SAND2021-8342PE

MLDL

Machine Learning and Deep Learning Conference 2021

Physics-based Deep Learning Driven CO_2 Flow Modeling and Data Assimilation for Real Time Forecasting

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- Funding Source (LDRD, DOE FE SMART Initiative)

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SMART Initiative

Science-informed Machine Learning to Accelerate Real Time (SMART) Decisions in Subsurface Applications

Real-Time Visualization
"CT" for the Subsurface

Rapid Prediction
Virtual Learning

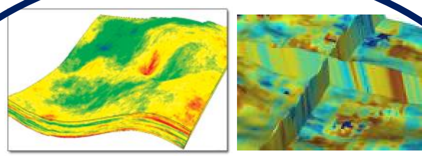
Real-Time Forecasting
"Advanced Control Room"

Transforming decisions through **clear vision** of the present and future subsurface.

- DOE Office of Fossil Energy & Carbon Management Project
- Specific goal: Machine learning-driven CO_2 modeling by combining fast ML-based forward modeling with ensemble-based (multiple) data assimilation (EnDA), resulting in real-time history matching of CO_2 operations and forecasting CO_2 and pressure plume development

Background: Building a Reservoir Model

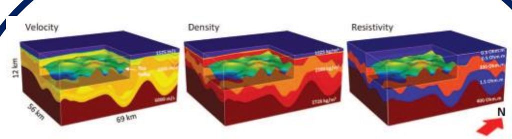
Task 6



Geological fracture model & properties

Flow/Transport Properties

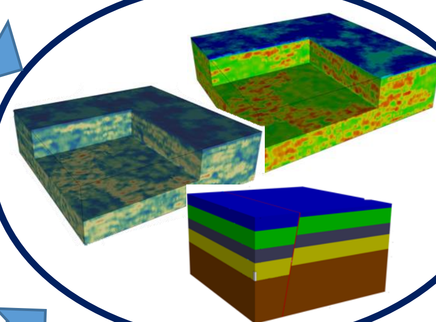
Task 2



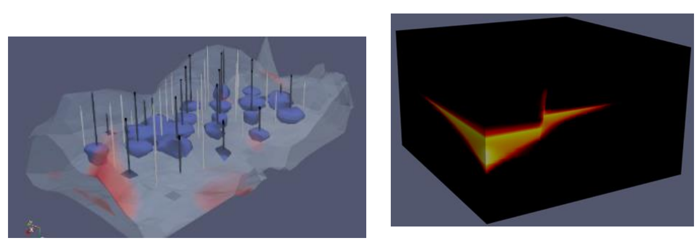
Rock Property models
Geophysical survey

Task 4 and Task 5

Reservoir model:
- Permeability/porosity/(fracture)
- Injection, production data
- Fluid property, water saturation



Fluid Plume Simulation



Task 3

K=f(σ)

Geomechanical model:
- **Stress**
- **Pore pressure**
- **Rock properties**

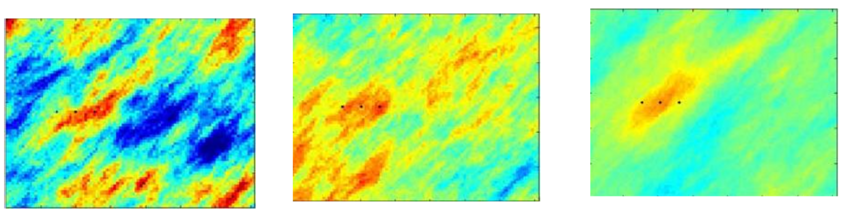
- Saturation/Pressure/Production/Displacement forecasting
- Update Reservoir model
- Development/monitoring decisions

Examples of Previous Work

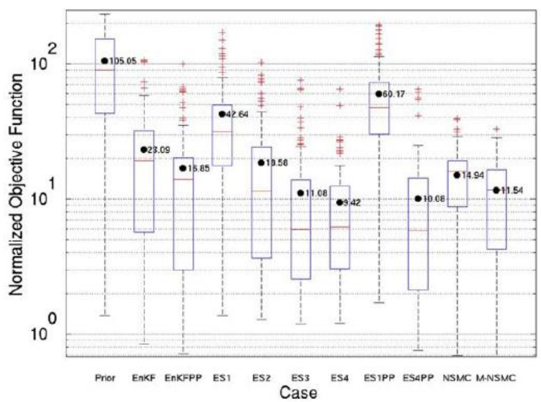
History matching/Data Assimilation (CO_2 Injection at Cranfield, MS)

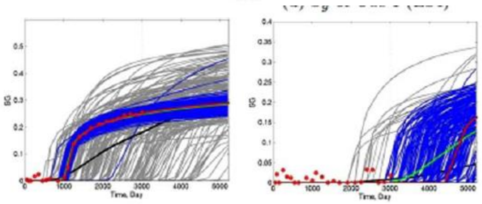
- Data: bottom hole pressure (BHP) at injection well and gas saturation at two obs. wells.
- Data integrated till 3000 days with prediction phase time of 5200 days.

Synthetic Truth | Calibration-cons-trained NSMC | Ensemble-based filtering method



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

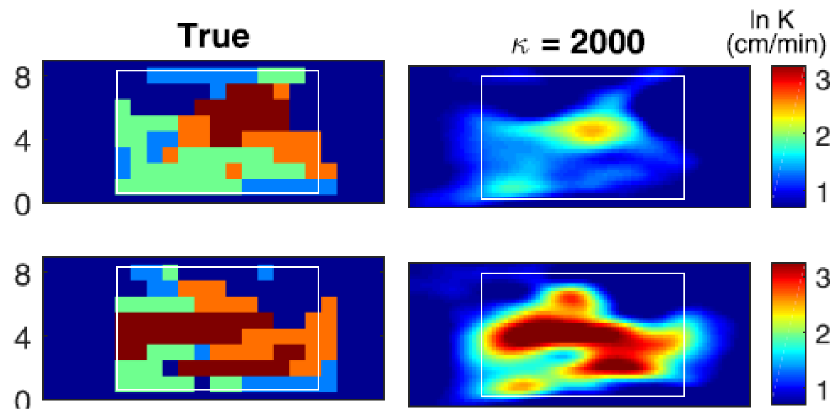




Tavakoli and Yoon et al. (WRR2013)

