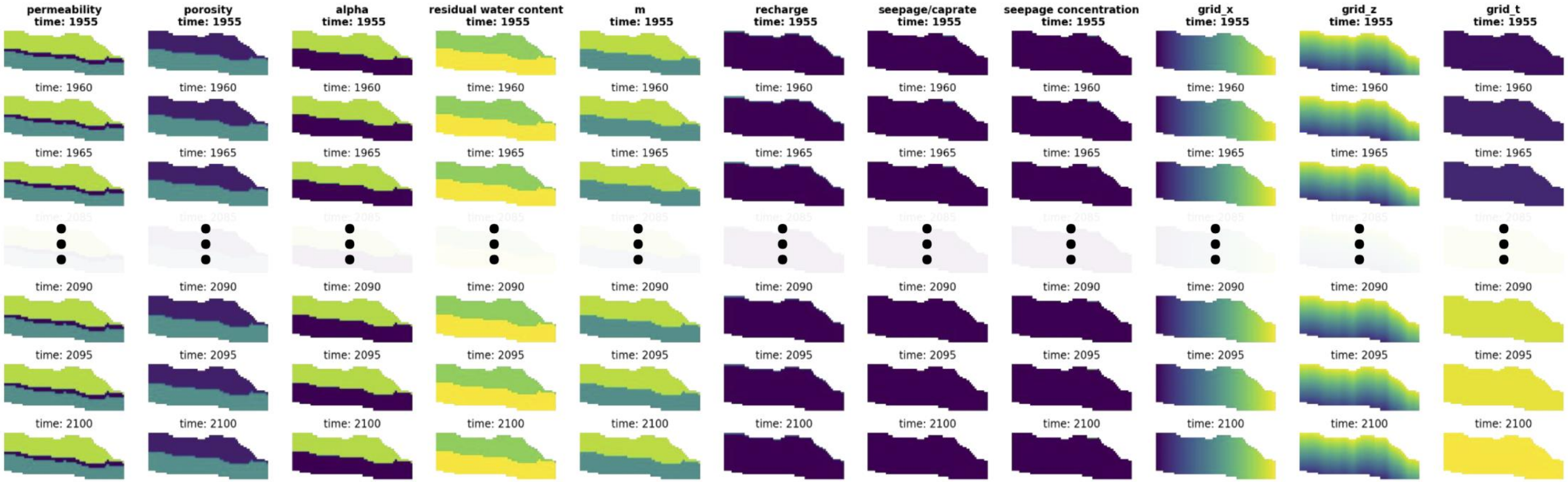
- Spatiotemporal variations
- Realistic climate projections (CMIP5)

Wang et al. 2022, Machine Learning and the Physical Sciences workshop, NeurIPS
Meray*, **Wang*** et al. 2023, Computers and Geosciences, under review

Surrogate modeling: Input and Output

Input parameters m(x,t): permeability, porosity, **recharge**, location, time, etc.

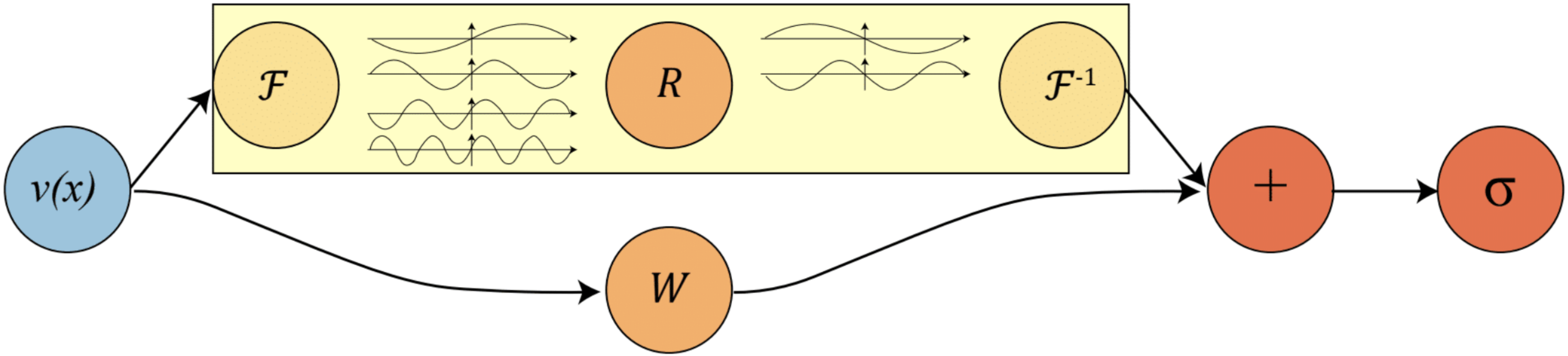
$n_x \times n_z \times n_t \times n_{input}$



