



# SMART-CS Initiative

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

**Task 5: Field Deployment – Dynamic Storage Reservoir Modeling**

**FECM Project Review Meeting  
August 28 – September 1, 2023**



# Task 5 –Dynamic Storage Reservoir Modeling

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**Goal: Provide real-time modeling, data assimilation and forecasting to support:**

- Field management -- to maximize storage while minimizing pressure buildup
- Induced seismicity risk assessment

## GCS Simulation Today:

- Human-labor intensive
- Heuristic exploration
- Slow and non-interactive
  
- Decision-Driven
- Ensemble Based



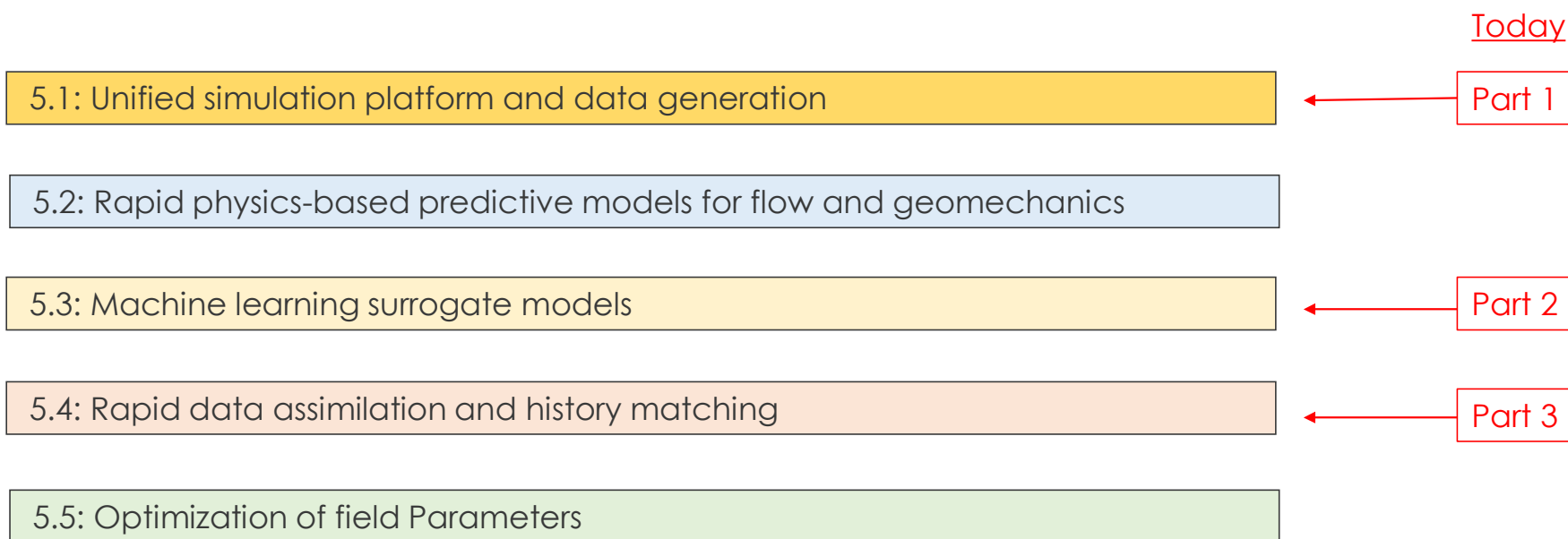
## SMART Vision:

- Human-labor efficient
- Automated workflows
- Highly interactive
  
- Decision-Driven
- Ensemble Based + *ML Acceleration*

# Task 5 –Dynamic Storage Reservoir Modeling

**Goal: Provide real-time modeling, data assimilation and forecasting to support:**

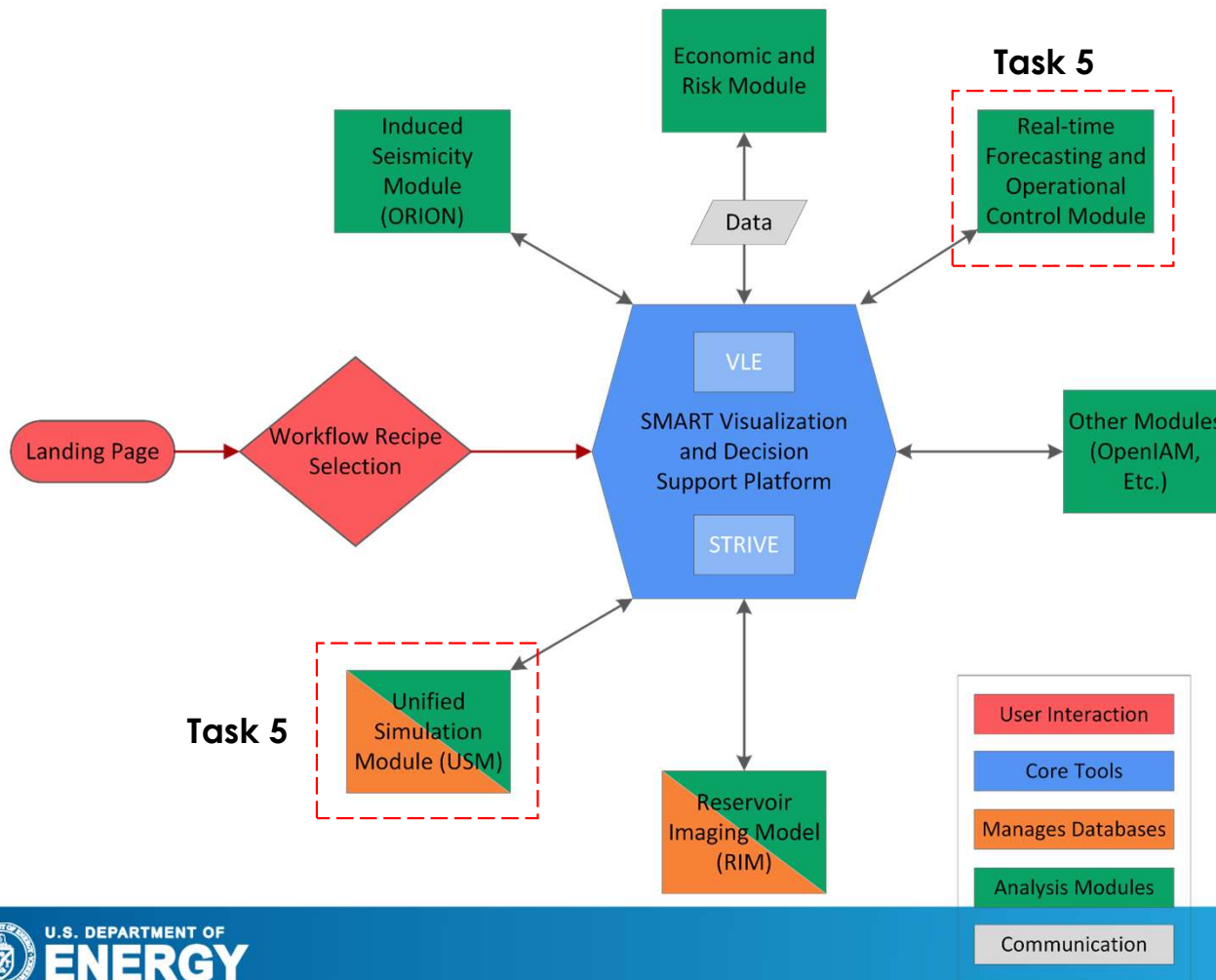
- Field management, to maximize storage while minimizing pressure buildup
- Induced seismicity risk assessment