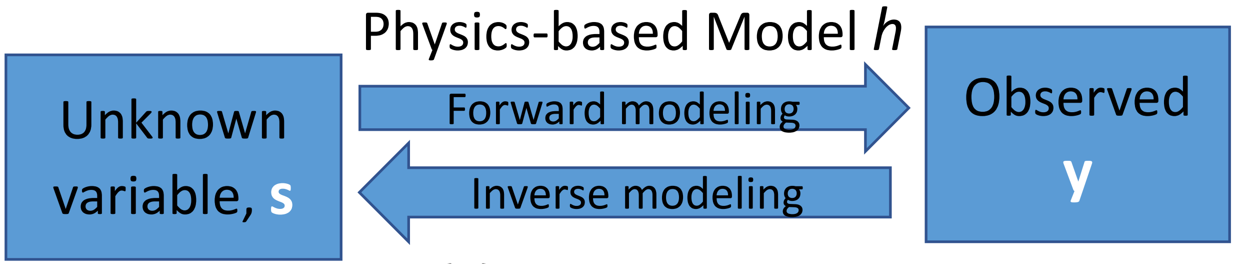
Tracer transport in 3D sandbox with MRI-based spatio-temporal data

Principal Component Geostatistical Approach (Jacobian-free Stochastic Inversion)



Lee and Yoon et al. (WRR2016)

Motivation for Deep Learning Based Approach



$$\mathbf{y} = h(\mathbf{s}), \qquad v \sim N(0, \boldsymbol{\Gamma}_{noise})$$

where

y := observations (n_{obs}); e.g., pressure, concentration

s := model parameters ($n_{unknowns}$) (e.g., permeability, porosity)

h := forward operators

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

1. **Computational burdens with matrix calculations**

   => ML-driven fast predictive reduced-order modeling

2. **# of forward model simulations**

   => Effective dimension reduction for data assimilation

Part 1: Forward ML Modeling

ML Methods for Model Training & Test Case

Toy Model Algorithms

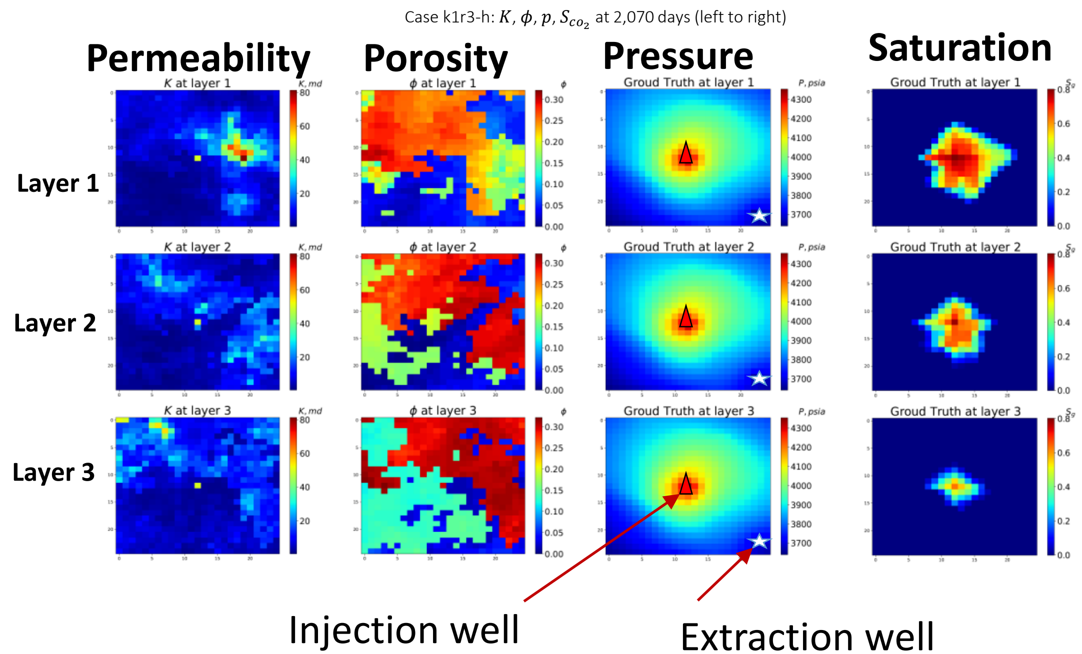
- Autoencoder
- Variational Autoencoder
- MLP

- CNN & variants
- LSTM & variants
- Physics informed
- Pix2pix

- Graph NN
- Gaussian process
- Decision trees

- CMG is a physics-based simulator
- Spatio-temporal data

3D Toy problem – Heterogeneous permeability
[3 permeability fields x and 9 injection rates]

