



Overview of SMART Initiative

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

Hema Siriwardane
DOE-NETL

Contributors: Hari Vishvanathan (LANL), Seyyed Housseni (UT BEG), David Alambaugh (LBNL), Christopher Sherman (LLNL), Alex Tartakovsky (UIUC), Jared Schuetter (Bettelle); Hongkyu Yoon (SNL), Joshua White (LLNL), Maruti Mudunuru (PNNL), David Morgan (NETL), Srikanta Mishra (TAMU).

**2024 FECM-NETL Carbon Management
Research Project Review Meeting**

Pittsburgh, PA

06 August 2024



Disclaimer



Science-informed Machine Learning to Accelerate Real Time (SMART)

Decisions in Subsurface Applications

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Our Motivation



Growing momentum for rapid commercial scale deployment of CCS

Develop relevant experience / understanding among stakeholders

Facilitate decision-making process during project planning, permitting, operations



Traditional analysis involves physics-based models

Data interpretation for characterization

Pre-injection planning and system design

Observational data integration for operational decision making



Recent focus on Machine Learning based computationally expedient alternatives



SMART- Initiative

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

VISION: Transform our ability to make better, informed decisions related to the subsurface through real-time visualization, forecasting, and virtual learning.

MISSION:

SMART Functionalities



Real-Time Visualization
"CT" for the Subsurface

Improve the ability to consolidate technical knowledge, site-specific characterization information, and real-time data in a digestible way.



ML-based Rapid Prediction
Virtual Learning

Enable the optimization of carbon storage reservoirs by creating a capability for "real-time" forecasting of carbon storage reservoir behaviour.



ML-based Real-Time Forecasting
"Advanced Control Room"

Enable improve the ability to understand and communicate expected subsurface behaviour during carbon storage operations to non-experts.

SMART Initiative

Science-informed **M**achine Learning to **A**ccelerate **R**eal **T**ime
(SMART) Decisions in Subsurface Applications

Task 2: Virtual learning to support permitting

Task 3: Advanced learning and computational methods

Task 4: Site-specific data management & imaging

Task 5: Site-specific storage reservoir modeling

Task 6: Site-specific decision support & visualization

Task 7: Site-specific data curation

Task 8: Geomechanical Modeling and Exploration
of Longer Term and Emerging Priorities

Technical Team

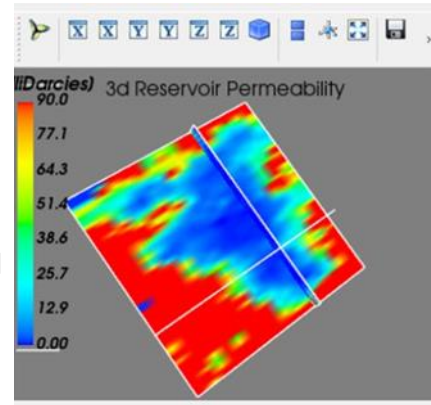


Current Progress

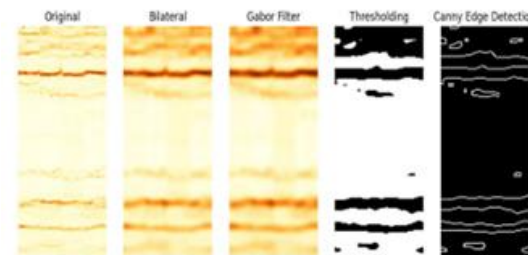
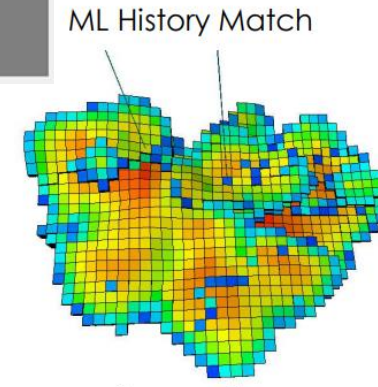


SMART Initiative

- SMART has developed a conceptual design of the SMART Visualization and Decision Support Platform.
- Several modules have been developed (Model Explorer – VLE, USM (Unified Simulation Module), STRIVE (SMART Tools Rapid Visualization Environment Module), ORION (Induced Seismicity Module), RTFO (Real-time Forecasting and Operational Control Module). Developments are continuing.
- Developed a Machine Learning (Transfer Learning) tool to forecast CO₂ plume saturation and pressure under operating conditions different from those used to train an earlier ML model.
- Developed a Machine Learning (ML) based algorithm for fault/fracture identification from FMI logs and passive seismic signatures to further refine the geomodel.
- Developed an ML-based data-assimilation/history matching frameworks for calibrating a site-specific dynamic model to pressure, saturation, temperature data.
- Developed Model Explorer tool to rapidly explore various modeled scenarios and impact of heterogeneity and/or uncertainty using ML-based fast predictive models.
- SMART-NRAP: Developed the Operational Forecasting of Induced Seismicity toolkit “ORION” (ORION), an open-source, observation-based ensemble forecasting toolkit, which is geared towards helping operators understand potential seismic hazards at a site.
- Developed a tool based on integrated computer vision and deep learning workflows for automating image log analysis, helping to rapidly and precisely detect fractures and baffles in subsurface formations.

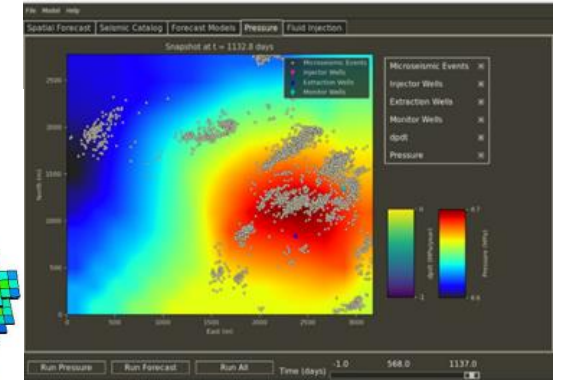


Virtual Learning Environment Module (VLE)

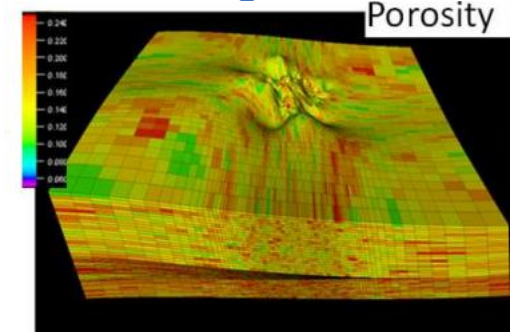


FMI-based Fracture, Bedding, and Baffles Identification using ML (FBBIML)

ORION (NRAP/SMART)