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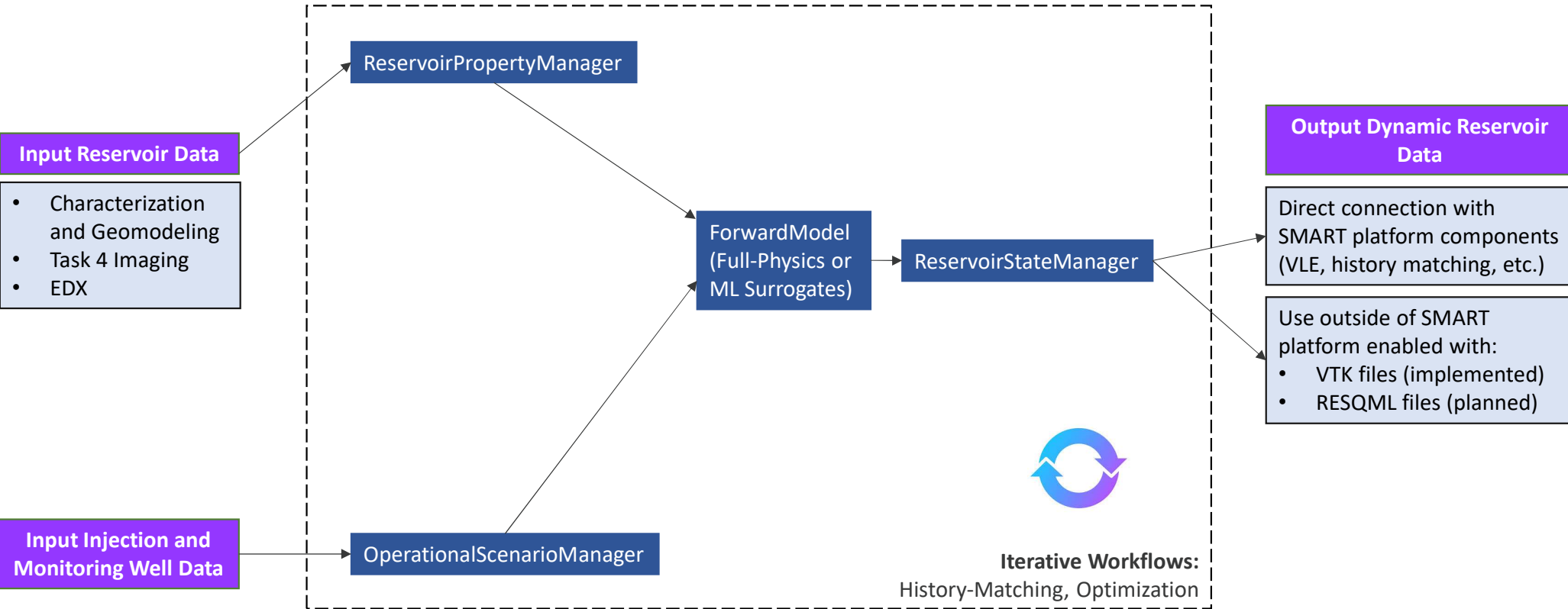
## Part 1: Unified Simulation Module

# Unified Simulation Module



**Objective:** Provide a unified way for a user to interact with reservoir simulation data and run simulation workflows

# Unified Simulation Module Data Flow



# Unified Simulation Module



Goal is a high-quality, shareable, enduring capability

## Quality control and documentation

- Code hosted on GitLab
- Installable Python package makes it easy to use
- Automated unit testing suite tests every commit pushed
- Standardized code formatting and style
- Sphinx documentation is automatically built
- Issue and milestone tracking
- *Following recommended software dev practices (Task 3)*

## Testing pipeline

Status	Pipeline	Triggerer	Stages
passed 00:00:28 1 month ago	forgot to include new DataManagerBase sourc... #930552655 feature/pickle → a8bec5e8 latest		✓
passed 00:00:28 1 month ago	applied yapf #930551570 feature/pickle → 55c1784d		✓
passed 00:06:27 1 month ago	Merge branch 'petrel-support' into 'main' #929529305 main → 68db821		✓ ✓
passed 00:03:08 1 month ago	switched tests to using a small 1D 2-cell grdec... #929526526 116 → e648725e latest merge request		✓
passed 00:00:28 1 month ago	switched tests to using a small 1D 2-cell grdec... #929526505 petrel-support → e648725e		✓

## Issue tracking

#9 - created 1 month ago by Jeffrey Burghardt - USM Deployment Enhancement	updated 1 month ago
#8 - created 1 month ago by Jeffrey Burghardt	
#7 - created 2 months ago by Christopher Sherman - USM Deployment priority: high	updated 1 month ago
#6 - created 2 months ago by Christopher Sherman - Initial USM Development priority: medium type: documentation	
#5 - created 2 months ago by Veronika Vasytkivska Enhancement type: optimization	
#3 - created 2 months ago by Kayla Kroll Enhancement	

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## Part 2: ML Surrogate Modeling



# ML Input Data

- Monthly pressure and saturation distributions at Illinois Basin Decatur Project (IBDP) site in 100 realizations of permeability and porosity fields (1.73M cells) with actual CO<sub>2</sub> injection rates

- Training (90 cases) and testing (10 cases)

- Input data

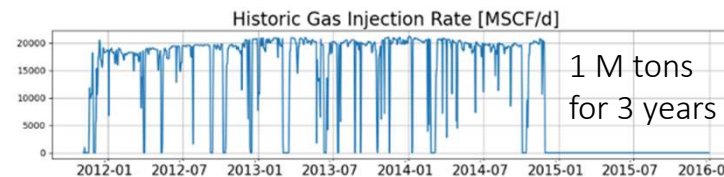
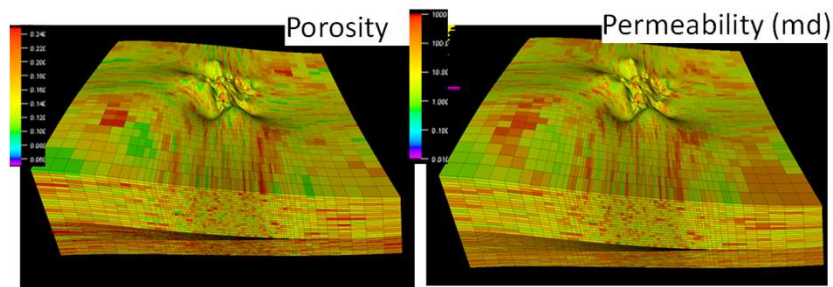
- Injection rate: (100, 50)
- Permeability: (100, 126, 125, 110, 3)
- Porosity: (100, 126, 125, 110)
- Topology: (100, 126, 125, 110)

- Output data

- Pressure: (, 50, 126, 125, 110)
- Saturation: (, 50, 40, 44, 94)

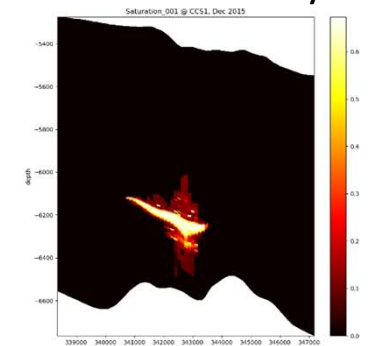
- Well data

- Injection rates: three perforation zones
- Monitoring: 6 multi-depth sensors

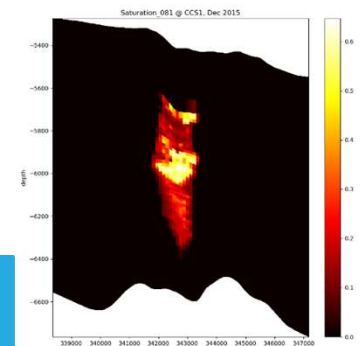


Example of porosity, permeability, and injection rates (input to ML models) & examples of CO<sub>2</sub> saturation distribution at 1 year after the end of injection (Eclipse)

80 cases with open fault horizontally



20 cases with closed fault horizontally



# ML Models

## Three primary goals:

- Computational efficiency to handle IBDP data (1.73M cells, 50 time steps, 100 realizations)
- Prediction accuracy
- Flexibility associated with input, output, portability, and potentially transfer learning

ORG	ML Method	Pressure RMSE (psi)	Saturation RMSE (-)*	Note
UT-BEG	UNet-MLP	<2	~0.016	Relatively big model (122M parameters, 23.6 hr training on 2 GPUs), handling full IBDP data
ORNL	Autoencoder-MLP (AE-MLP)	~20-25	~0.018	Latent space based approach, 2D slice model for pressure
SNL	Modified DeepONet with subsampling (DeepONet)	~2	~0.018	Subsampling for computational efficiency (~ 1hr training on 1 GPU & 2.2M parameters), handling full IBDP data
LANL	Fourier Neural Operator (FNO-1)	~5	~0.015	2D input due to data size on single GPU
LLNL	Fourier Neural Operator (FNO-2)	~4	~0.015	32 GPUs for ML training with full IBDP data (2 & 1 hrs for P & S)
UIUC	Karhunen-Loeve-Deep Neural Network (KL-DNN)	<2	~0.020	Domain needs to be coarsened in both space and time due to big IBDP data