Output parameters y(x,t): tritium concentration, hydraulic head

$n_x \times n_z \times n_t \times n_{output}$

Surrogate modeling: Fourier Neural Operator



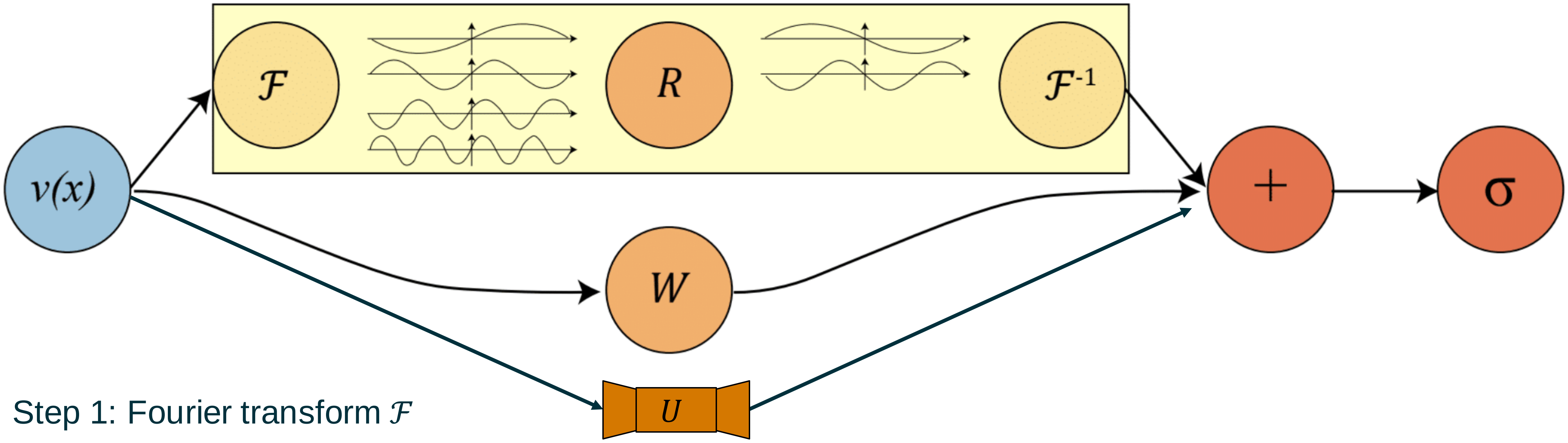
Step 1: Fourier transform $\mathcal{F}$

Step 2: Linear transform on the lower Fourier modes R

Step 3: Inverse Fourier transform $\mathcal{F}^{-1}$

Li et al. 2021, Wen et al. 2022

Surrogate modeling: Fourier Neural Operator + U-Net



Step 1: Fourier transform $\mathcal{F}$

Step 2: Linear transform on the lower Fourier modes R

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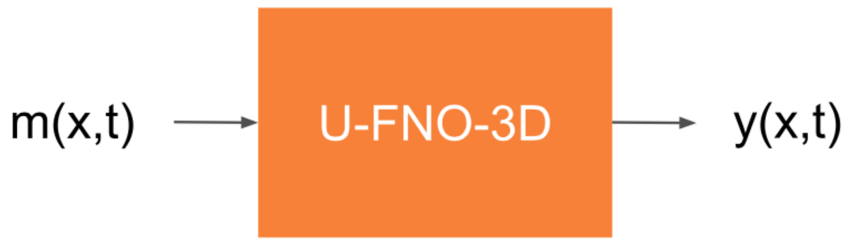
Li et al. 2021, Wen et al. 2022

Surrogate modeling: two different architectures

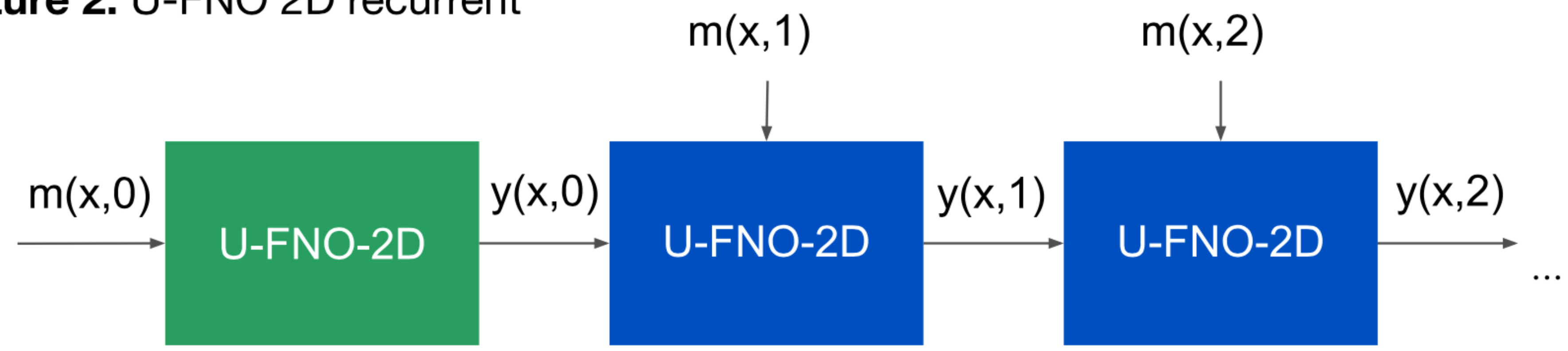
a)

Architecture 1: U-FNO 3D



b)

Architecture 2: U-FNO 2D recurrent



Learn physics for Δt

Surrogate modeling: Physics-informed loss function

$$\mathcal{L}(y,\hat{y}) = \underline{\mathcal{L}_{MRE}(y,\hat{y}) + \beta_1 \mathcal{L}_{der}(y,\hat{y})} + \beta_2 \underline{\mathcal{L}_{plume}(c',\hat{c'})} + \beta_3 \underline{\mathcal{L}_{BC}(\hat{y})}$$

