



# CO<sub>2</sub> Storage Site Characterization using Deep Generative Models

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## Introduction

In this work, we present a fast Machine Learning (ML)-based inverse modeling for real-time subsurface history matching and forecasting. The work aims to support CO<sub>2</sub> related operations and forecasting CO<sub>2</sub> and pressure plume development for DOE Science-informed Machine Learning to Accelerate Real Time (SMART) initiative. The proposed method utilizes one of the current efficient data assimilation methods, i.e., *Hierarchical Bayesian with Gaussian Prior* (through power-transformation of unknowns). In Bayesian framework, the prior uncertainty of subsurface unknown properties, e.g., permeability field, is typically parameterized as log-normal with mean and covariance. However, there are two major challenges for high-dimensional applications:

- the number of (expensive) forward model simulations
- computational burdens for high-dimensional matrix-matrix computations.

To address these challenges, we use deep-generative model-based data assimilation methods for large-scale carbon storage site characterization and forecast. Variational AutoEncoder (VAE) and novel Wasserstein Generative Adversarial Networks are used to learn the approximate distribution from multipoint geostatistics-derived training images as prior and accelerated data assimilation is performed on the low-dimensional latent space in a Bayesian framework. Numerical examples with synthetic 2D permeability fields with fluvial channels confirm that our proposed method provides promising subsurface site characterization with reliable uncertainty quantification.

## Model Reduction

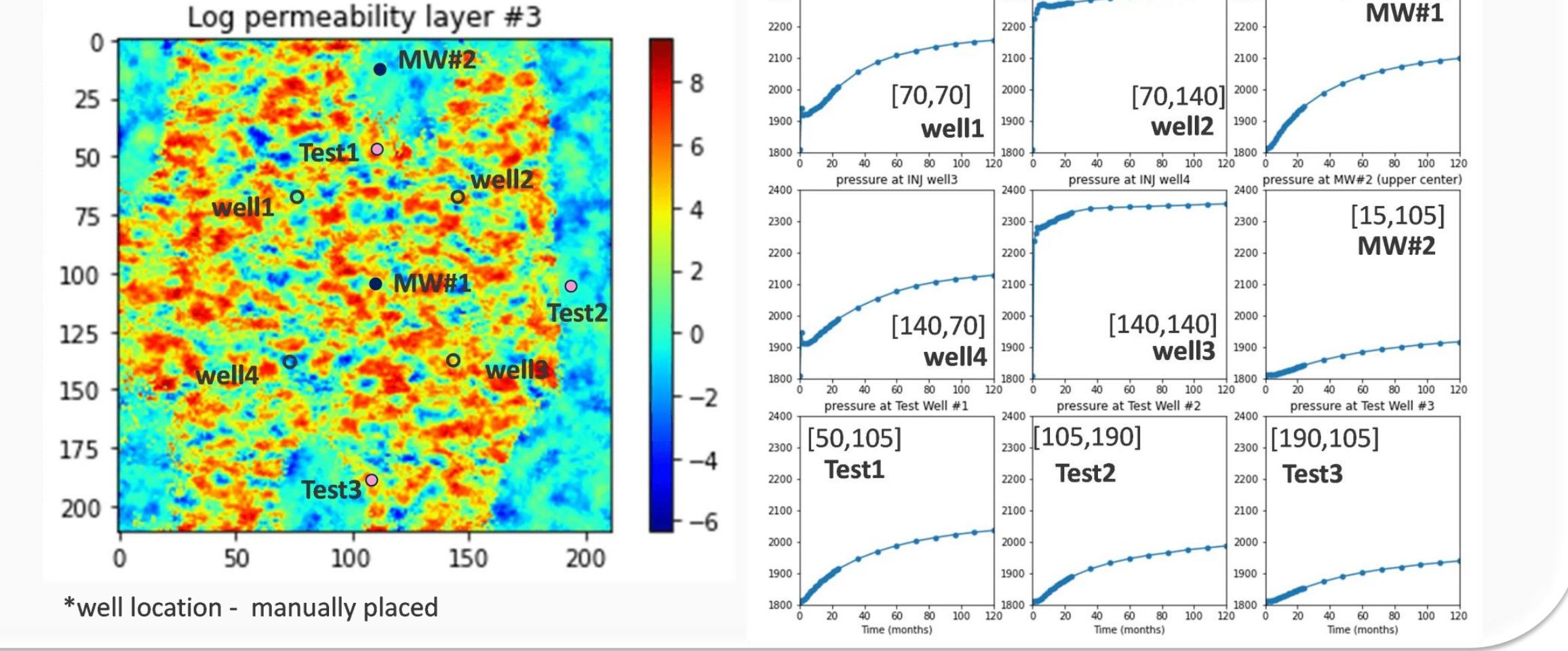
### Forward modeling:

$$\mathbf{y} = \mathbf{F}(\mathbf{m}) \approx \mathbf{F}(\mathbf{G}(\mathbf{z}))$$