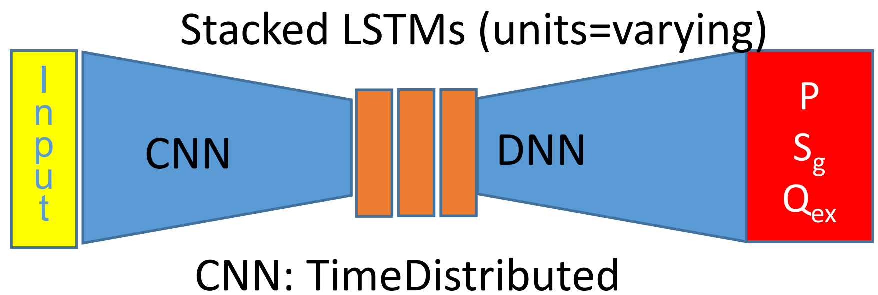


25x25x3 layers

DL for Forward Model Prediction

- **Stacked DL architecture:**

- CNN-LSTM-DNN

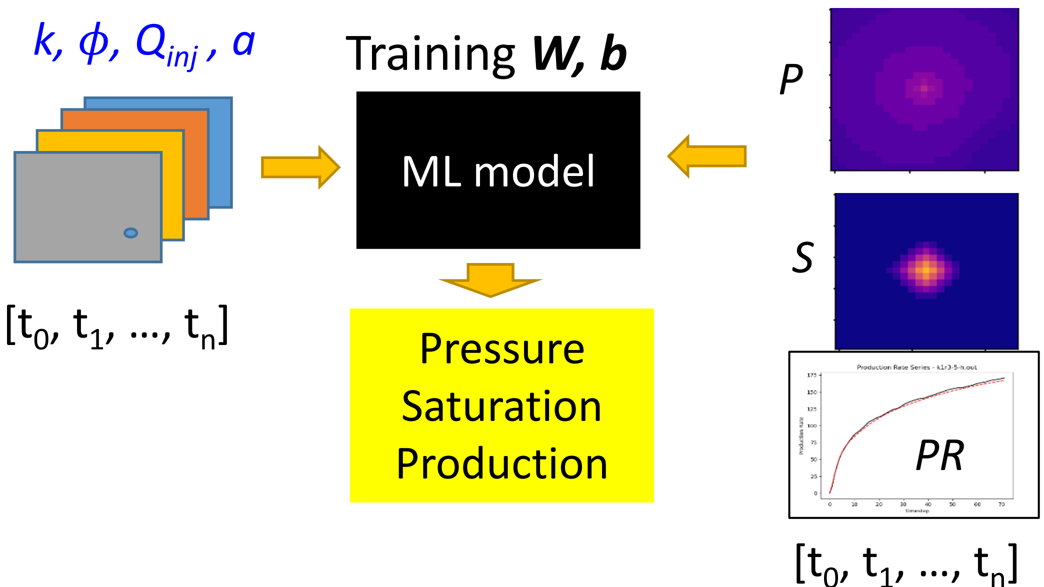


Input:

k, ϕ, Q_{inj}, a (active zone)

Output:

Pressure, Saturation, Well production



Physics-Based Loss Functions

- **Loss functions can be constructed through governing equations**
  - Physical constraints, theoretical equations, and relations can be incorporated for data-driven model (e.g., trained model)
  - We incorporated different terms from governing equations into the loss functions
  - Flux, mass conservation, known quantities are used

Governing equations for two phase flow

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

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

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

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

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

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

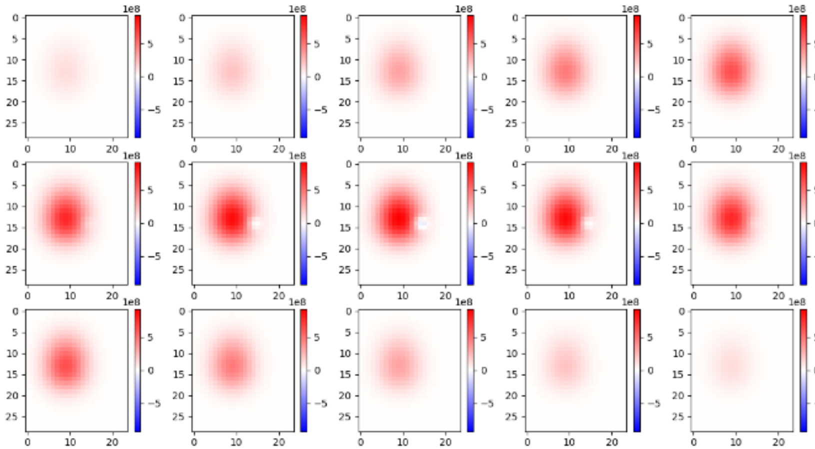
$+\lambda_{bhp} * \boxed{MSE(\hat{P}_{bhp}, P_{bhp})} + \lambda_{pr} * \boxed{MSE(\hat{P}_{bhp}, P_{bhp})}$

Model Input

• Pressure & Production Rate model

- Small model domain
  - Horizontal 29 x 24 cells (subsampling: every 10 cells in each x & y) from 290 x 240 original domain
  - 15 depth layers (whole layers)
  - Yearly data (up to 99 yrs) from monthly data
- Two injection wells and one (passive) production well
  - Cumulative injection amount over time
  - Radial Basis function to distribute injection amount
- 32 training/validation sets & 4 testing sets
- Binary active zone (also for saturation & production rate)
  - Zeros for inactive zones used in loss function

Distribution of radial basis function

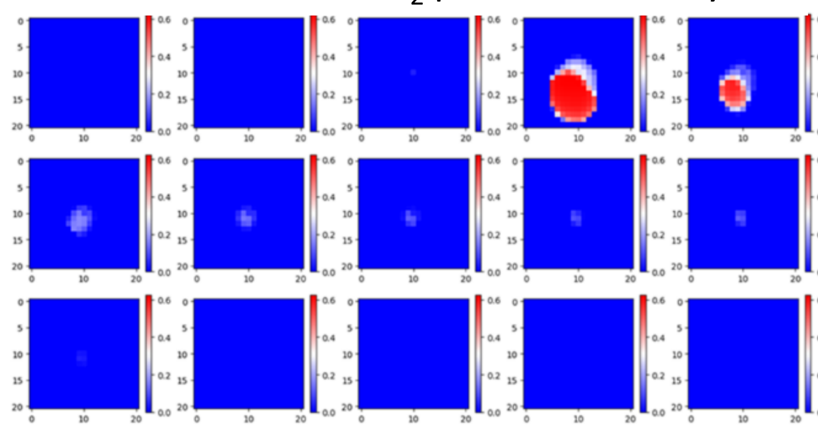


Weights: High, medium, low radial distance & point source at wells

• CO_2 Saturation model

- Small model domain
  - Two horizontal 21 x 21 cells around two injection wells where CO_2 plumes spread (subsampling: every 4 cells)
  - 15 depth layers (whole layers)
  - Yearly time interval (a total of 100 = initial + 99 yrs) from monthly data
- Injection rate
  - Cumulative injection amount over time at well locations

Distribution of CO_2 plume at t = 99 yrs



Yoon et al. (in prep)

