An encoder-decoder ConvLSTM surrogate model for simulating geological CO_2 sequestration with dynamic well controls

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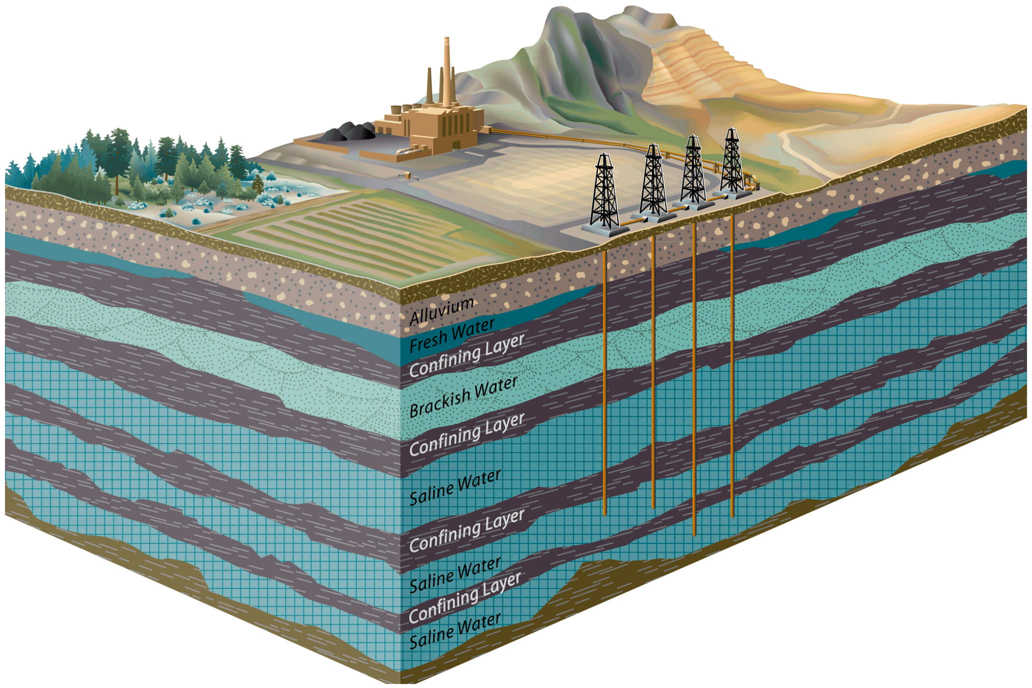
1. Introduction

Geological Carbon Sequestration (GCS)



Multiphase, Multicomponent

Complex Thermodynamics

CO_2 flow in porous media

Geological Heterogeneity

Coupled Multi-physics Process

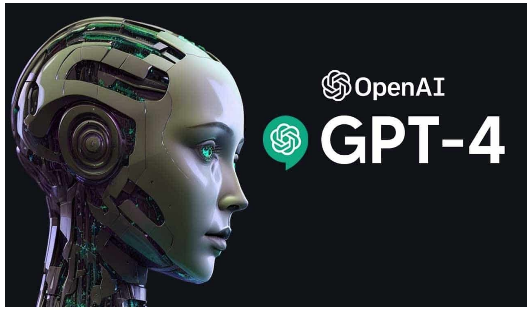
- A promising strategy for mitigating climate warming
- Injection of SC-CO_2 into subsurface reservoirs (e.g. deep saline aquifers)

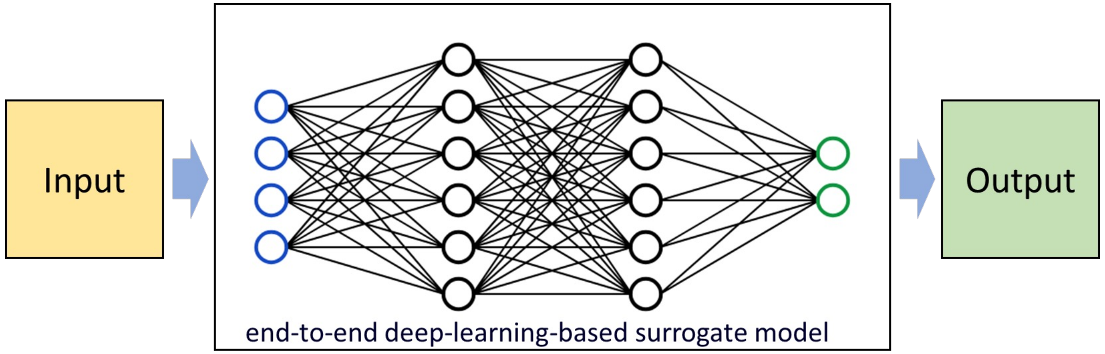
× Challenge to characterize CO_2 migration

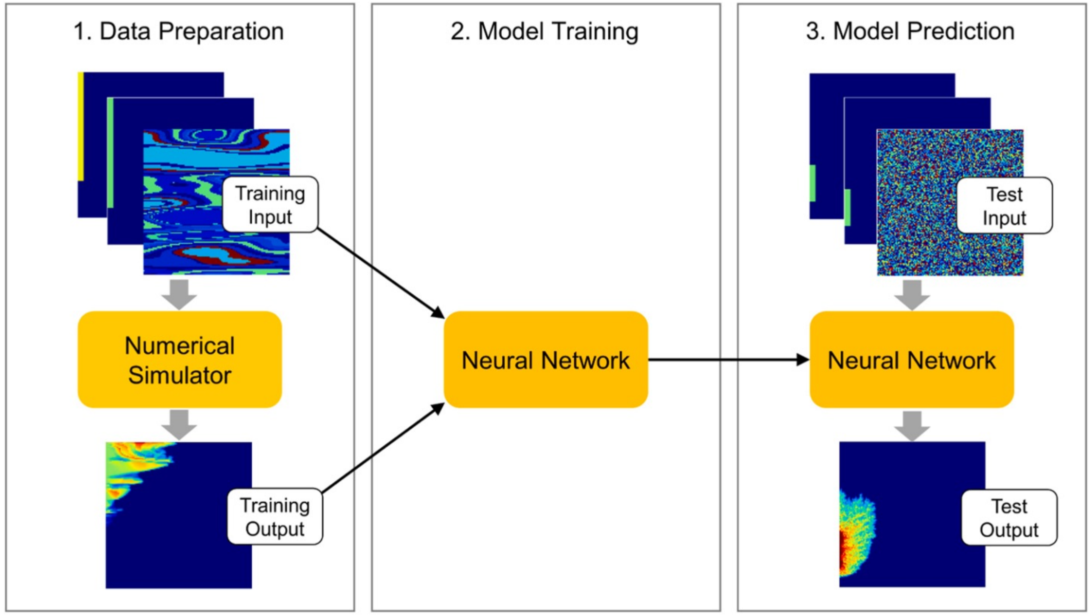
× Inefficient to run simulation for optimization/ inverse problems