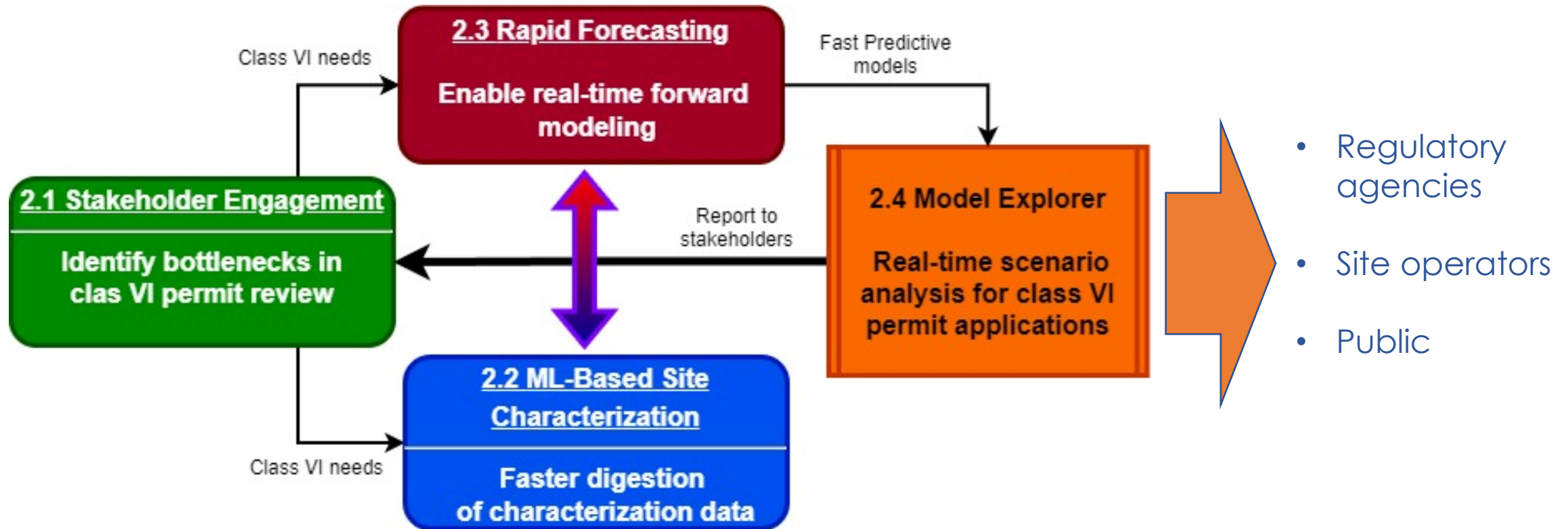


Data Assimilation and History Matching with ML



IBDP SNL Model

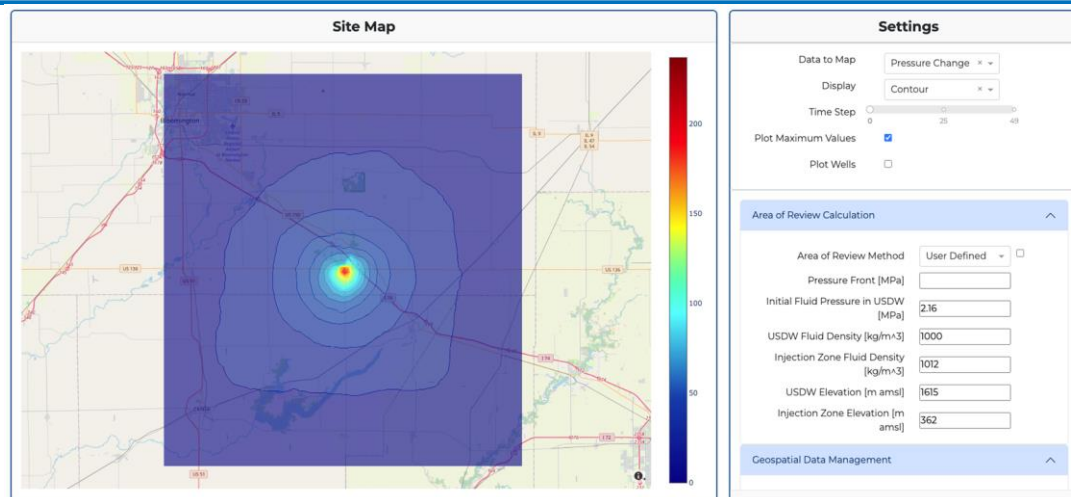
TASK 2: Wiring Diagram –Virtual Learning for Permitting



TASK 2: Example tools

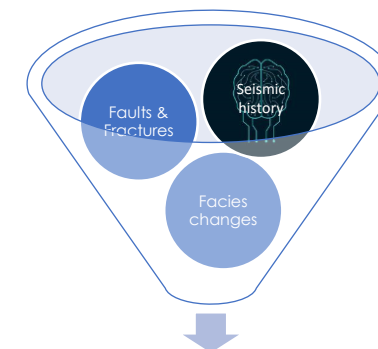
Tool: Model Explorer

Highlight # 1: AoR & Corrective Action - Dynamic Simulation



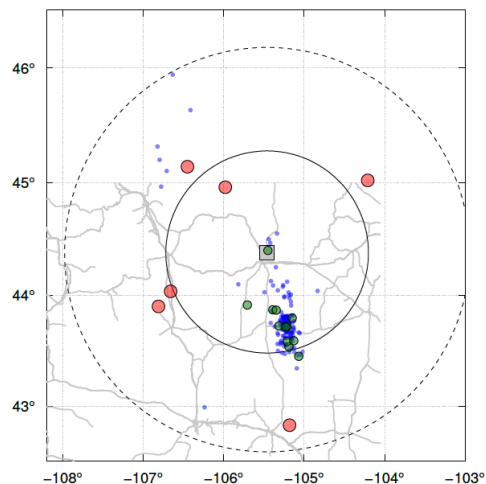
Tool: SmartSeis

Highlight # 2: Site Characterization – Seismicity Detection →



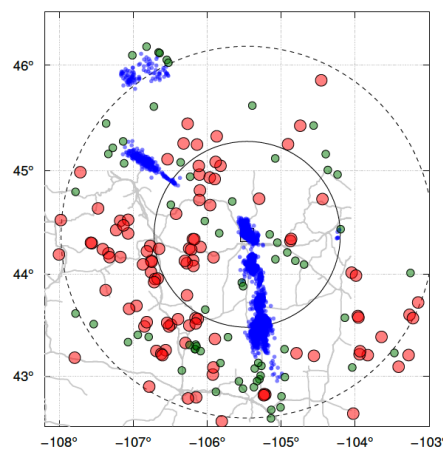
Site Characterization

Conventional detection



- Explosion
- Earthquake
- Unknown source type
- CCS Site

ML detection



Conventional methods

- Using catalogs /traffic light
- Biased and hindered by noise
- Slow

ML based method

- Uses trained models (detects ~40 times more events)
- Remove bias and noise
- Fast

Task 3, Advanced Learning and Computational Approaches

Activities

- **1: Software Quality Assurance (QA)**

- Ensure that any software in Phase 2 meets a set of agreed upon quality and reliability standards, allowing those tools to satisfy any requirements dictated by the application in which they are being used

- **2: Cross-activity Integration**

- Identify overlaps in techniques and methodologies developed during Phase 1 and adapting them for ease of applicability by 2A and 2C teams

- **3: Advanced Machine Learning Methods**

- Focus on AI/ML methods that can make SMART transformational ML models and overcome challenges identified in Phase I

- **4: Advanced Computational Approaches**

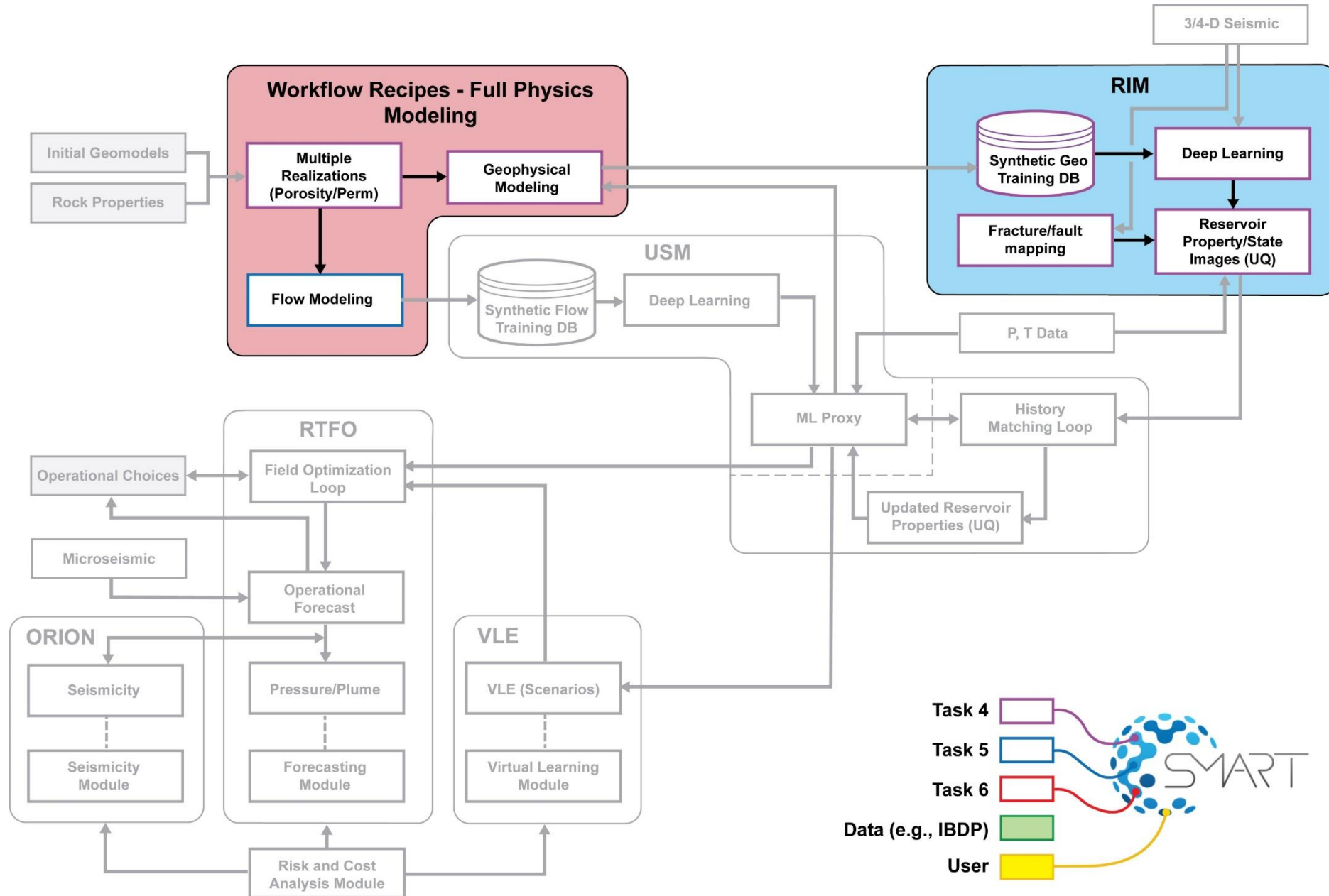
- Focus on advanced methods to enhance performance (accuracy, efficiency, privacy) that could not be achieved by a single ML method