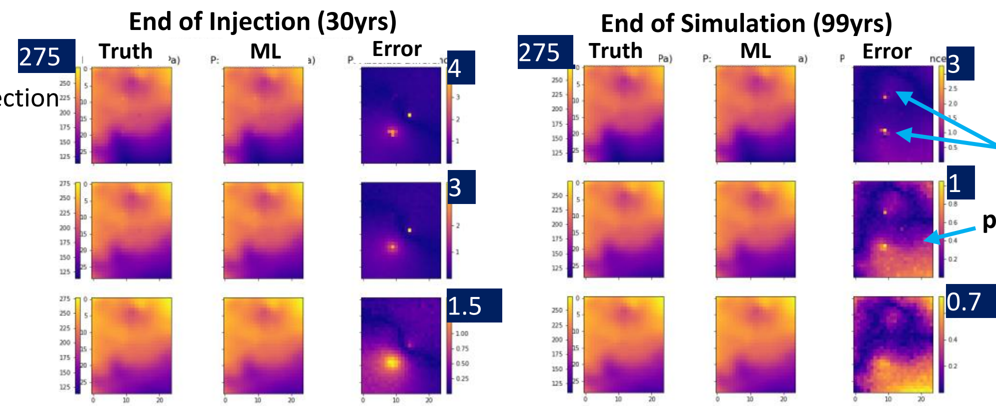
Results – Pressure & Production Rate

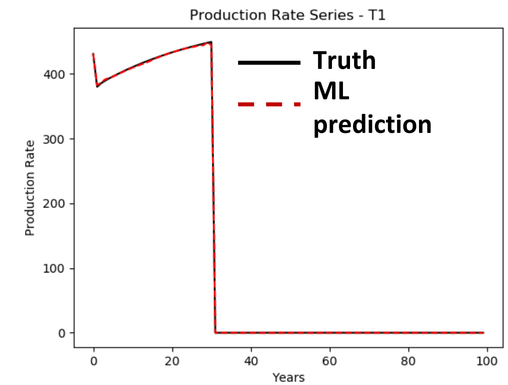
Moderate injection rate Test case 1

Bottom of Injection layer

Top of Injection reservoir

Top of secondary reservoir



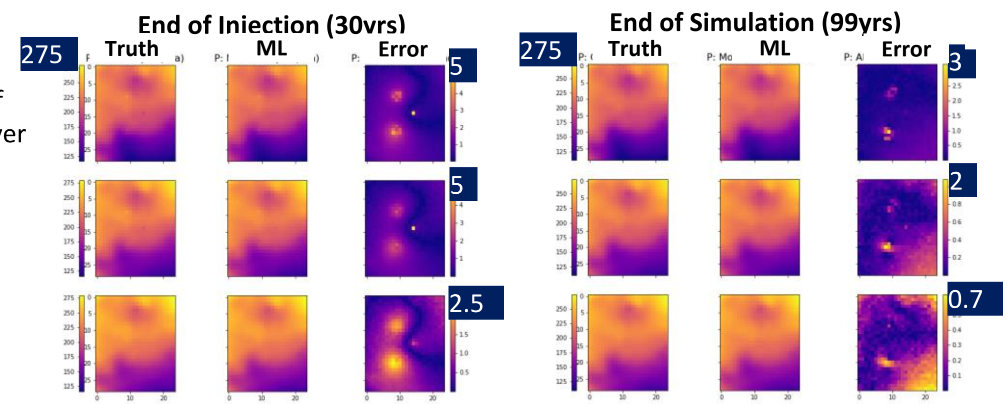


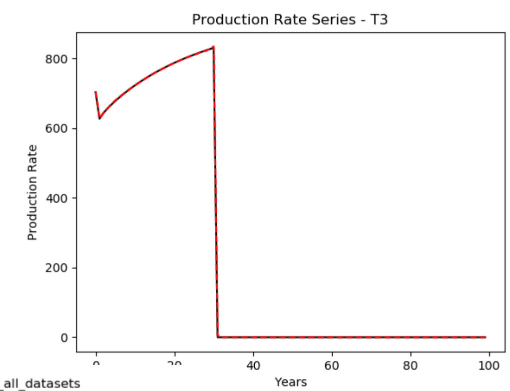
High injection rate Test case 3

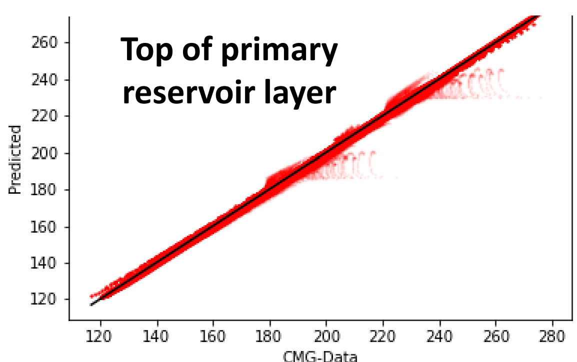
Bottom of Injection layer

Top of Injection reservoir

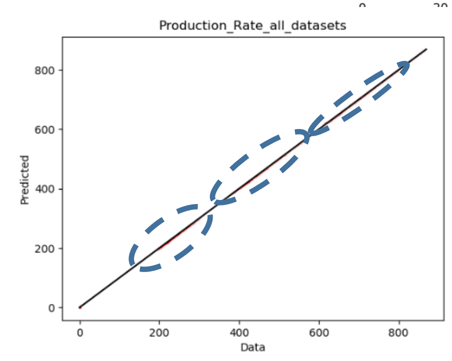
Top of secondary reservoir







Parity plot (All 40 datasets)

