DeepPore Dynamics

Omar AlSuqri, Shamim Karimi pashaki, Oluwaseun Olabode, Nathalie Pinheiro, Alex Trenam

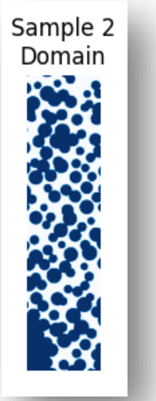
Outline

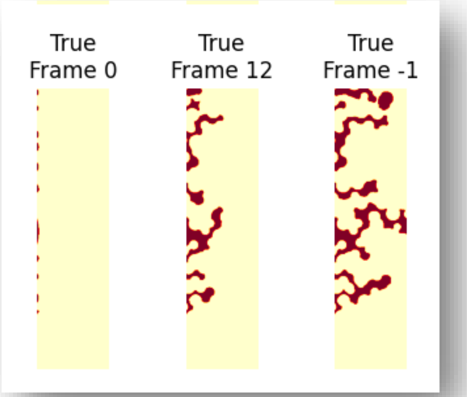
- Challenge and background
- Our approach – diffusion models
- Model parameters and results
- Iterative single time step iterations
- Next steps

The Challenge

- Building innovative AI models to predict CO_2 invasion in a porous rock matrix.

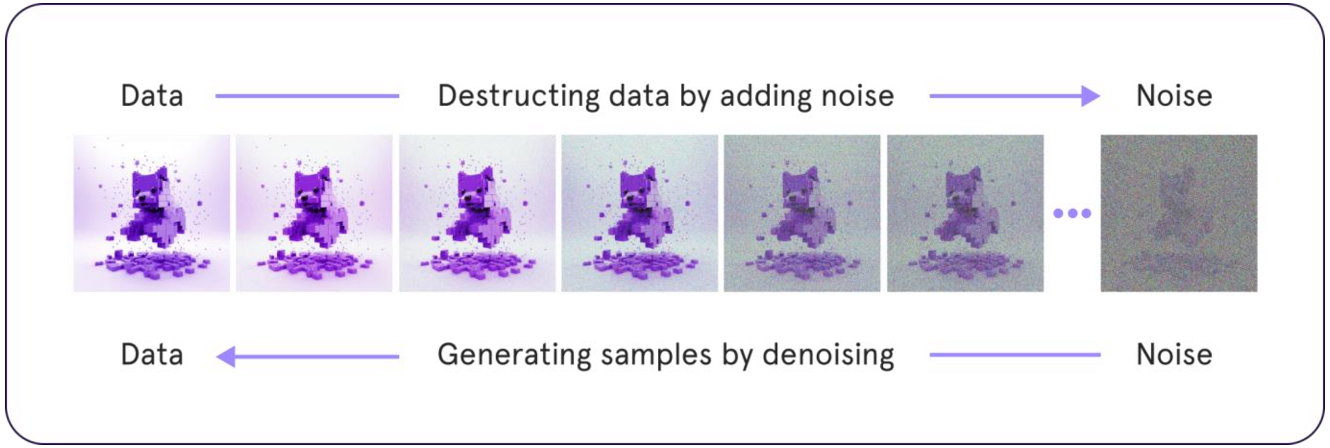
- Data:
    - Domain arrays.
    - Invasion arrays.