Task 3, Advanced Learning and Computational Approaches

Accomplishments

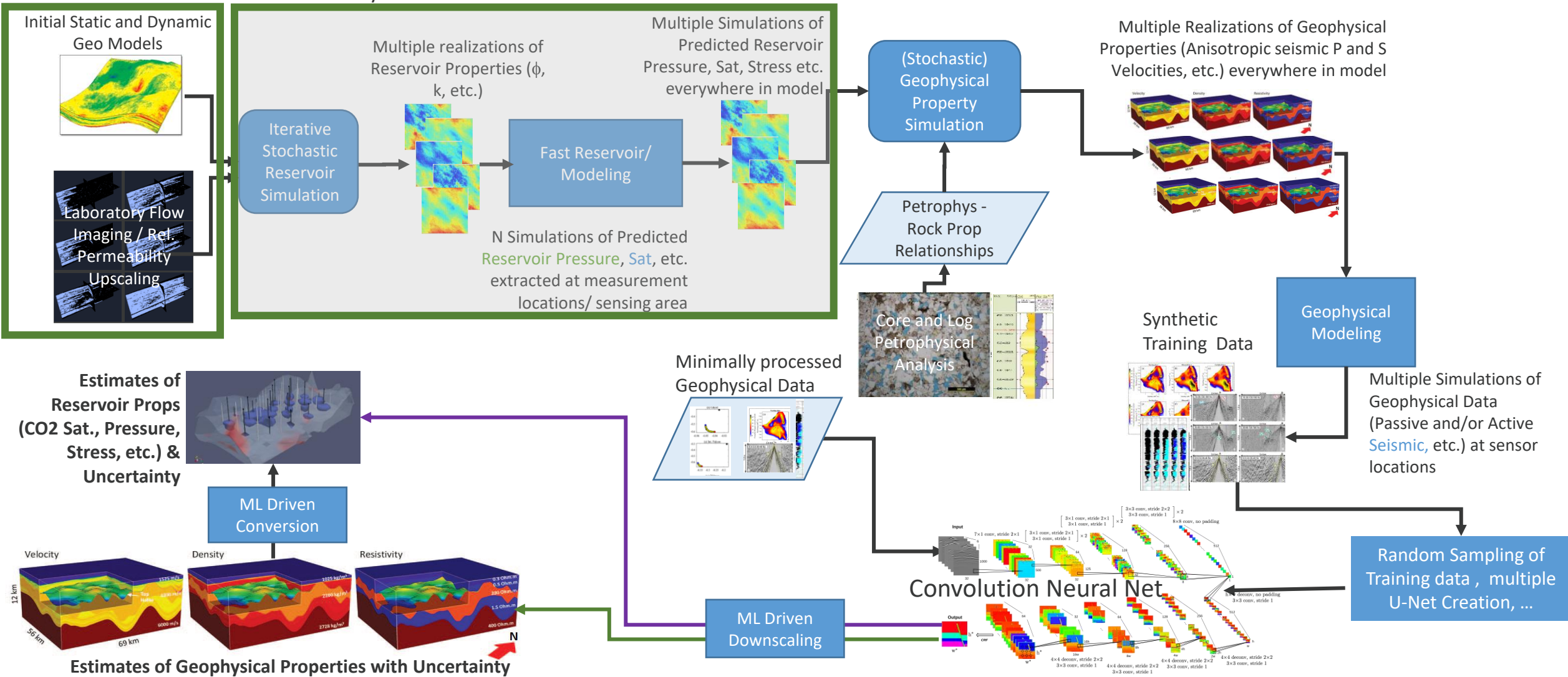
- **Advanced ML Methods & Advanced Computational Approaches**
 - Topic Area: Fast and Flexible Solutions for Fluid Flow Prediction
 - Built flexible models that leverage advanced approaches (e.g., Neural Operators) to handle the dynamic evolution of pressure, saturation, and stress and can serve as the basis to expand to solve other field prediction problems
 - DeepONet
 - Fourier Neural Operator
 - Graph Neural Operator
 - PICKLE
 - HGGNN
 - Wafer Scale Engine Field Equation Application Programming Interface
 - These models also allow for the incorporation of physics and scientific knowledge to increase the user confidence and understanding of the model reasoning processes
 - Models tested on the clastic shelf dataset, with some models also being tested on IBDP

TASK 4: Wiring Diagram –Data Organization and Imaging



Task 4 - Reservoir Property Imaging Workflow for Any Type of Geophysical Data

Provided by TASK 5 via Universal Data and Mod Platform

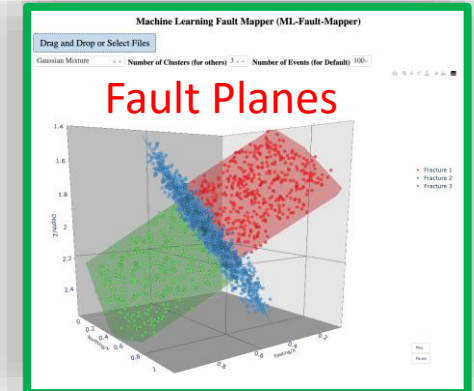
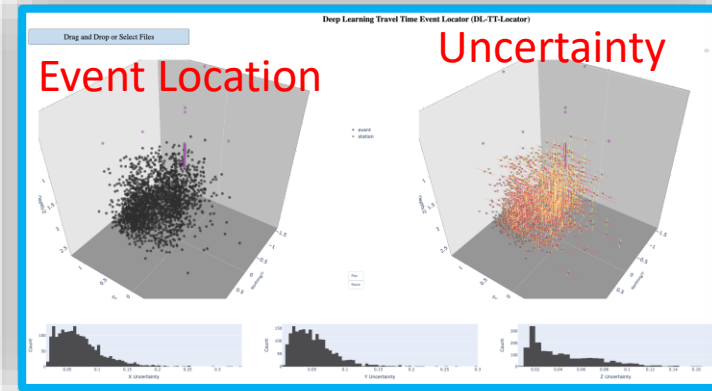
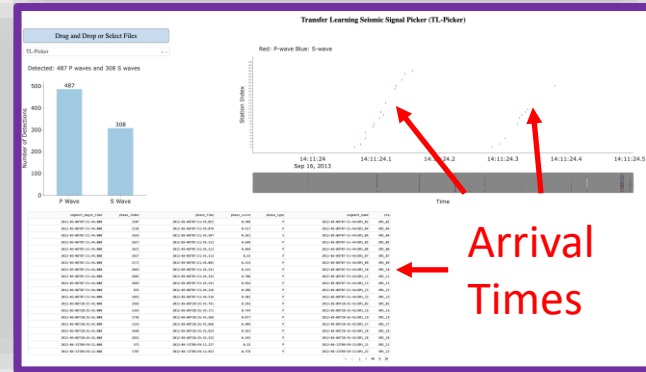


