SAND2022-15848C

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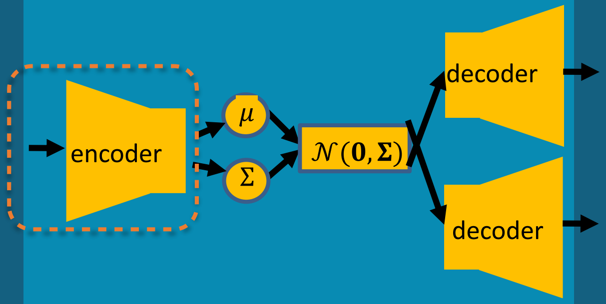
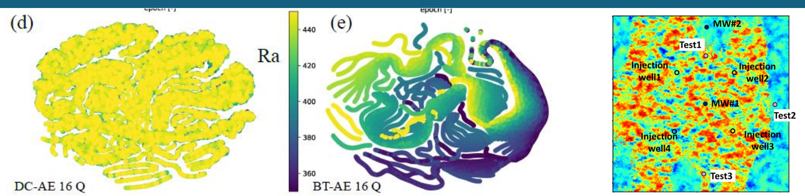
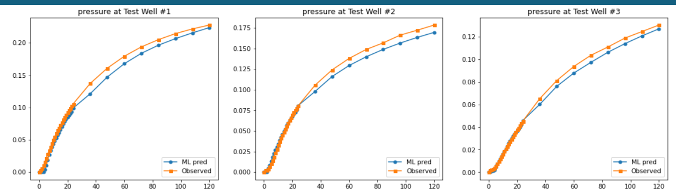
Machine Learning-Driven Poroelasticity Modeling and Real-time Data Assimilation







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CouFrac Conference, Berkeley, 2022

SAND2022-XXXX

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U.S. DEPARTMENT OF ENERGY NNSA

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Collaborators

- Jonghyun Harry Lee (U. of Hawaii at Manoa) – Deep learning for inverse modeling
- Meen (Teeratorn) Kadeethum (SNL) – Reduced order modeling
- Jack Ringer, Vincent Liu, Daniel Lizama, Rachel Willis (SNL interns) – Image, PINN, & waveform data analysis
- Joe Hogge (SNL) – DOE SMART Initiatives

Motivation for Deep Learning Based Approach

Two major challenges for high-dimensional forward and inverse problems for real-time forecasting

1. **Computational burdens with matrix calculations (e.g., Jacobian)**

   => Effective dimension reduction

2. **# of forward model simulations for inverse modeling**

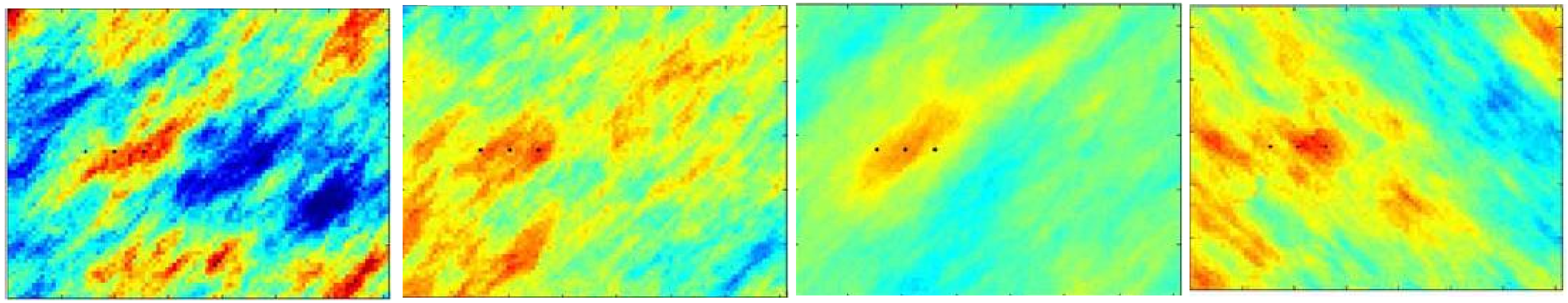
   => (ML-driven) fast, reduced order predictive modeling

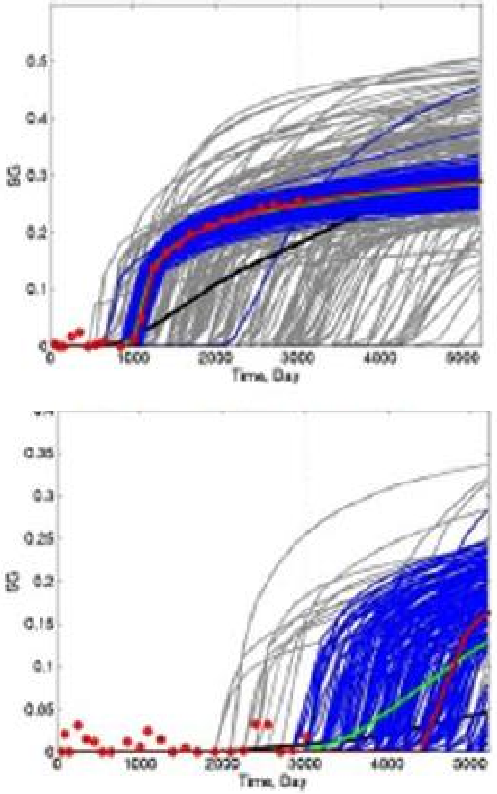
Specific Goals: Machine learning-driven CO_2 modeling by combining fast ML-based forward modeling with (ensemble-based) data assimilation (EnDA), resulting in real-time history matching of CO_2 operations and forecasting CO_2 and pressure plume development

Parameter estimation and uncertainty quantification

History matching
(CO_2 Injection at Cranfield, MS)

Synthetic Truth | Calibration-constrained NSMC | Ensemble-based filtering method | With incorrect prior data





Algorithm
Ensemble Kalman filter
Ensemble smoother
Ensemble smoother with multiple data assimilation
Ensemble Kalman filter with pilot point
ES4 with pilot point
Null-space Monte Carlo[b]
Multiple calibration-constrained NSMC

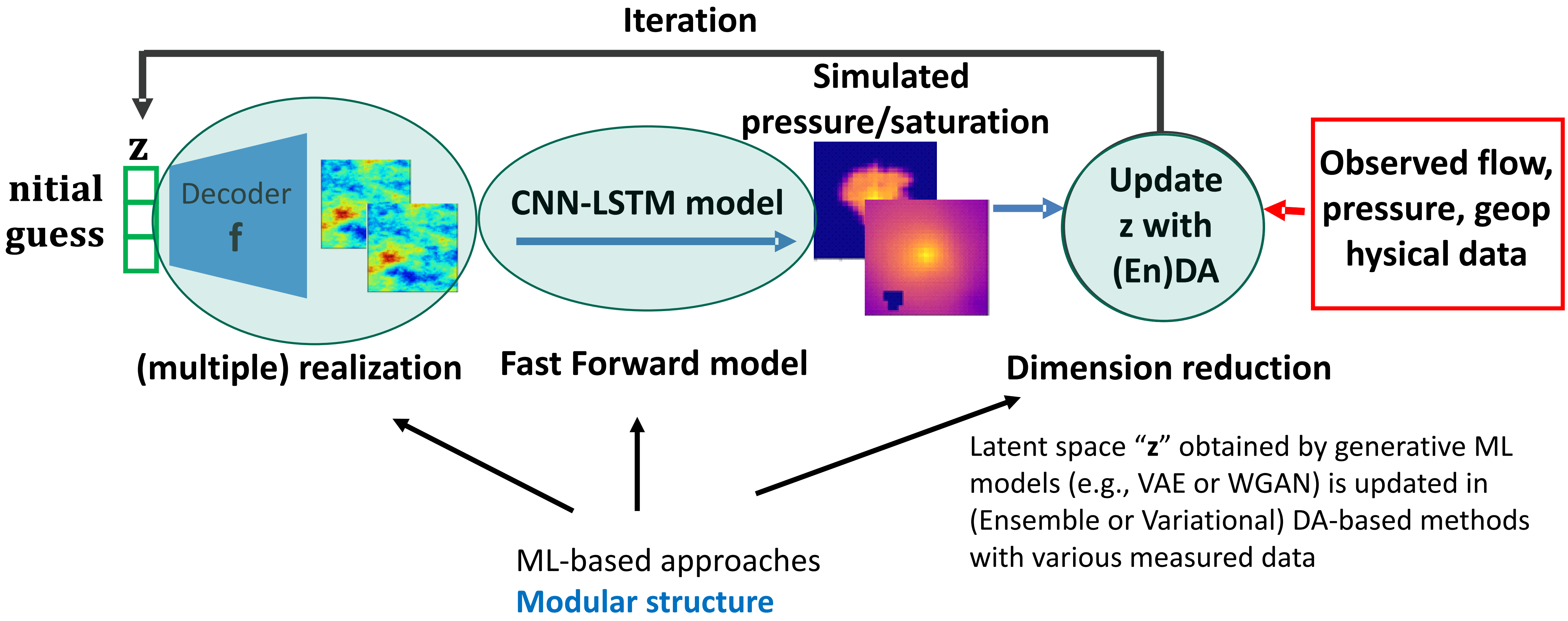
- With limited observation data, solutions with incorrect prior data can match the observed data well ➔ more spatially representative data (e.g., geophysical sensing data, tracer test)
- Another possible solution => more robust ensemble member generation using machine learning

Tavakoli et al. (WRR2013)
Yoon et al. (WRR2013)

Yoon et al. (2007), Yoon & McKenna (2013)
Lee and Yoon et al. (WRR2016)

ML-based Data Assimilation Framework

- Data assimilation in low dimensional latent space of unknown parameters with dim(z)
- Forward model executions can be significantly reduced



Latent space "**z**" obtained by generative ML models (e.g., VAE or WGAN) is updated in (Ensemble or Variational) DA-based methods with various measured data

Kang et al. (WRR, in press), Bao et al. (in prep), Yoon et al. (in prep)

- **ML-based Forward Model**
- ML-based Data Generation
- Data Assimilation
- Summary

ML for Forward Models

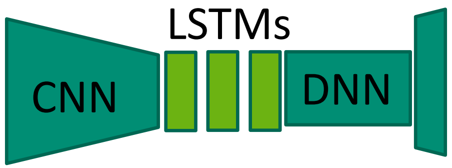
Models for pressure, CO_2 saturation, and water production rate

CNN-LSTM-DNN

Input

- **Permeability and porosity (x,y,z)**
- **Cumulative injection over time**
- **Injection rates/time**
- **Activity binary zone**

ML architecture



CNN, DNN: TimeDistributed

- CNN: Convolutional Neural Network
- LSTM: Long Short Term Memory
- DNN: Dense neural network
- AE: Autoencoder

Output

P & S_{co2} (x,y,z,t)
Q_{prod}(t)

Dimension reduction & interpolation

Physics-Based Loss Functions

- **Loss functions can be constructed through governing equations & physical constraints**
  - We incorporated different terms from governing equations into the loss functions
  - Flux, mass conservation, known quantities are used

Governing equations for two phase flow

$$\frac{\partial(\emptyset \rho_w S_w)}{\partial t} = \nabla\left(\rho_w \frac{k_{rw}\boldsymbol{k}}{\mu_w}(\nabla P_w - \rho_w g z)\right) + \boldsymbol{q}_w$$

$$\frac{\partial(\emptyset \rho_{nw} S_{nw})}{\partial t} = \nabla\left(\rho_{nw} \frac{k_{rnw}\boldsymbol{k}}{\mu_{nw}}(\nabla P_{nw} - \rho_{nw} g z)\right) + \boldsymbol{q}_{nw}$$