1. Introduction

Deep Learning Techniques and Surrogate Modeling



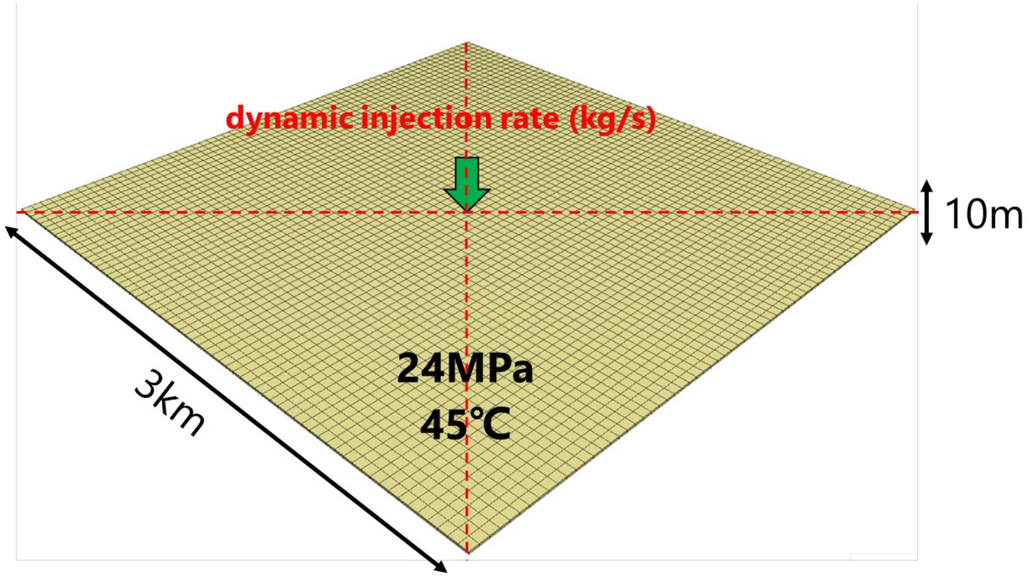




Wen et al., 2021

- ✓ An image-to-image task with end-to-end fashion
- ✓ Fast inference time (within milliseconds)
- ✓ Advantageous in optimization / inverse problems

2. Methods: governing equations & numerical model



Property	Value
Model Size	3km*3km*10m
Mesh	64*64*1
Boundary Condition	Open Flow
Thermal Effect	Neglected
Relative Permeability	Corey
Capillary Pressure	van Genuchten

- **Mass conservation for each component κ**

$$\frac{\partial}{\partial t}M^\kappa = -\nabla \cdot \boldsymbol{F}^\kappa + Q^\kappa$$

- **Mass accumulation**

$$M^\kappa = \phi \sum_\beta S_\beta \, \rho_\beta X_\beta^\kappa$$

- **Mass flux**

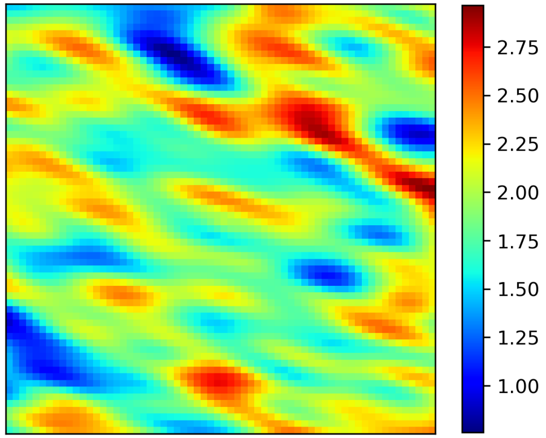
$$\boldsymbol{F}^\kappa = \sum_\beta X_\beta^\kappa \, \boldsymbol{F}_\beta$$

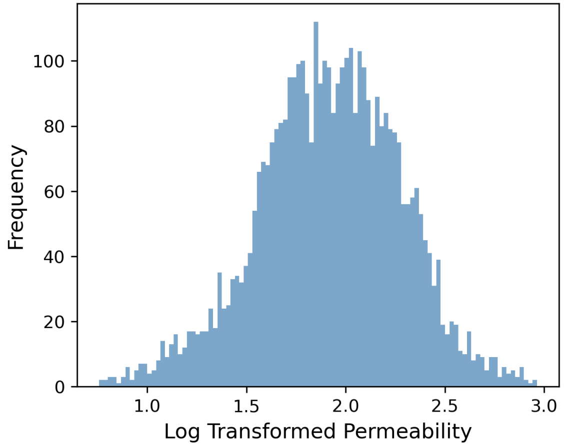
- **Multiphase Darcy's law**

$$\boldsymbol{F}_\beta = -k\frac{k_{r\beta}\rho_\beta}{\mu_\beta}(\nabla p_\beta - \rho_\beta \boldsymbol{g})$$

Methods: dataset generation

Gaussian Random Field





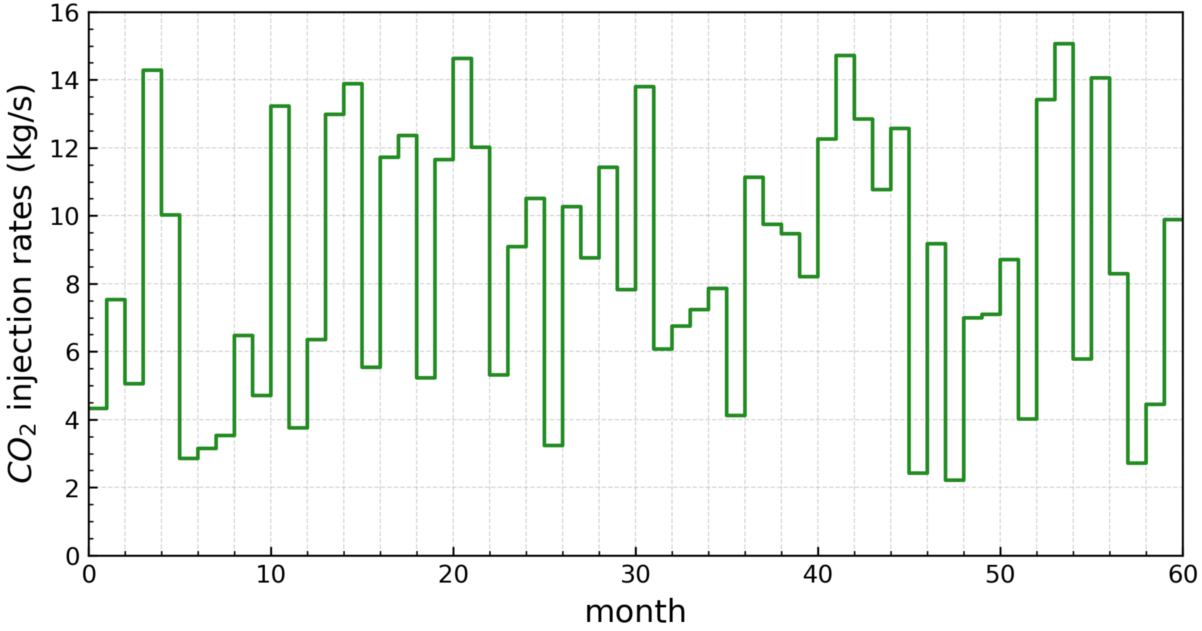
by GSTools

- Permeability follows a log-normal distribution
- Anisotropy permeability fields
- Porosity is correlated to permeability (Zhong et al., 2019):