Task 4 – Fault/Fracture Imaging

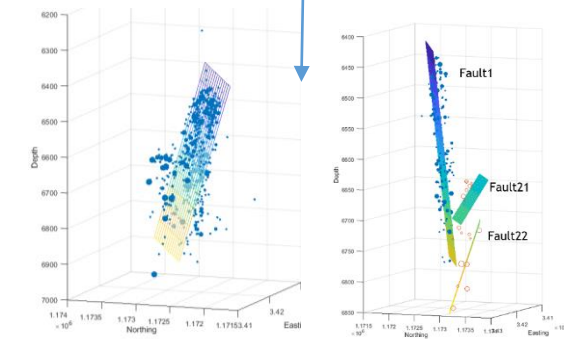
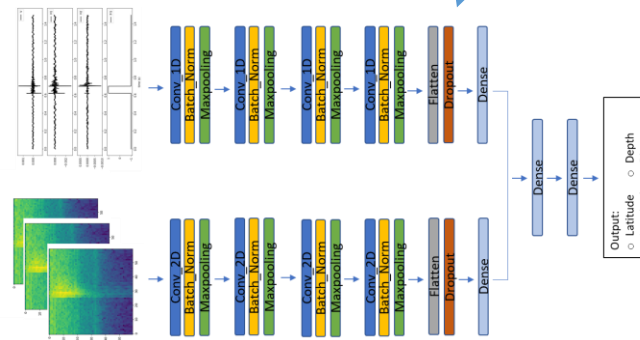
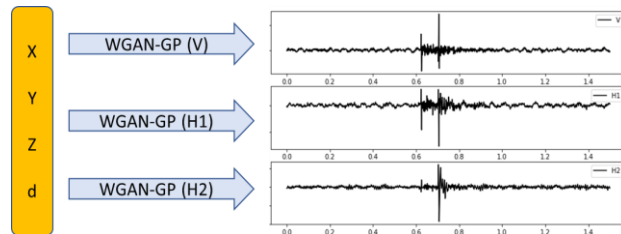
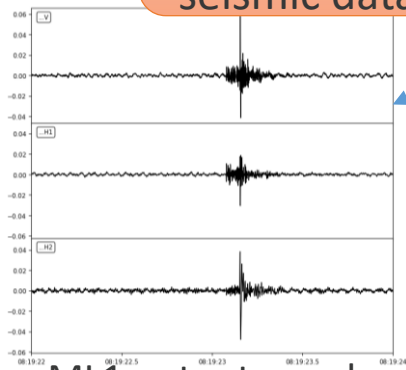
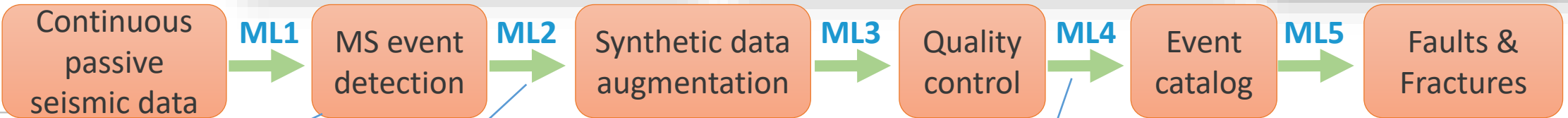
ORNL Workflow



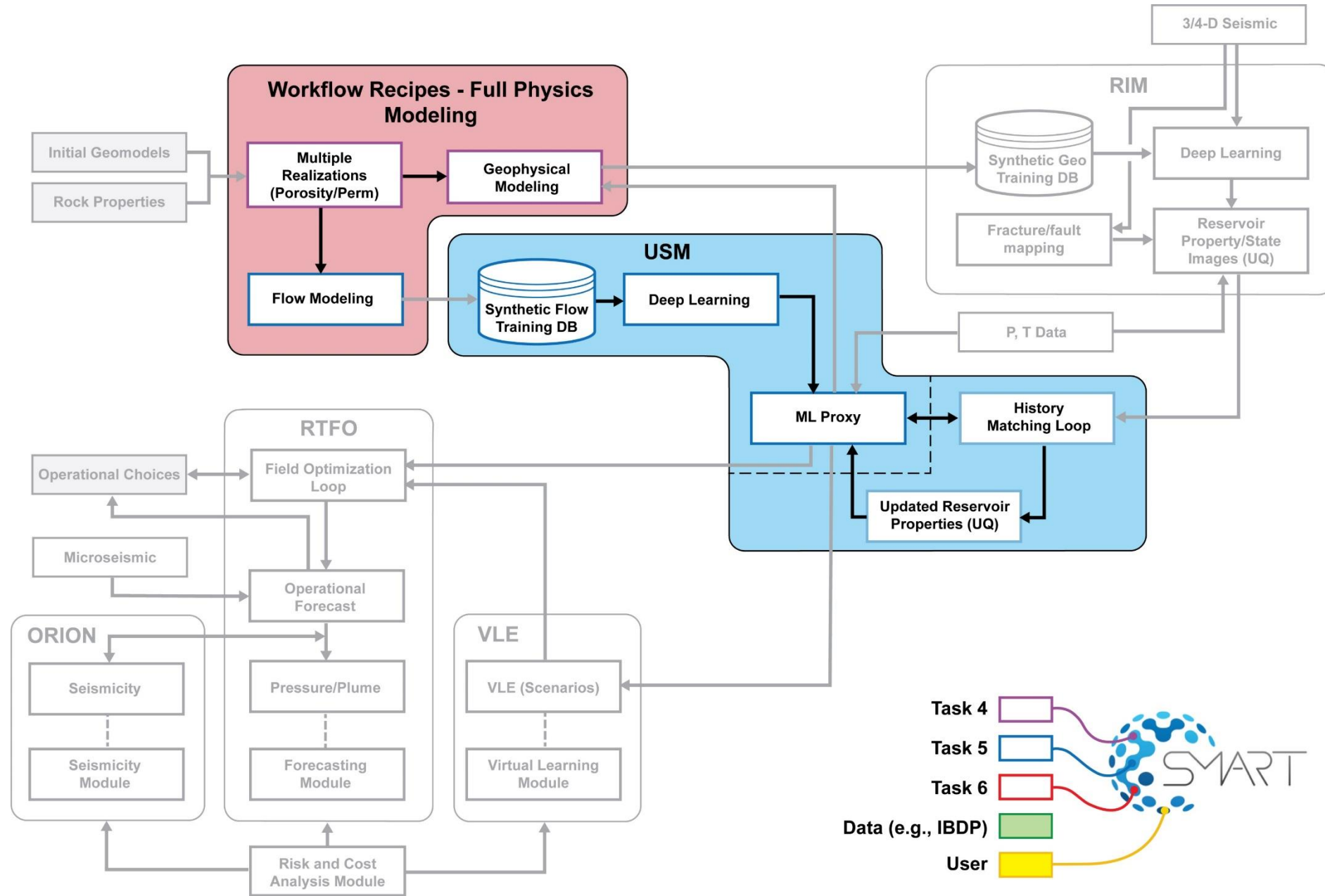
ORNL developed a workflow with three AI applications to improve the speed and reduce the cost of fault and fracture imaging for carbon storage sites.



SNL Workflow



TASK 5: Wiring Diagram –Storage Reservoir Modeling



Task 5 –Dynamic Storage Reservoir Modeling

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

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

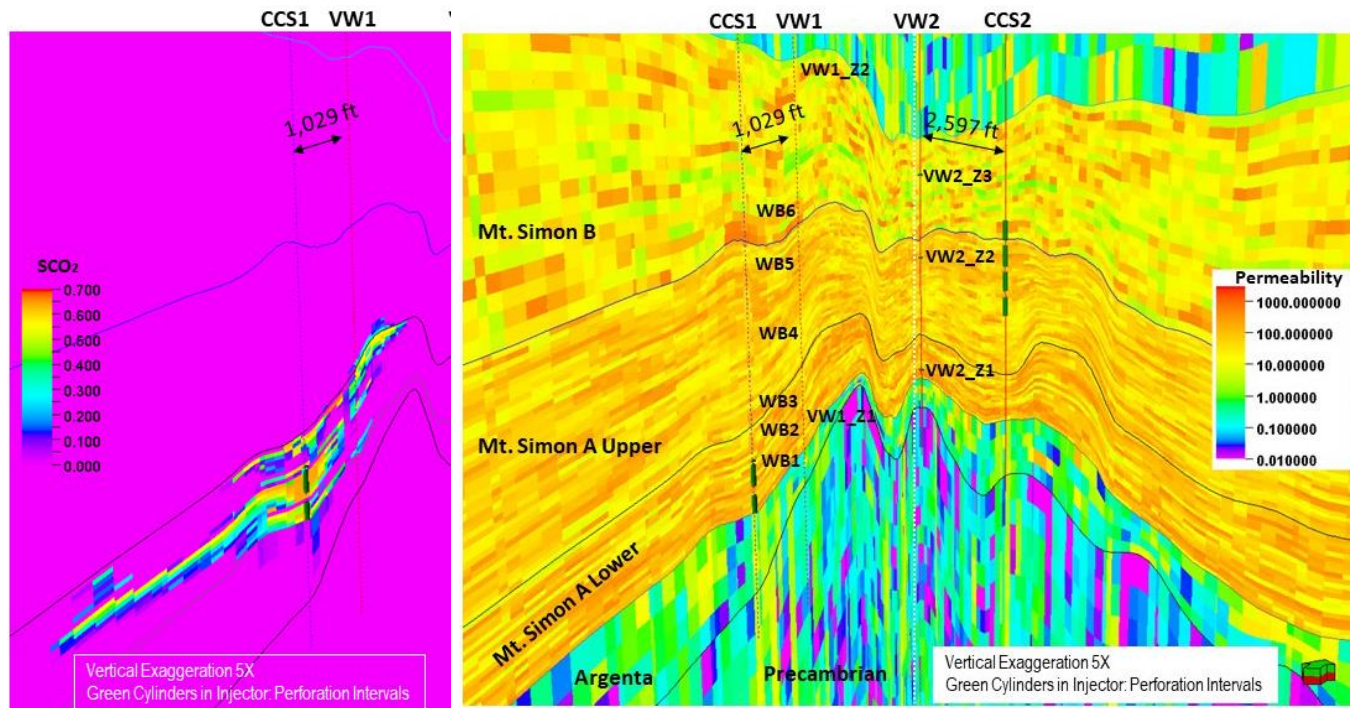


Figure: Physics-based simulation of CO₂ saturation plume at the end of 3 years injection (left) at the Illinois Basin-Decatur Project (IBDP) site with a geologic model (right)