Loss= $MSE(\hat{P}, P) + MSE(\hat{S}_{nw}, S_{nw}) + MSE(\hat{q}_{pr}, q_{pr})$

$+ \lambda_{flux} * MSE(\widehat{Flux}, Flux)$

$+ \lambda_{mass} * MSE\left(\frac{\partial\widehat{(M_{nw})}}{\partial t}, \frac{\partial(M_{nw})}{\partial t}\right)$

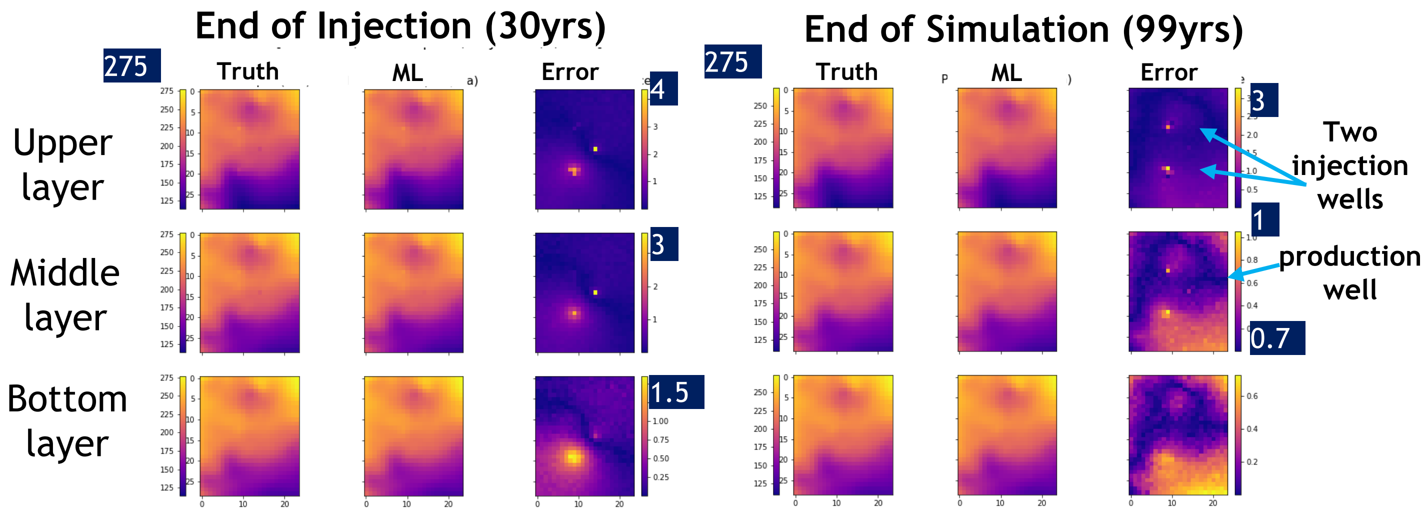
$+ \lambda_{binary} *$ Binary Crossentropy $(\hat{S}_{nw}, S_{nw})$

$+ \lambda_{bhp} * MSE(\hat{P}_{bhp}, P_{bhp}) + \lambda_{pr} * MSE(\hat{P}_{bhp}, P_{bhp})$

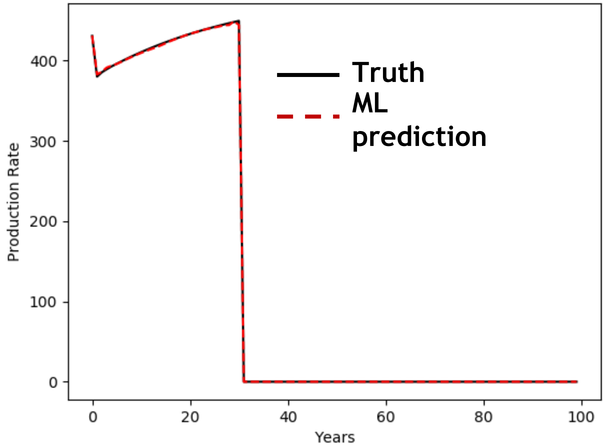
MSE: Mean Square Error

Results – Pressure, CO_2 Saturation & Production Rate

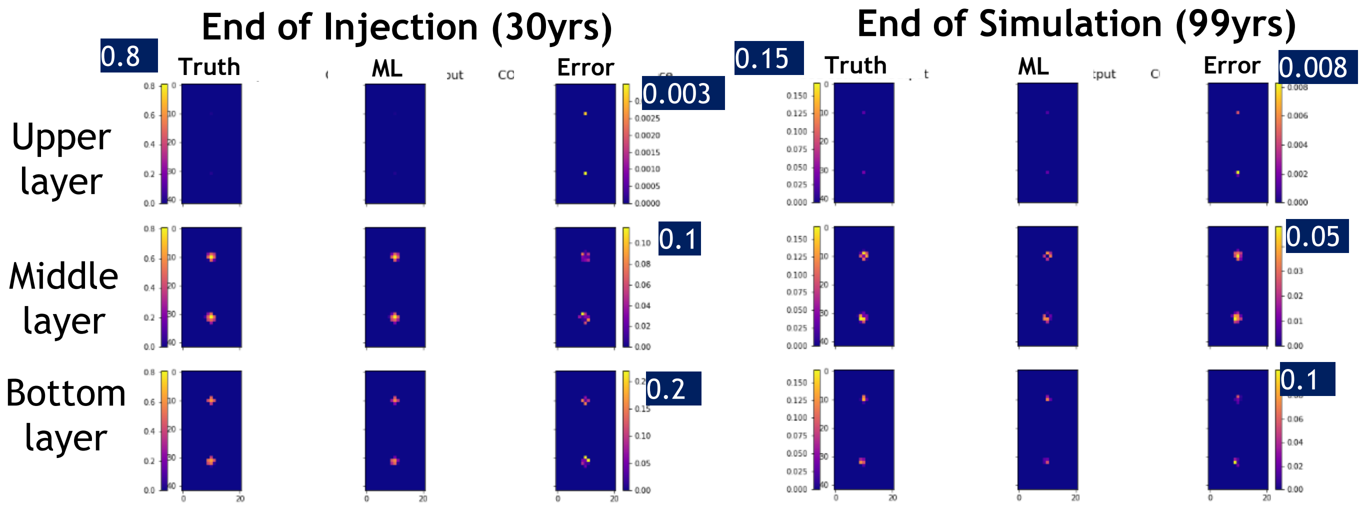
Pressure



Production Rate



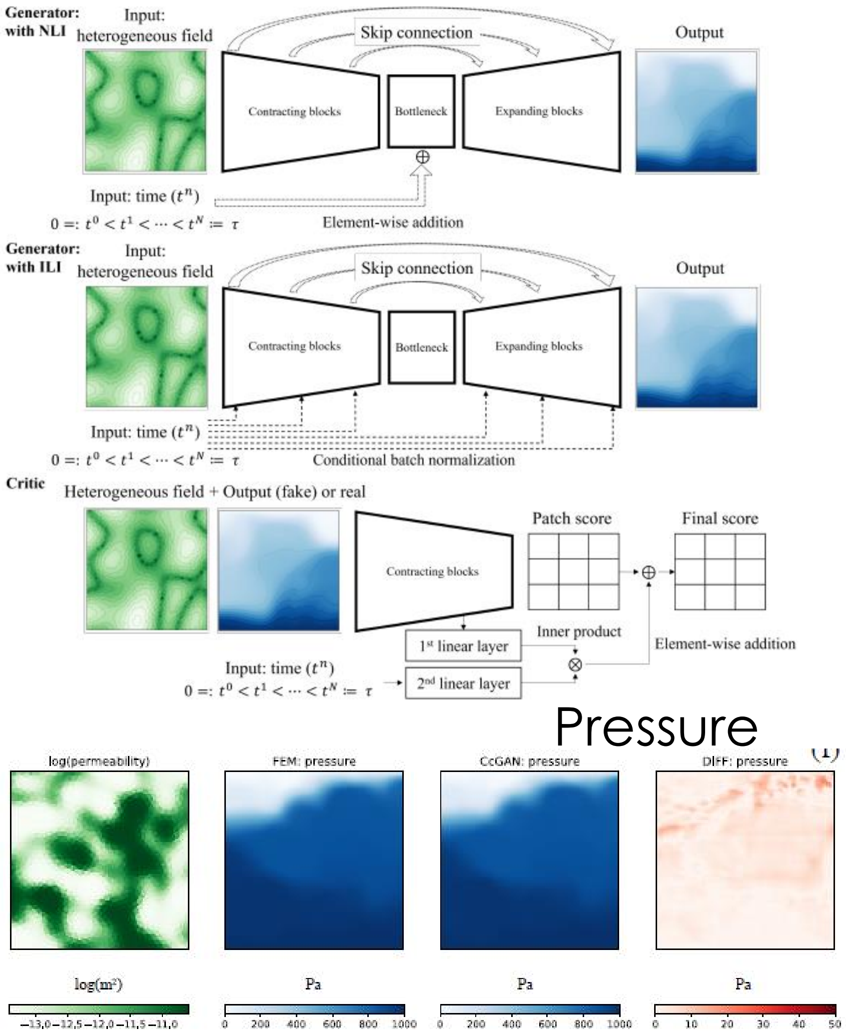
CO_2 Saturation



- Trained models has high prediction accuracy for all quantities

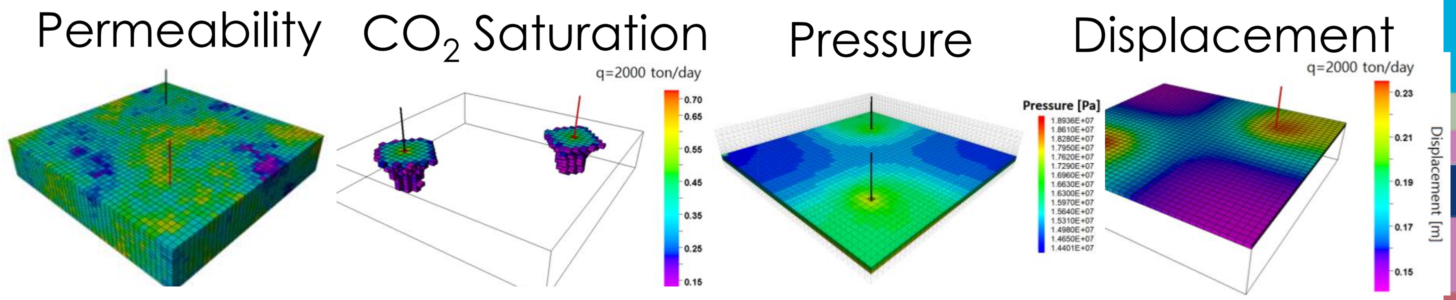
ML approaches for coupled poro-elasticity processes

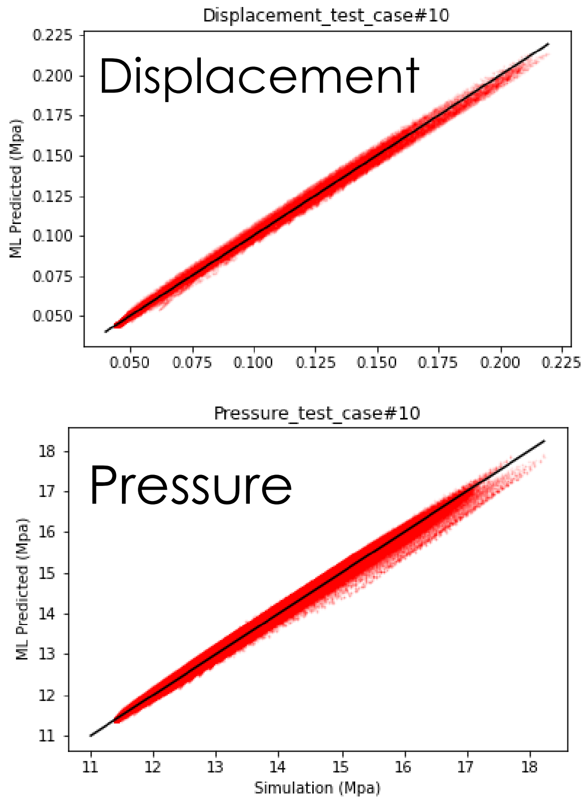
- Continuous conditional generative adversarial networks (CcGAN) for time-dependent PDEs