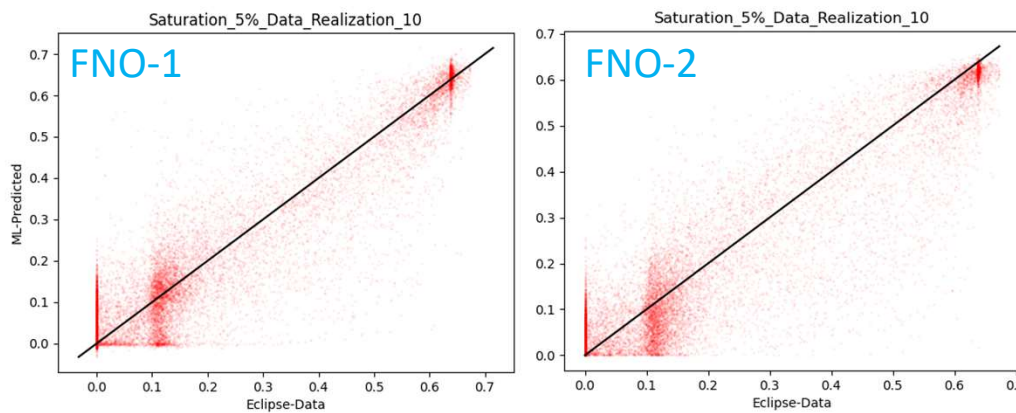
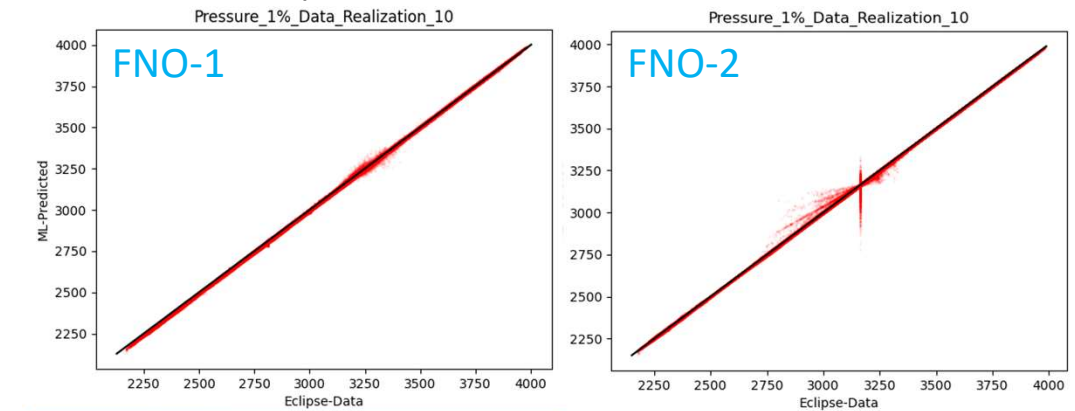
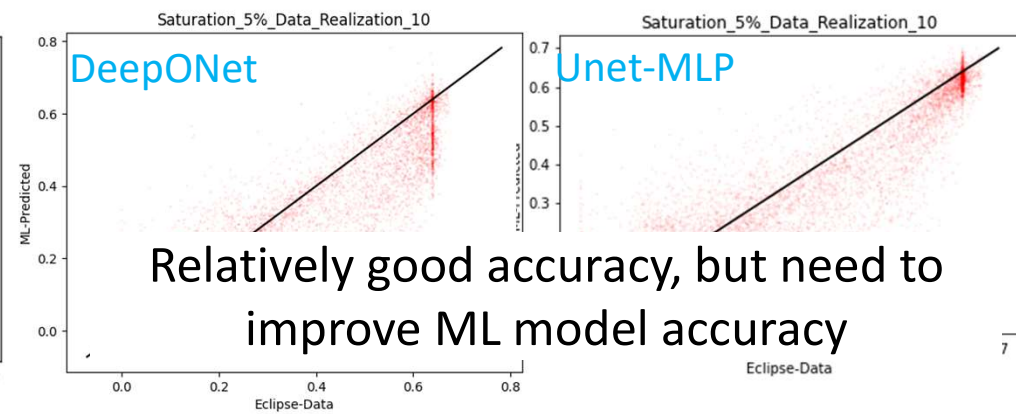
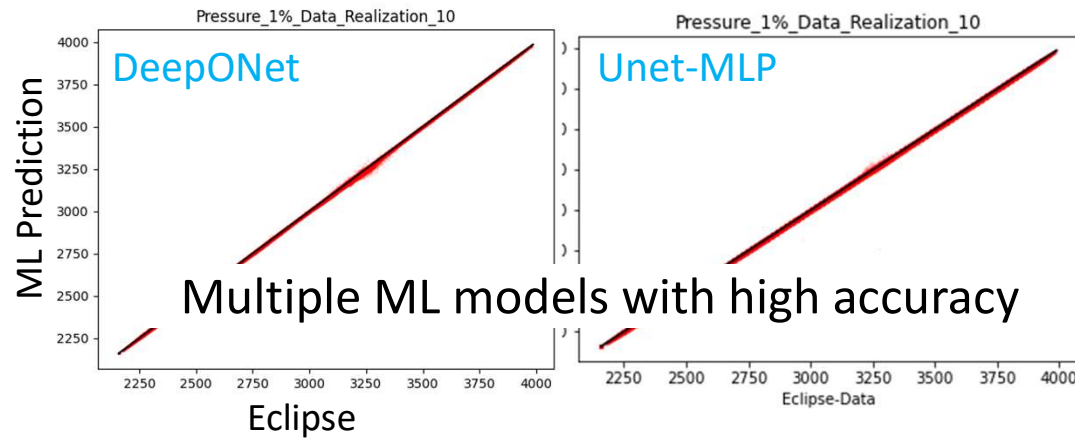
\* Saturation evaluation was performed over the central part (~10%) of pressure model domain

\* Challenge for saturation ML models: a majority of saturation data are zeros

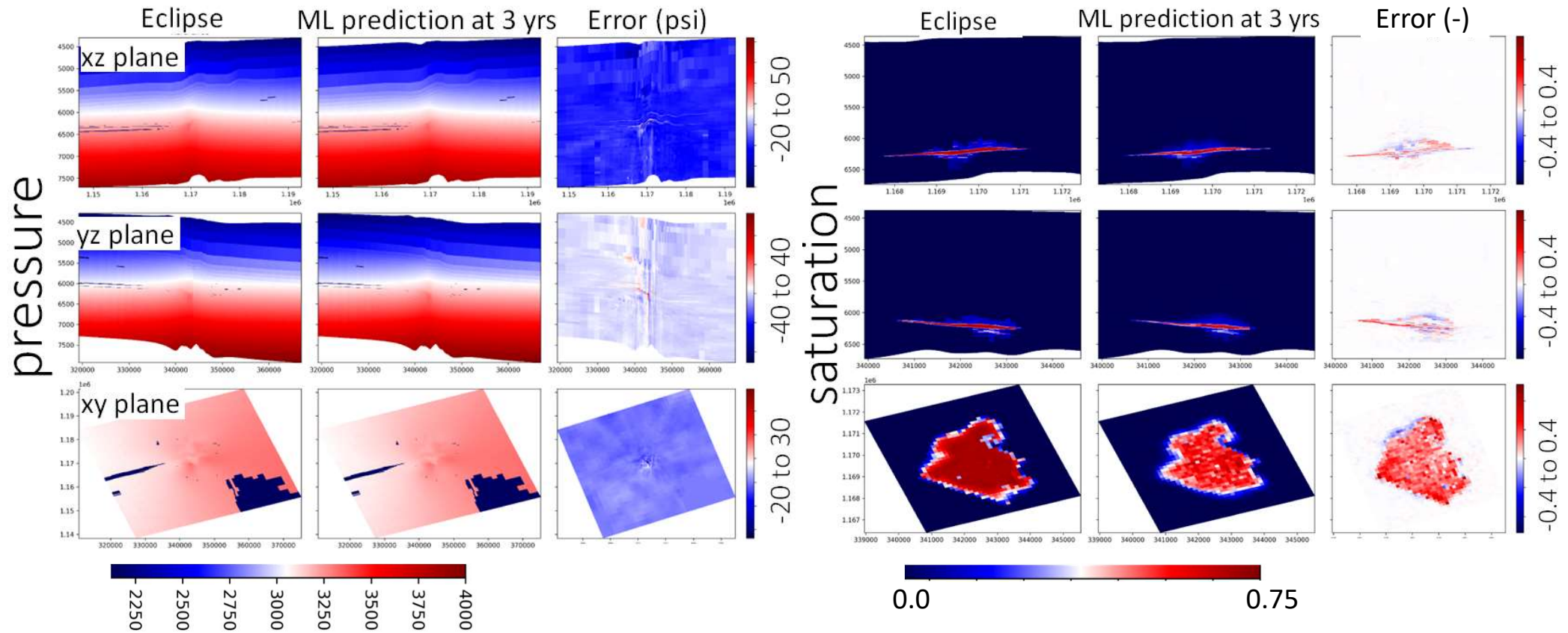
# Pressure & Saturation Prediction (realization 10)