- $\mathbf{y}$  is a (nobs x 1) simulated observation vector,
- $\mathbf{F}$  is a flow model that produces outputs at obs. locations
- $\mathbf{m}$  is a (m x m) permeability matrix,
- $\mathbf{G}$  is a generator or deterministic map from  $\mathbf{z}$  to  $\mathbf{s}$
- $\mathbf{z}$  is a (k x k) latent space matrix.

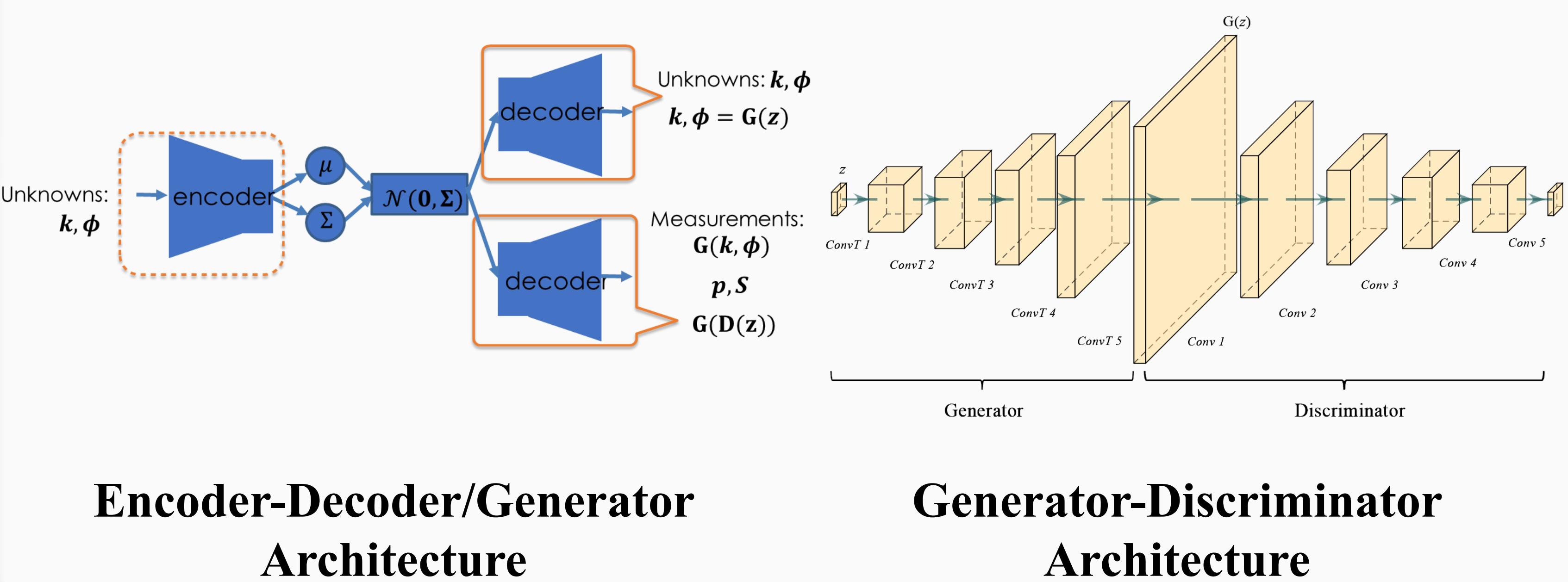
$\mathbf{G}(\mathbf{z})$  can be obtained from any generative models and here we used Variational AutoEncoder (VAE) and Wasserstein Generative Adversarial Networks (WGANs).