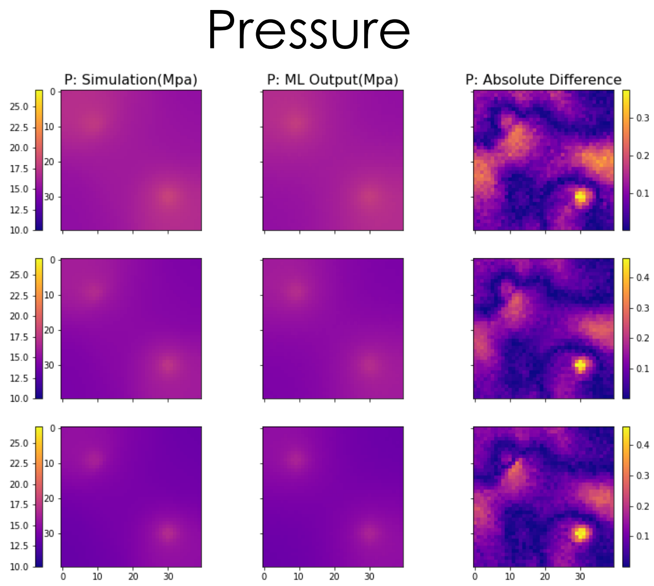


Kadeethum et al. (AWR, 2022; Sci. Rep. 2022)

- CNN-LSTM-DNN reduced order modeling for coupled processes



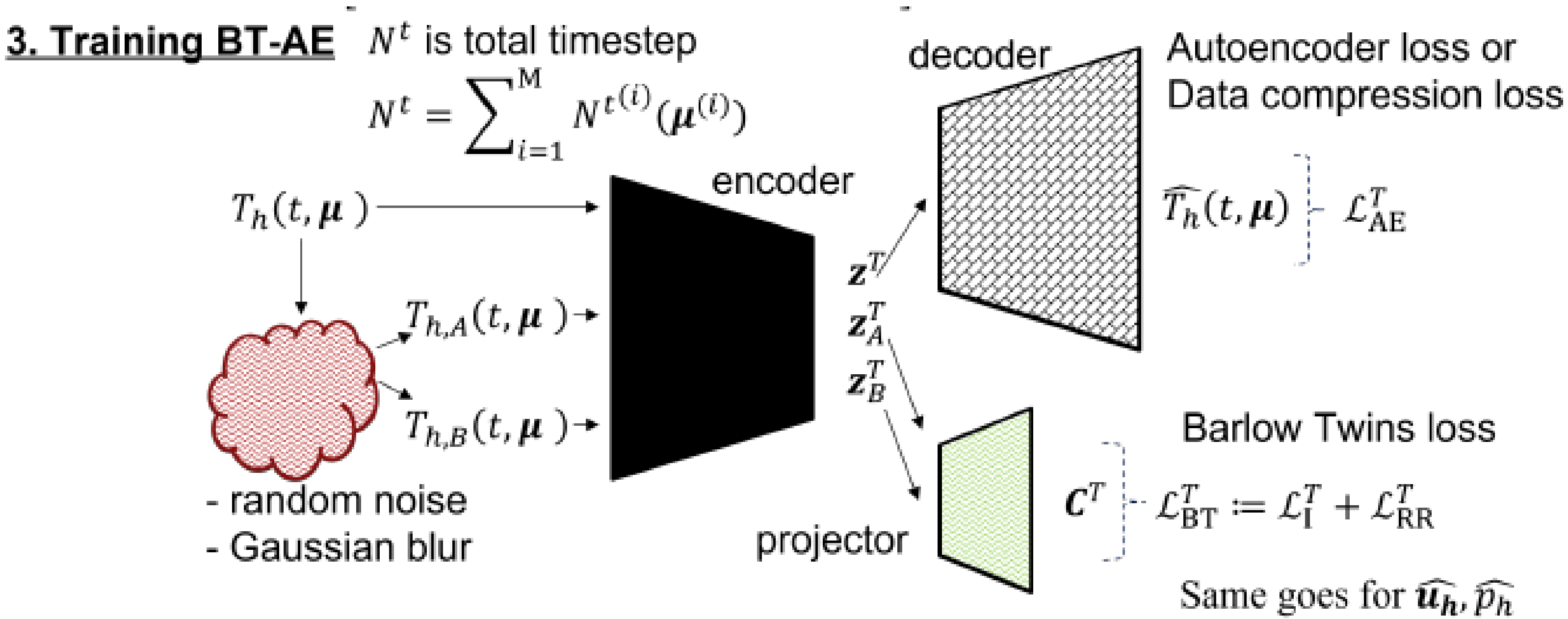




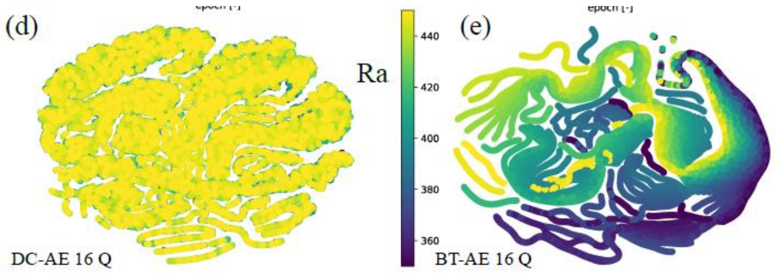
Yoon et al. (in prep for GRL)

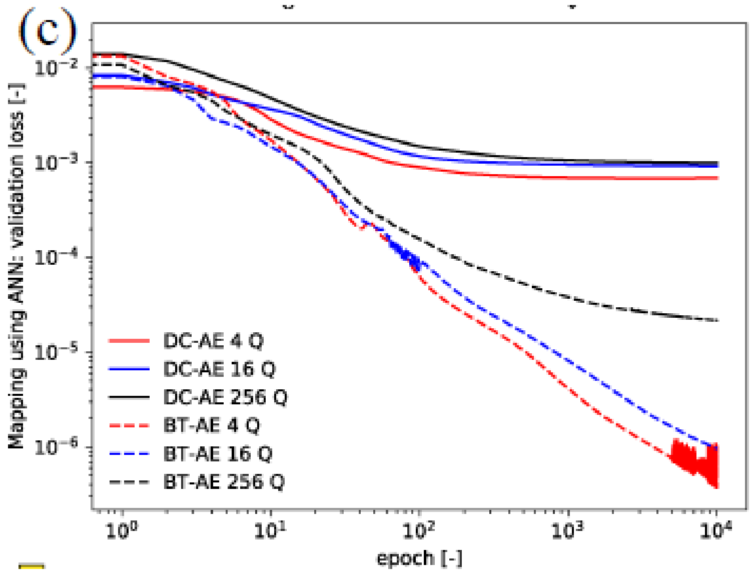
Ongoing Progress

Self supervised ML (Barlow Twins)



DC-AutoEncoder BT-AE





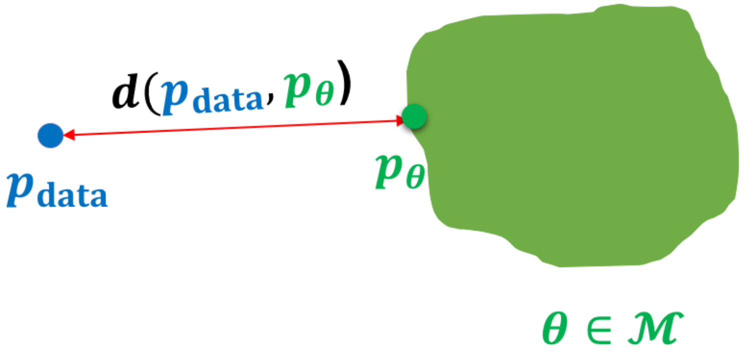
Kadeethum et al. (Sci. Rep., Accepted)

- ML-based Forward Model
- **Generative Models**
- Data Assimilation
- Summary

Generative Model as Prior modeling

- Expression power of NNs (as universal approximator)
- Approximate the data distribution using NNs given access to the data D
- Use the generative model for downstream inference

$\mathbf{x}^{(j)} \sim p_{\text{data}}$
$j = 1, 2, \ldots, |\mathcal{D}|$

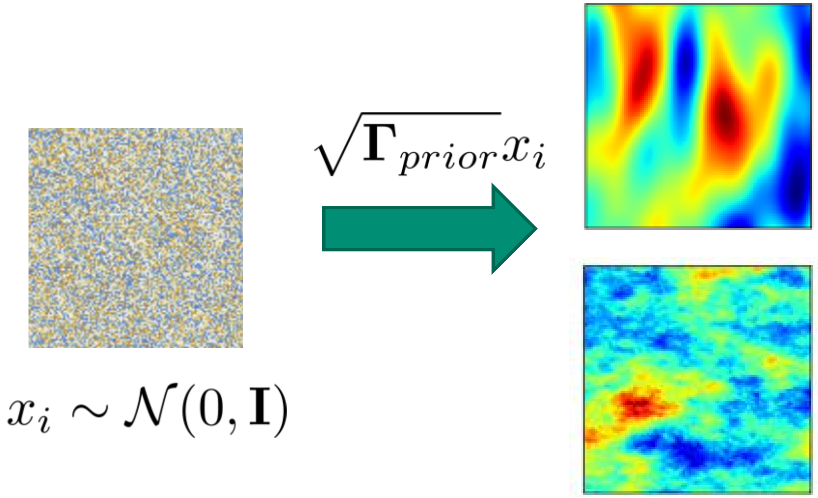


Model family

$$\min_{\theta \in \mathcal{M}} dist(p_{data}, p_{\mathrm{NN}(\theta)})$$

Generative Model Example

- Generative Model Example: Gaussian Sampling $\sim N(0, \boldsymbol{\Gamma}_{prior})$



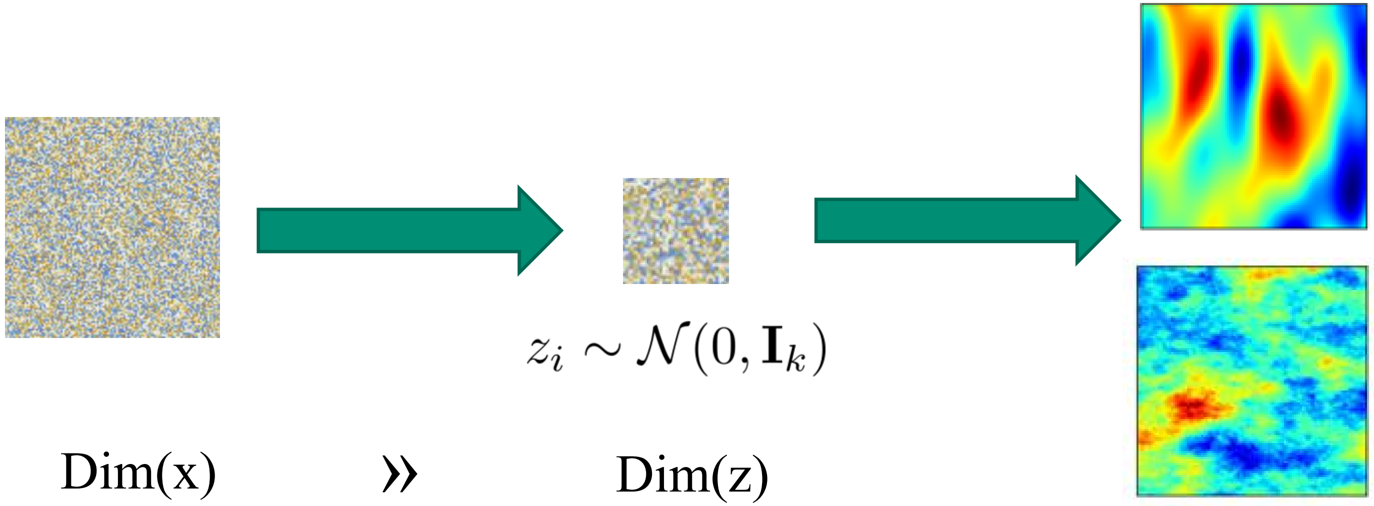
$$s = G(x) = \sqrt{\Gamma_{\text{prior}}} x$$