Simulated data-driven: Mean relative error on output and corresponding derivatives

$$\mathcal{L}_{MRE}(y,\hat{y}) = \frac{\|y-\hat{y}\|_2}{\|y\|_2} \quad \mathcal{L}_{der}(y,\hat{y}) = \frac{\|\partial y/\partial x - \partial \hat{y}/\partial x\|_2}{\|\partial y/\partial x\|_2} + \frac{\|\partial y/\partial z - \partial \hat{y}/\partial z\|_2}{\|\partial y/\partial z\|_2}$$

Simulated data-driven: Derivatives on the plume boundary

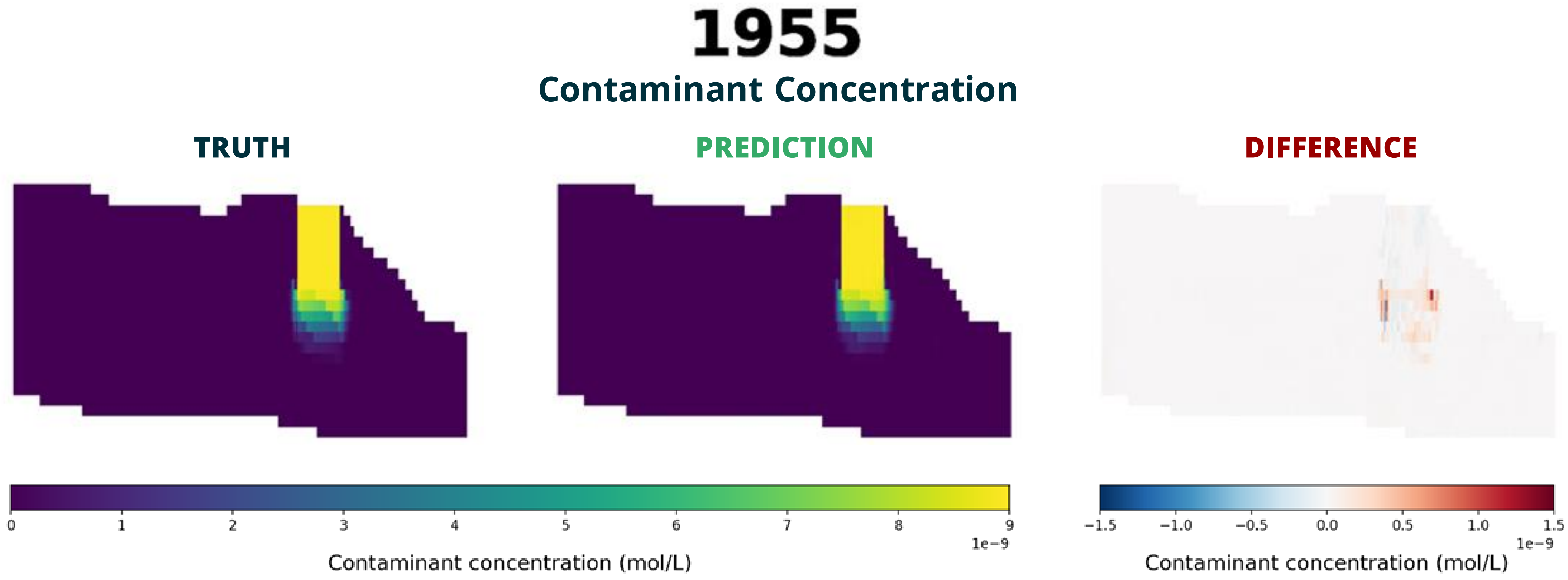
$$\mathcal{L}_{plume}(c',\hat{c'}) = \frac{\|\partial c'/\partial x - \partial \hat{c'}/\partial x\|_2}{\|\partial c'/\partial x\|_2} + \frac{\|\partial c'/\partial z - \partial \hat{c'}/\partial z\|_2}{\|\partial c'/\partial z\|_2}$$

Physics-informed: No flow boundary condition for hydraulic head

$$\mathcal{L}_{BC}(\hat{y}) = \|\hat{q}_x|_{\partial D}\|_2 + \|\hat{q}_z|_{\partial D}\|_2 + \|\partial \hat{h}|_{\partial D}\|_2$$