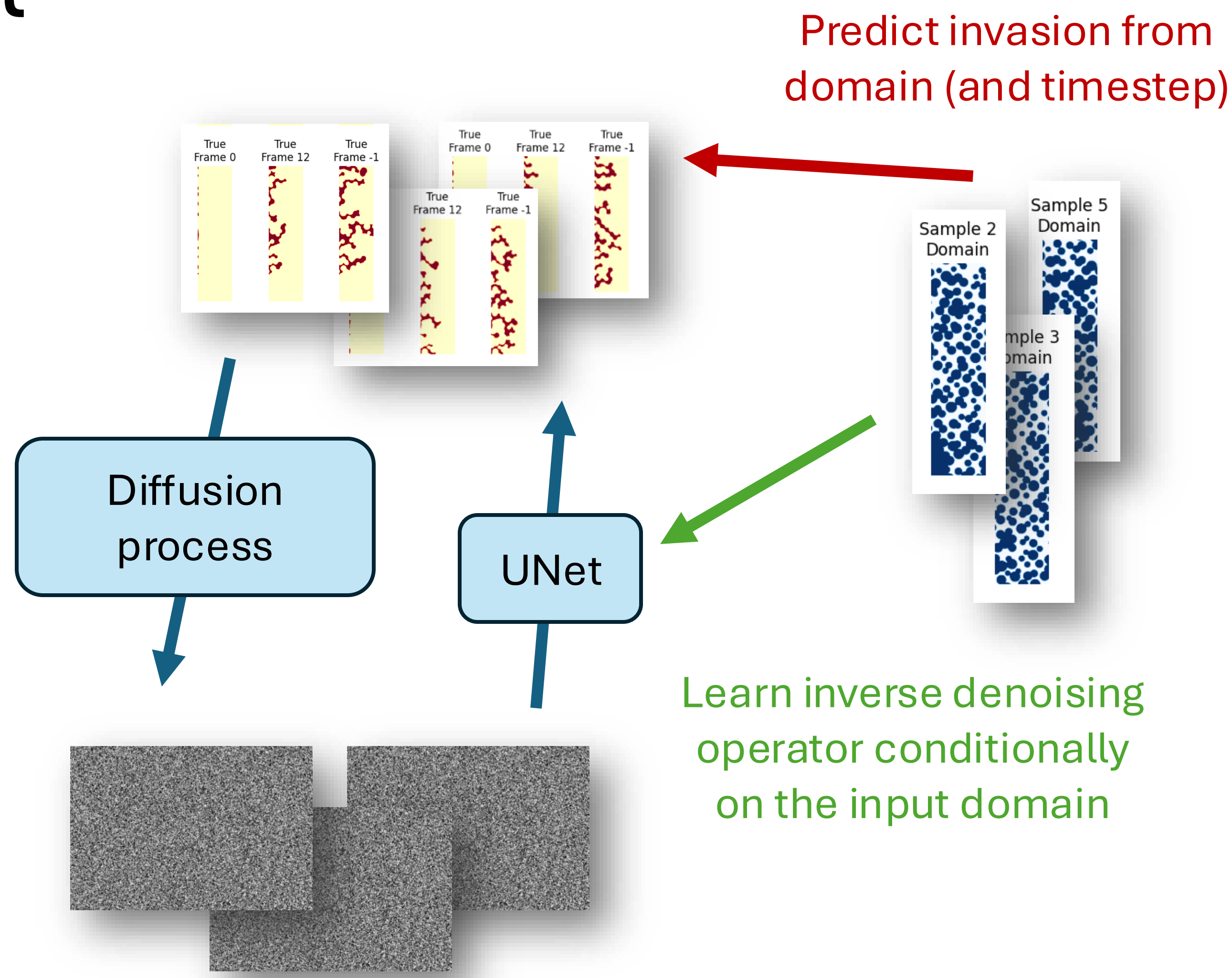
Diffusion models

- First introduced for image generation in Ho et al. (2020)
- Generative approach, outperforming GANs – Dhariwal et al. (2021)
- Work well for creating images from noise and a prompt



- Recent works have shown good results using diffusion models to predict fluid flow past an obstacle of varying shape – Hu et al. (2024)