$$\phi = 0.05\log_{10}(k) + 0.15.$$

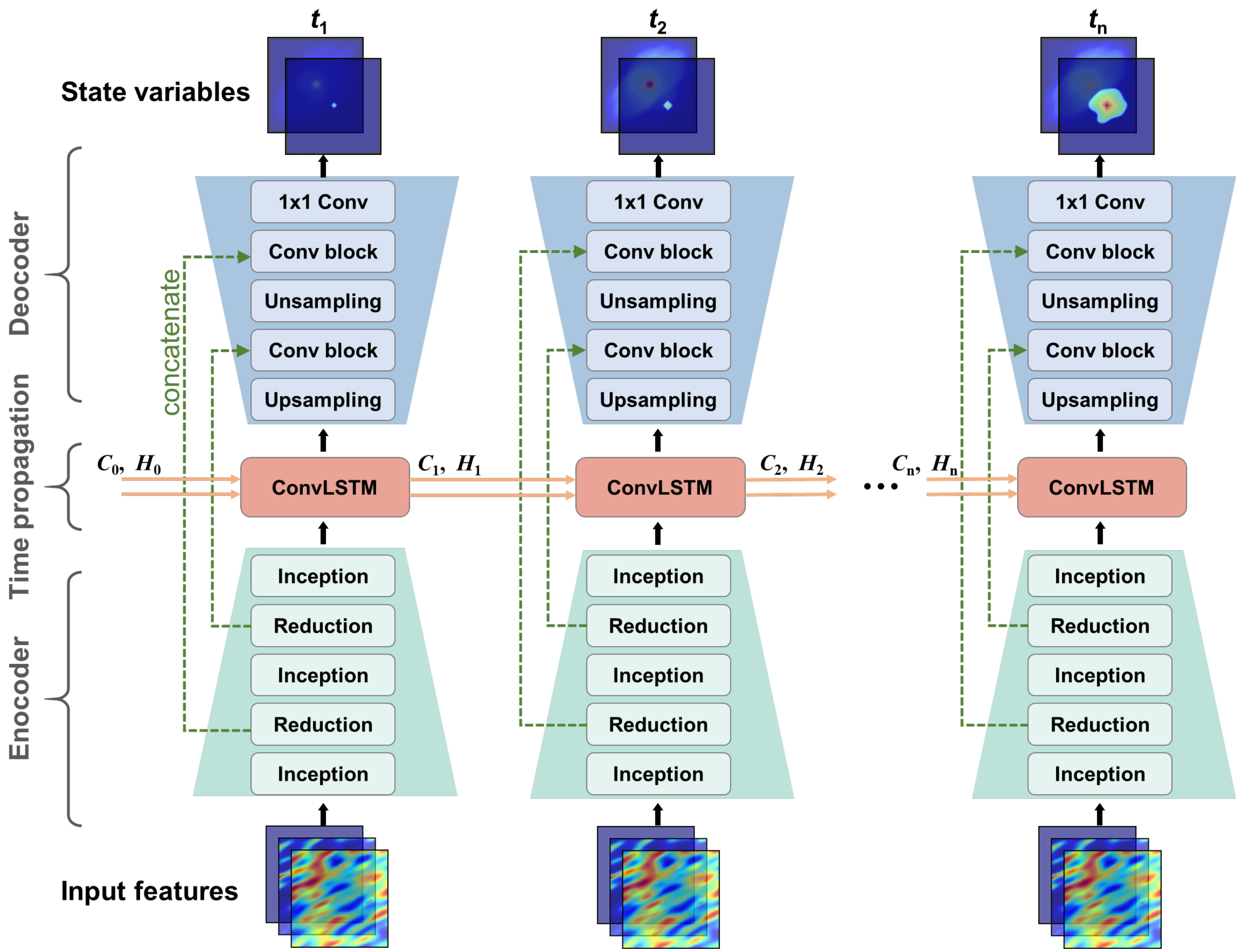
- 5000 cases in total

Dynamic Well Controls

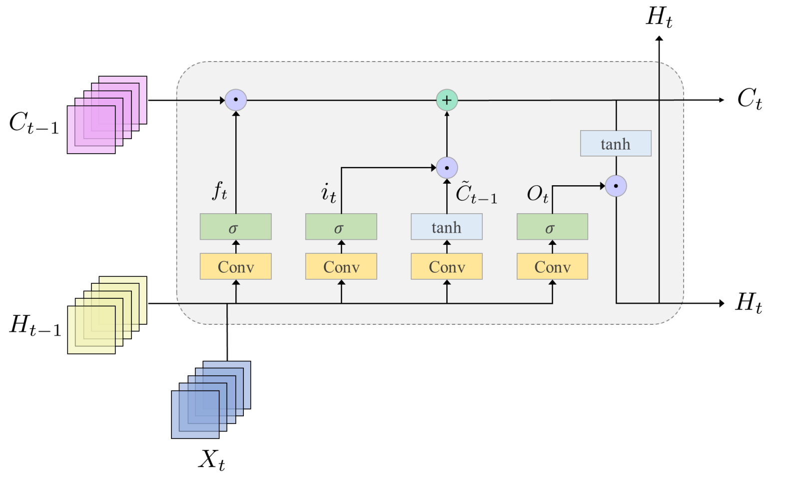


- monthly injection rate sampled via Latin-Hypercube Sampling

Methods: Encoder-Decoder ConvLSTM



Convolution Long Short-Term Memory

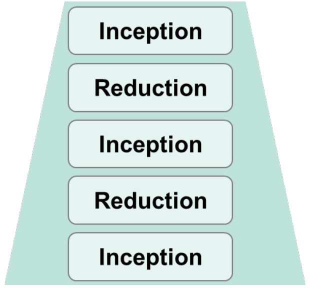


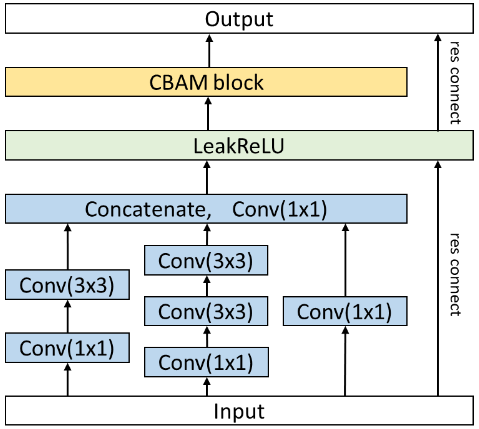
$$
\begin{aligned}
\mathbf{i_t} &= \mathrm{Sigmoid}\left(\mathrm{Conv}\left(\mathbf{x_t};\mathbf{w_{xi}}\right)+\mathrm{Conv}\left(\mathbf{h_{t-1}};\mathbf{w_{hi}}\right)+\mathbf{b_i}\right)\\
\mathbf{f_t} &= \mathrm{Sigmoid}\left(\mathrm{Conv}\left(\mathbf{x_t};\mathbf{w_{xf}}\right)+\mathrm{Conv}\left(\mathbf{h_{t-1}};\mathbf{w_{hf}}\right)+\mathbf{b_f}\right)\\
\mathbf{o_t} &= \mathrm{Sigmoid}\left(\mathrm{Conv}\left(\mathbf{x_t};\mathbf{w_{xo}}\right)+\mathrm{Conv}\left(\mathbf{h_{t-1}};\mathbf{w_{ho}}\right)+\mathbf{b_o}\right)\\
\mathbf{g_t} &= \mathrm{Tanh}\quad\left(\mathrm{Conv}\left(\mathbf{x_t};\mathbf{w_{xg}}\right)+\mathrm{Conv}\left(\mathbf{h_{t-1}};\mathbf{w_{hg}}\right)+\mathbf{b_g}\right),\\
\mathbf{c_t} &= \mathbf{f_t}\odot\mathbf{c_{t-1}}+\mathbf{i_t}\odot\mathbf{g_t}\\
\mathbf{h_t} &= \mathbf{o_t}\odot\mathrm{Tanh}(\mathbf{c_t})
\end{aligned}
$$

- ✓ capturing time-varying features
- ✓ alleviating gradient exploding or vanishing