Tritium concentration on test set

Physics-informed surrogate model runs **600x** faster than Amanzi-ATS



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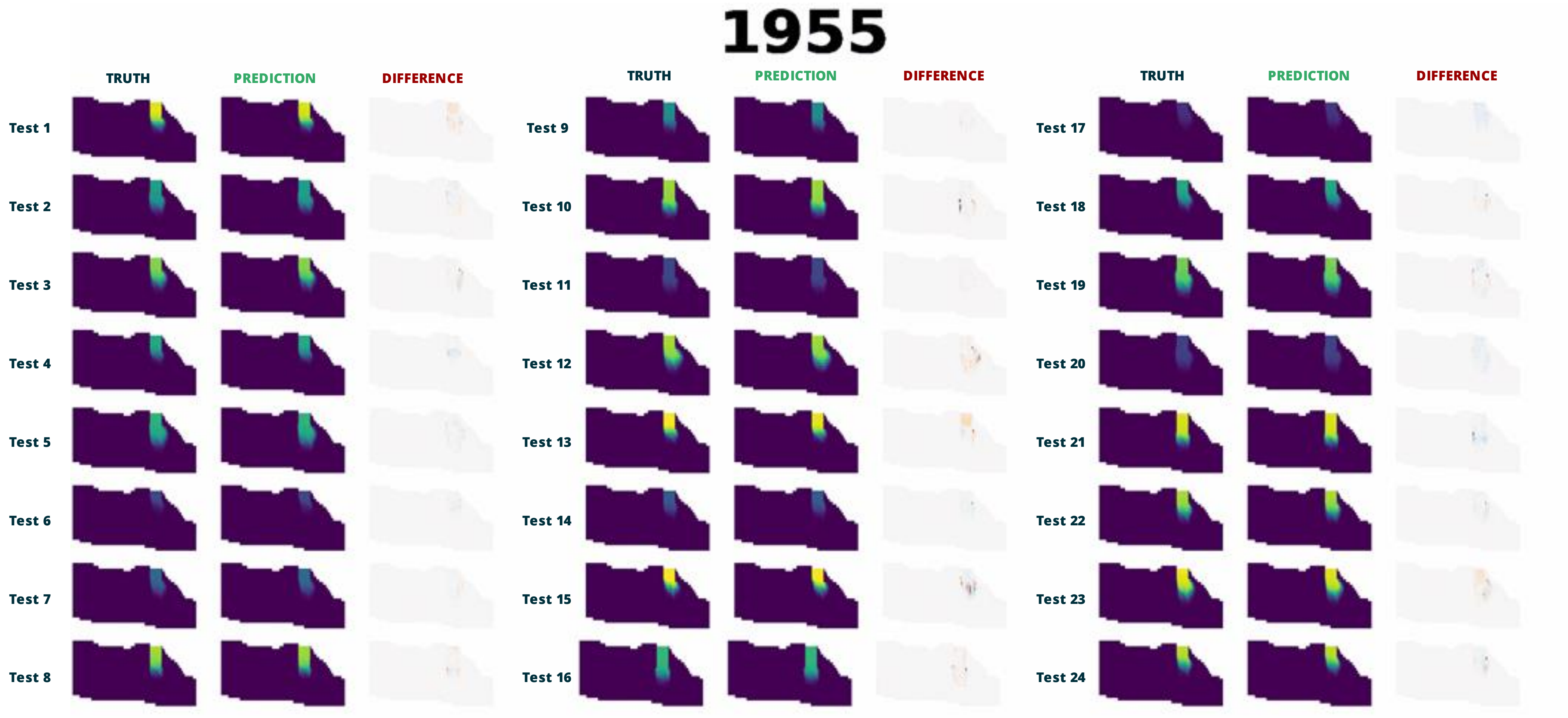
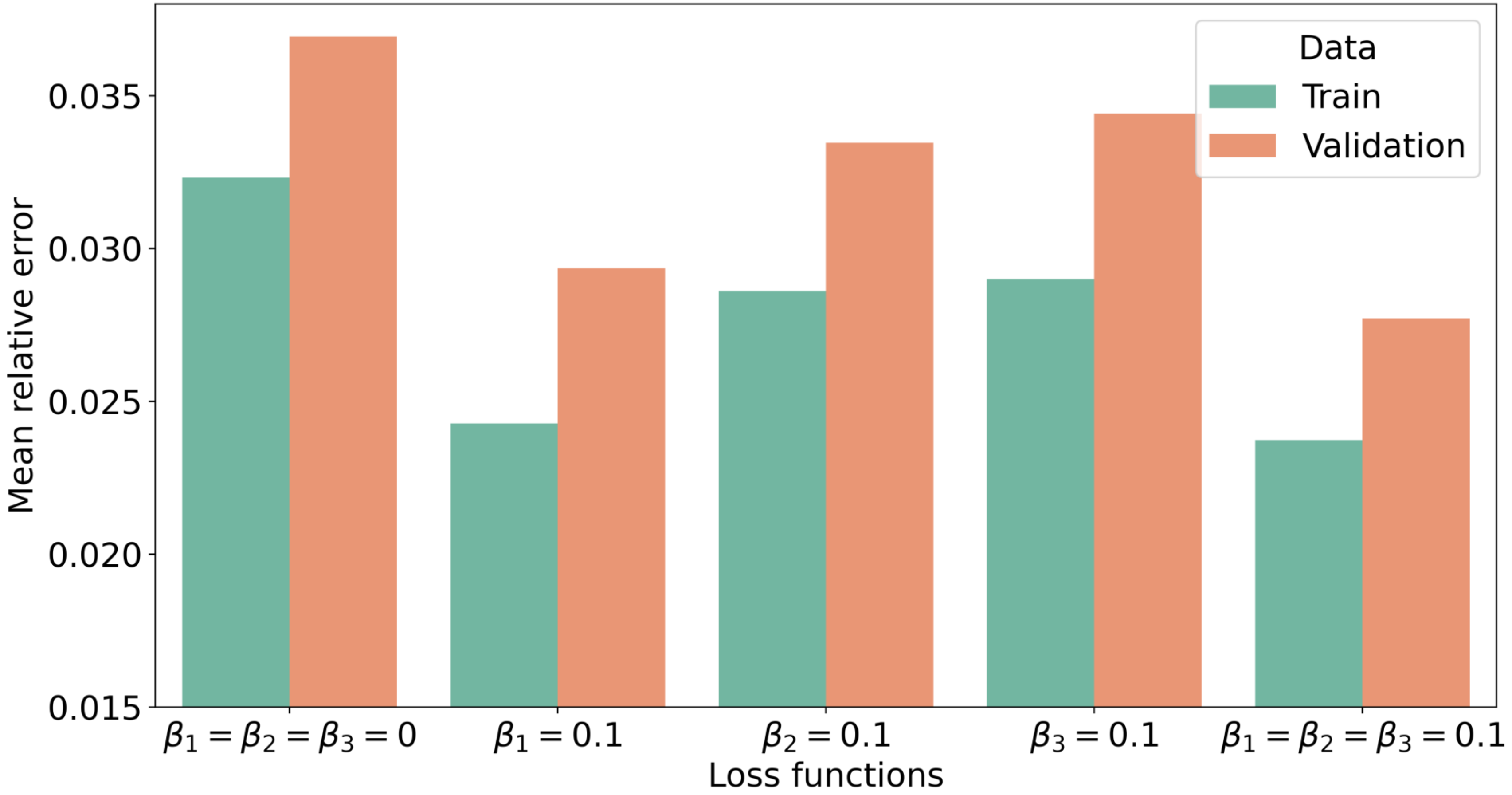