- Normalizing Flow:

$$P_x(x) = P_z(z) \left| \det \left(\frac{\partial G(z)}{\partial z} \right) \right|^{-1}$$

Generative Model as Dimension Reduction

- Generative Model Example: Gaussian Sampling $\sim N(0, \boldsymbol{\Gamma}_{prior})$



$z_i \sim \mathcal{N}(0, \mathbf{I}_k)$

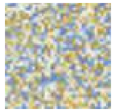
Dim(x) » Dim(z)

$$s_i = \sqrt{\boldsymbol{\Gamma}_{prior}} x_i \approx \sqrt{\boldsymbol{\Gamma}_k} z_i$$

$$y = h(s) = h(\sqrt{\boldsymbol{\Gamma}} x) \approx h(\sqrt{\boldsymbol{\Gamma}_k} z)$$

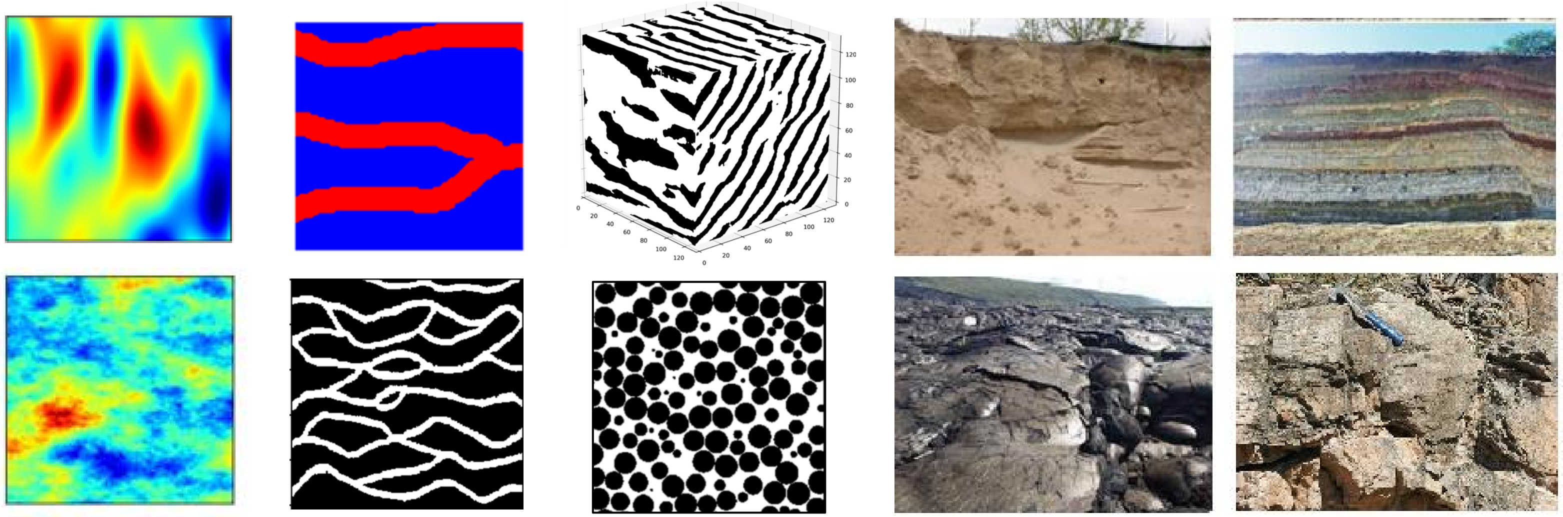
Generative Model with NNs

- Gaussian $N(0, \mathbf{\Gamma}_{prior})$ and other complex distributions with NNs
- Variational autoencoders, generative adversarial networks, and so on…

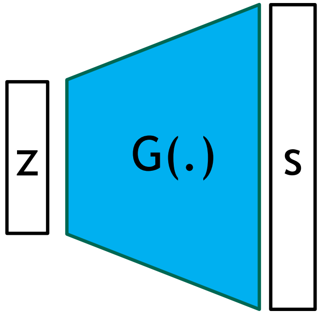


$z_i \sim \mathcal{N}(0, \mathbf{I}_k)$

$G_{NN}(z_i)$

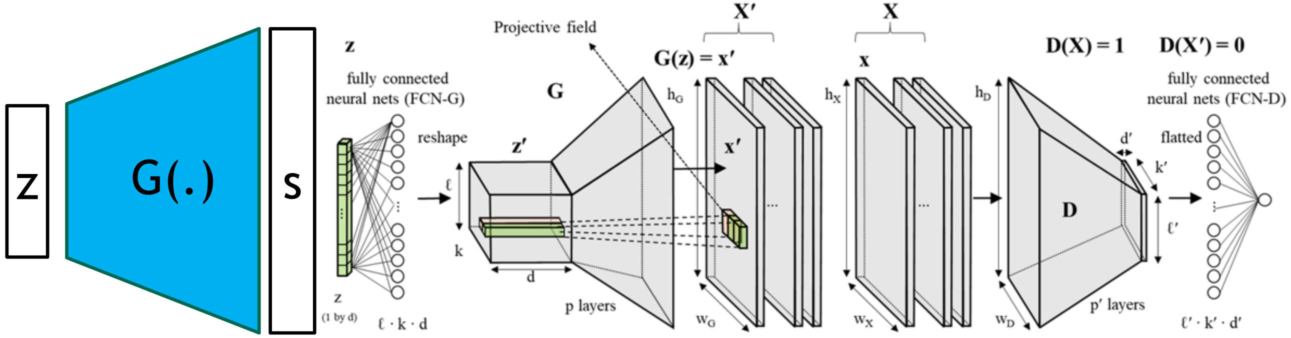


dim(z) << dim(s)



Deep Learning-based Prior Modeling

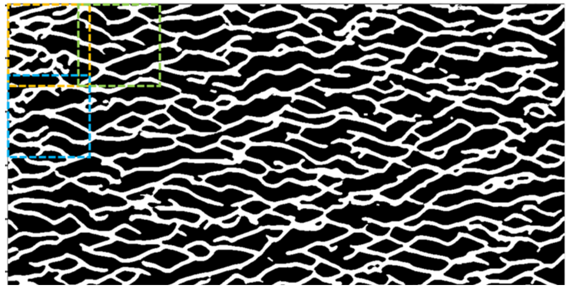
Spatially Assembled GAN (SAGAN)



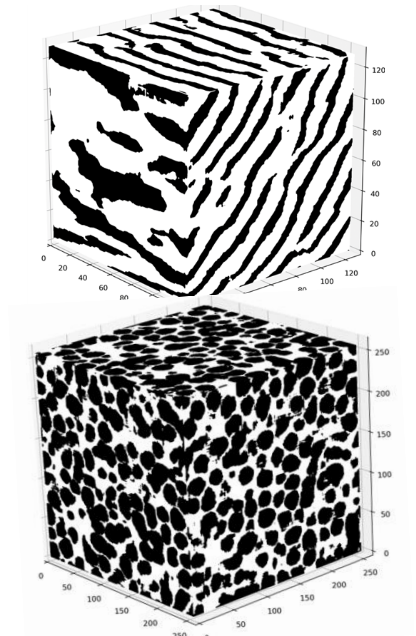
Training image (TI)

Training/
Generation

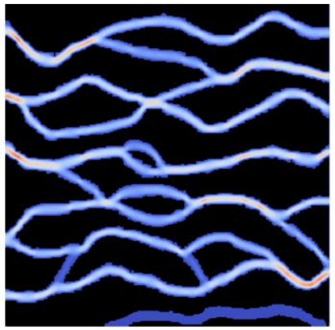
Generated image (GI)



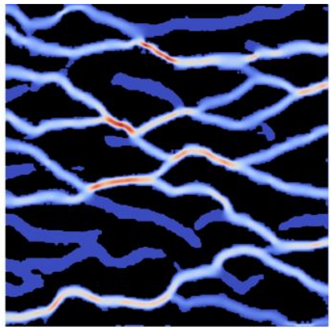
Generated earth images



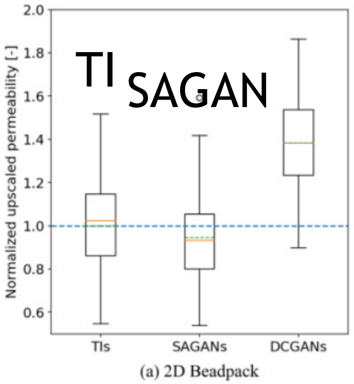
Training image



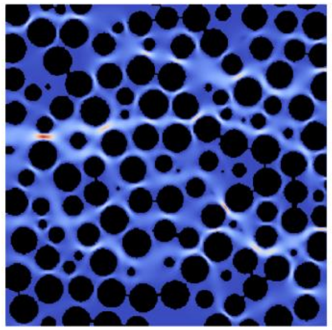
Generated image



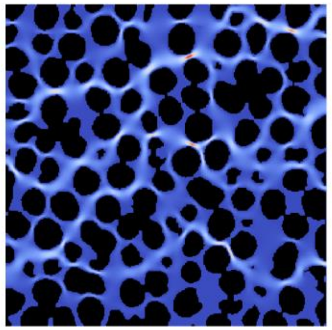
Perm. distribution



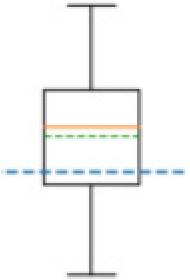
Training image



Generated image



SAGAN

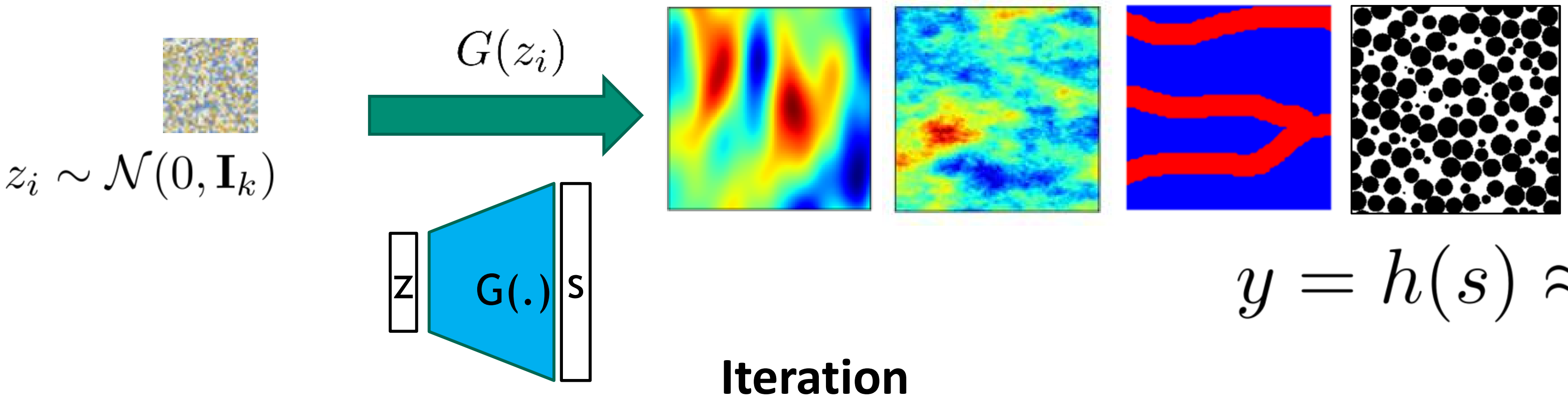


Velocity field & permeability distribution: Pore-scale simulations with training image (TI) and realization