[<https://edx.netl.doe.gov/dataset/illinois-state-geological-survey-isgs-illinois-basin-decatur-project-ibdp-geological-models>]

Carbon Storage Simulation

Workflows Today:

- Strong physical basis
- Decision-driven
- Ensemble-based

- Human-labor intensive
- Slow and non-interactive
- Heuristic optimization

SMART Vision:

- Strong physical basis
- Decision-driven
- Ensemble-based

- Human-labor efficient
- Highly interactive
- Automated workflows
- Rapid data assimilation

Task 5 –Dynamic Storage Reservoir Modeling

Key Idea: Use ML models, trained on physical simulations, to create a rapid surrogate

- Learns physical-basis embedded in full-physics models
- Is exposed to a broad array of possible surface configurations (porosity, permeability, baffles)
- Achieve prediction accuracy, training efficiency (with 1.73 M cells of IBDP model), and portability of trained models in an interactive user interface (i.e., unified simulation module)

Saturation Plume Comparison for Run 10 at Time 36
(Extent for Saturation Change > 0.01)

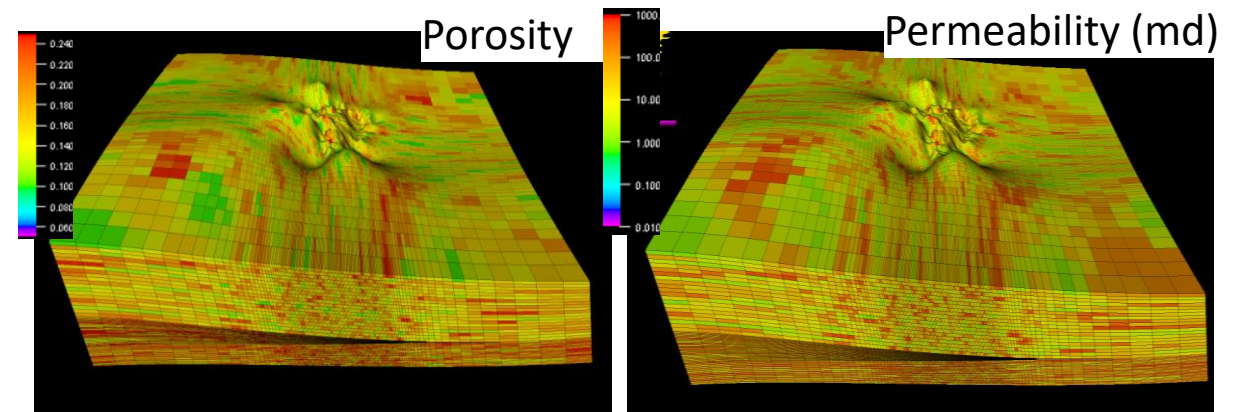
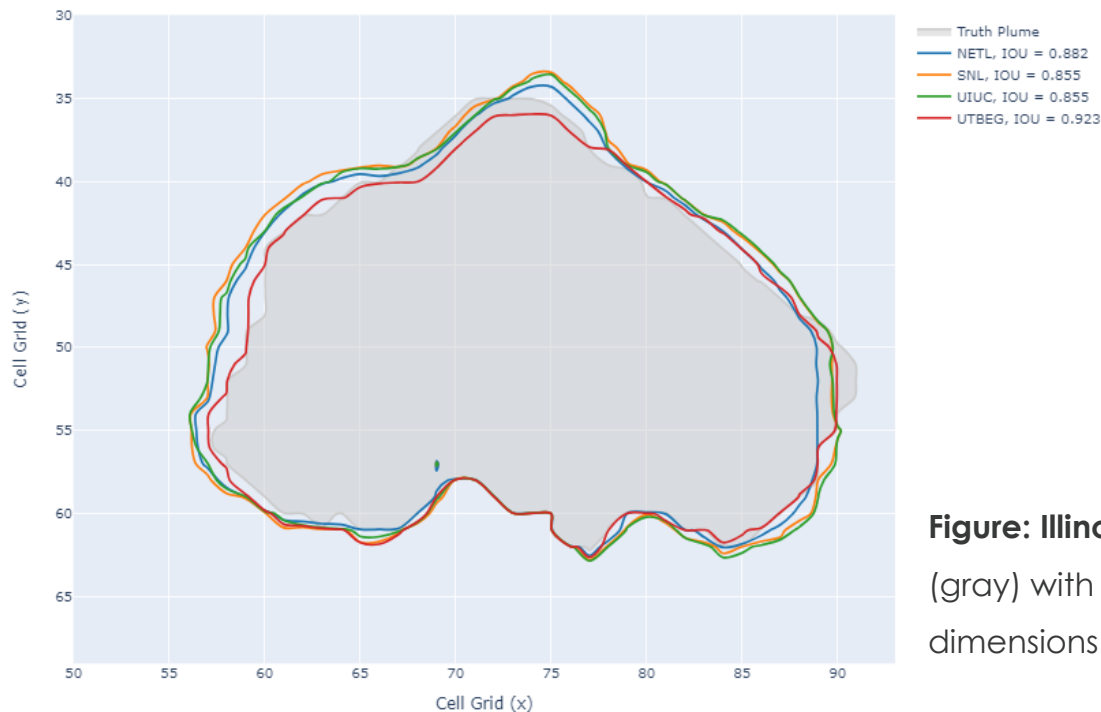
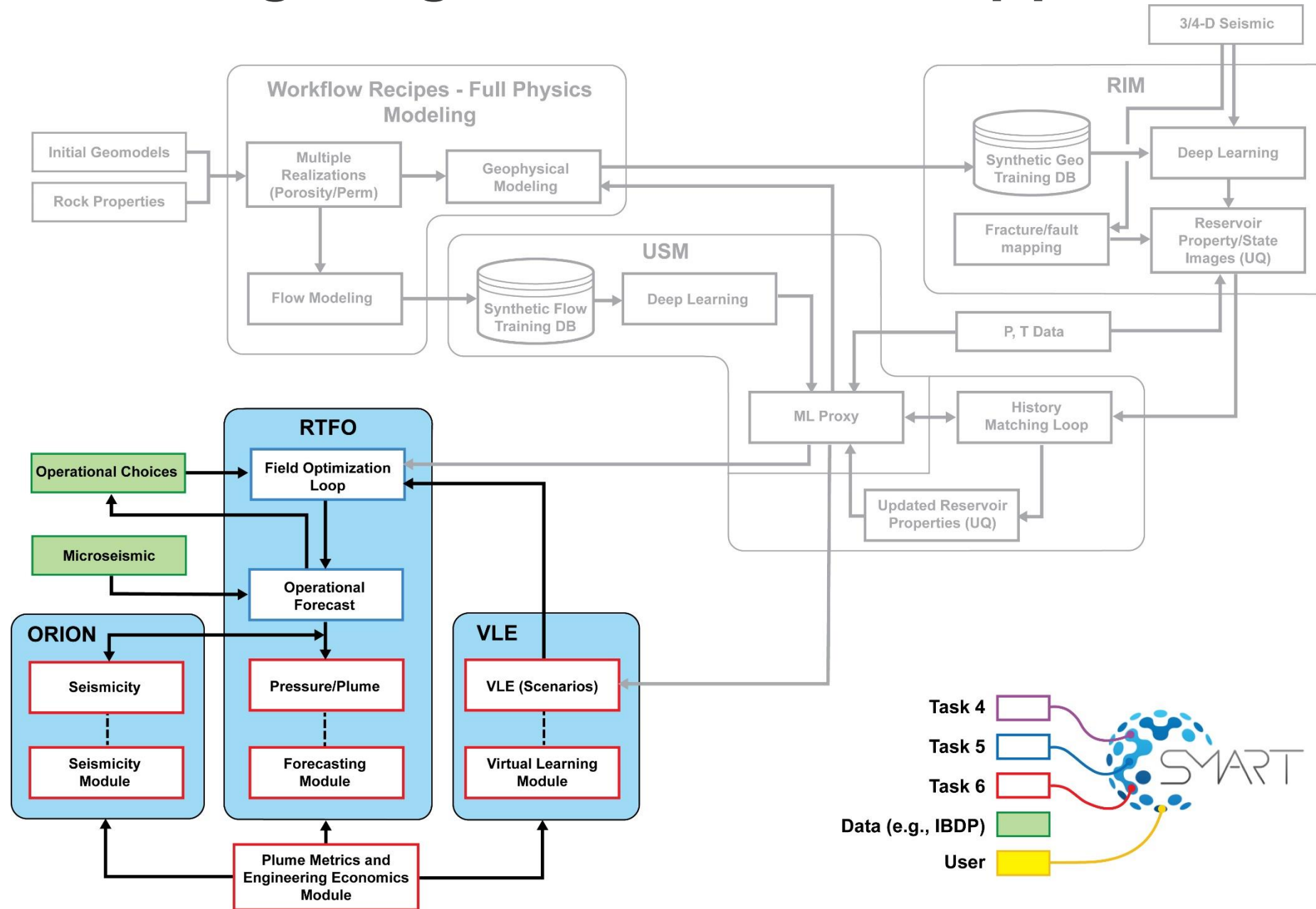
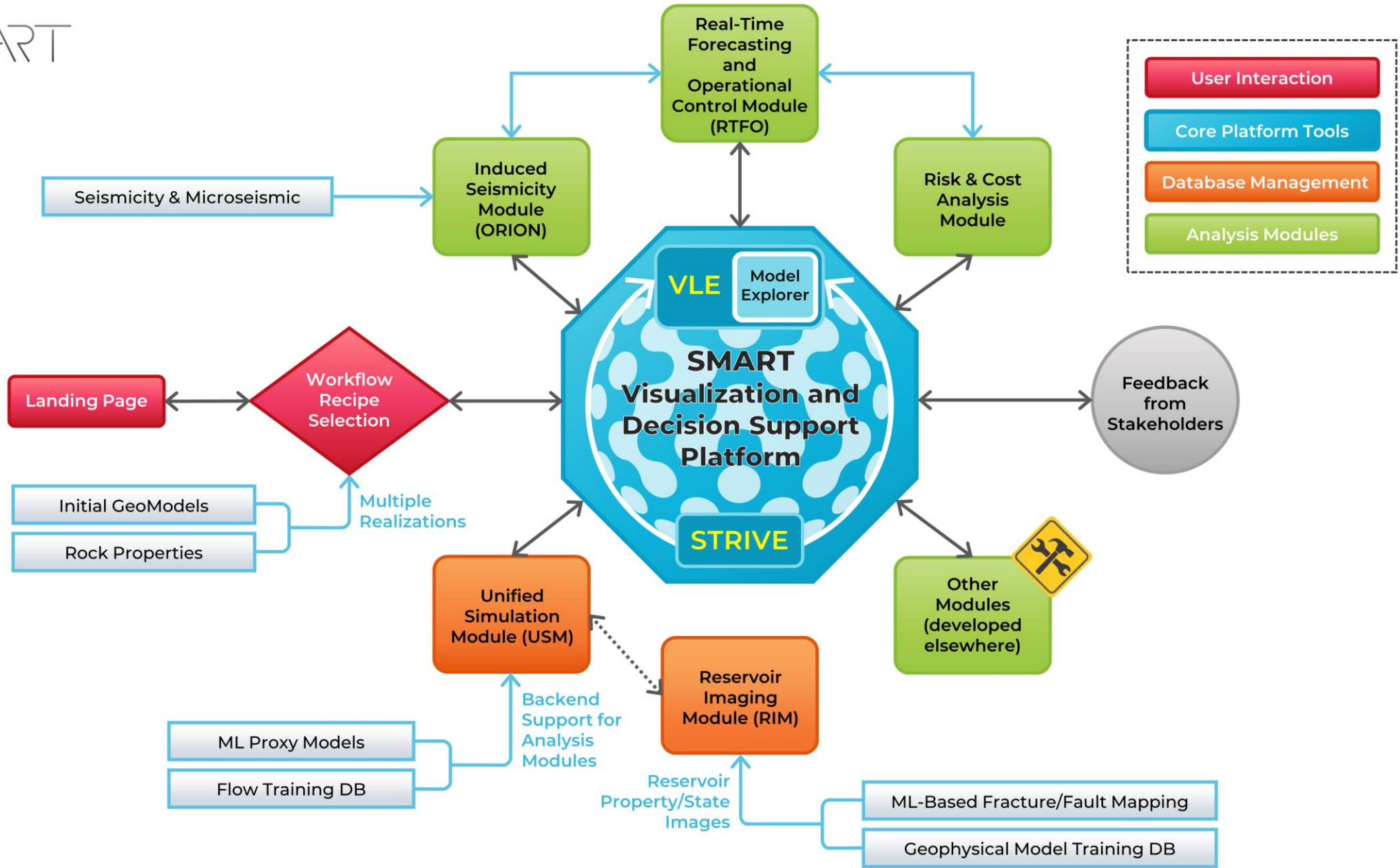