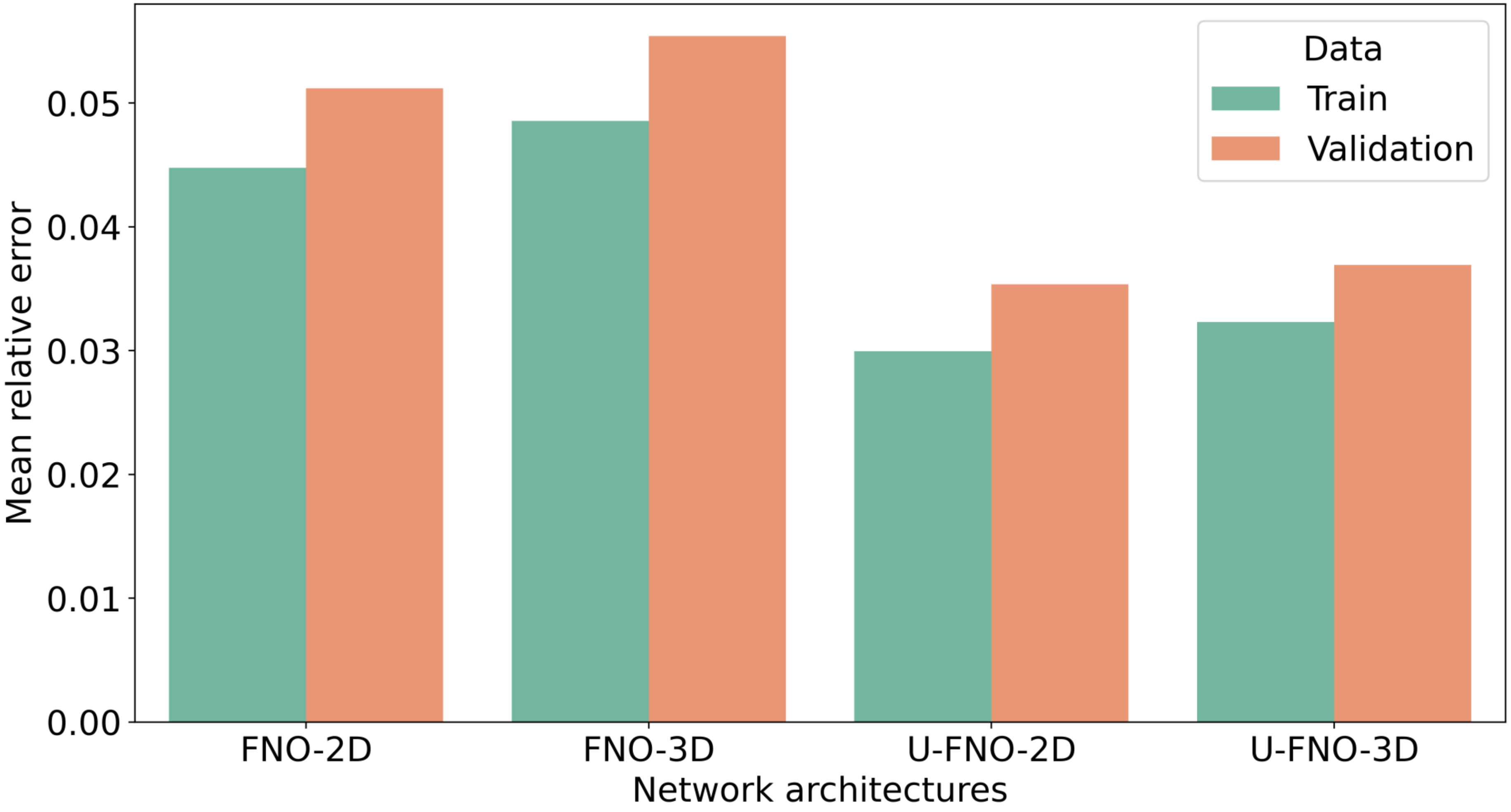
Performance: multiple loss functions

$$\mathcal{L}(y,\hat{y}) = \mathcal{L}_{MRE}(y,\hat{y}) + \beta_1\mathcal{L}_{der}(y,\hat{y}) + \beta_2\mathcal{L}_{plume}(c',\hat{c'}) + \beta_3\mathcal{L}_{BC}(\hat{y})$$