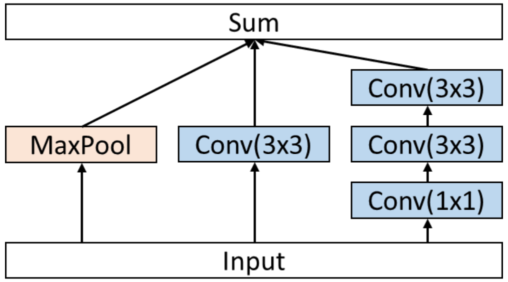
Methods: Encoder-Decoder ConvLSTM

Encoder



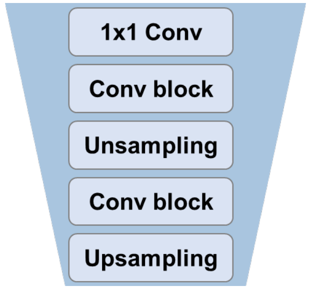


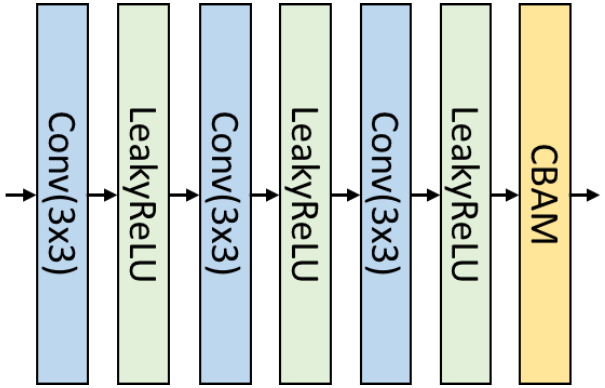
Inception block
hierarchical feature



Reduction block
dimension reduced 1/2

Decoder

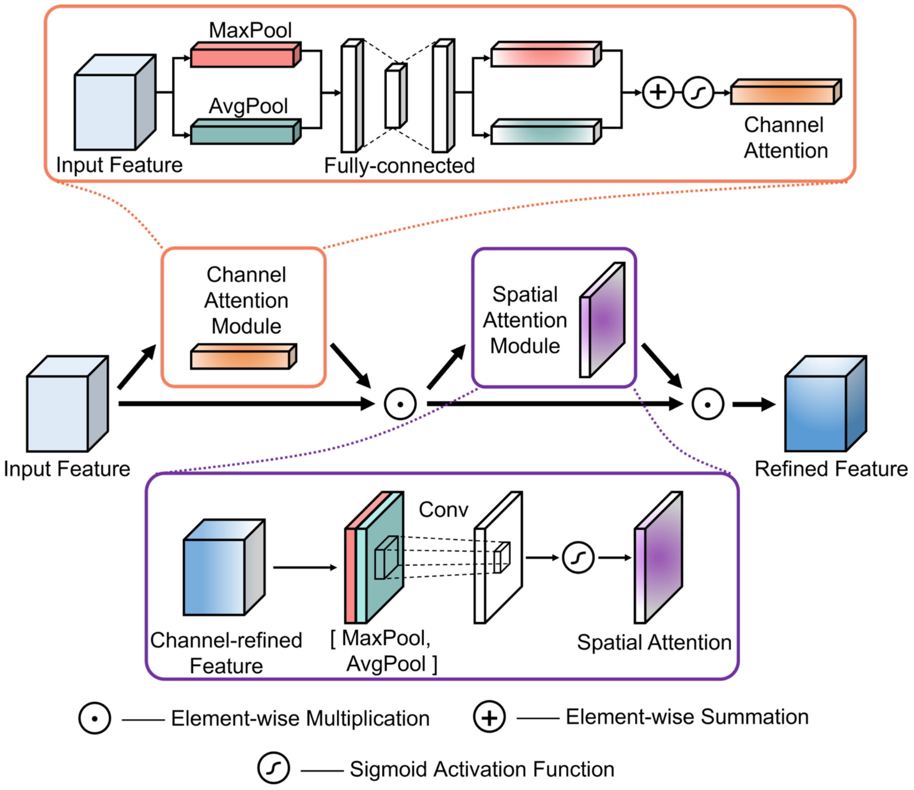




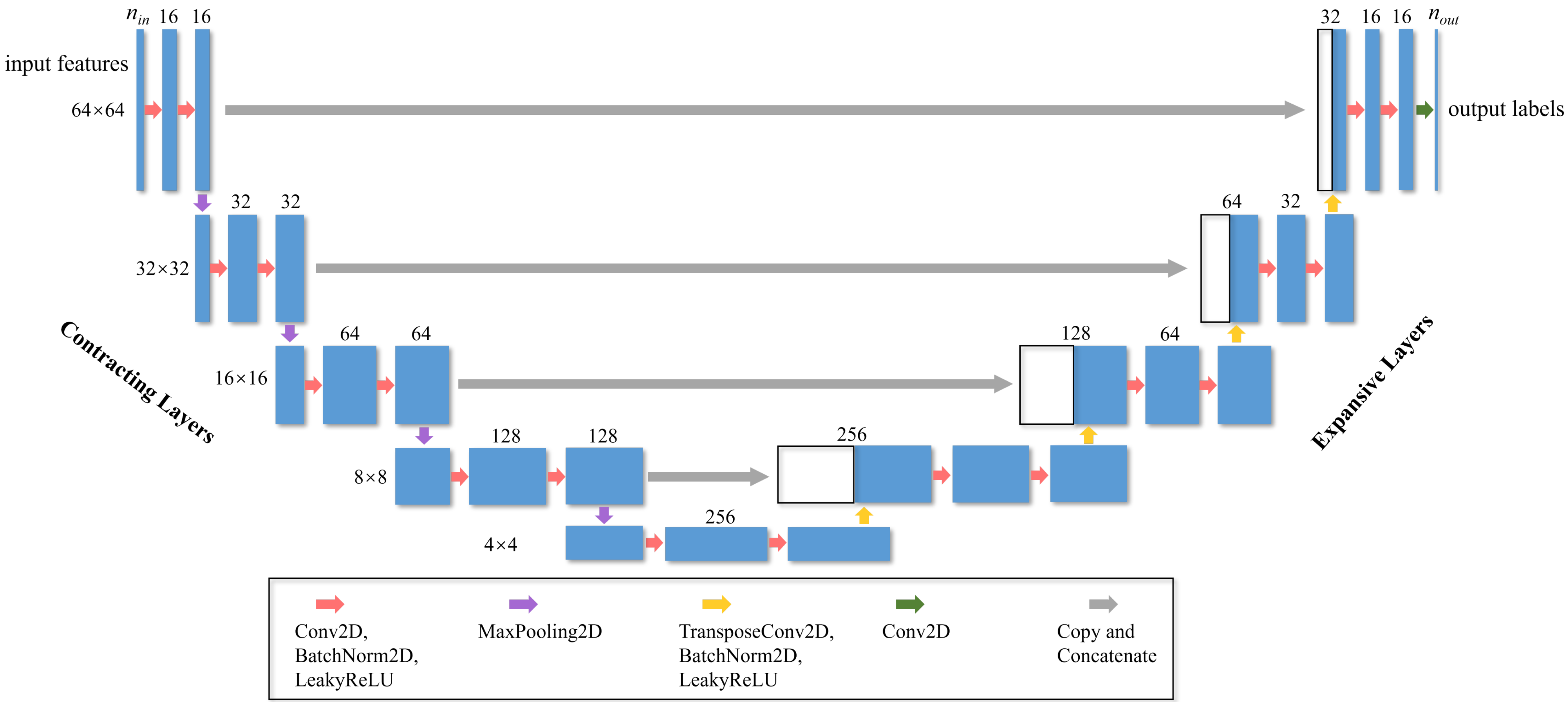
Conv block

CBAM

Convolutional Block Attention Module
(Woo et al., 2018)



Methods: benchmark with U-Net



Methods: model training

$$L(\theta) = \boxed{\frac{1}{n_s}\frac{1}{n_t}\sum_{i=1}^{n_s}\sum_{t=1}^{n_t}\left\|y_i^t - \hat{y}_i^t\right\|_p} + \boxed{\lambda_1 \frac{1}{n_s}\frac{1}{n_t}\sum_{i=1}^{n_s}\sum_{t=1}^{n_t}\sum_{j=1}^{k}\left\|D^j y_i^t - D^j \hat{y}_i^t\right\|_p} + \boxed{\lambda_2 \frac{1}{n_s}\frac{1}{n_{t_i}}\sum_{i=1}^{n_s}\sum_{t=1}^{n_{t_i}}\left\|y_i^t - \hat{y}_i^t\right\|_p}$$

L1 for pressure
L2 for saturation

Gradient loss

Temporal penalty

ED-ConvLSTM model summary. n_t denotes the channel for time step.

Name	Type	Output shape
Input		n_t, 64, 64, 3
Encoder 1	Inception Residual Block	n_t, 64, 64, 16
Encoder 2	Reduction Block	n_t, 32, 32, 16
Encoder 3	Inception Residual Block	n_t, 32, 32, 64
Encoder 4	Reduction Block	n_t, 16, 16, 64
Encoder 5	Inception Residual Block	n_t, 16, 16, 128
ConvLSTM	Convolutional LSTM Layer	n_t, 16, 16, 128
Decoder 1	Upsampling Block	n_t, 32, 32, 128