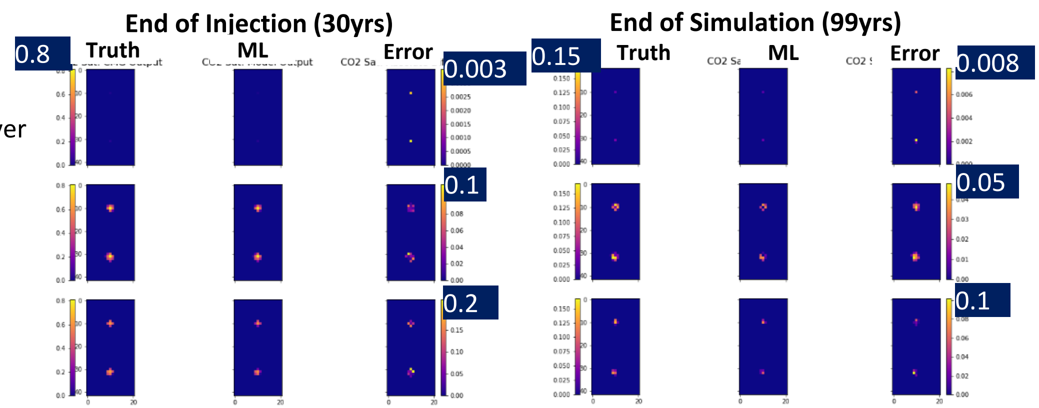


Results – CO_2 Gas Saturation

Below Injection layer

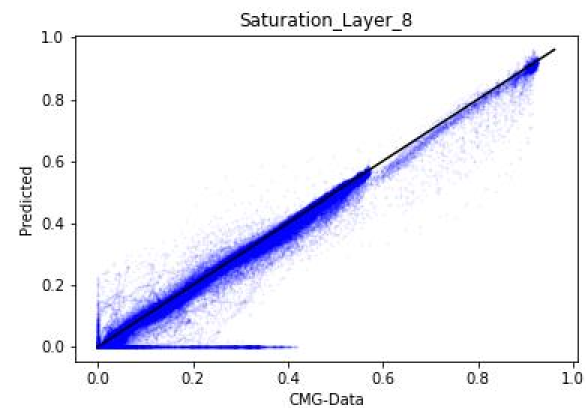
Top of Injection reservoir

Top of secondary reservoir



Moderate injection rate Test case 1

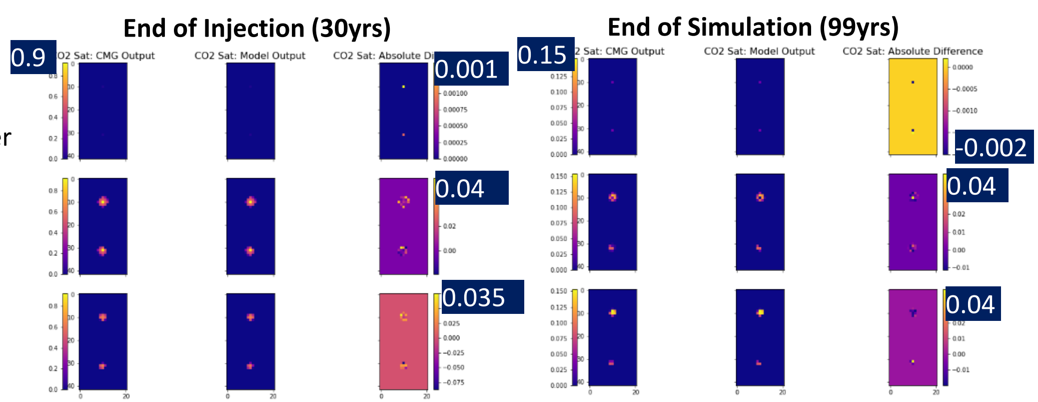
Top of primary reservoir layer



Below Injection layer

Top of Injection reservoir

Top of secondary reservoir



High injection rate Test case 3

Machine Learning Model Performance

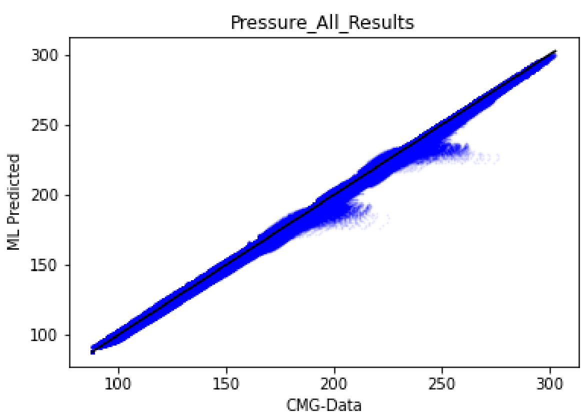
Output	RMSE	Unit	Min	Max	Training time*
Pressure	0.609	bar	87.966	302.795	1.77 hrs
Saturation	0.0089	--	0	0.92624	2.28 hrs
Production	1.687	STB	0	864.489	1.48 hrs

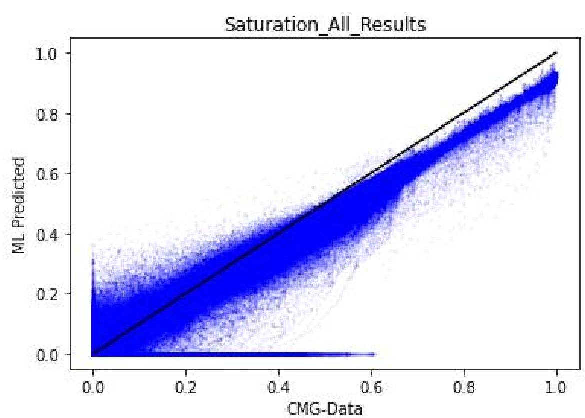
* 1 NVIDIA GPU (Quadro 5000)

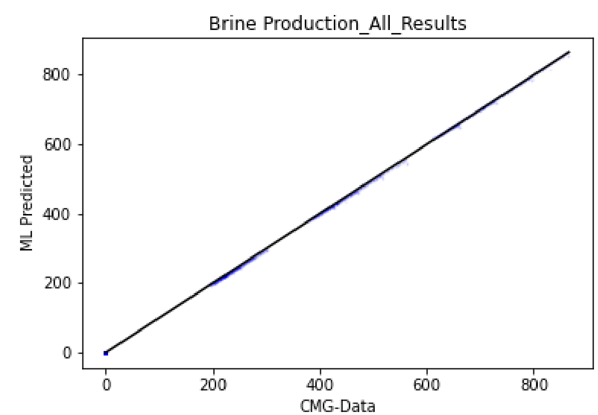
All trained models executed within 1 second

STB: Stack Tank Barrel

Parity plot (All 40 datasets)







Part 2:
Variational Autoencoder for Data Assimilation

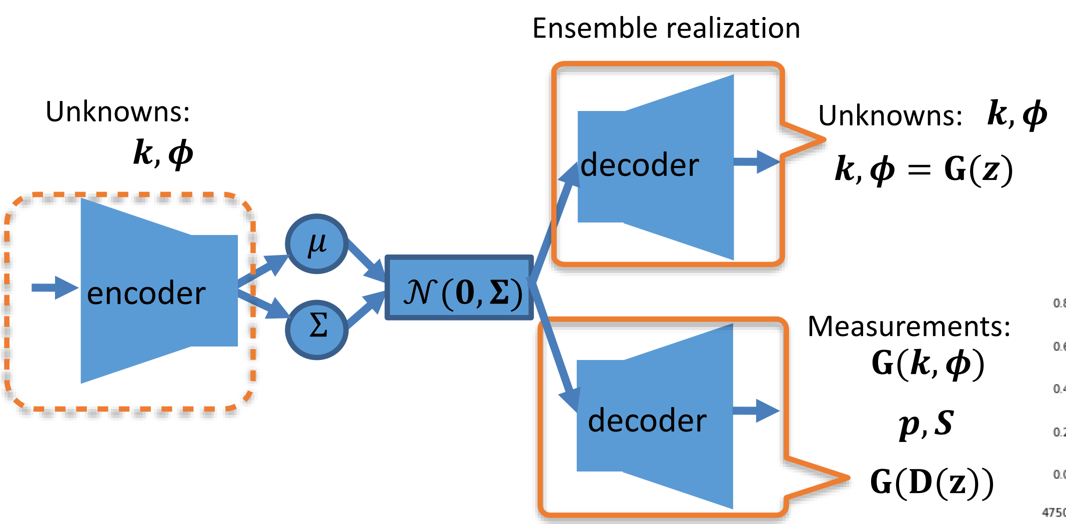
Variational AutoEncoder(VAE) & Ensemble-based data assimilation (EnDA)