Pressure plot with 1% of entire data

Saturation plot with 5% of entire data

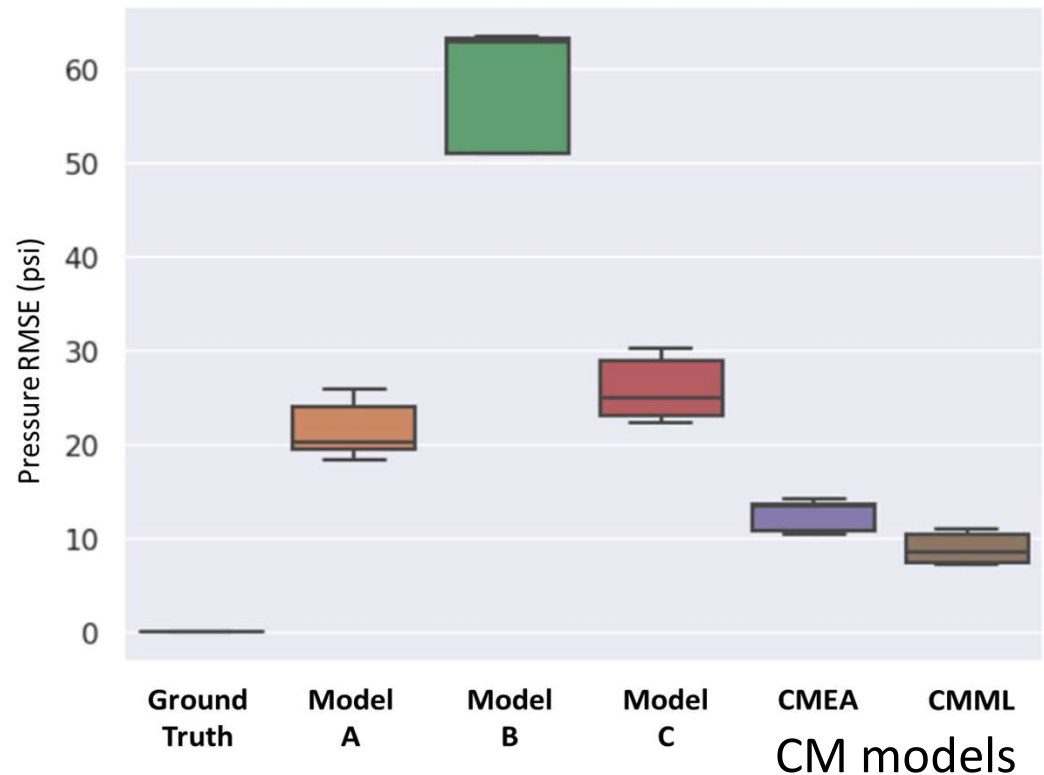


# Snapshots of Pressure and Saturation



# ML Committee Machine (CM)

- **CM**: an ensembled approach to aggregate predictions of multiple ML models into a final decision
- For this demo, a few simple neural network models A-C for pressure at IBDP site are used
- CMs (CMEA and CMML) performed better than individual ML models



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**Part 3:** Accelerated History Matching and Plume Visualization with Machine Learning

# Authors and Contact Information

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*Petroleum Engineering*

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# Objective and Challenges

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- Development and application of ML-assisted tools and workflows for **field-scale application and validation** of geologic carbon storage
  - Rapid forecasting of CO<sub>2</sub> plume evolution constrained by observed distributed temperature and pressure data while accounting for data sparsity and geologic uncertainties
- Current Challenges
  - Expensive forward simulation: multiphase, compositional and coupled flow
  - Repeated simulations for model calibration and uncertainty analysis
  - Traditional history matching is time consuming -- often takes weeks/months and is not amenable to real time decision-making



# Proposed Workflow: Outline of Steps

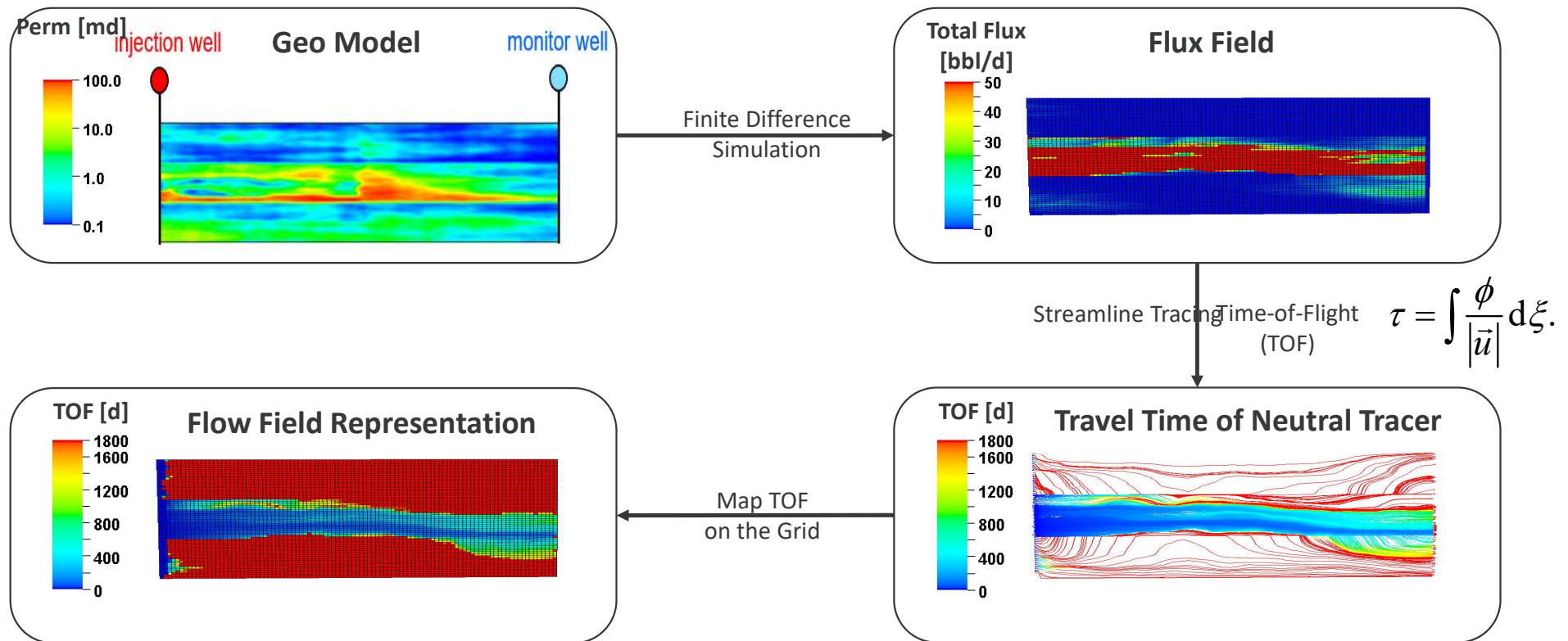
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- Dimensionality and computational time reduction for the training data
  - Single Time-of-Flight map representing CO<sub>2</sub> propagation
- Neural Network Training
  - Variational autoencoder (VAE) to compress time of flight images using latent variables
  - Regression model to estimate autoencoder latent variables based on the monitoring data
- Prediction of CO<sub>2</sub> plume images
  - Estimate Time-of-Flight map from monitoring data (pressure and temperature at the injection and monitoring wells)

# Data Dimensionality and Computational Time Reduction: Single Time-of-Flight Map Representing CO<sub>2</sub> Propagation

Time of Flight (TOF): Travel time of a neutral tracer along streamlines representing the flow field and fluid transport



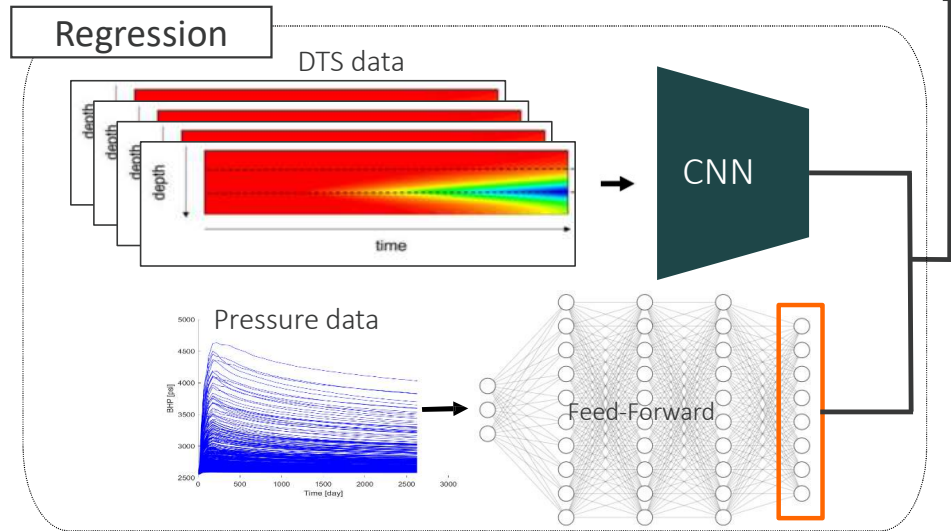
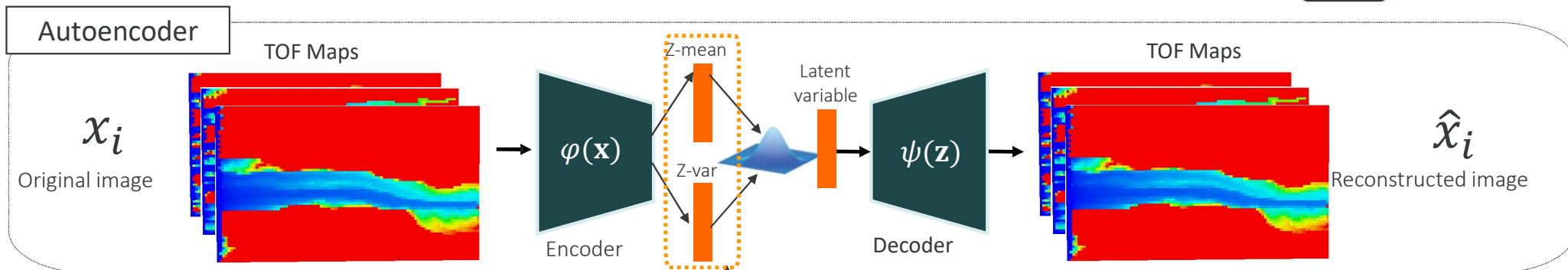
# Proposed Workflow: Outline of Steps