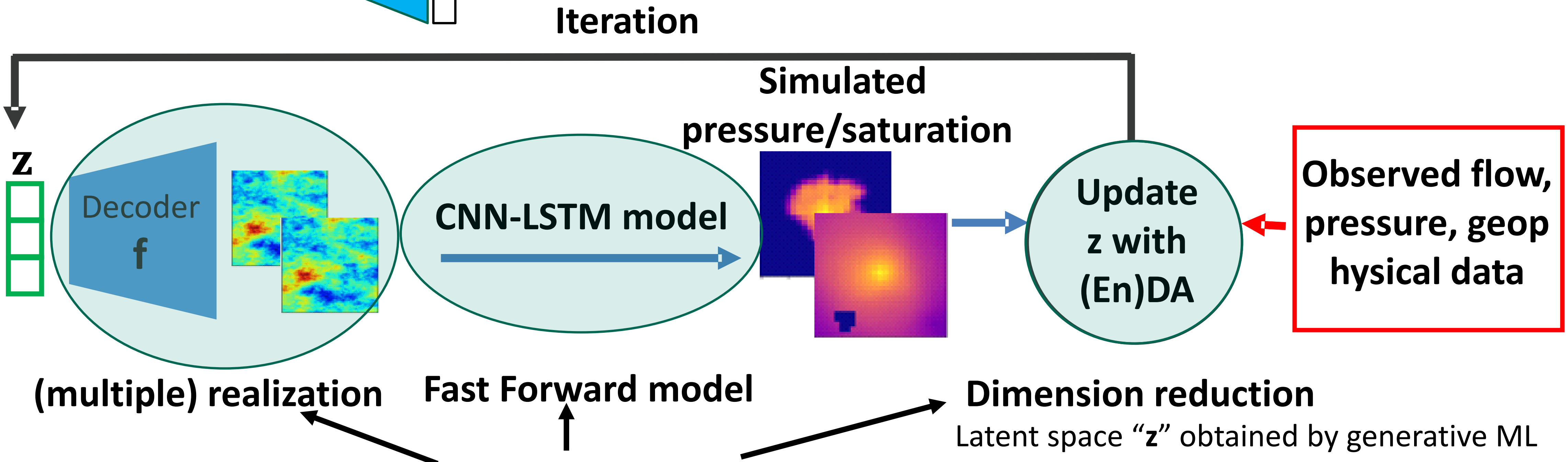
Kim et. al., *JCH* 2021

- ML-based Forward Model
- ML-based Data Generation
- **Data Assimilation**
- **Summary**

ML-based Data Assimilation Framework



$$y = h(s) \approx h(G(z))$$



ML-based approaches

Modular structure

Latent space "**z**" obtained by generative ML models (e.g., VAE or WGAN) is updated in (Ensemble or Variational) DA-based methods with various measured data

Kang et al. (WRR, In press), Bao et al. (in prep), Yoon et al. (in prep)

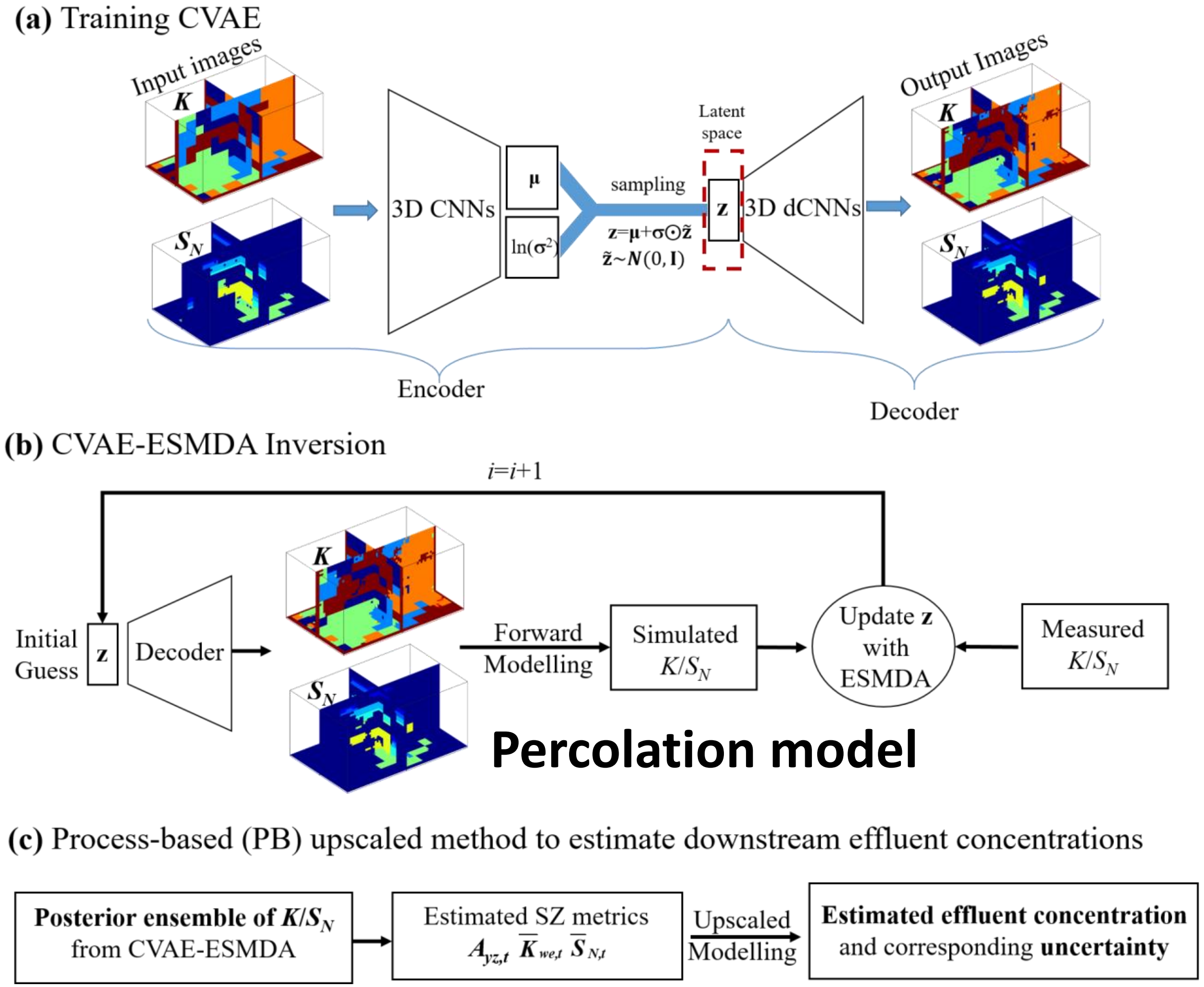
Remarks

- Then the original inverse problem becomes $P_x(x) = P_z(z)\left|\det\left(\frac{\partial G(z)}{\partial z}\right)\right|^{-1} \approx C P_z(z)$

$$p(\mathbf{z}) \sim \exp\left(\underbrace{-\frac{1}{2}(\mathbf{y}-\mathbf{h}(\mathbf{G}(\mathbf{z})))^\top \mathbf{\Gamma}_{\text{error}}^{-1}(\mathbf{y}-\mathbf{h}(\mathbf{G}(\mathbf{z})))}_{\text{likelihood}} \underbrace{-\frac{1}{2}(\mathbf{z}-\mathbf{z}_{prior})^\top \mathbf{\Gamma}_{\text{prior}}^{-1}(\mathbf{z}-\mathbf{z}_{prior})}_{\text{prior}}\right)$$

- Prior modeling beyond popular Gaussian models (e.g., Matérn Kernel)
- By construction, we know prior covariance in latent space (e.g., identity)
- Inversion performed on *smaller* latent space of unknown parameters
- Only require "dim(z)" forward model executions at each iteration instead of dim(s) or dim(obs)

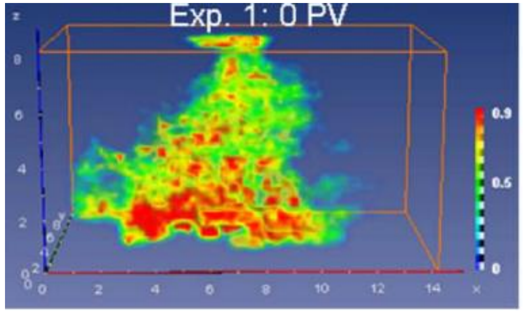
Convolutional Variational AutoEncoder-Ensemble Smoother with Multiple Data Assimilation (CVAE-ESMDA)



Percolation model

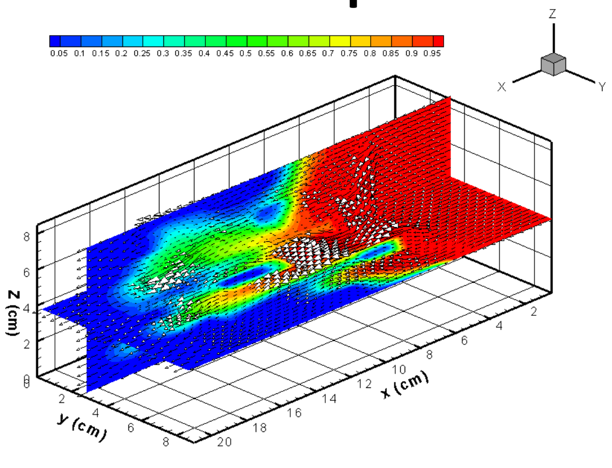
Kang et al. (WRR, In press)

DNAPL saturation in a sandbox



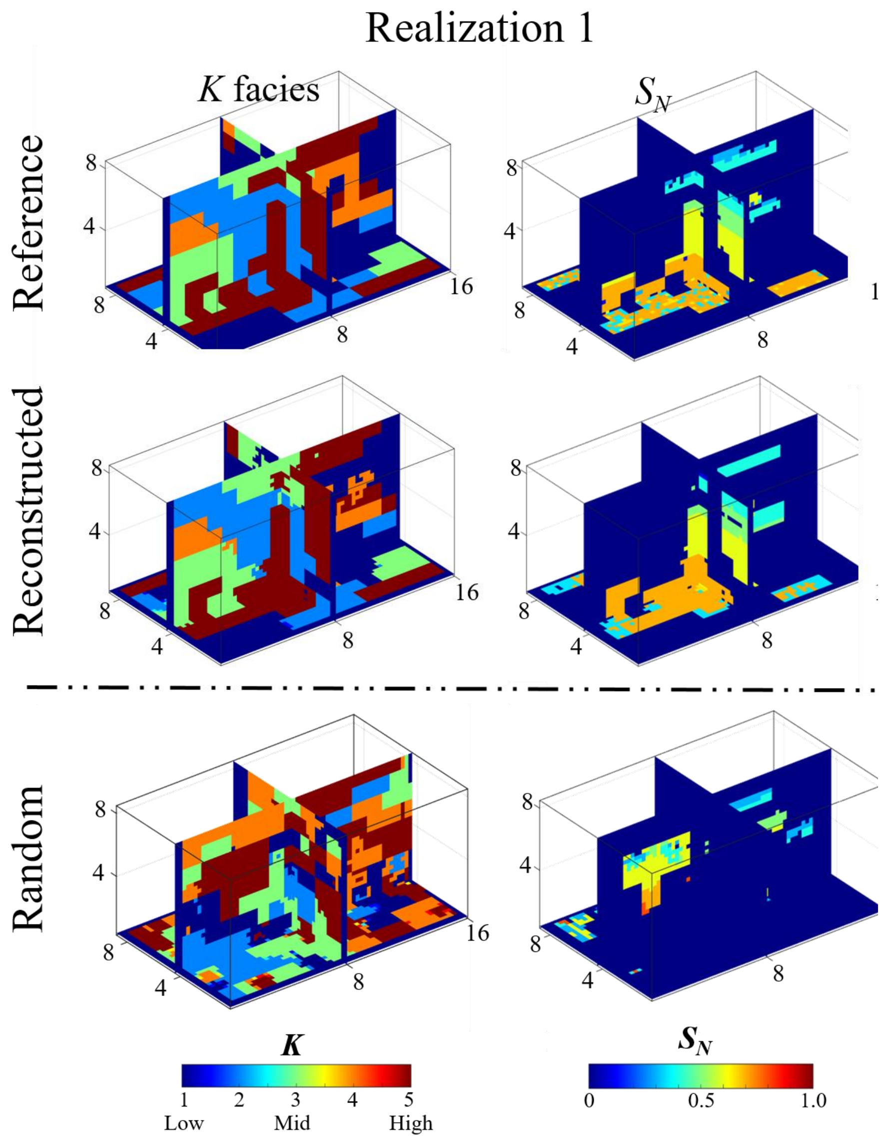
Zhang et al. (JCH 2007)