### Clastic Shelf MODEL:

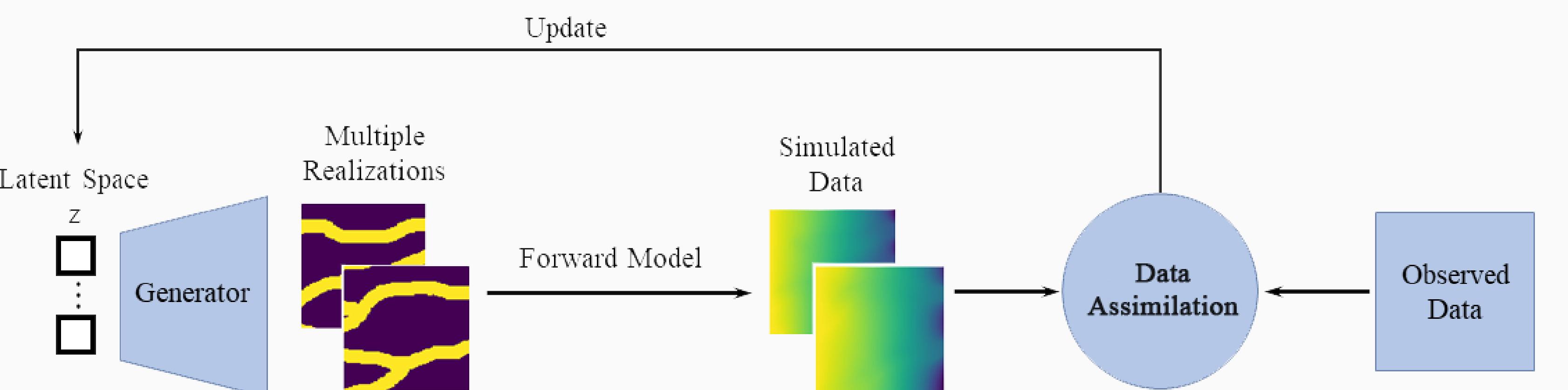


\*well location - manually placed

## Deep Generative Model Architecture



## Data Assimilation with Deep Generative Models



### Main Conceptual Idea

$$\begin{aligned} \text{Forward problem: } \mathbf{y} &= \mathbf{F}(\mathbf{m}) \\ \text{with data assimilation framework:} \\ \mathbf{m}^{i+1} &= \mathbf{m}^i + \mathbf{C}_{MD}^i (\mathbf{C}_{DD}^i + \alpha_i \mathbf{C}_D)^{-1} (\mathbf{d}_{uc}^i - \mathbf{d}^i) \\ \mathbf{d}_{uc}^i &= \mathbf{d}_{obs} + \sqrt{\alpha_i} \mathbf{C}_D^{1/2} \mathbf{I}_d \end{aligned}$$

where  $\mathbf{C}_{MD}^i$  is the cross-covariance between the model parameters and simulated data,  $\mathbf{C}_{DD}^i$  is the auto-covariance of the simulated data,  $\mathbf{C}_D$  is the observation error covariance,  $\mathbf{d}^i$  is the simulated data,  $\mathbf{d}_{uc}^i$  is the perturbed observation data, and  $\alpha_i$  is an inflation factor.

with any (nonlinear) dimension reduction:

$$\begin{aligned} \mathbf{y} &= \mathbf{F}(\mathbf{G}(\mathbf{z})), \dim(\mathbf{z}) \ll \dim(\mathbf{m}) \\ \mathbf{z}^{i+1} &= \mathbf{z}^i + \mathbf{C}_{ZD}^i (\mathbf{C}_{DD}^i + \alpha_i \mathbf{C}_D)^{-1} (\mathbf{d}_{uc}^i - \mathbf{d}^i) \end{aligned}$$

VAE/WGAN is our choice since it constructs the prior  $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