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# Neural Network Training



Loss function:

$$L = L_{VAE} + \underbrace{\frac{1}{Nz} \sum_{j=1}^{Nz} |\sigma_j^2 - \hat{\sigma}_j^2|^2}_{\text{Image reconstruction loss}} + \underbrace{\frac{1}{Nz} \sum_{j=1}^{Nz} |\mu_j - \hat{\mu}_j|^2}_{\text{Bottleneck loss}}$$

$$L_{VAE} = \frac{1}{N} \sum_{i=1}^N |x_i - \hat{x}_i|^2 - \frac{1}{Nz} \sum_{j=1}^{Nz} \frac{1}{2} [1 + \log(\sigma_j^2) - \sigma_j^2 - \mu_j^2]$$

# Proposed Workflow: Outline of Steps

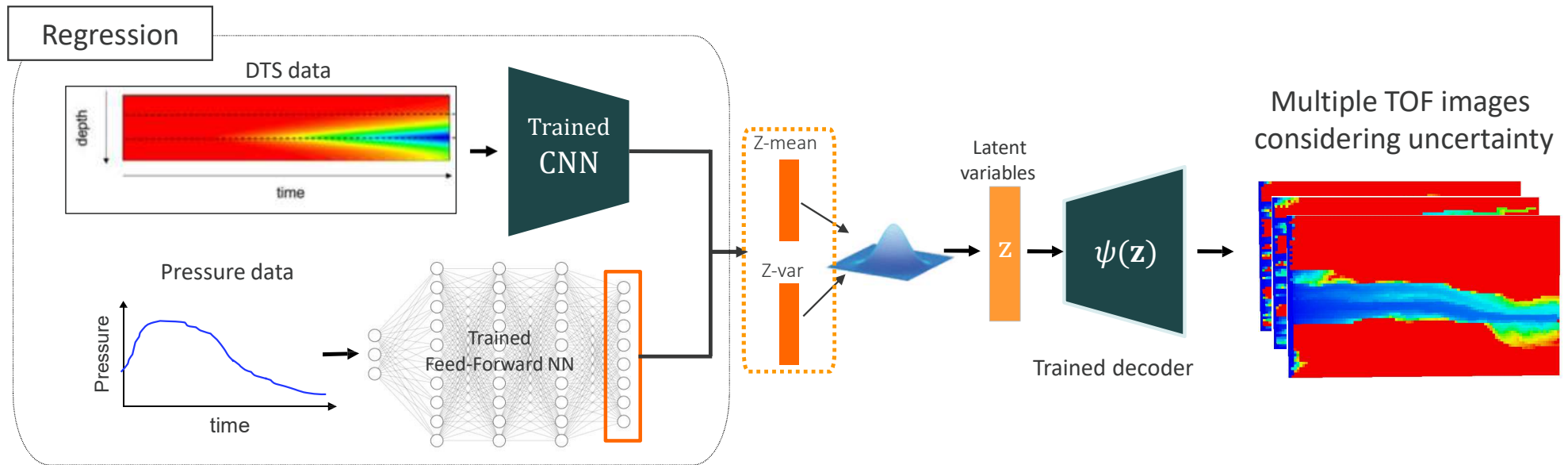
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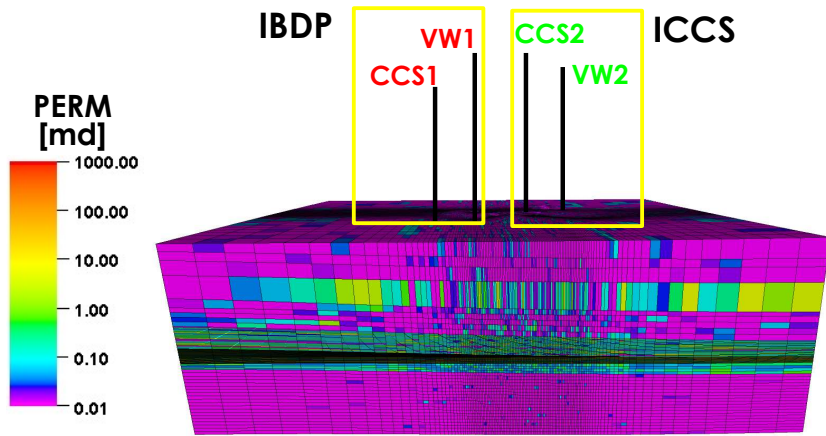
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# Prediction of CO2 Onset Time Map

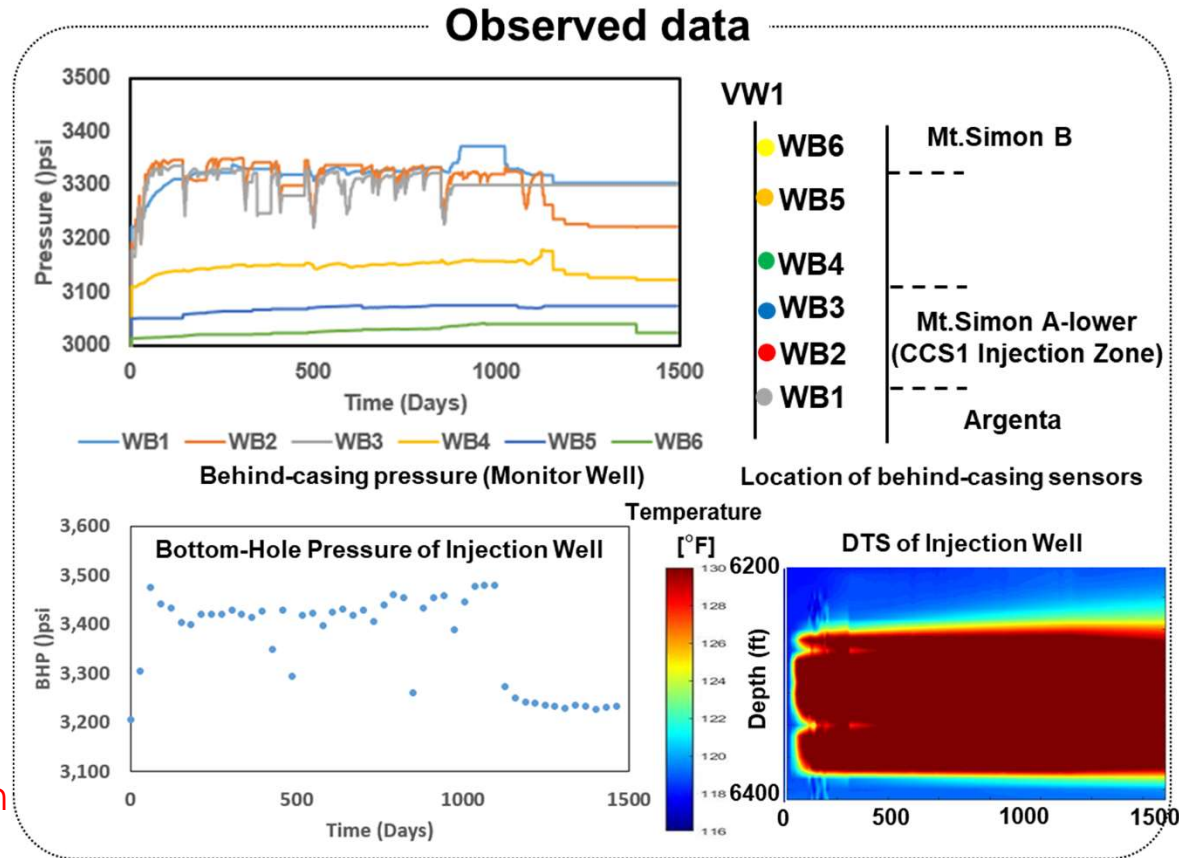
Predict the Time-of-Flight map based on the field monitoring measurements