The Model

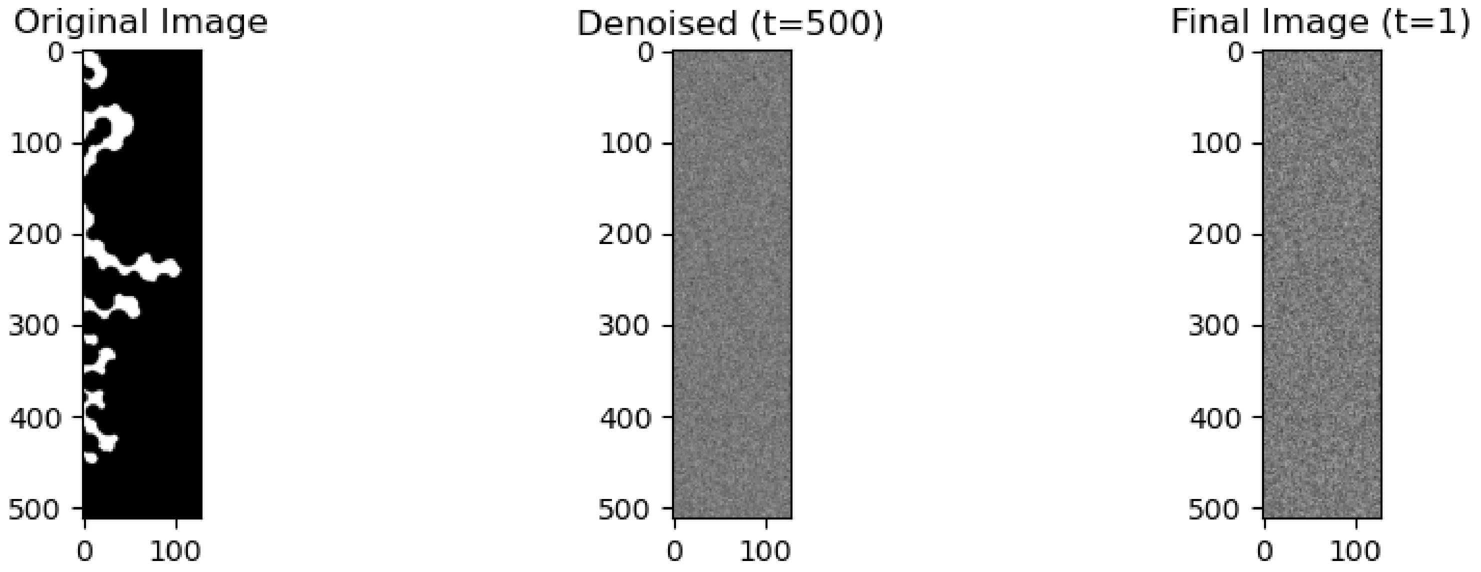

Predict invasion from domain (and timestep)
True Frame 0
True Frame 12
True Frame -1
Sample 2 Domain
Sample 5 Domain
Diffusion process
UNet
Learn inverse denoising operator conditionally on the input domain