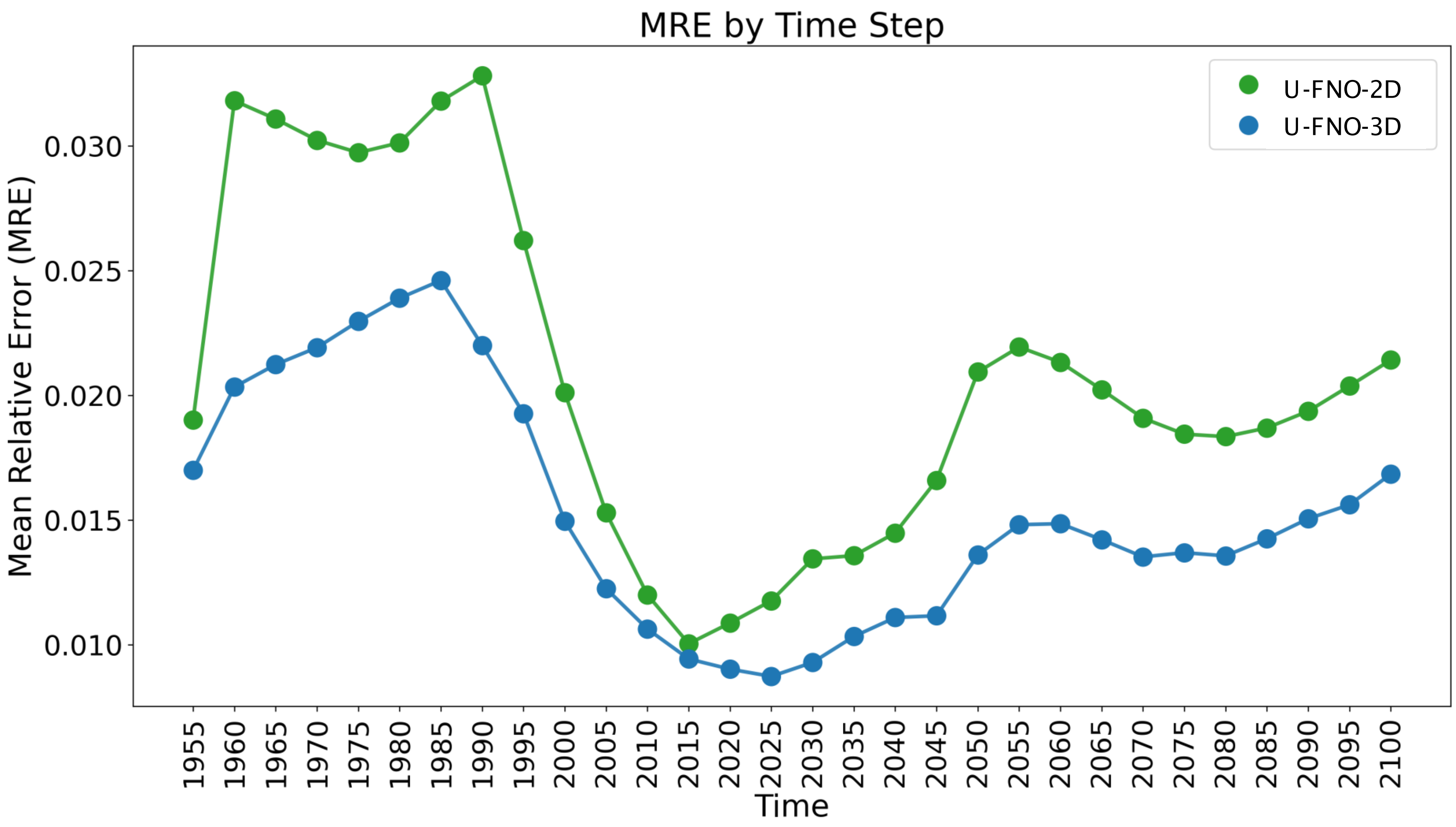
Performance: multiple different architectures