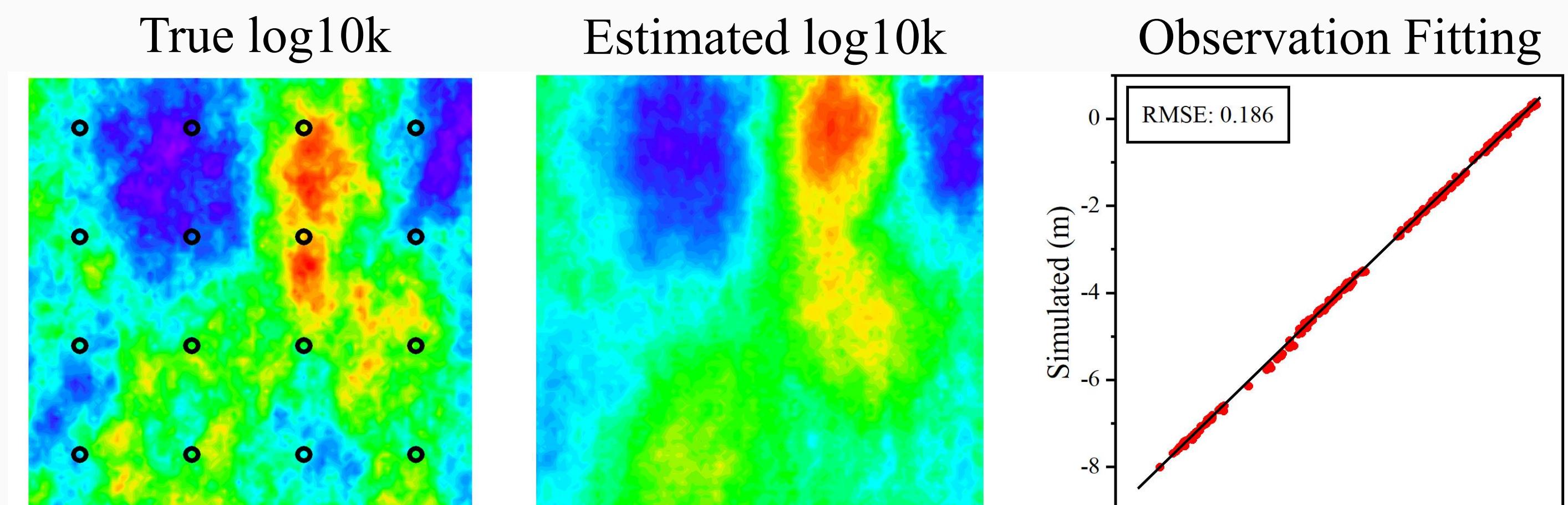
- Covariance can be directly computed with Adjoint method and Fast Linear Algebra (i.e., Variational Inference) or can be approximated with Ensemble via Ensemble Smoother.
- Depending on the choice (variational inference or Ensemble approximation), one would need a few hundreds of forward modeling evaluation

## Experimental Results

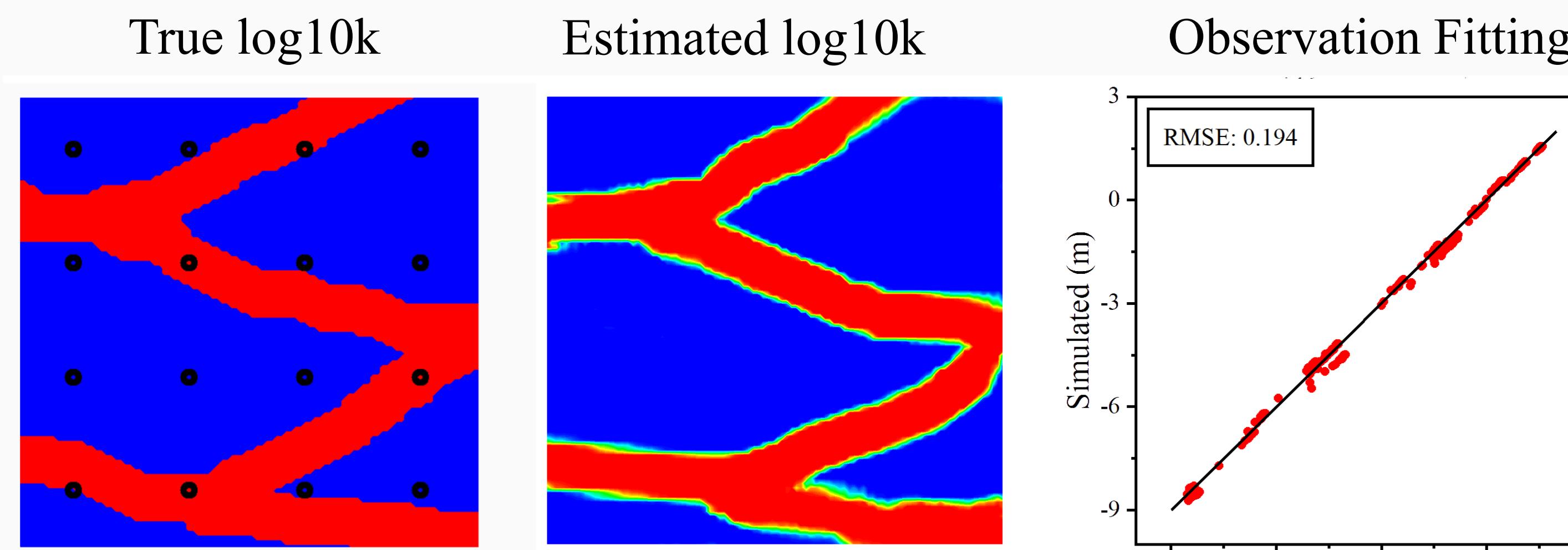
### Validation with Single Phase Flow Application

Here we used USGS MODFLOW as “full” physics single phase flow model. 96 x 96 unknown k field has been compressed to 3x3 latent dimension through WGAN. 16 wells hydraulic tomography was applied to obtain pressure data.