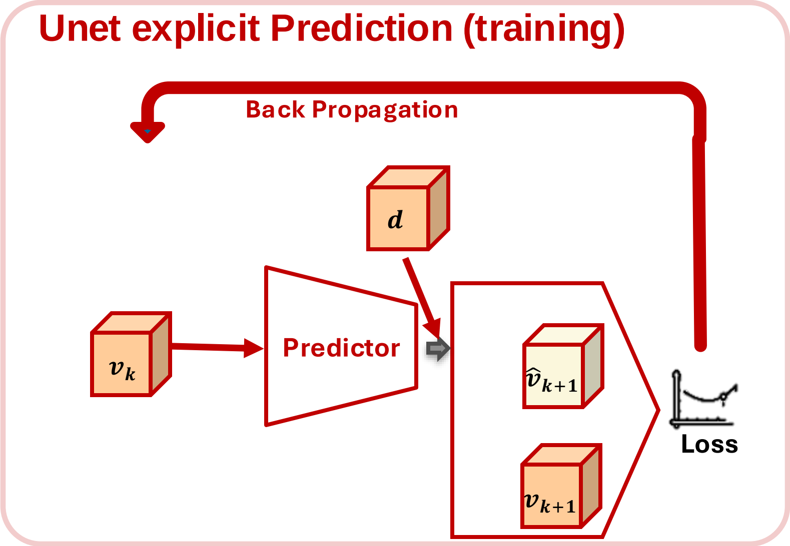
Diffusion Models Parameters

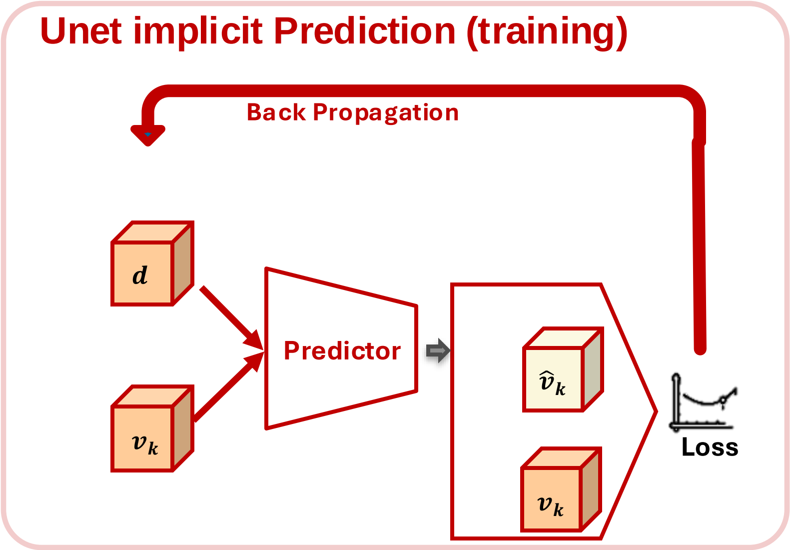
Time steps	Epochs	Data Size	Training time
1000	10	177	9 hrs

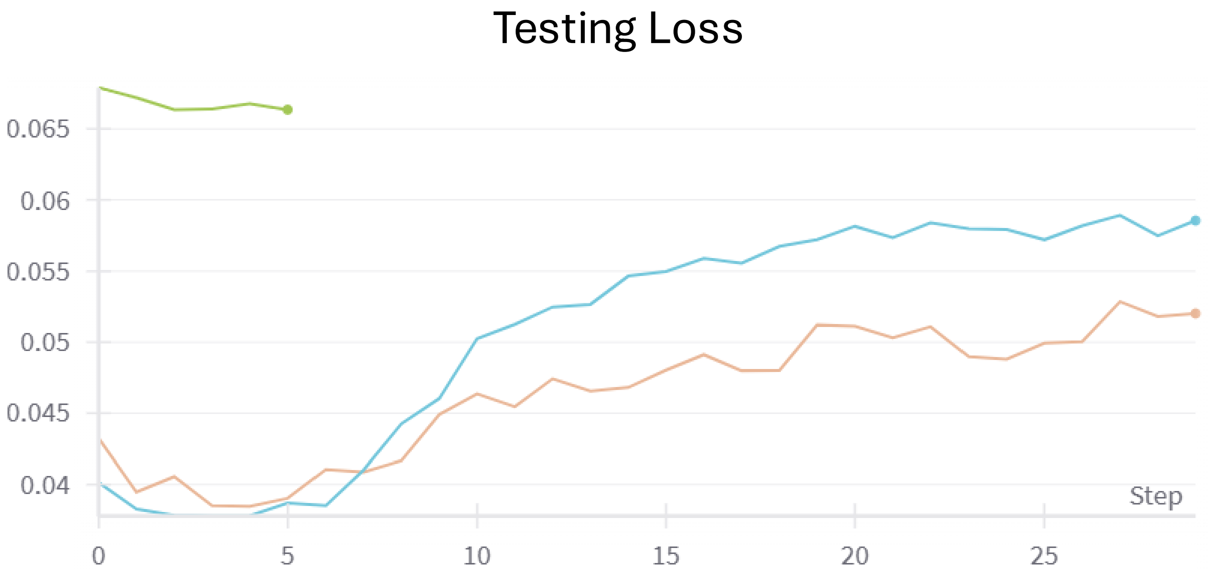
Results

- The training loss ended with a MSE of 0.004
- The validation loss have an average value of about 0.0025.