Decoder 2	Convolutional Block	n_t, 32, 32, 64
Decoder 3	Upsampling Block	n_t, 64, 64, 64
Decoder 4	Convolutional Block	n_t, 64, 64, 32
Decoder 5	1 × 1 Convolutional Layer	n_t, 64, 64, 1
Output		n_t, 64, 64, 1

U-Net model summary

Name	Type	Output shape
Input		64, 64, 4
Encoder 1	Conv2d/Conv2d/MaxPool2d	32, 32, 16
Encoder 2	Conv2d/Conv2d/MaxPool2d	16, 16, 32
Encoder 3	Conv2d/Conv2d/MaxPool2d	8, 8, 64
Encoder 4	Conv2d/Conv2d/MaxPool2d	4, 4, 128
Conv	Conv2d/Conv2d	4, 4, 256
Decoder 1	TransposeConv2d/Conv2d/Conv2d	8, 8, 128
Decoder 2	TransposeConv2d/Conv2d/Conv2d	16, 16, 64
Decoder 3	TransposeConv2d/Conv2d/Conv2d	32, 32, 32
Decoder 4	TransposeConv2d/Conv2d/Conv2d	64, 64, 16
Conv	1 × 1 Conv2d	64, 64, 1
Output		64, 64, 1

use 24 time steps to train, predict all the 60 time steps when testing

Results: evaluating metrics

Coefficient of determination

$$R^2 = 1 - \frac{SS_{RES}}{SS_{TOT}} = 1 - \frac{\sum_i (y_i - \hat{y}_i)^2}{\sum_i (y_i - \overline{y})^2}$$

Normalized root mean square error

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}} \quad NRMSE = \frac{RMSE}{(y_{max} - y_{min})}$$

Mean structural similarity index

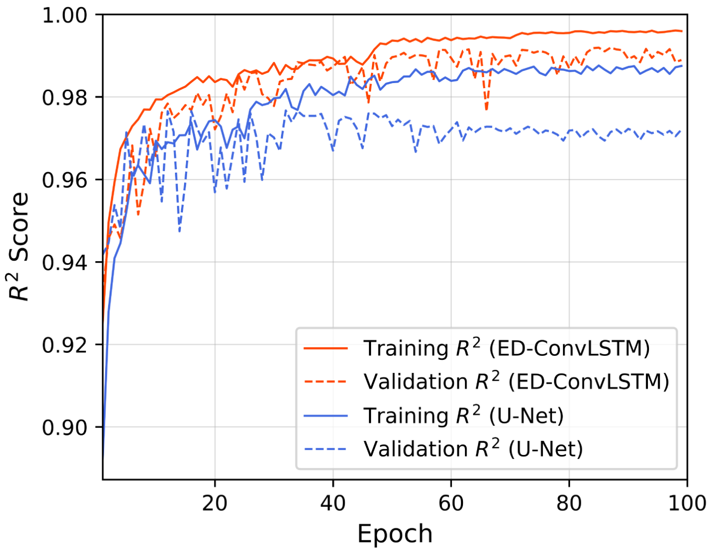
$$SSIM = \frac{1}{M} \sum_{m=1}^{m} \frac{(2\mu_{u,m}\mu_{v,m} + K_1^2)(2\sigma_{uv,m} + K_2^2)}{(\mu_{u,m}^2 + \mu_{v,m}^2 + K_1^2)(\sigma_{u,m}^2 + \sigma_{v,m}^2 + K_2^2)}$$