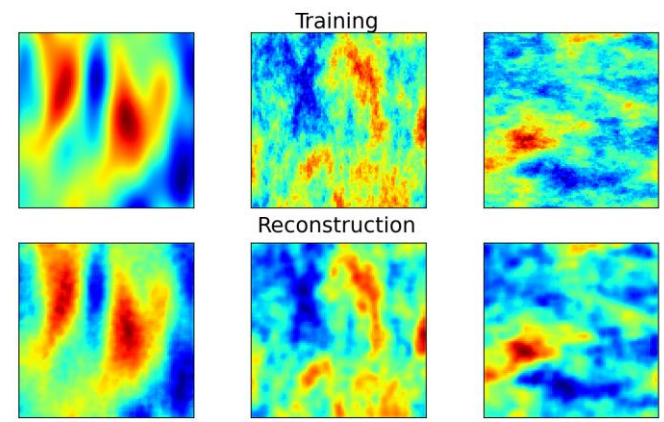
Objective: real-time history matching of CO_2 operations and forecasting CO_2 and pressure plume development

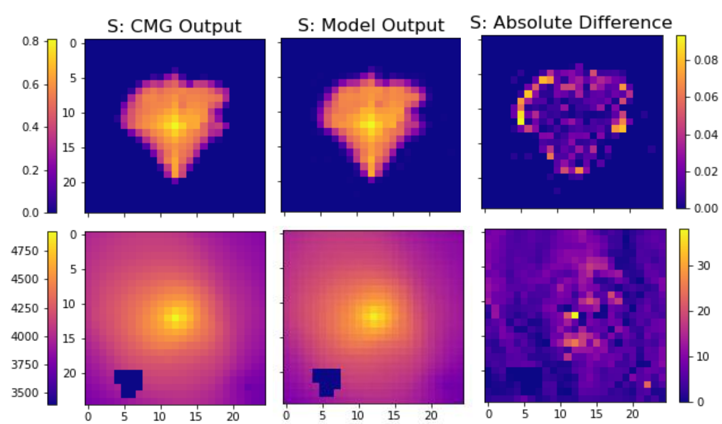
- Deep Learning-based nonlinear projection approach to accelerate the stochastic inversion.
- VAE and its decoder to map the permeability k to the latent vector z ***whose dimension is much smaller than the original dimension of k*** while ensuring a good approximation accuracy.

Variational AutoEncoder(VAE)-based Inversion

- **VAE to construct data-driven nonlinear dimension reduction model:**
  - Data assimilation in **small nonlinear latent space of unknown parameters with dim(z)**
  - Only require "**dim(z)**" forward model executions at each iterations instead of dim(m) or dim(obs)
  - Can encode **prior beyond Gaussian**







Variational AutoEncoder(VAE)-based Inversion

Formulation for (optimization-based) Data Assimilation with VAE-based prior

Forward problem: $\mathbf{y} = \mathbf{G}(\mathbf{m})$

with l Gauss Newton iterations from $\mathbf{m}^0 = \mathbf{m}_{prior}$

$$\boldsymbol{m}^{l+1} = \boldsymbol{m}^0 + \mathbf{C}_{\text{prior}}\mathbf{J}\left(\mathbf{J}\mathbf{C}_{\text{prior}}\mathbf{J}^{\mathrm{T}} + \mathbf{C}_{\mathbf{obs}}\right)^{-1}\left(\mathbf{y} - \mathbf{G}(\mathbf{m}^l) + \mathbf{J}(\boldsymbol{m}^l - \boldsymbol{m}^0)\right)$$

With any (nonlinear) dimension reduction G of m

$$\boldsymbol{y} = \mathbf{G}(\mathbf{D}(\mathbf{z})), \mathbf{dim}(\boldsymbol{z}) \ll \mathbf{dim}(\boldsymbol{m})$$

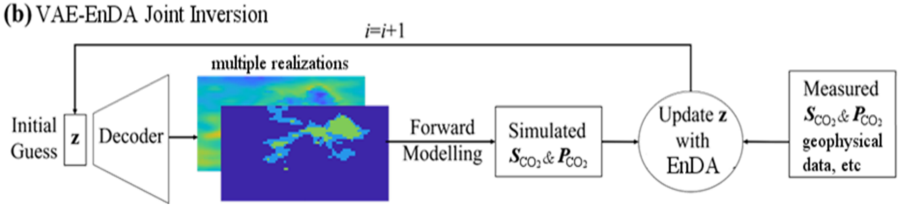
$$\mathbf{z}^{l+1} = \mathbf{z}^l + \alpha\left(\mathbf{J}_\mathbf{z}^{\mathbf{T}}\mathbf{C}_{\text{obs}}^{-1}\mathbf{J}_\mathbf{z} + \mathbf{C}_{\text{prior}_\mathbf{z}}^{-1}\right)^{-1}\left(\mathbf{y} - \mathbf{G}\left(\mathbf{D}(\mathbf{z}^l)\right) - \mathbf{C}_{\text{prior}_\mathbf{z}}^{-1}\mathbf{z}^l\right)$$

with step length (learning rate α). And the posterior covariance is given as

$$\mathbf{C}_{\boldsymbol{posterior}_\boldsymbol{z}} = \left(\mathbf{J}_\boldsymbol{z}^{\mathbf{T}}\mathbf{C}_{\boldsymbol{obs}}^{-\mathbf{1}}\mathbf{J}_\mathbf{z} + \mathbf{C}_{\boldsymbol{prior}_\boldsymbol{z}}^{-\mathbf{1}}\right)^{-\mathbf{1}}$$