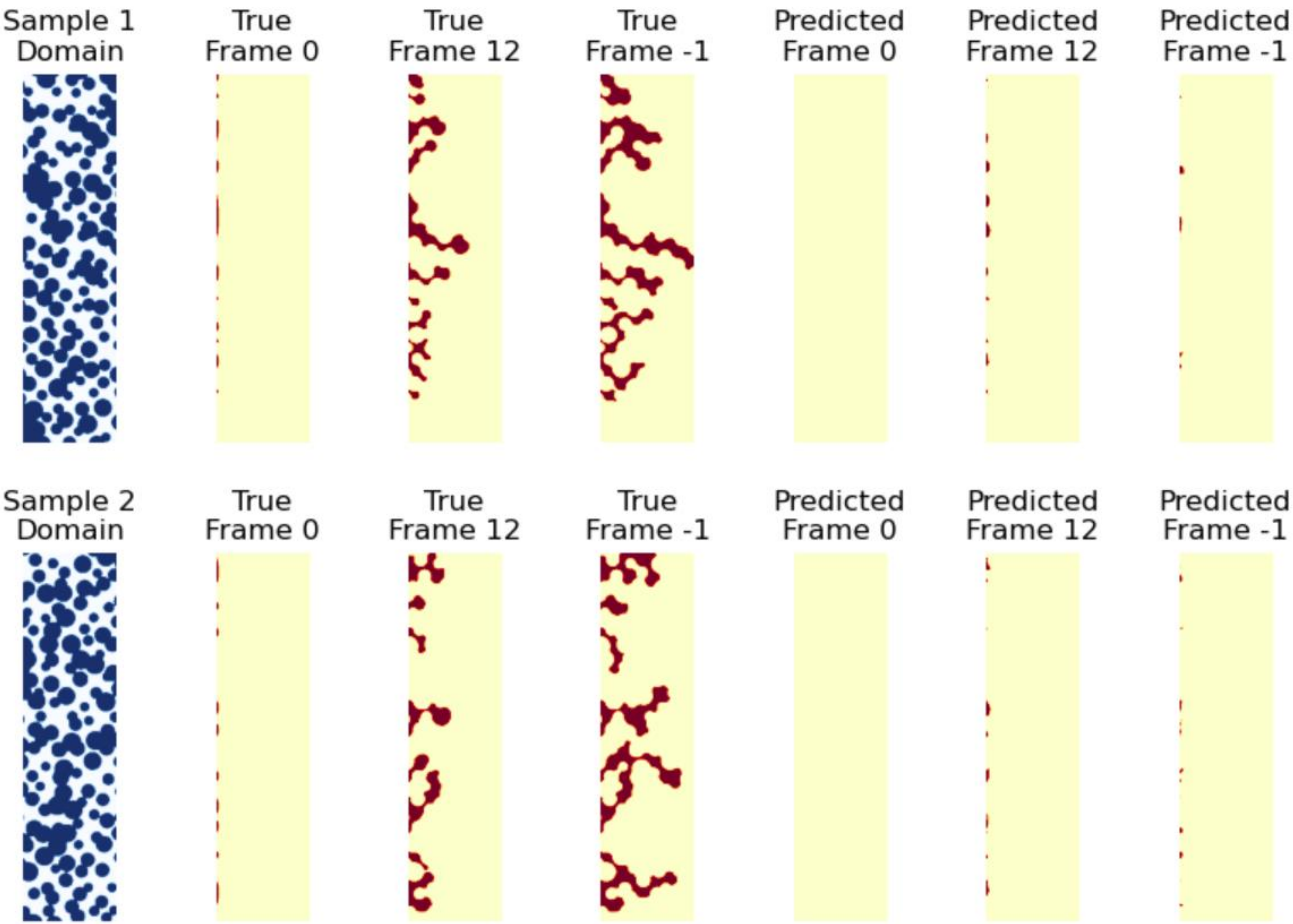




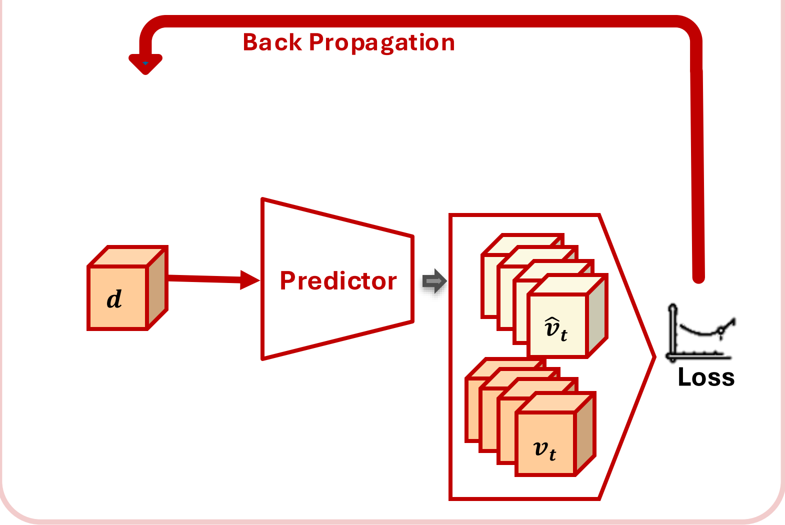


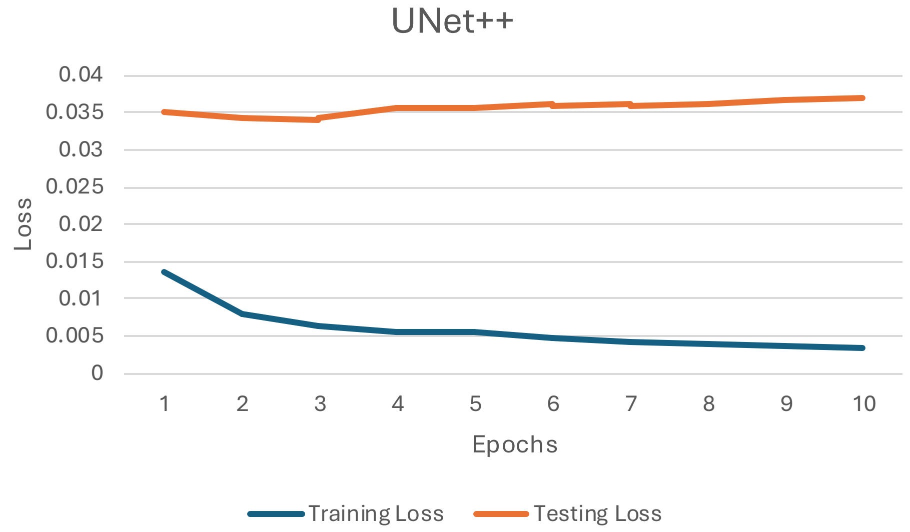
Unet explicit: 1timestep input (previous t), domain as mask
Unet explicit: 1timestep input (previous t), domain as mask, subsamples
Unet implicit: 2 inputs (guess t, domain)

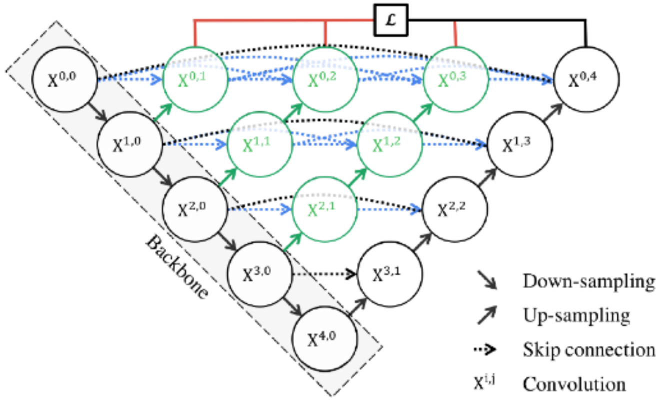
Unet explicit: 1timestep input (previous t), domain as mask