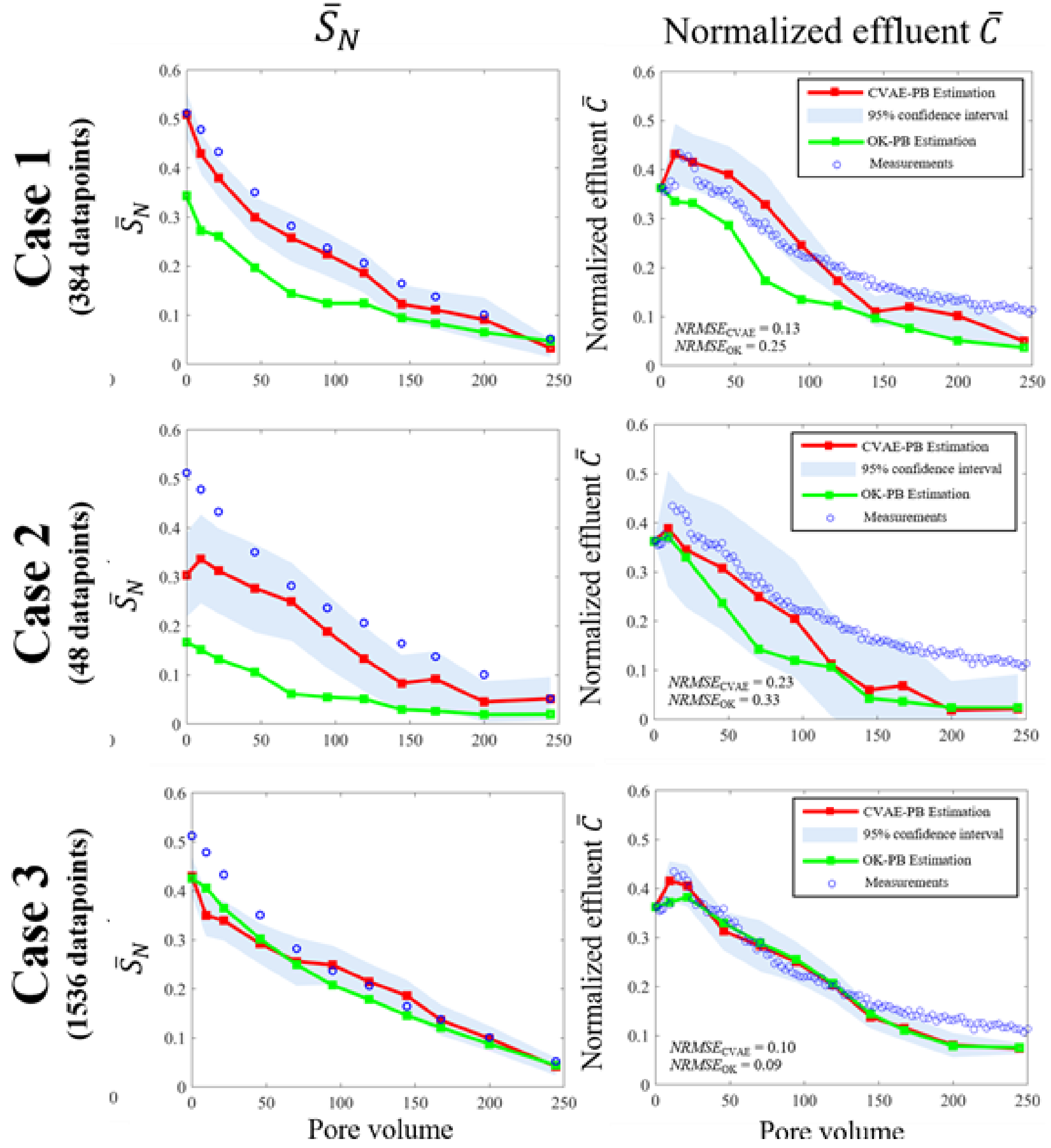
Tracer transport



Yoon et al. (WRR 2008, 2013)

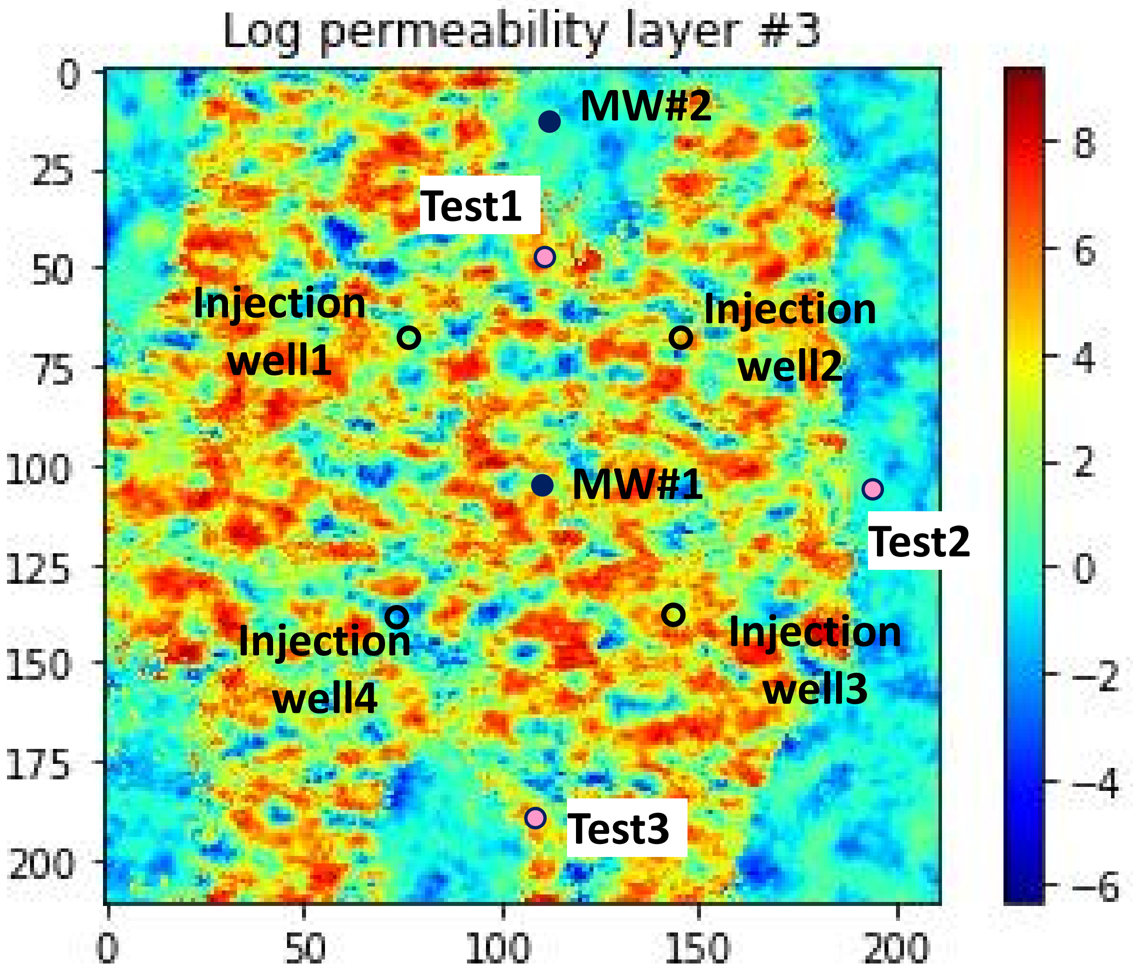
CVAE-ESMDA: K and S_{NAPL} fields, Normalized Concentration



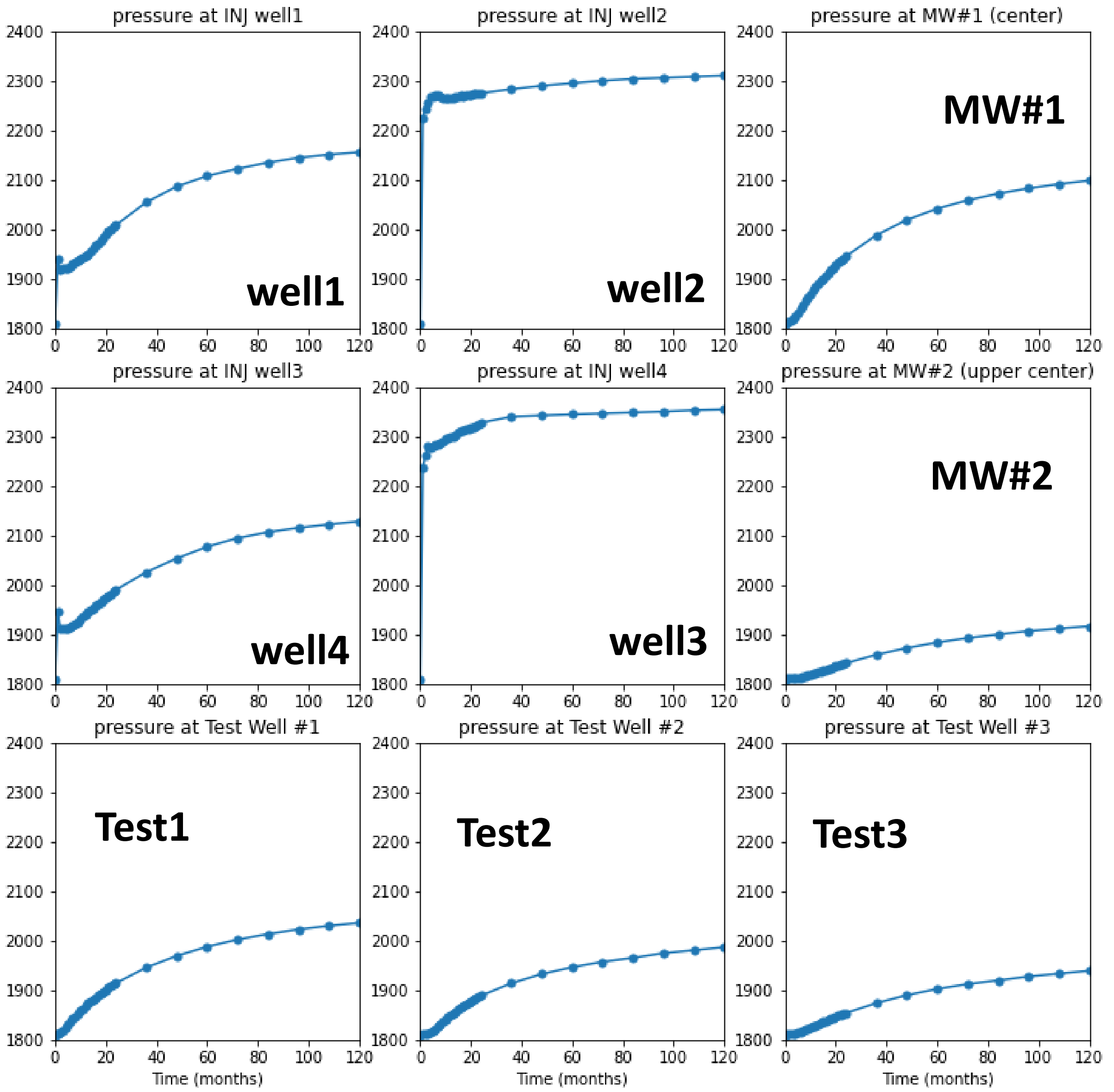


Kang et al. (WRR, In press)