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

(b) VAE-EnDA Joint Inversion



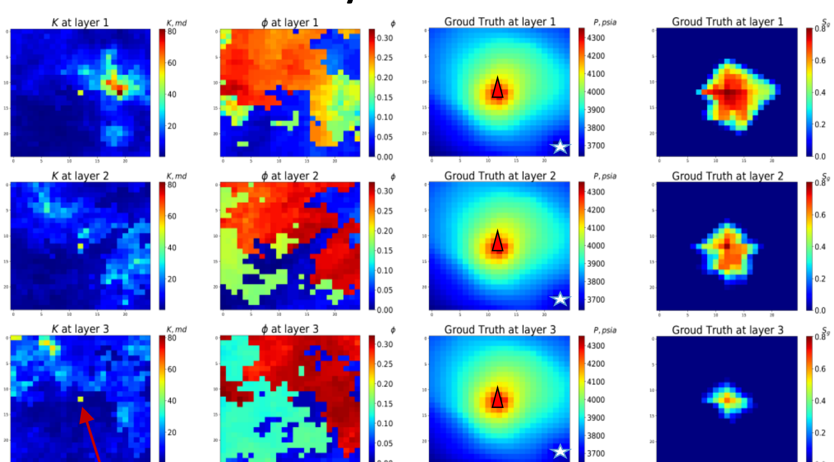
Latent space "**z**" obtained by VAE, i.e., deep learning-based encoder will be updated in EnDA-based methods for data assimilation with various measured data.

Description of the data used

- **High fidelity numerical simulator to generate multiphase CO_2 flow in 3D heterogeneous field**
  - Heterogeneous material properties (permeability & porosity)
  - Injection & extraction well operations
  - CO_2 saturation, pressure, and production in space and time

- 3D Toy problem (25x25x3)
[a total of 27 cases with 3 permeability fields x 9 injection rates]

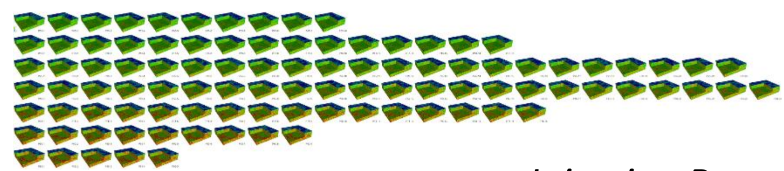
Permeability **Porosity** **Pressure** **Saturation**



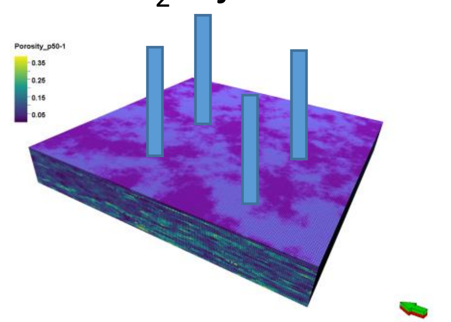
CO_2 injection well

Water extraction well

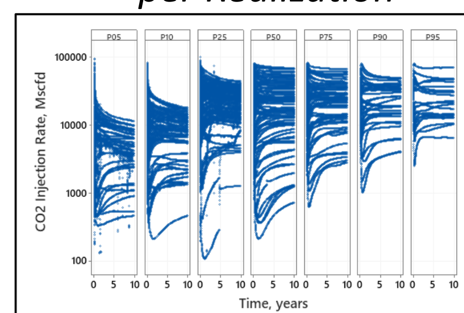
- Field scale-based permeability distribution
- 100 realizations based on probability (P05/10/25/50/75/90/95)



Four CO_2 injection wells



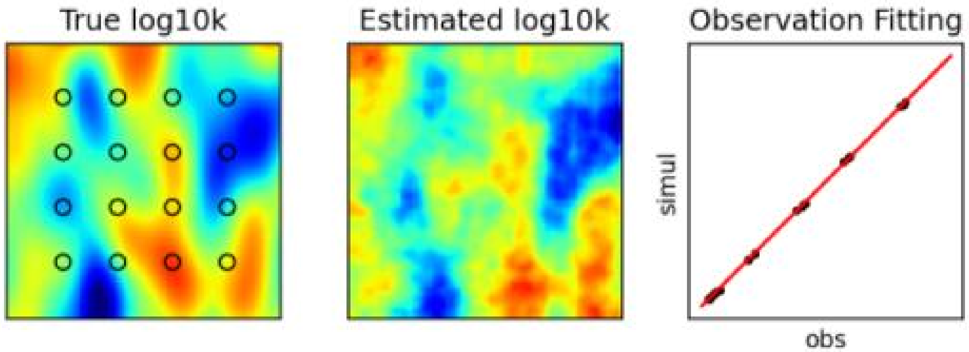
Injection Rate per Well per Realization



** Visualizations provided by LLNL. Data generated by EERC (Courtesy: Nick Azzolina)*

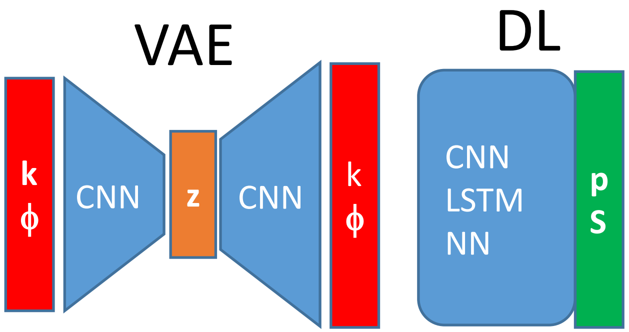
Results I: Single phase flow

- Inversion example using a single-phase flow model:
  - Here we used a "full" physics single phase flow model
  - 10,000 (100x100) unknown permeability (**k**)
    => latent space (**z**) with 32 latent dimension
  - 16 observation wells with head data
  - **33** forward model runs/iteration to construct Jacobian
  - Initial guess: any guesses converged
  - Only 3-4 iterations required due to accurate gradient information in latent space