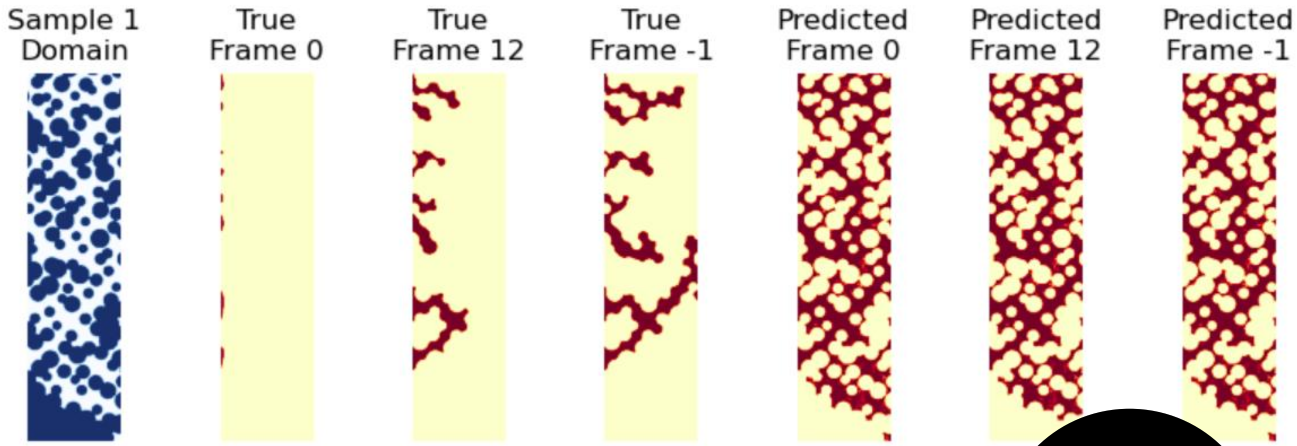


Unet++ Prediction – Multiple output (training)