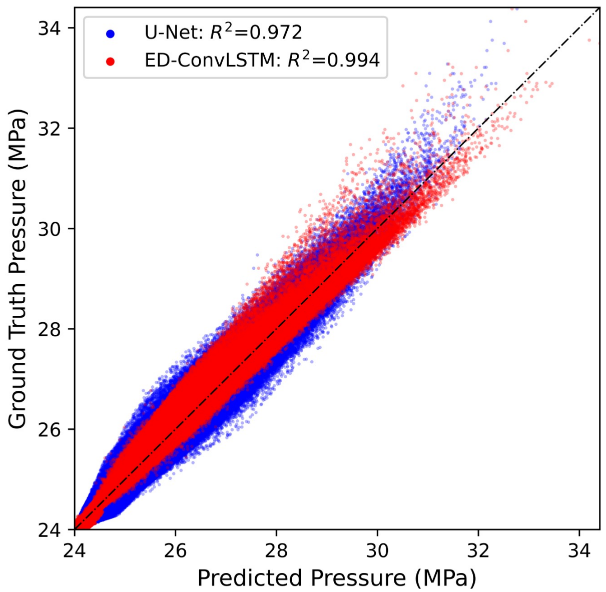
Normalized absolute percentage error

$$NAPE = \frac{||y - \hat{y}||}{y_{max} - y_{min}} * 100$$

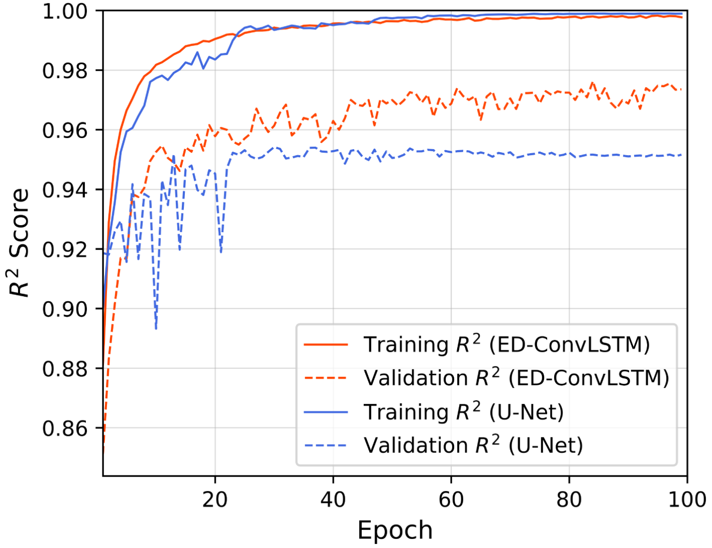
Results: training curves & overall R^2

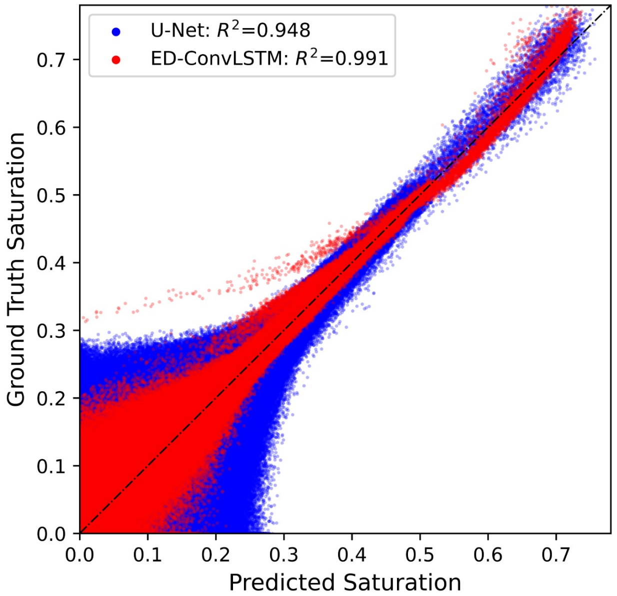
pressure:





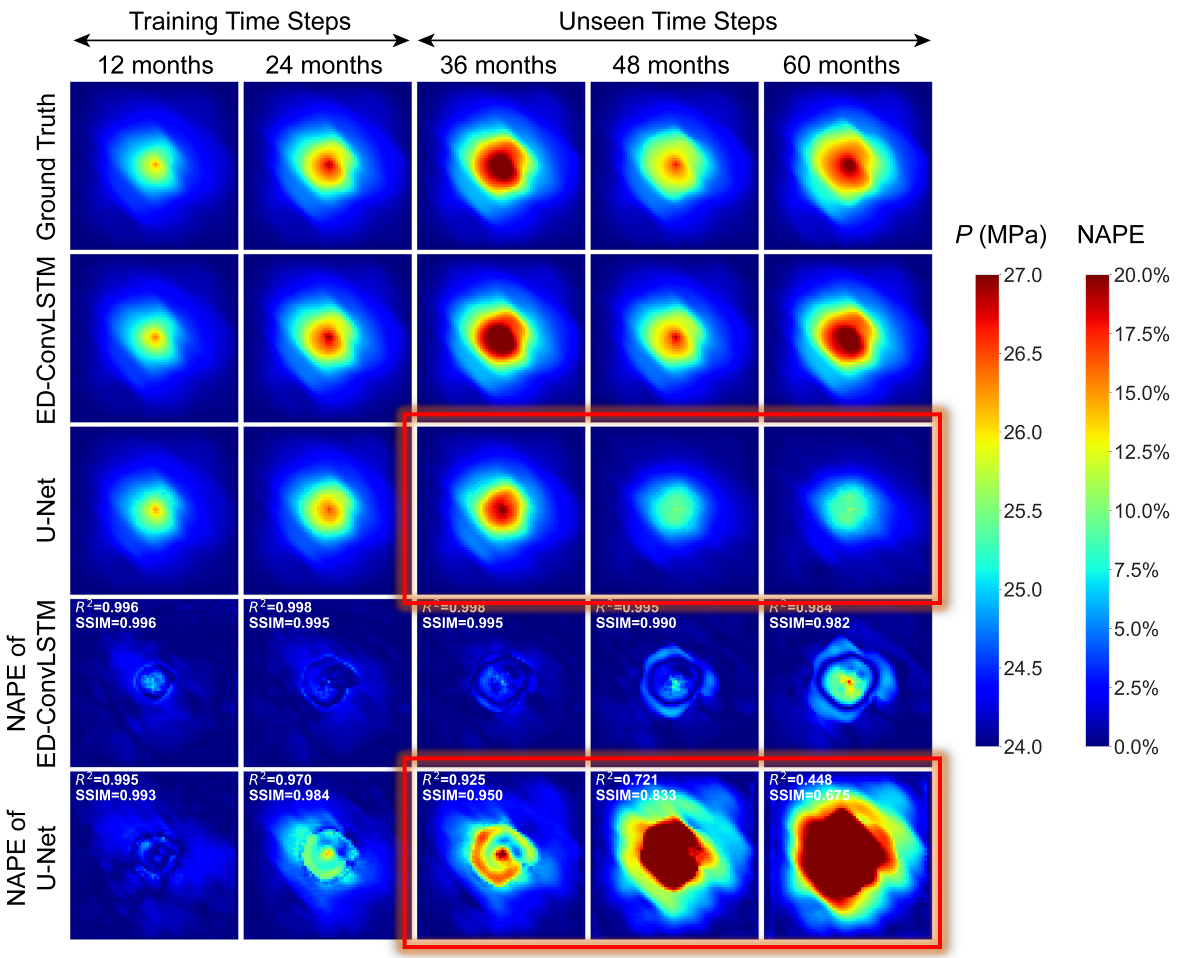
saturation:



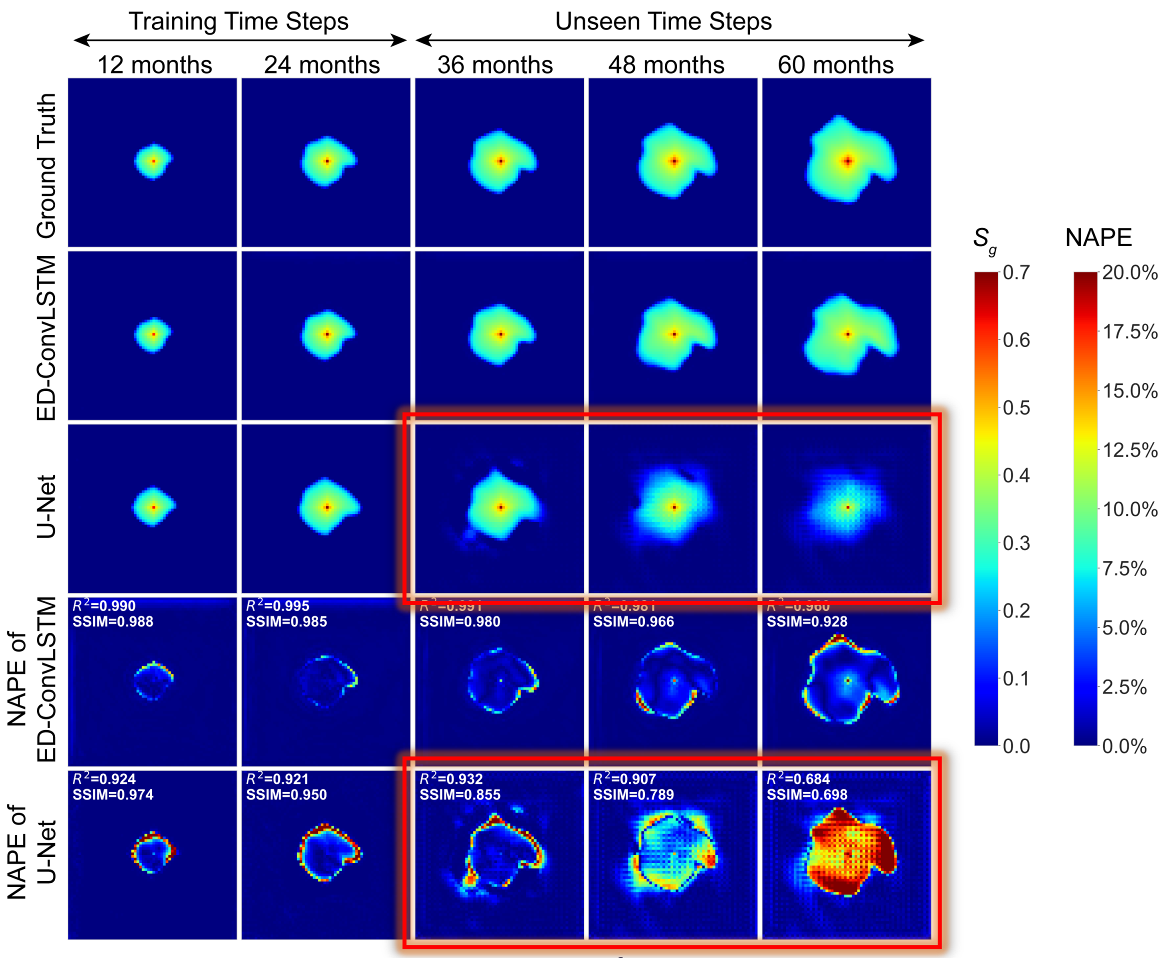


Results: extrapolate to unseen time steps

✓ ED-ConvLSTM exhibits a better match with ground truth compared with U-Net, especially at unseen time steps