Well locations & pressure profile over time for DA

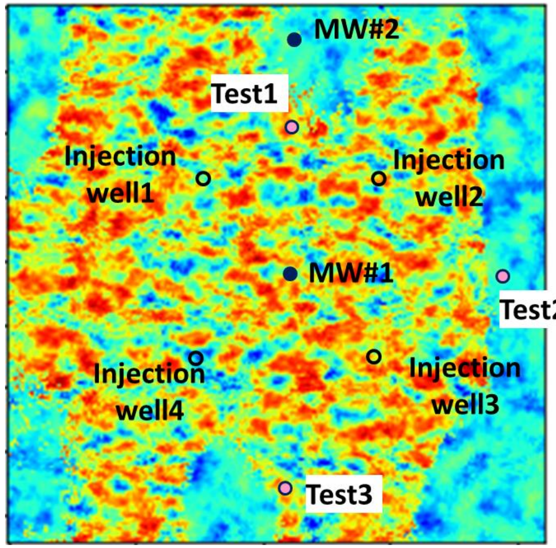


CO_2 injection through 4 wells

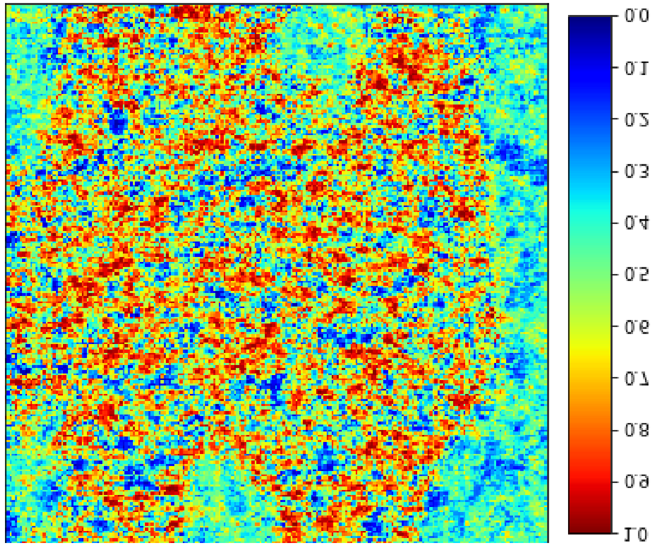


VAE-Inversion

Truth

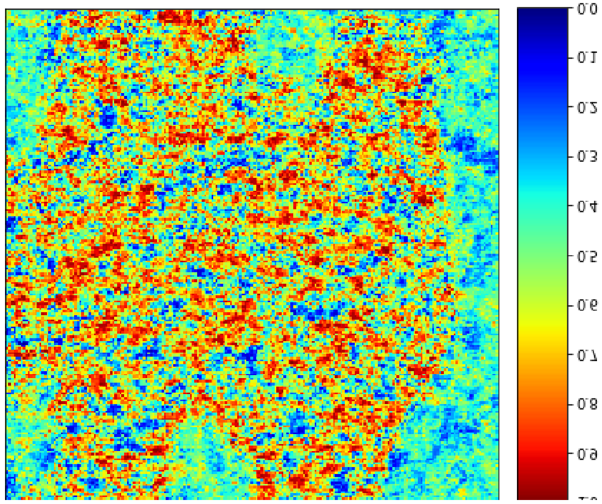


Estimated

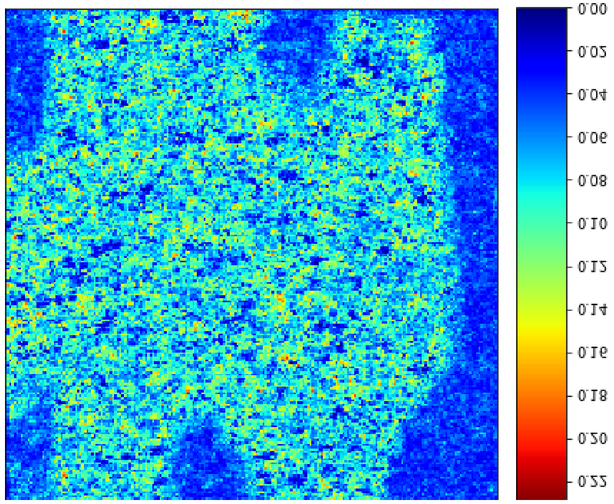


Posterior Analysis (normalized)

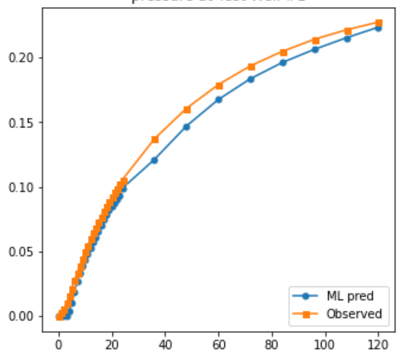
Mean of 1,000 realizations



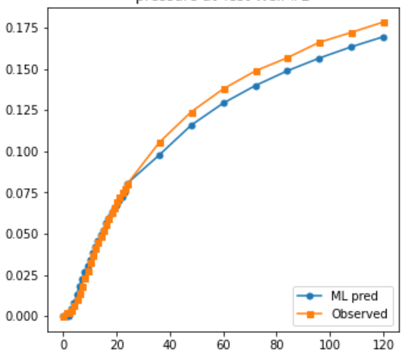
Standard deviation



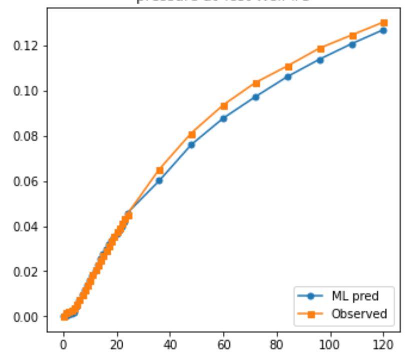
Test #1



Test #2

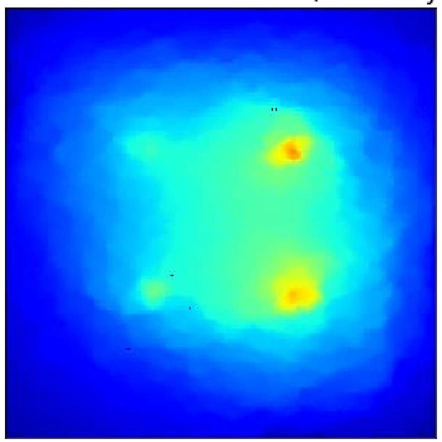


Test #3



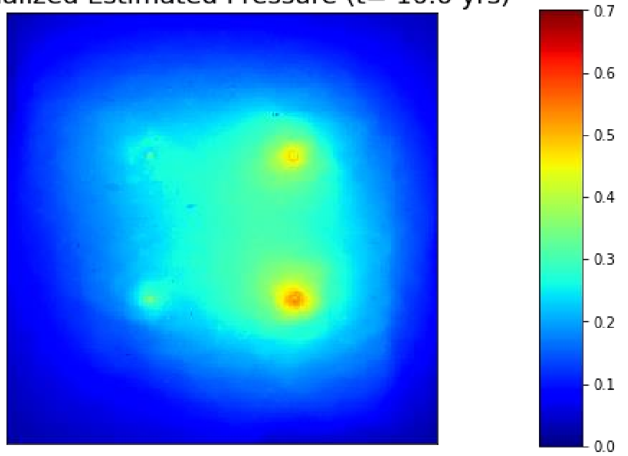
Truth

Normalized CMG Pressure (t= 10.0 yrs)

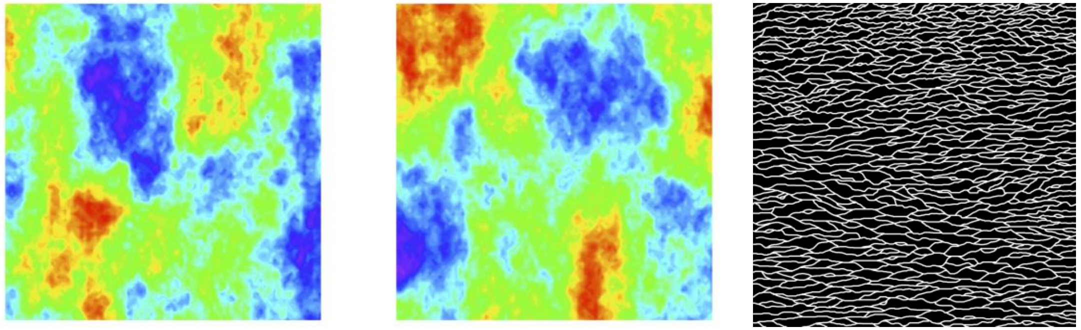


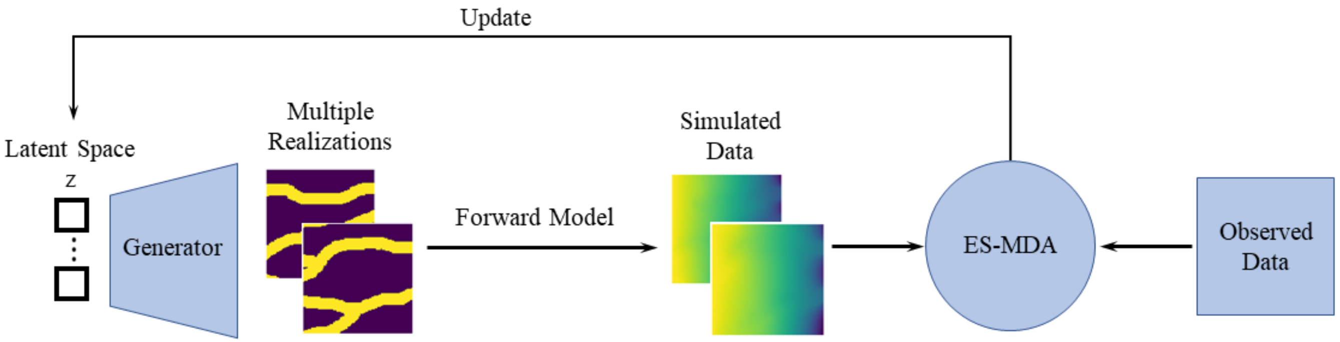
Estimated

Normalized Estimated Pressure (t= 10.0 yrs)