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

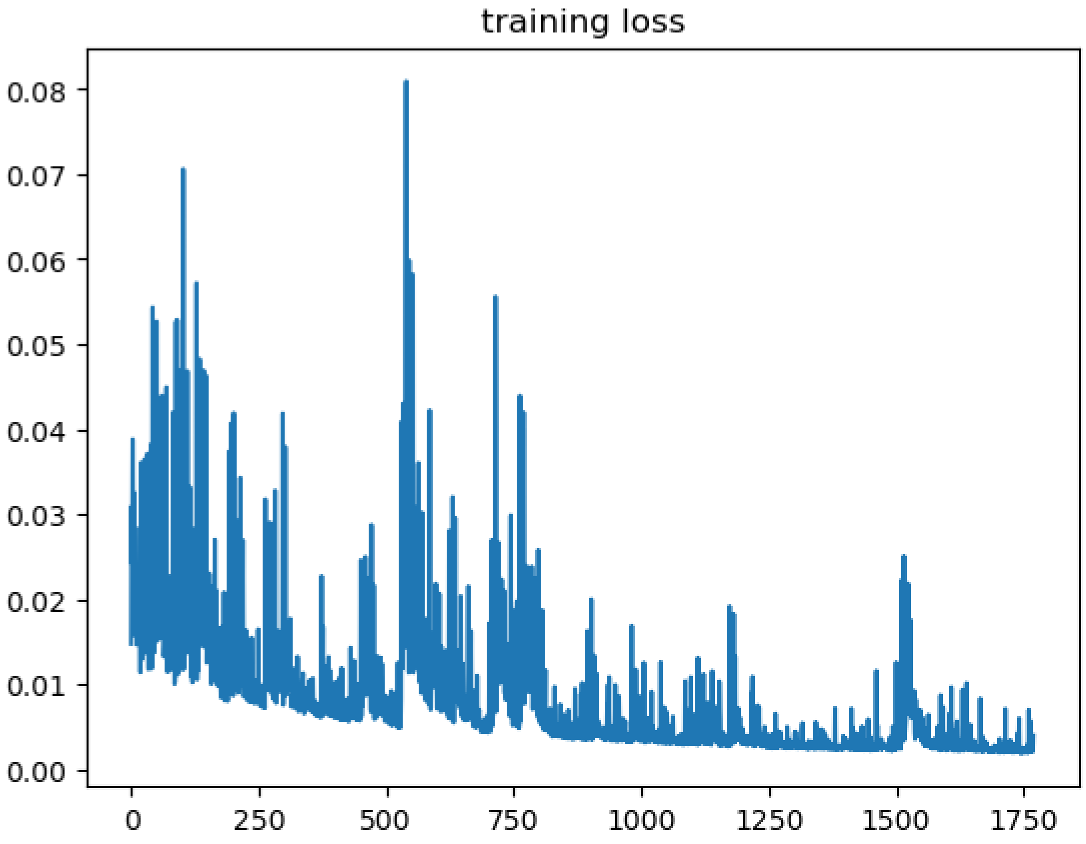
Next steps

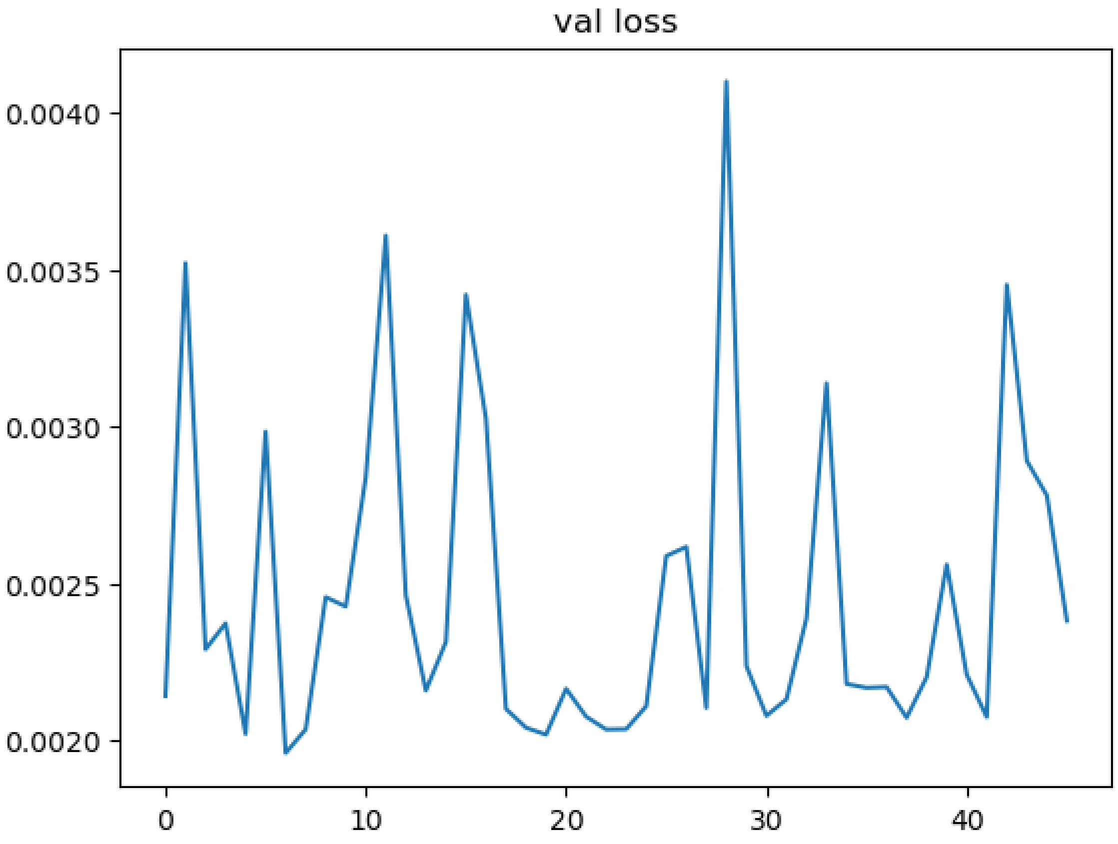
- Diffusion:
  - Correct the model and generate close denoised realizations.
  - Enhance the training by trying a different neural network.
  - Apply the domain data at the end to make sure that generated CO_2 are not located out of the pores.
- Assessing whether applying 3D Conv layers in the Unet generates better results, or adding LSTM instead of the Unet to integrate time sequence better.
- Try time embedding using Feature-wise Linear Modulation (FiLM)

$$y = \gamma(t) \cdot x + \beta(t)$$

Thank you

Appendix


training loss
0.08
0.07
0.06
0.05
0.04
0.03
0.02
0.01
0.00
0
250
500
750
1000
1250
1500
1750


val loss
0.0040
0.0035
0.0030
0.0025
0.0020
0
10
20
30
40