# IBDP Model Description and Data Availability

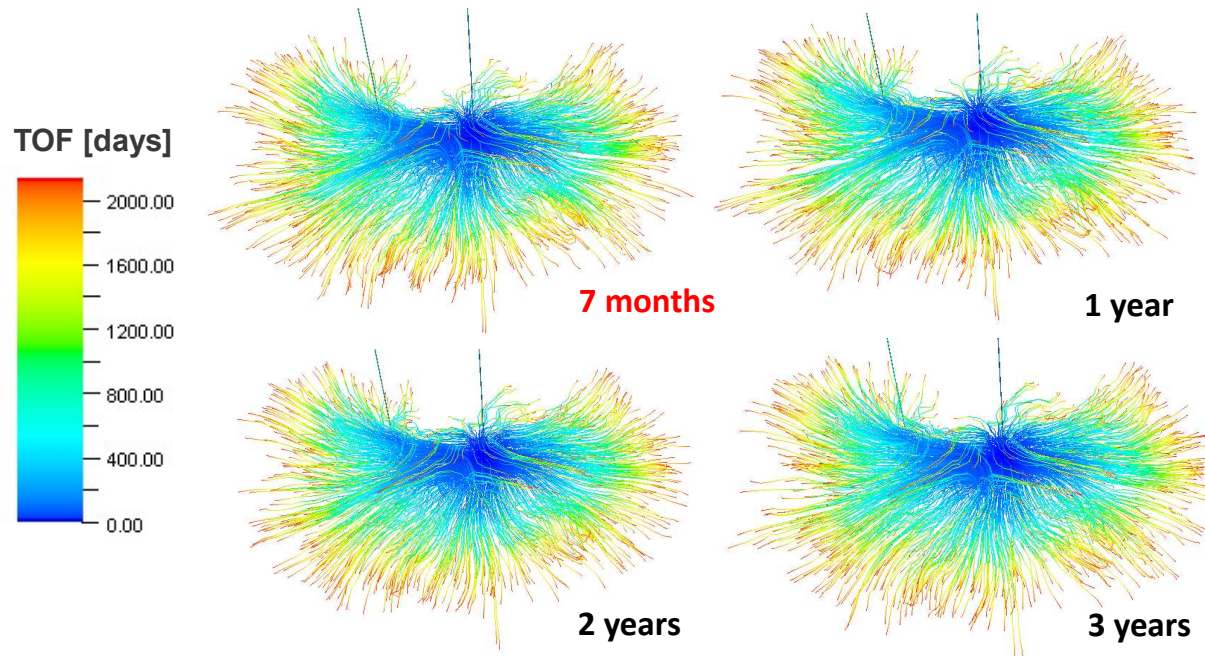


- Grid: 126 \* 125 \* 110 (1.73 Million Cells)
- ECLIPSE Compositional Model (E300)
- Thermal Option
- CO2STORE Module
- Simulation Period: 2011-2015
- Run Time: 12 hours with 32 Cores Parallel run



# Time of Flight Calculations :Validation of Flux Field Stabilization

- **Challenge:** Run time for a full simulation is too long (12 hrs) and unfeasible for training data generation purposes (hundreds of simulations)
- **Solution:** Calculate time of flight when the flow field is stabilized



Selected simulation period:  
7 months (flux field has been stabilized)

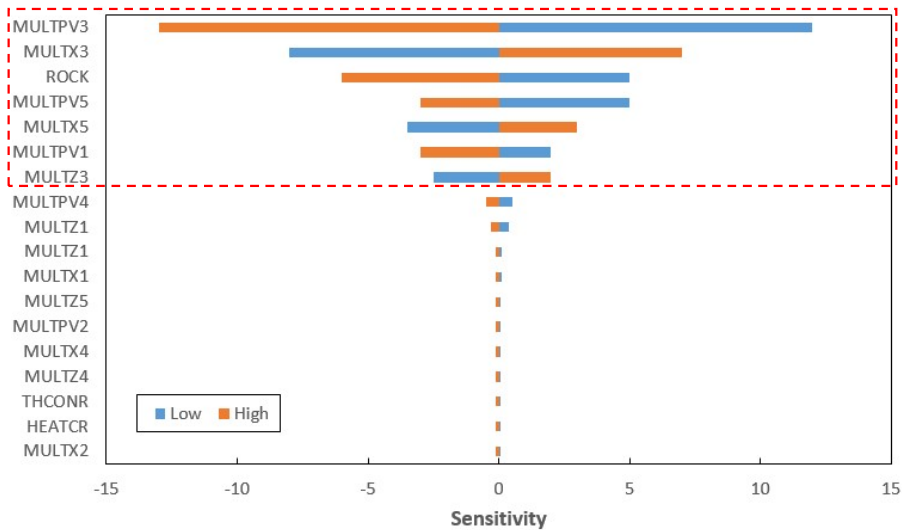
Run Time: 12 hrs **1 hr**



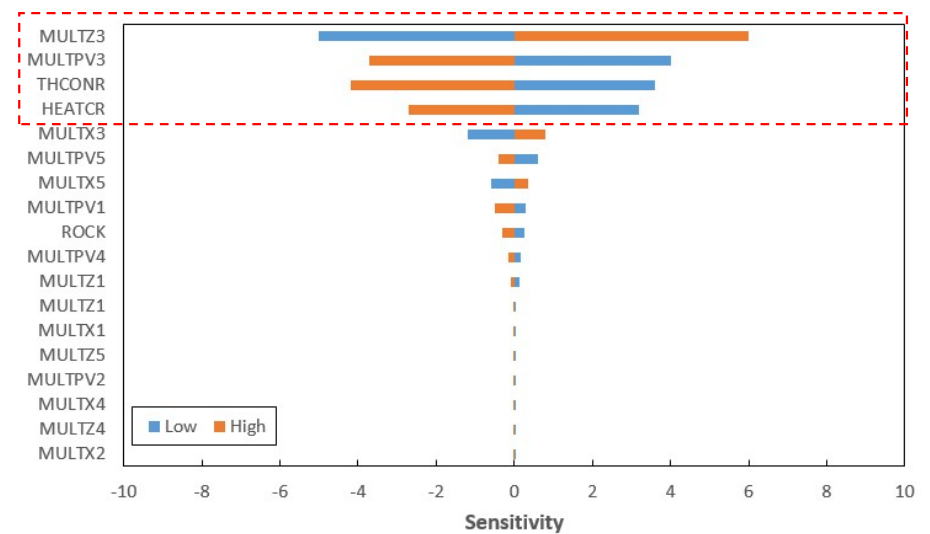


# Sensitivity Analysis for Training Data Generation

Pressure Responses (injection well + monitoring well)



DTS (injection well)

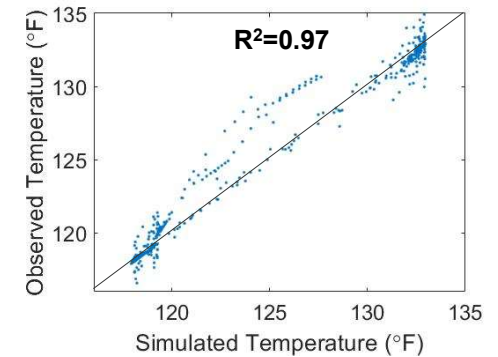
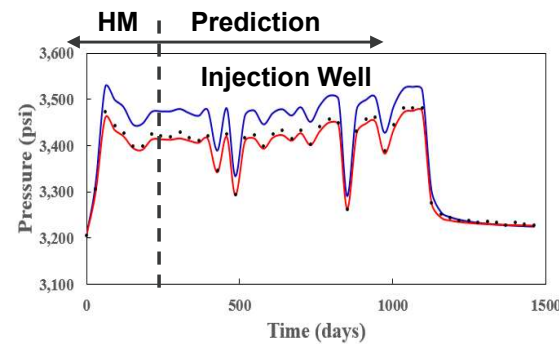
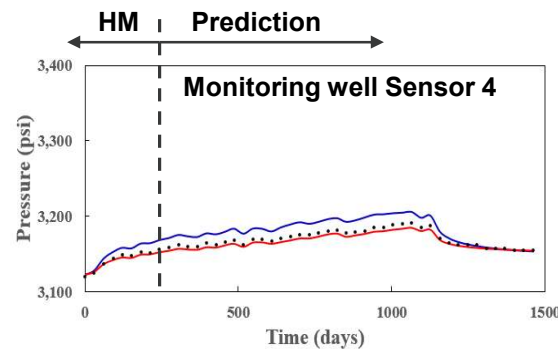
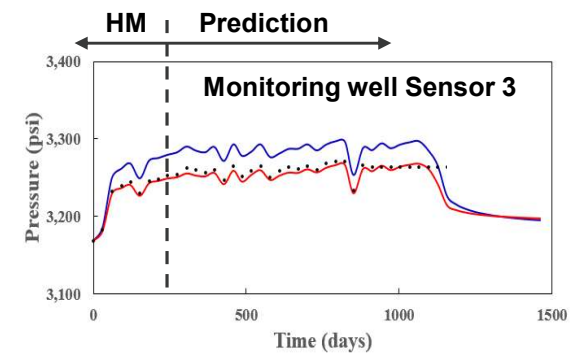
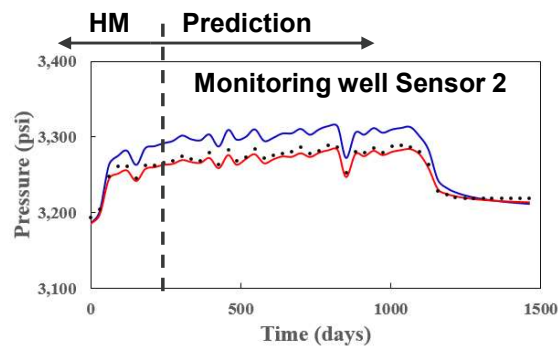
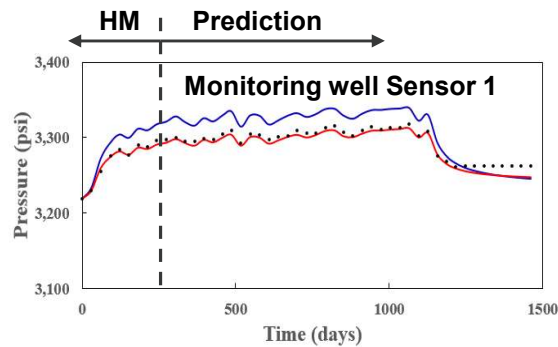