Figure: Illinois-Basin Decatur Test. Comparison of physic-based model (gray) with four ML models (lines), showing predicted saturation plume dimensions (plan view) on test case for IBDP.

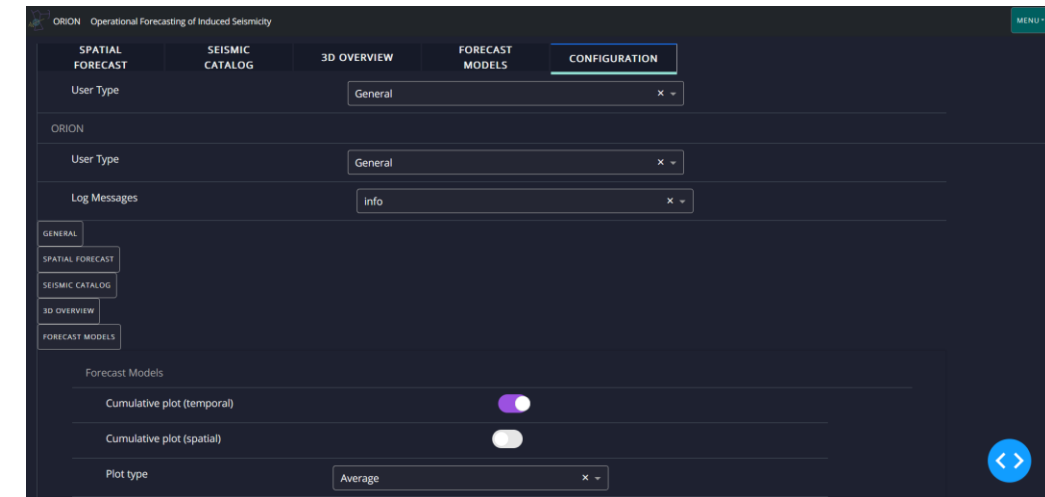
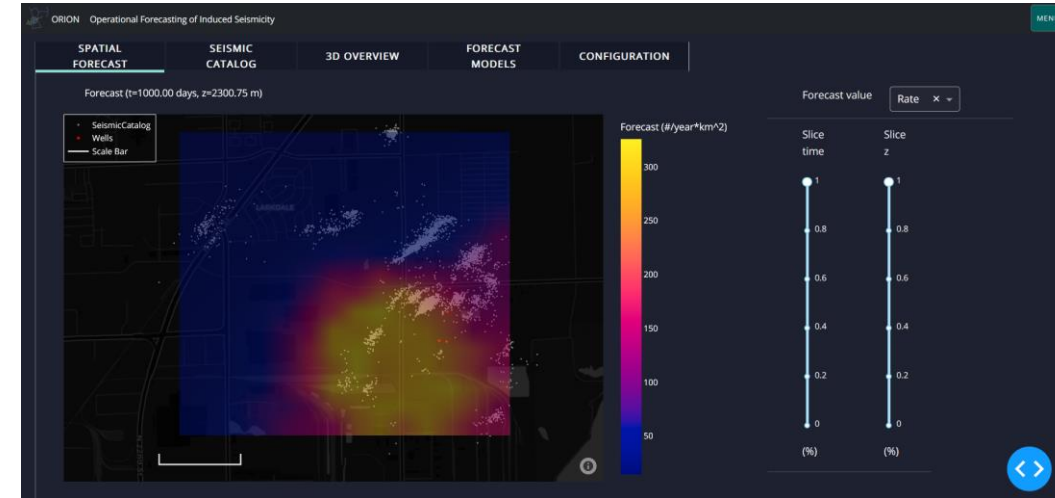
TASK 6: Wiring Diagram – Decision Support & Visualization