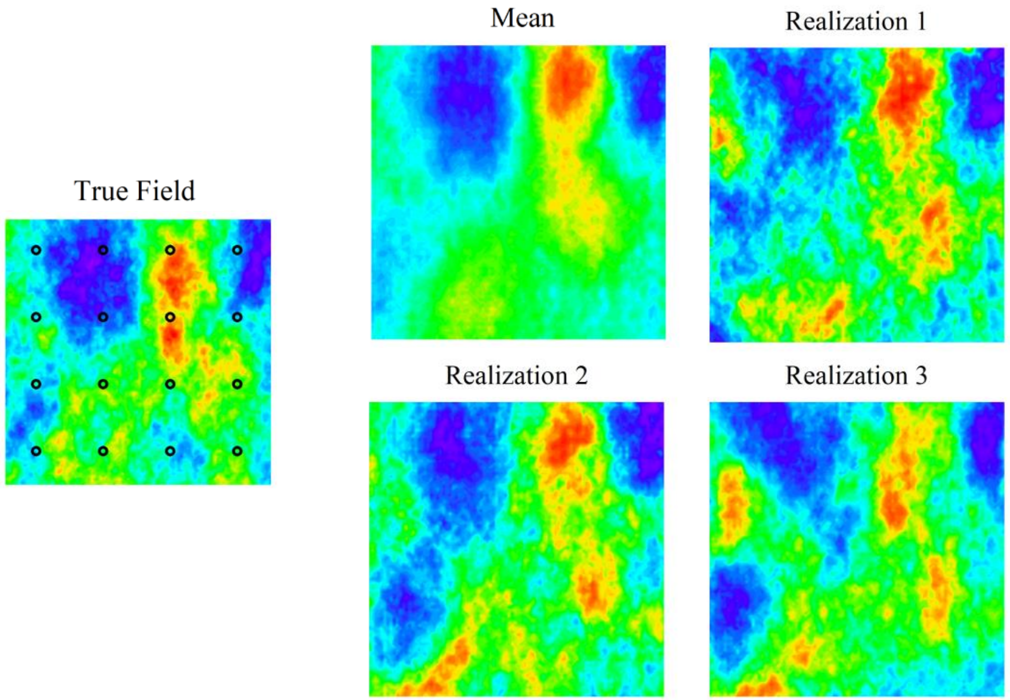


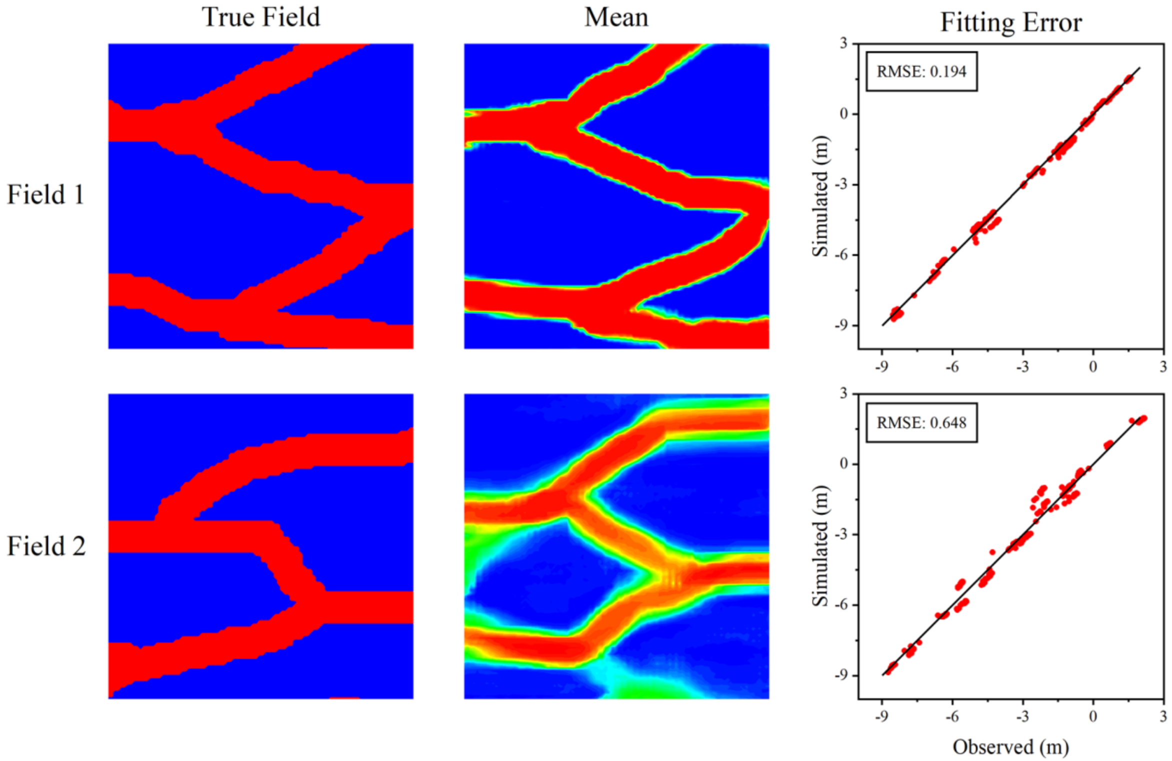
Data Assimilation (ES-MDA) with WGAN prior





Training Images for 1) Gaussian and 2) channelized aquifer



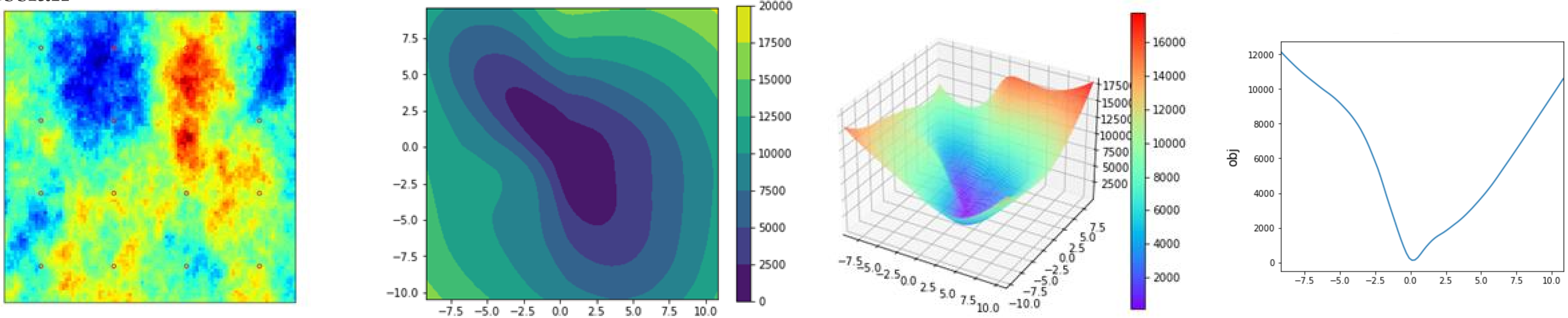


Bao et al., in prep

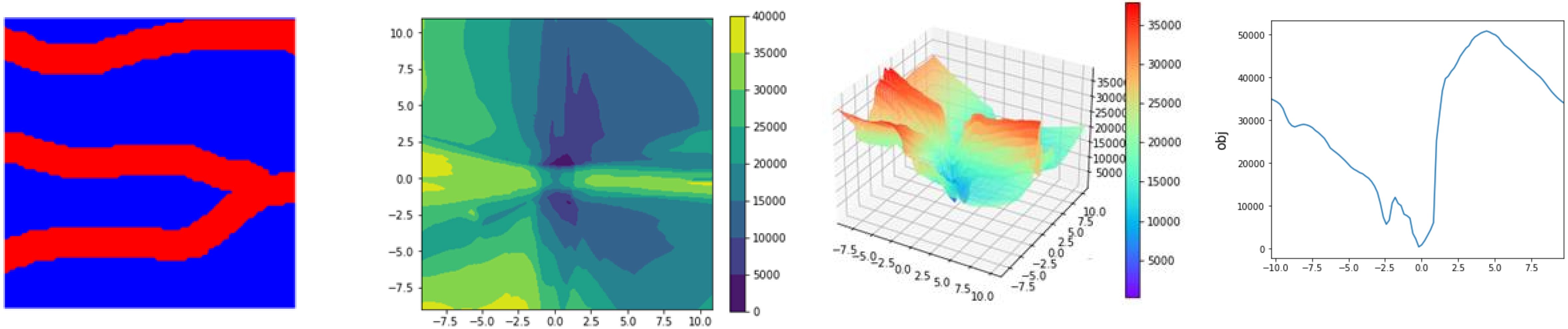
Challenges: GAN-based prior

Objective function: -log(post)

Gaussian



Non-Gaussian



Bao et. al., *to be submitted*

Summary

- Data assimilation in the latent space with deep learning methods (VAE, WGAN) and fast deep learning-based forward modeling can achieve real-time history matching of CO_2 operations and forecasting pressure plume development.

- Latent space optimization including optimal choice of the nonlinear dimension reduction requires further study with more realistic and various types of observed data.

- ML/DL with domain knowledge can lead to dramatic improvement in spatio-temporal data analytics and decision making for optimal monitoring system development.

Thank you!

Any questions?

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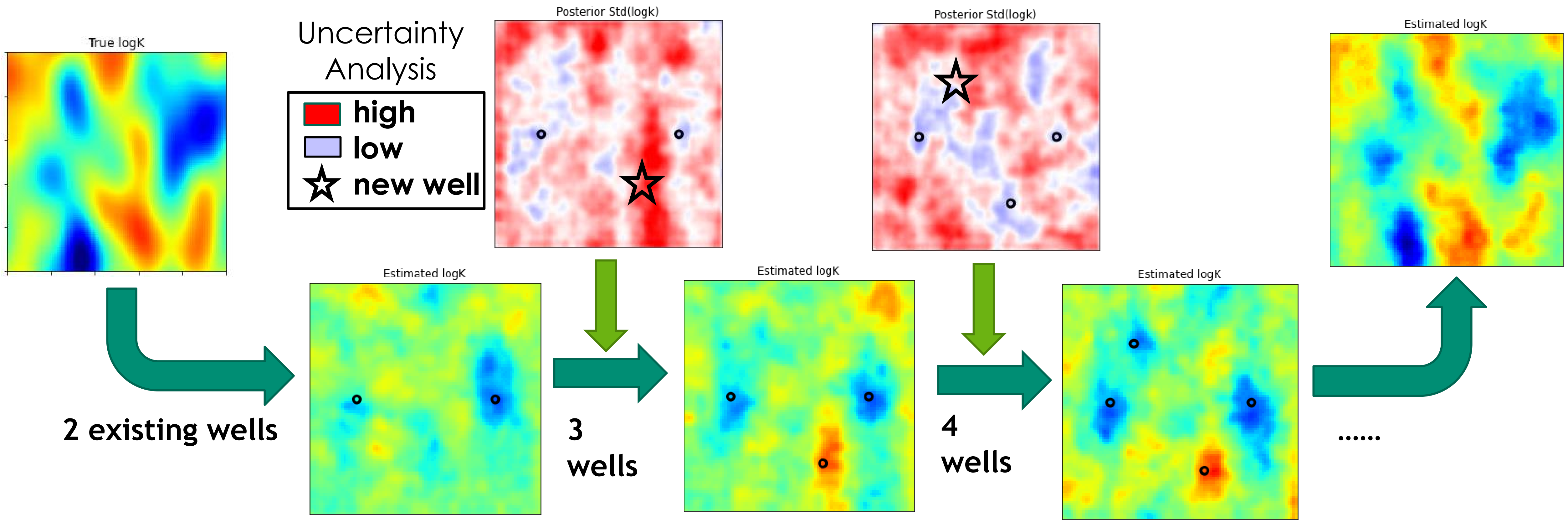
Preliminary Result: Optimal Monitoring Well Placement



- By computing posterior covariance and <u>maximize the information gain</u> (e.g, D optimality) in the small latent space, our data assimilation method can accelerate Optimal Experiment Design (OED) problems and identify next "best" well locations

Physics-Informed Neural Networks (PINNs) for PDEs

- A form of neural networks known as **Physics-Informed neural networks** (PINN) to solve **partial differential equations** (PDEs) involved in fluid flow and reactive transport.
- A main idea of PINNs is to **incorporate governing equations of physics** in the form of **partial differential equations** (PDEs) **into the loss** via automatic differentiation (AD)

Input: Concentration data + head loss and conductivity +
Advection-Diffusion-Reaction equation + Darcy Equation
Prediction: Permeability field is estimated inversely