With 30 epochs



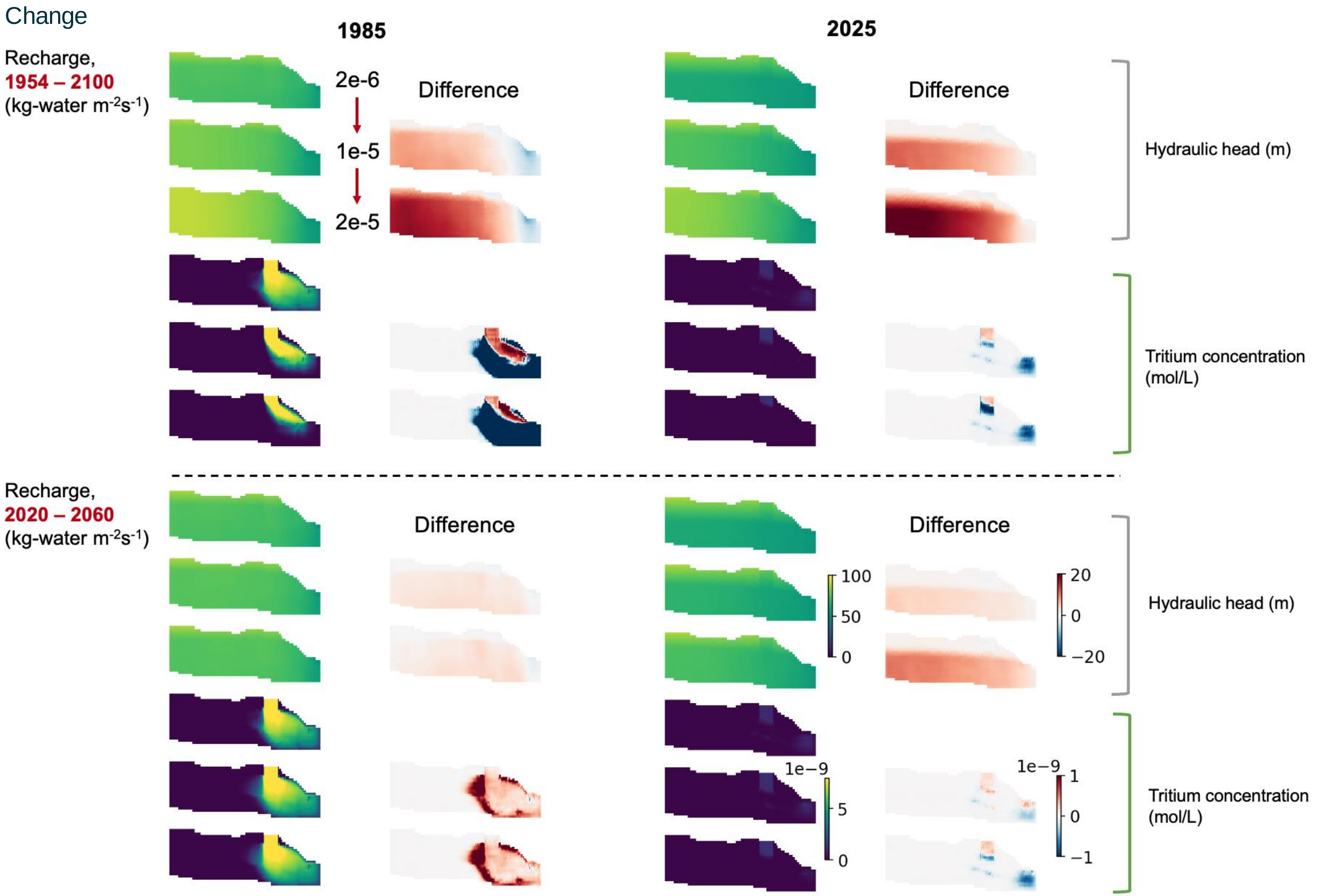
Performance: multiple different architectures