Operational Forecasting Of Induced Seismicity (ORION) SMART AND NRAP

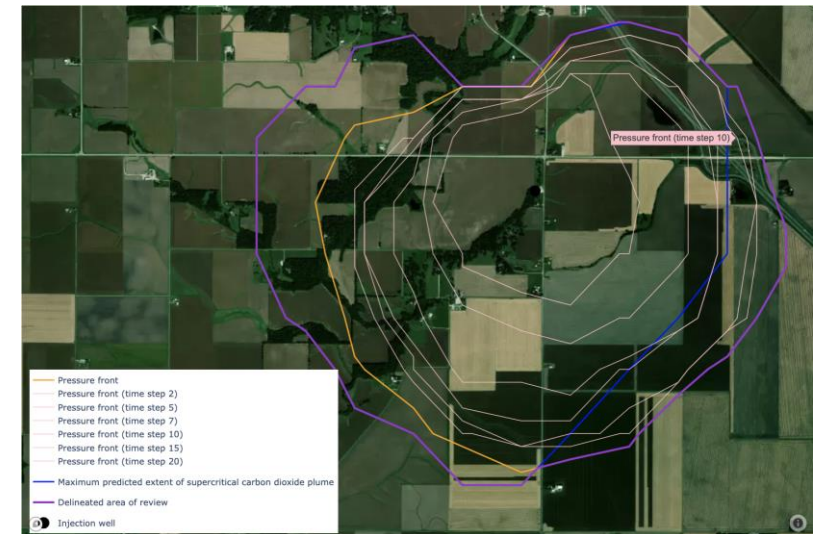
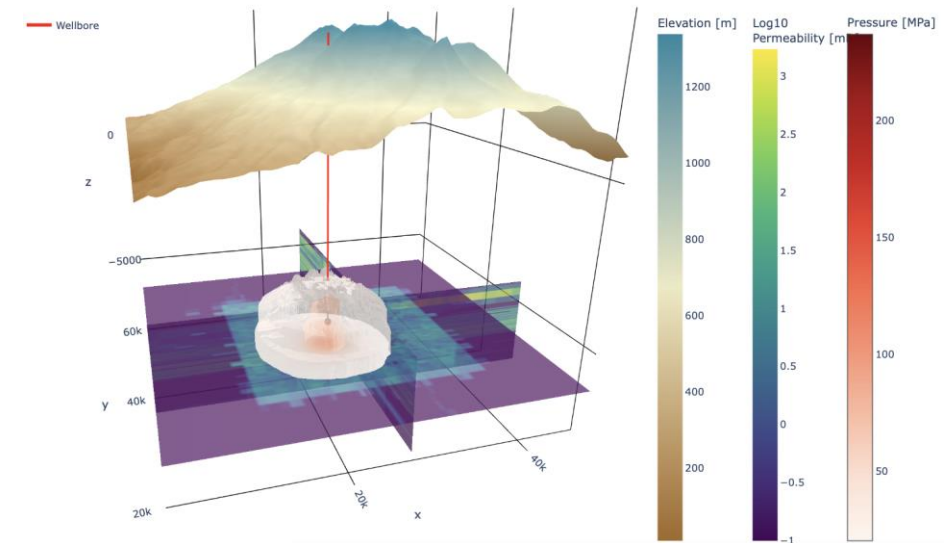
- ORION serves as the Induced Seismicity Module for Platform
- Key inputs:
 - Observed seismic activity
 - Pressure model
 - Geologic model
- Outputs:
 - Independent seismic forecast models that are based off different physical assumptions, statistics, and ML (in development)
 - An ensemble seismic forecast
 - Visualizations to assist end-users understanding of seismic activity / risks



Model Explorer Module

Why is Model Explorer important, and how can it accelerate the Class-VI permitting process?

- Allows for quick visualization of the model inputs, output, and other types of data integration, where multiple sets of technical information (e.g., site characterization data and modeling input) can be visualized and evaluated in an integrated fashion.
- Calculates and maps Area of Review (AoR) in real-time in response to model inputs. Able to display the evolution and maximum predicted extent of the supercritical CO₂ plume, pressure front, and the combined AoR.
- AoR calculation is based on a pressure-front that can be user defined or determined using the suggested EPA methods.



TASK 8 – Geomechanical Modeling

- Full-physics poromechanical and fault reactivation modeling capabilities are increasingly mature, but they remain computationally expensive and see limited application in industry.
- Ensembles of physics-based poromechanical simulations to train a rapid ML surrogate and efficient transfer learning

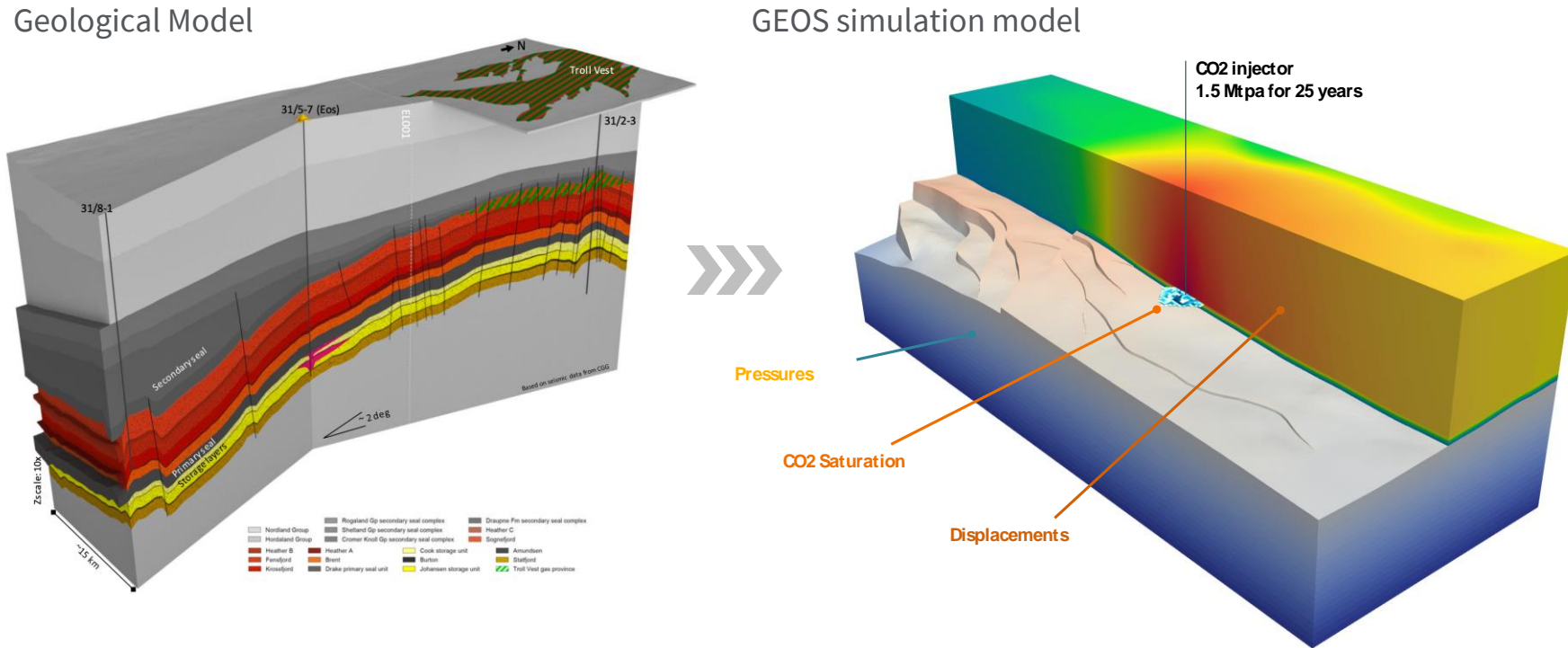


Figure: GEOS poromechanical simulation of the Northern Lights injection project [courtesy TotalEnergies].

Hackathon: EY24 Early win – SMART platform development and outcomes

- SMART platform development hackathon was held at PNNL Seattle Campus (July 9-10, 2024)
- Platform developers from PNNL, LLNL, and NETL
- **Objectives:**
 - Using STRIVE, integrating key SMART modules into the platform.
 - Develop workflow recipes and establish coupling between modules within the SMART platform.
- **Outcomes:**
 - Functional SMART platform landing page with integrated SMART modules.
 - Established preliminary workflows and module coupling within the platform.
 - A demo at DOE-FECM meeting on early prototype of SMART platform and key functionalities.