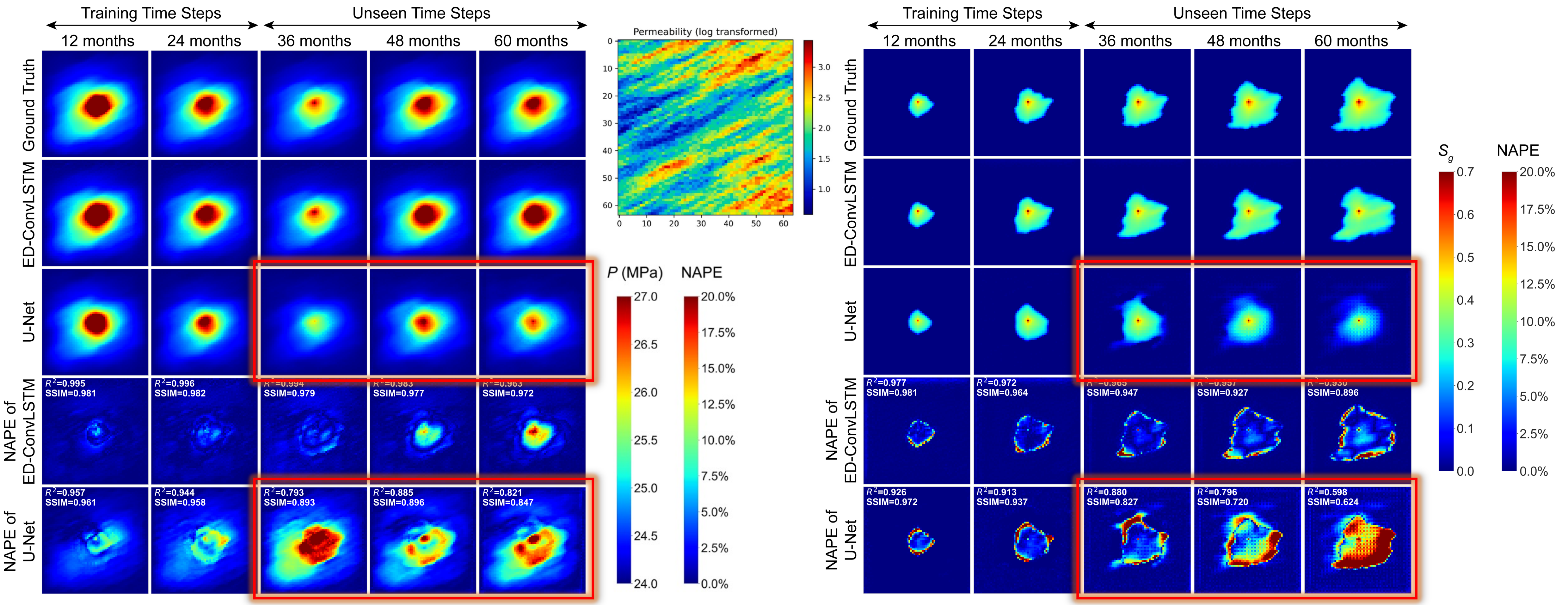
pressure



saturation

Results: generalize to out-of-distribution geo-parameters

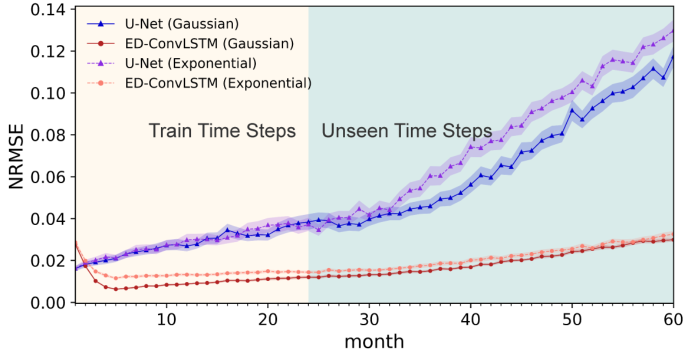
✓ ED-ConvLSTM can generalize well to exponential random permeability fields



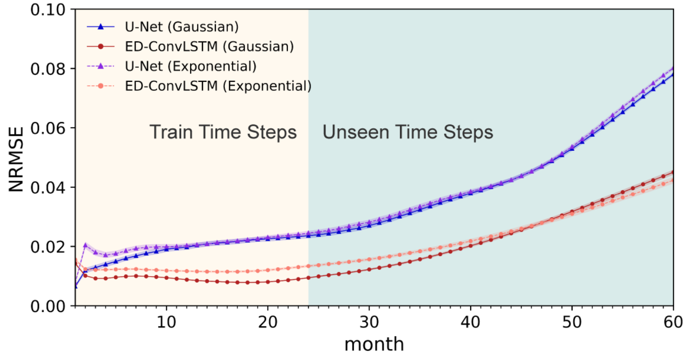
pressure

saturation

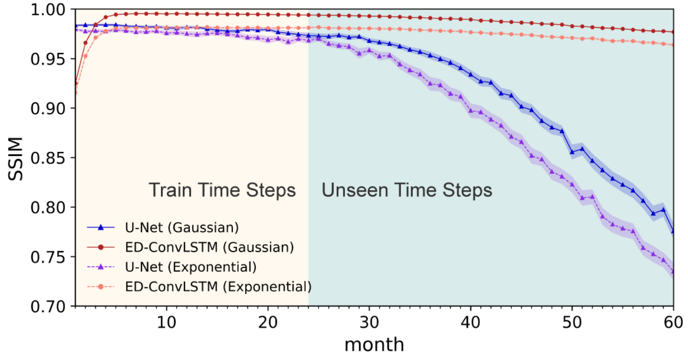
Discussion



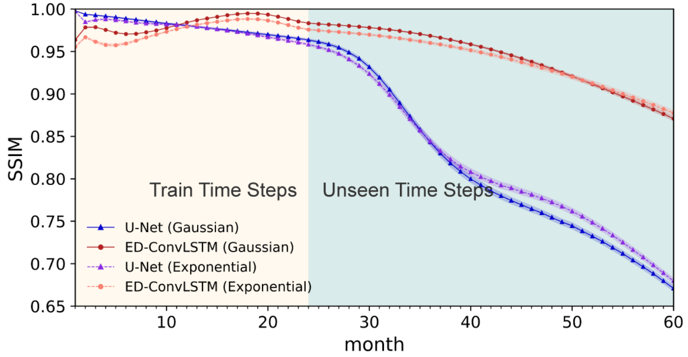
(a) NRMSE of pressure through time.



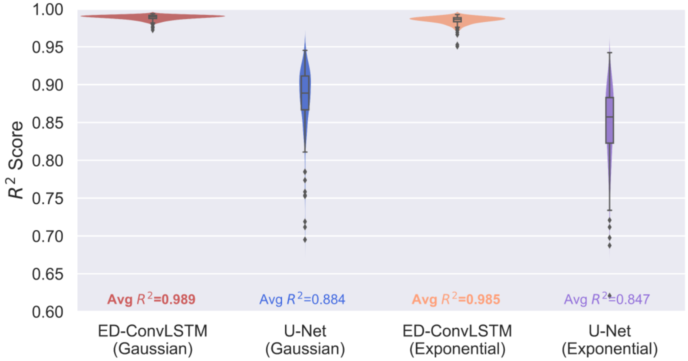
(b) NRMSE of saturation through time.



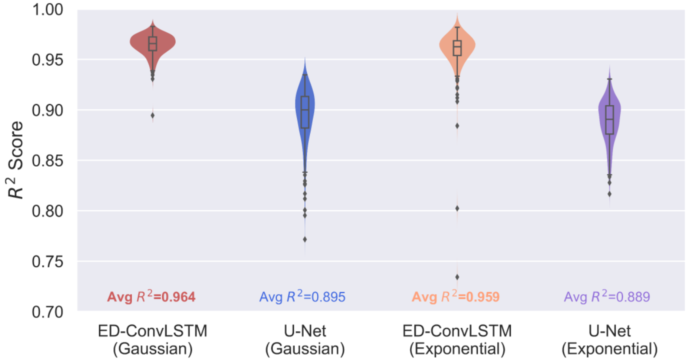
(c) SSIM of pressure through time.



(d) SSIM of saturation through time.



(e) R^2 score of pressure.



(f) R^2 score of saturation.

➢ Ablation study:

	R^2 for pressure	R^2 for saturation
ED-ConvLSTM	0.9890	0.9642
ED-ConvLSTM without CBAM module	0.9764	0.9298
ED-ConvLSTM without penalty loss terms	0.9884	0.9135

➢ Computation efficiency:

	Training time (minute)	Inference time (second/case)
ED-ConvLSTM	246	0.7
U-Net	60	1.4
Numerical simulation	–	91.8

- ✓ Stable performance throughout time and across different geological / engineering setups
- ✓ 130x speedup compared to full-order model

Conclusions & Remarks

Conclusions:

1. A data-driven surrogate model for GCS with dynamic well controls is proposed based on an encoder-decoder convolutional-LSTM architecture. It is able to make more decent predictions compared with U-Net.
2. Due to the convolutional-LSTM backbone, the model is capable of extrapolating to unseen time steps.
3. The effective feature extraction blocks enables the model to generalize well to out-of-distribution geological settings.

Future directions:

1. Realistic 3D reservoirs with multiple wells
2. Physical constraints
3. Parallel computing: Transformers

Thank you !

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https://github.com/fengzhao1239/ED-ConvLSTM