Selected Parameters: MLTPV1/3/5, MULTX3/5, MULTZ3, Rock Compressibility, Rock/Fluid Thermal Conductivity, Rock Heat Capacity

# Pressure and Temperature Matching Comparison

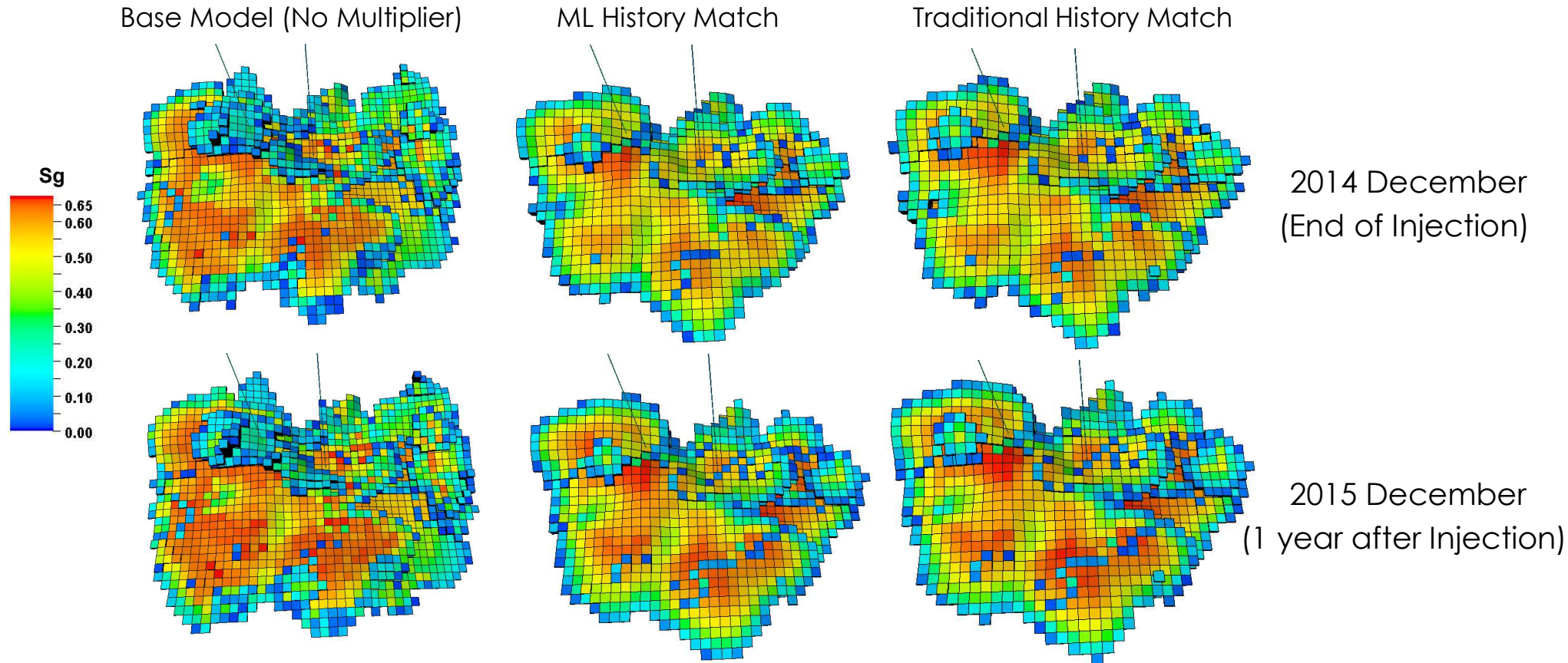


Significant speed-up: 5 hours for training, seconds for model calibration/predictions as opposed to traditional history matching that can take days or weeks.



# 3D CO<sub>2</sub> Saturation Contour Comparison

Contour generated from CO<sub>2</sub> saturation map with a threshold of 1%



# Summary

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- Proposed ML assisted workflow and application to the IBDP site shows promising results with orders of magnitude speed up
- Incorporated thermal effects to integrate DTS data and utilized Time-of-Flight to reduce computational time substantially
- Future Opportunities
  - Leverage Oil Industry Experience: Fast Marching Method for Coupled Flow, Streamlines for visualization, Storage/CO2 Sweep Optimization via Rate control

**Questions?**

# Acknowledgements

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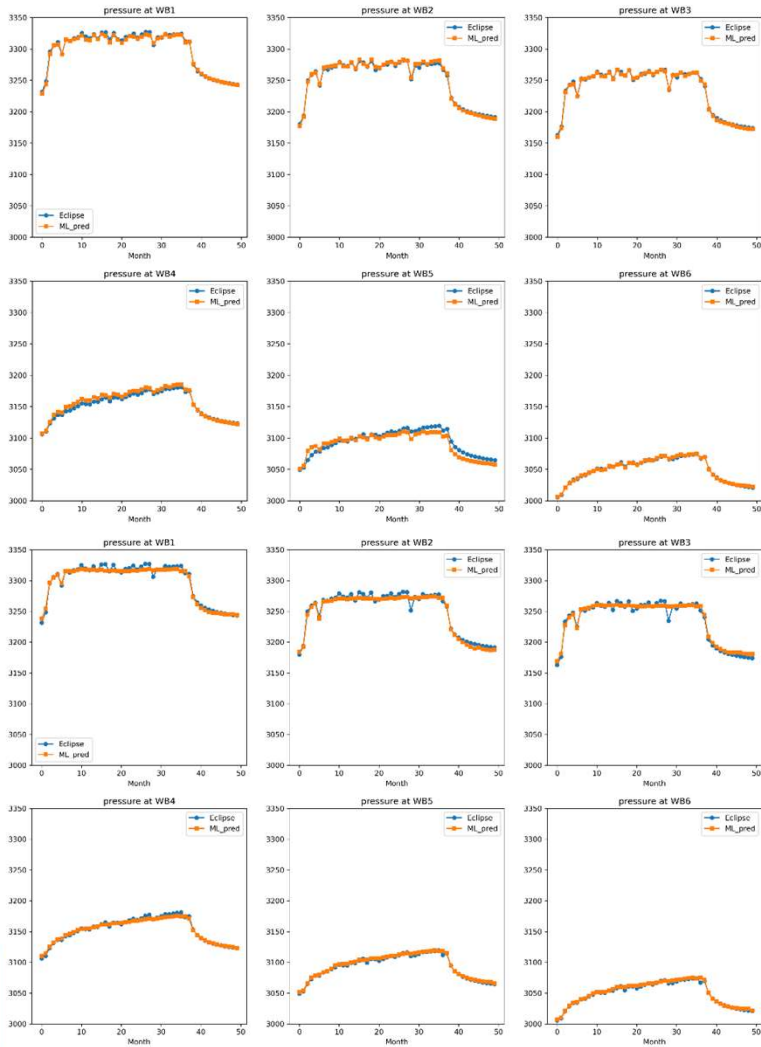
## Funding:

- This work was funded by the SMART Initiative through the DOE Office of Fossil Energy and Carbon Management and the Bipartisan Infrastructure Law.