#### Gaussian Fields

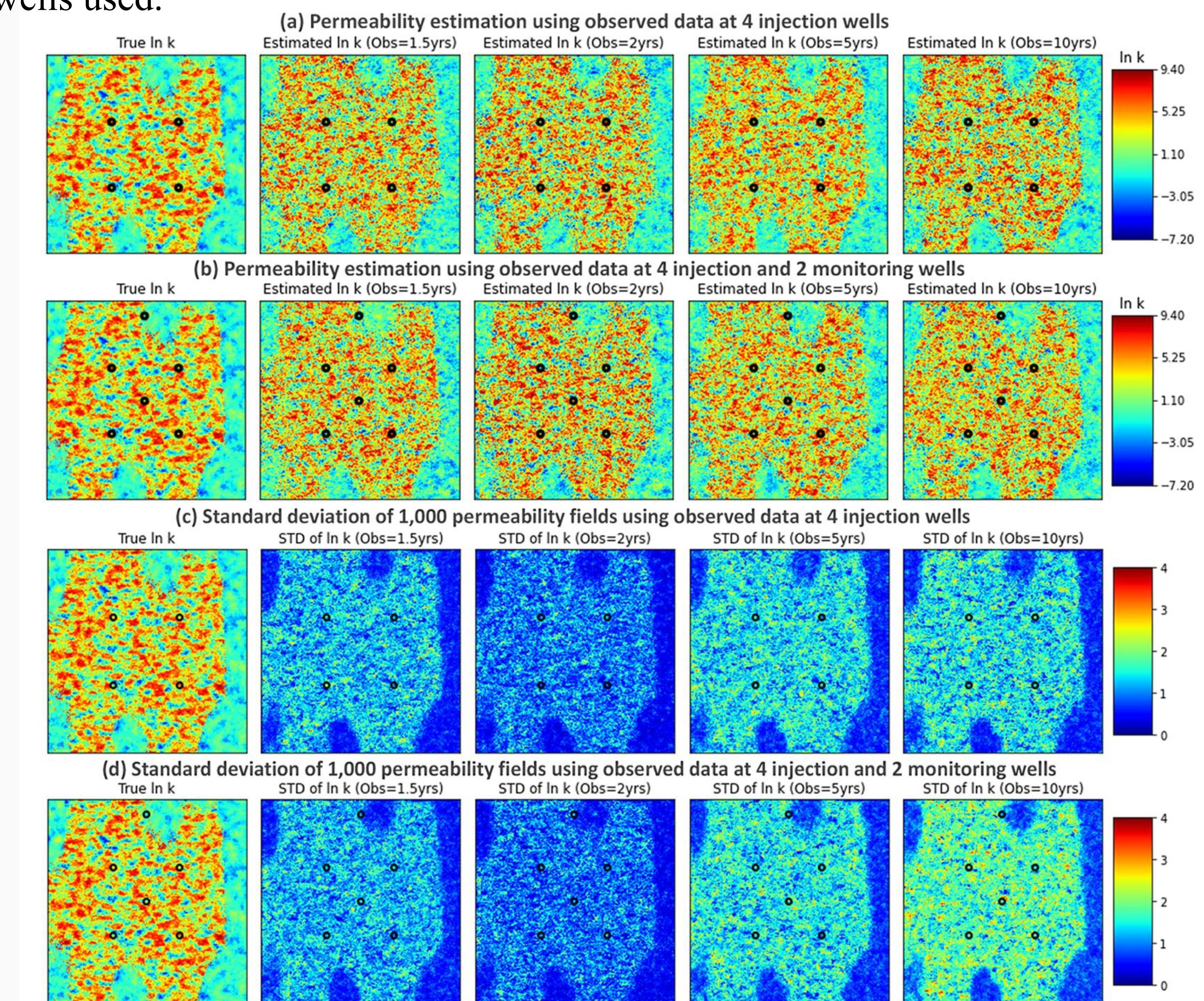


#### Channelized Fields



#### Multi-Phase Flow Application using Clastic Shelf Data

Here we used CMG for CO<sub>2</sub> injection simulation. 211 x 221 unknown k field has been compressed to 32 latent dimension through VAE. 4 injection/2 monitoring wells used.



## Acknowledgement

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