With 150 epochs



Architecture for future projections

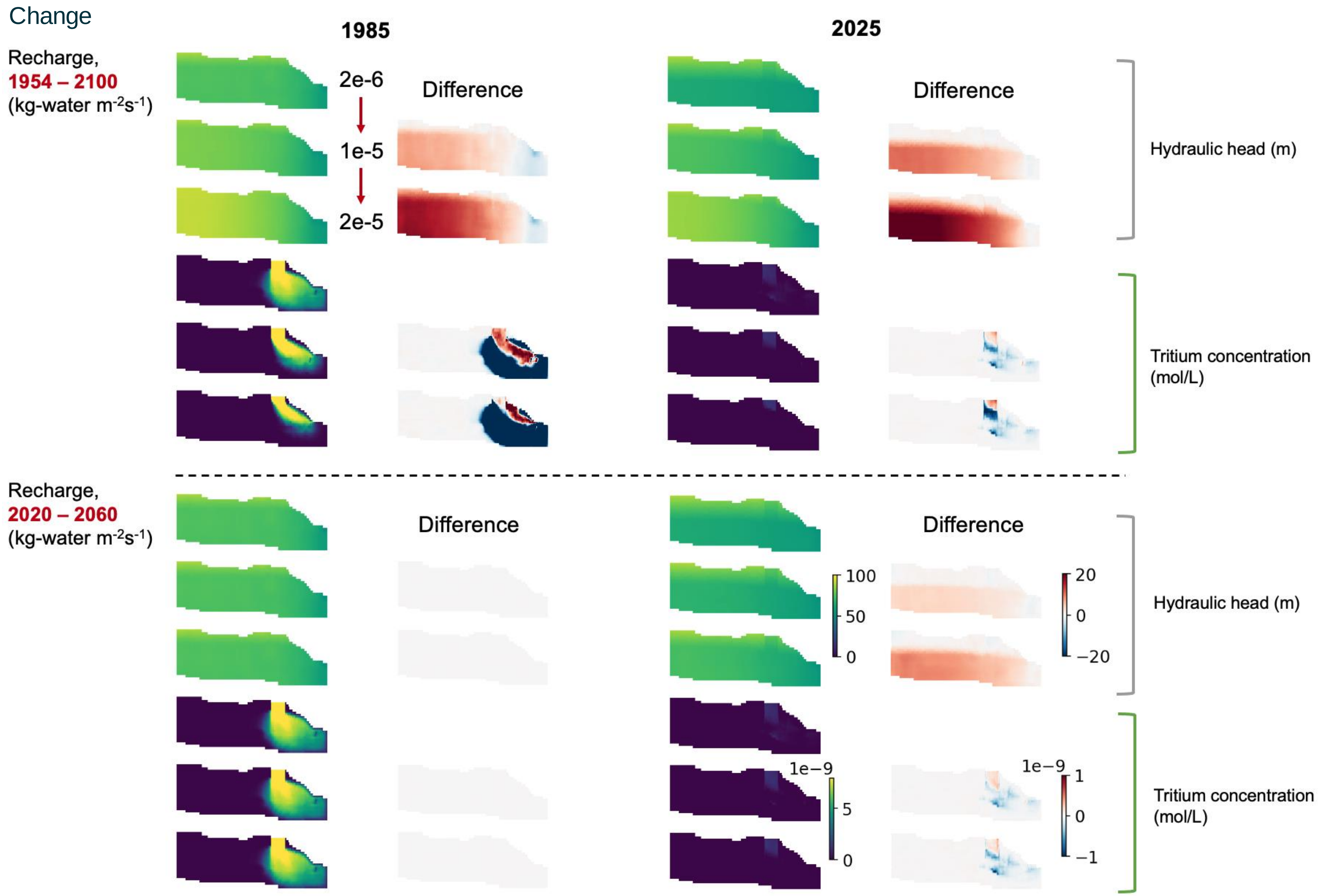
U-FNO-3D



Changing the future recharge impacts the **historical** prediction

Architecture for future projections

U-FNO-2D

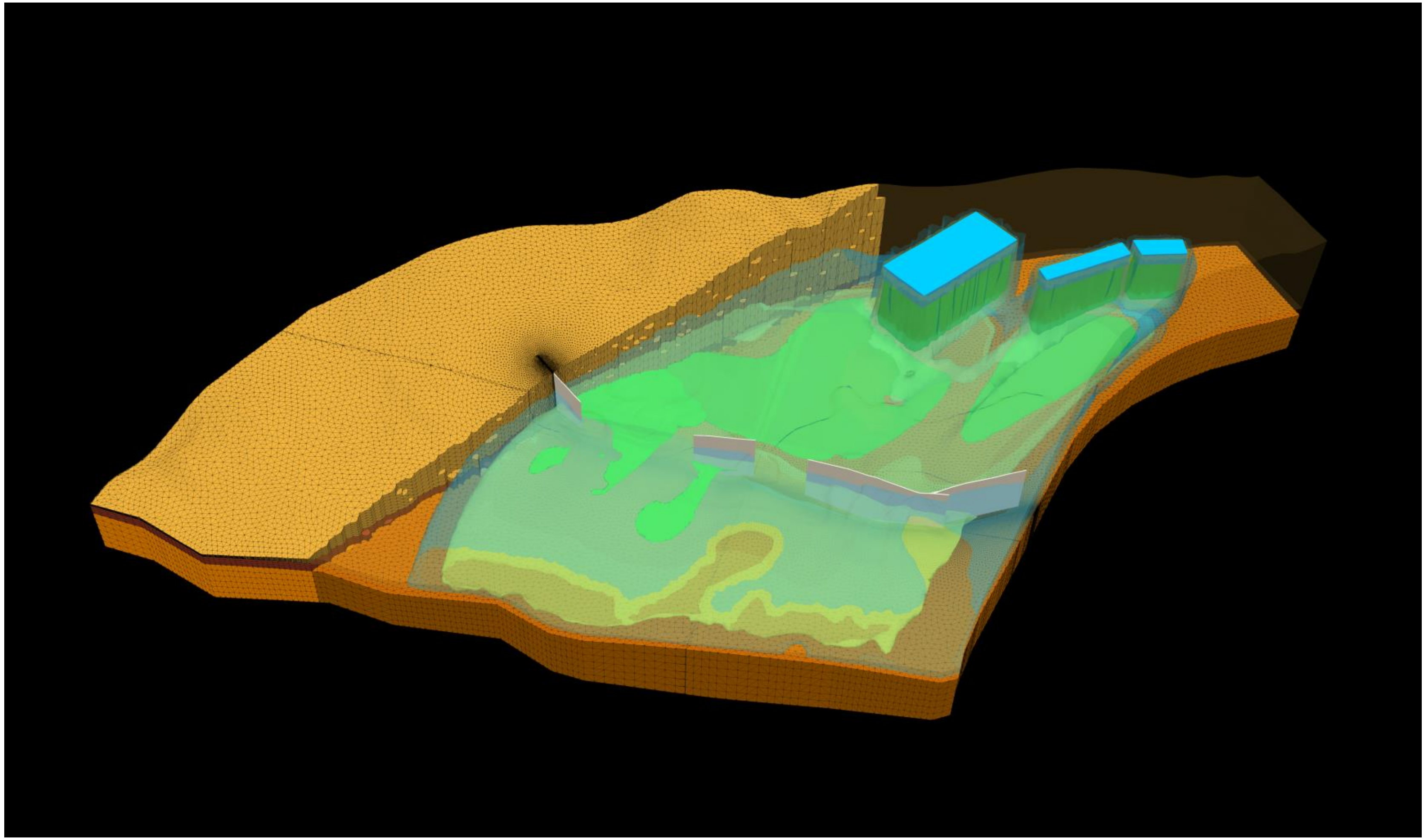


Changing the future recharge **only** impacts the future prediction

Conclusion

- We propose two different architectures U-FNO-2D (recurrent) and U-FNO-3D.
- We design the custom loss functions including:
  - Simulated data-driven loss
  - Physics-informed loss
- U-FNO-3D has more parameters for better training and predictions
- U-FNO-2D is well-suited for predicting the future climate perturbation impacts

Future surrogate modeling with full 3D model



What is next?

Integrate in-situ long-term monitoring data and support remediation decisions