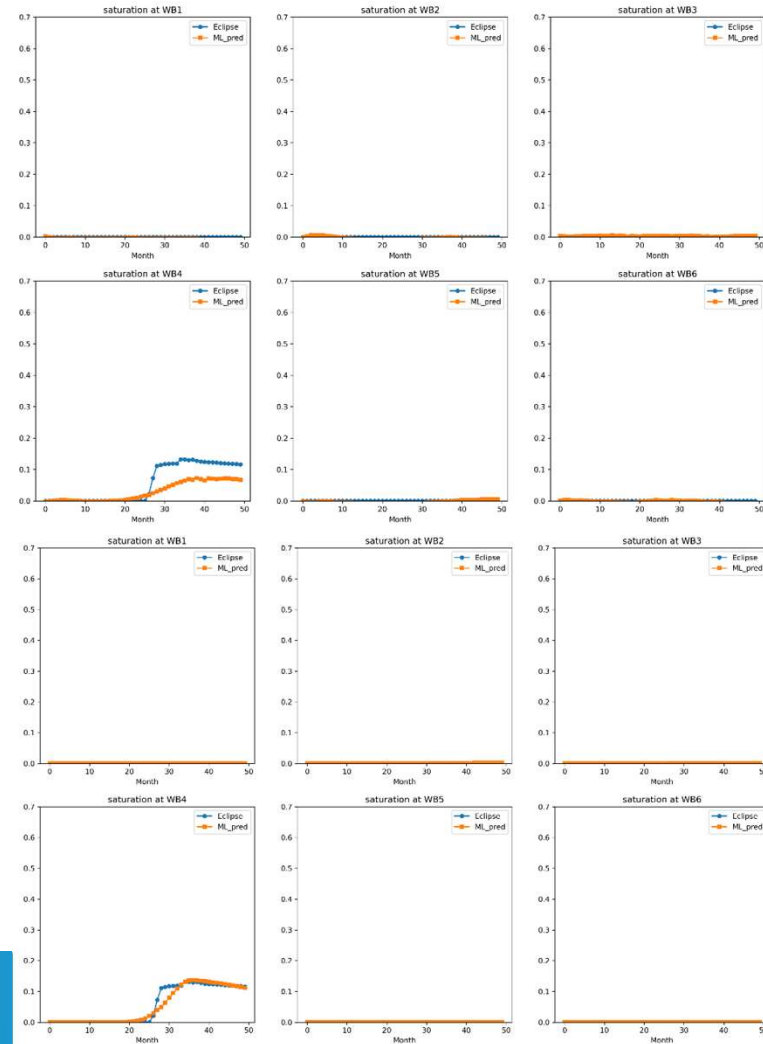
## Auspices:

- Portions of this work were performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07-NA27344.
- Portions of this work were performed under the auspices of the U.S. Department of Energy by Pacific Northwest National Laboratory under contract DE-AC05-76RL01830.
- Portions of this work were performed under the auspices of the U.S. Department of Energy by Sandia National Laboratories under contract DE-NA0003525.
- Portions of this research were executed through the NETL Research and Innovation Center's Carbon Storage Program

# Pressure (psi) & Saturation (-) at six different depths in monitoring well (realization 10)

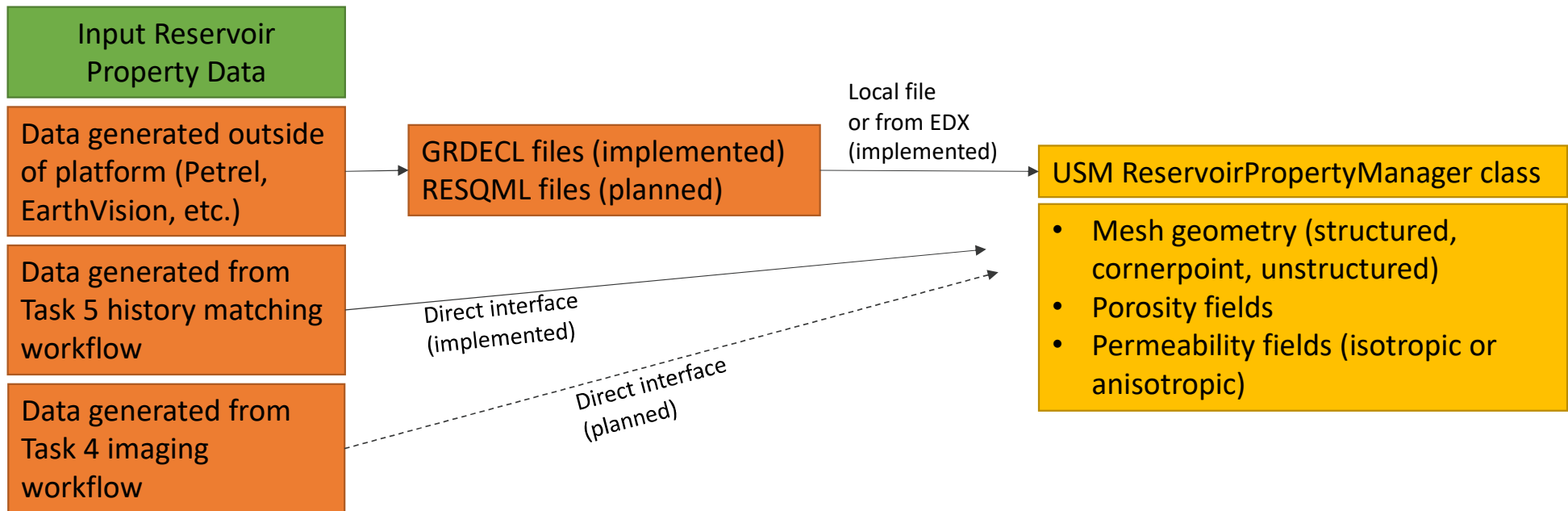


SNL



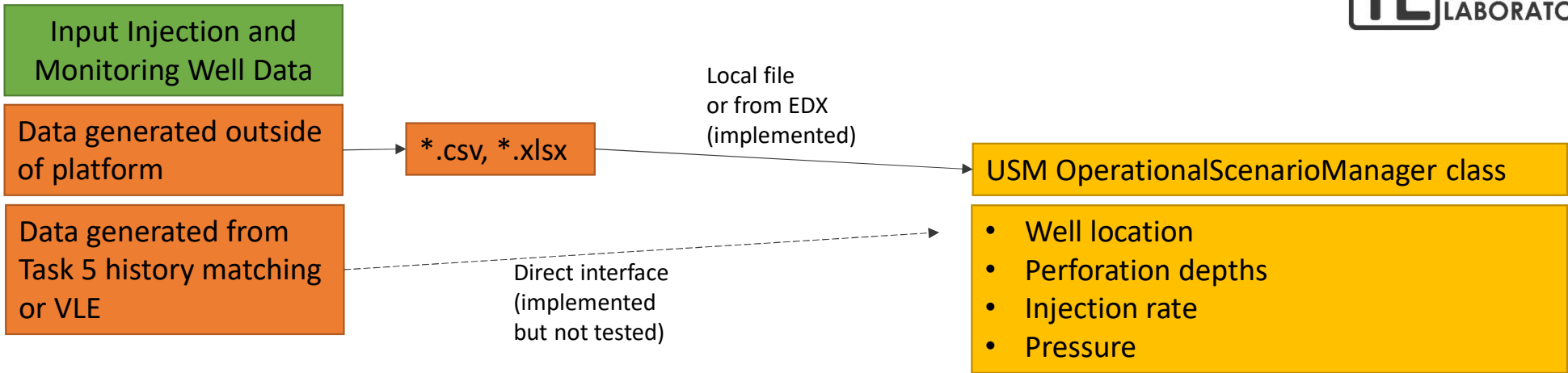
UT-BEG

# Unified Simulation Module

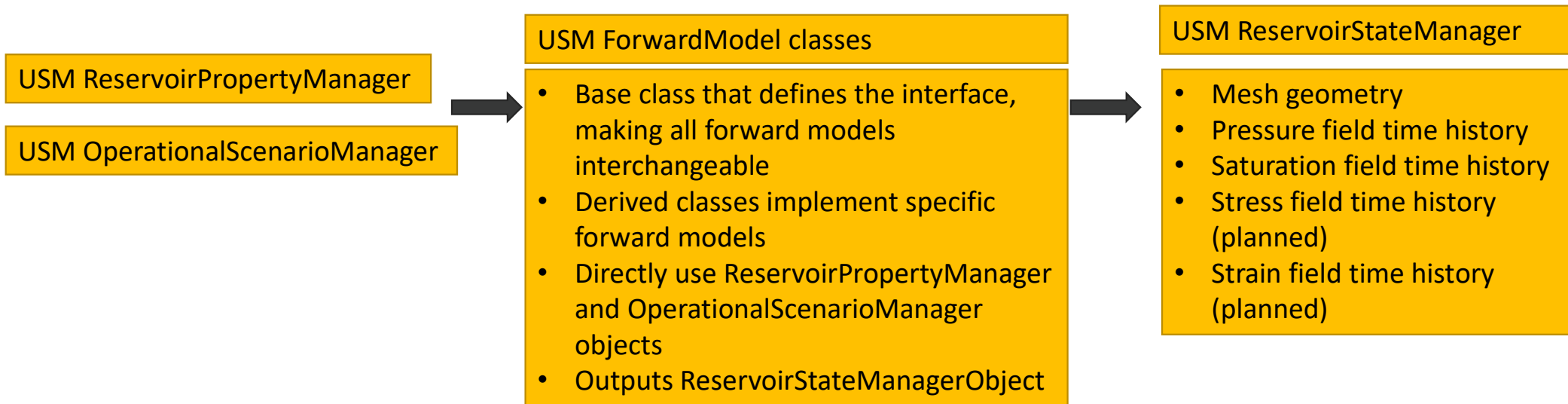




# Unified Simulation Module



# Unified Simulation Module



# Unified Simulation Module