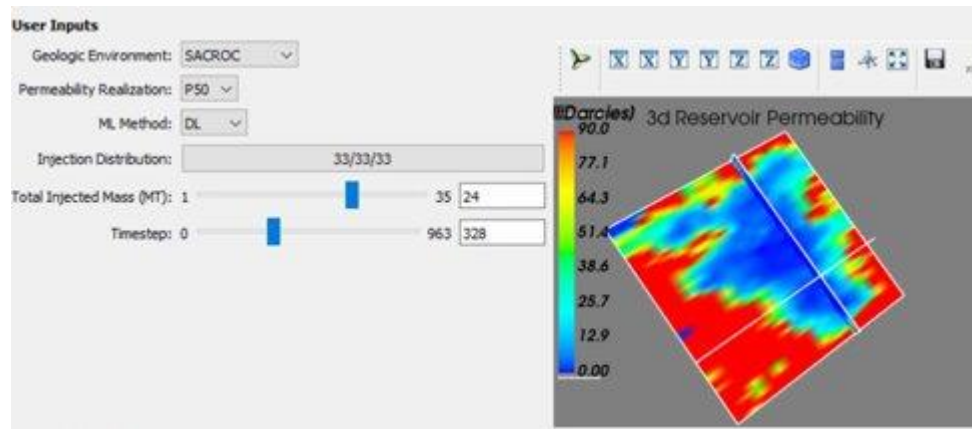
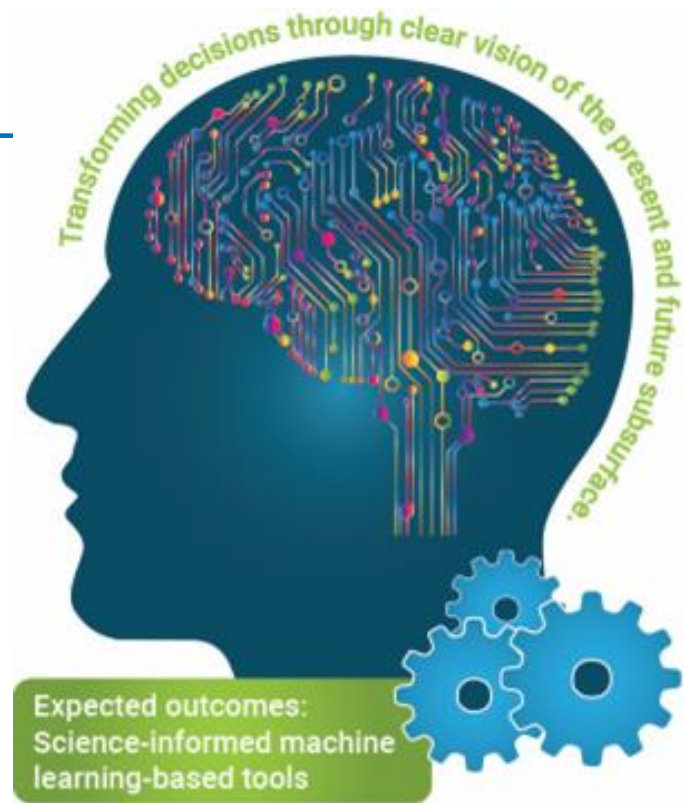
How Can SMART Assist CCS Projects?

- SMART tools can be applied for (a) virtual learning during the pre-injection permitting phase, and (b) ML-assisted operational decision making & visualization.

- **Virtual Learning** - During pre-injection permitting phase, rapid exploration and communication of the impact of data and model uncertainties and “what-if” scenarios on system evolution after CO₂ injection.

- **Operational Decision Making and Visualization**

- Rapid interpretation of geophysical images for improved visualization of subsurface rock and fluid properties and dynamic model updates.
- Near (real) time optimization of CO₂ injection operations using fast predictive models that are regularly calibrated to observations of pressure, temperature, saturation etc.



AI/ML at Work for CCS: Example

The **Virtual Learning Environment (VLE)** is an exploratory tool which uses ML predictions to rapidly inform an end user of how a given reservoir simulation would likely change in response to altered inputs.

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

Decision-makers

Project Engineers

Regulators

High-level Executives

Landowners/Public

Phases

Site/Field Selection

Permitting

Development

Operations

Closure

Questions

- ① Where is the CO₂ now?
- ② How do I move the CO₂ where I want it to be?
- ③ Is the project safe?
 - Will it leak, and if so, where?
 - Will it cause induced seismicity?

Rapid predictive analysis
and stakeholder outreach

Better imaging and
subsurface visualization

Faster model calibration
and operational forecasting

SMART Presentations at FECM Meeting, Pittsburgh, PA

Program Details (Tuesday, August 6, 2024)

10:30 a.m. - 12:10 a.m.	SMART Session 1 – Computational and Visualization Advances 7 Presentations
1:25 p.m. – 3:25 p.m.	SMART Session 2 – Field Applications 6 Presentations
4:00 p.m. - 5:20 p.m.	SMART Session 3 – Applications 4 Presentations
5:45 p.m. - 7:45 p.m.	SMART – Poster Session 18 Poster Presentations
5:45 p.m. - 7:45 p.m.	SMART – Tool Demonstration Session 11 Tool Demonstrations

SMART Presentations at FECM Meeting, Pittsburgh, PA

2024 Program Details (Tuesday, August 6, 2024)

10:30 a.m. - 10:40 a.m.	SMART Initiative Overview Hema Siriwardane, National Energy Technology Laboratory
10:40 a.m. - 10:55 a.m.	ML-based Dimension Reduction Strategies Seyyed Hosseini and Hongsheng Wang, University of Texas Bureau of Economic Geology
10:55 a.m. - 11:10 a.m.	Physics-Informed Machine Learning Alexandre Tartakovsky, University of Illinois Urbana-Champaign
11:10 a.m. - 11:25 a.m.	Transfer Learning for Multi-Physics Problems Hongkyu Yoon, Sandia National Laboratory
11:25 a.m. - 11:40 a.m.	Model Explorer for Virtual Learning Maruti Mudunuru and Ashton Kirol, Pacific Northwest National Laboratory
11:40 a.m. - 11:55 a.m.	Induced Seismicity Forecasting with ORION Kayla Kroll and Chris Sherman, Lawrence Livermore National Laboratory
11:50 a.m. - 12:10 p.m.	SMART Visualization and Decision Support Platform (FWP-1025011) Maruti Mudunuru, Pacific Northwest National Laboratory, Chris Sherman, Lawrence Livermore National Laboratory and Patrick Wingo, National Energy Technology Laboratory

SMART Presentations at FECM Meeting, Pittsburgh, PA

2024 Program Details (Tuesday, August 6, 2024)

1:25 p.m. - 1:45 p.m.	Comparison of ML-Based Proxy Modeling Strategies Jared Schuetter, Battelle Memorial Institute
1:45 a.m. - 2:05 a.m.	ML-Based Data Assimilation and History Matching Masahiro Nagao, Texas A&M University and Akhil Data-Gupta, Texas A&M University
2:05 a.m. - 2:25 a.m.	ML-Based Optimization for CO2 Injection Bailian Chen, Los Alamos National Laboratory
2:25 a.m. - 2:45 a.m.	ML-Based Rock Properties and Seismic Volume Enhancement Athanasios (Athos) Nathanail and Manika Prasad, Colorado School of Mines
2:45 a.m. - 3:05 a.m.	ML-Based Fracture and Fault Identification Youzuo Lin, University of North Carolina
3:05 a.m. - 3:25 a.m.	ML-Based Rock Physics Modeling and Reservoir Imaging (FWP-FP00014427) David Alumbaugh, Lawrence Berkeley National Laboratory

SMART Presentations at FECM Meeting, Pittsburgh, PA

2024 Program Details (Tuesday, August 6, 2024)

4:00 p.m. - 4:20 p.m.	Comparison of ML-Based Proxy Modeling Strategies Jared Schuetter, Battelle Memorial Institute
4:20 p.m. – 4:40 p.m.	ML-Based Data Assimilation and History Matching Masahiro Nagao, Texas A&M University and Akhil Data-Gupta, Texas A&M University
4:40 P.m. – 5:00 p.m.	Overview of the NRAP/SMART Technoeconomic and Liability Evaluation for Storage (TALES) Model David Morgan and Chung-Yan Shih, National Energy Technology Laboratory
5:00 P.m. - 5:20 p.m.	USM - Unified Simulation Module in SMART Jeff Burghardt and Wenjing Wang, Pacific Northwest National Laboratory

Concluding Remarks

- SMART motivation, structure, organization, wiring diagrams
- **Goal** ⇒ Empower various stakeholders with advanced ML and related tools that can accelerate decision-making
- Outcomes of SMART expected to be publicly available
- Each Task will present its key accomplishments from EY23

**Thank you for
your attention**