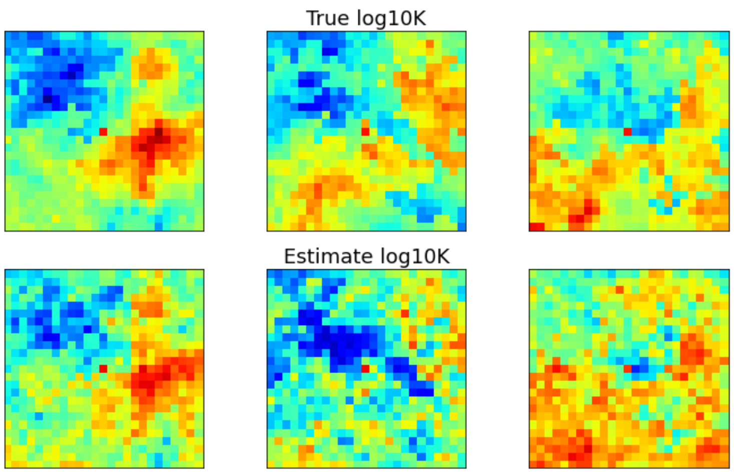


Results II: Multiphase Flow

- Use a simple 3D problem to demonstrate VAE-based inversion
  - the latent space is constructed based on both (k,ϕ) and (P, S)
  - the cost of the trained reduced order model ~O(1 sec)
  - can run optimization-based inversion or stochastic Newton MCMC for full posterior pdf characterization of the latent space

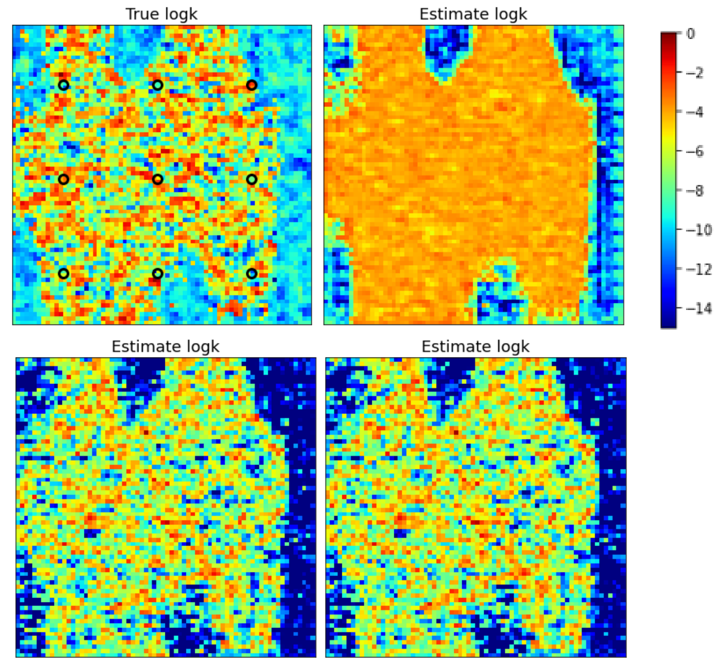


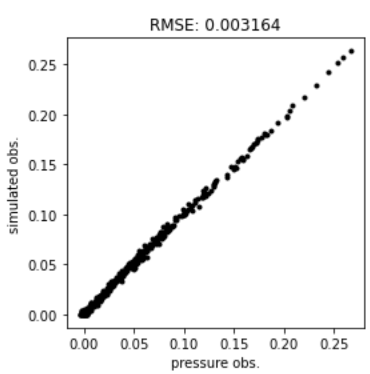
- Inversion example using DL-based reduced order model for multi-phase flow with nonlinear dimension reduction:
  - ML trained reduced order model with 3D toy problem
  - 25x25x3 unknown **k** => **z** with 32 latent dimension
  - 720,000 noisy transient pressure observations
  - **33** forward model runs/iteration to construct Jacobian
  - Initial guess: Perturbed field with ~10% error
  - Only **~3 min inversion time** on a single core laptop
  - Convergence with any (reasonable) initial guesses due to data-driven prior!

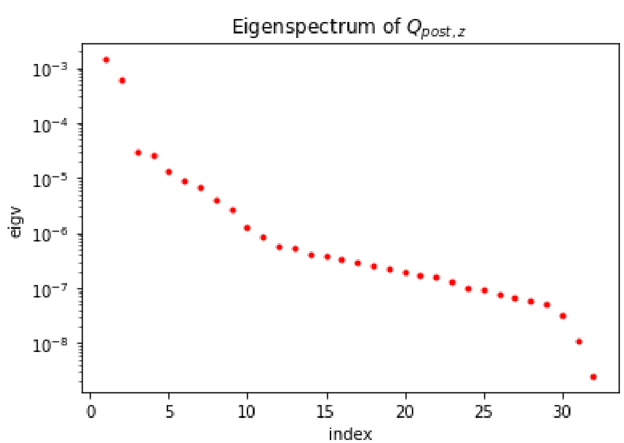


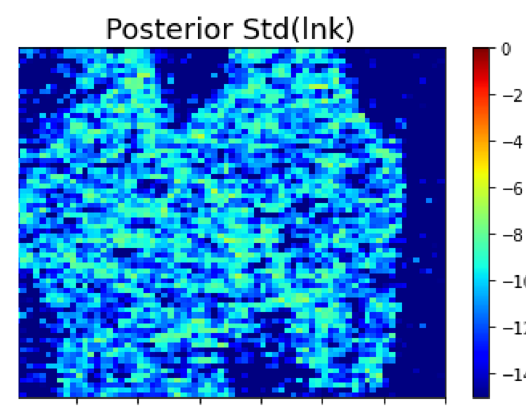
Multiphase Flow at Realistic Reservoir

- Use a realistic 2D problem to demonstrate VAE-based inversion
  - the latent space is constructed based on k and Pressure
  - the cost of the trained reduced order model ~O(1 sec)
- Inversion example :
  - 71x71 unknown **k** => **z** with 32 latent dimension
  - 9 observation wells for time series pressure data & permeability (hard data)
  - Latent space was constructed from training data
  - Initial guess: Zero mean & STD
  - Only **~3 min inversion time** on a single core laptop
  - Inversion in the latent space identifies the k structures well!









Conclusions

Variational autoencoder for real-time history matching of CO_2 operations and forecasting CO_2 and pressure plume development with fast deep learning-based forward modeling.

Latent space optimization with interpretability including optimal choice of the nonlinear dimension reduction requires further study.

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