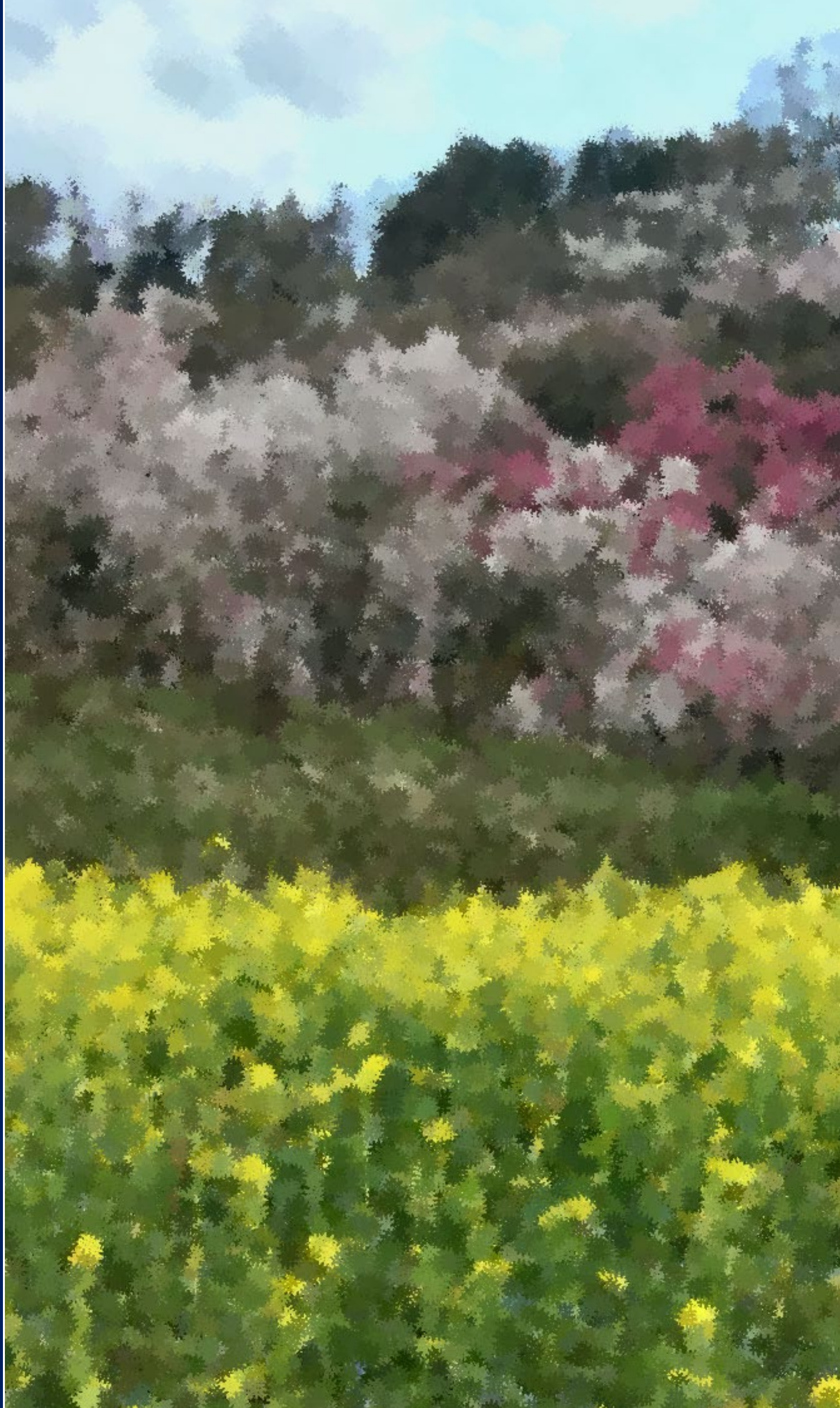
Advanced Environmental Monitoring Systems (ALTEMIS)
New Paradigm of Long-Term Monitoring

Haruko Wainwright

Nuclear Science and Engineering; Civil and Environmental Engineering

Massachusetts Institute of Technology



NSE
Nuclear Science & Engineering at MIT
science : systems : society

MIT | Civil and Environmental Engineering

ALTEMIS Collaborators

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- Carol Eddy-Dilek – Project Lead
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- Holly VerMeulen
- Emily Fabricatore

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Massachusetts Institute of Technology

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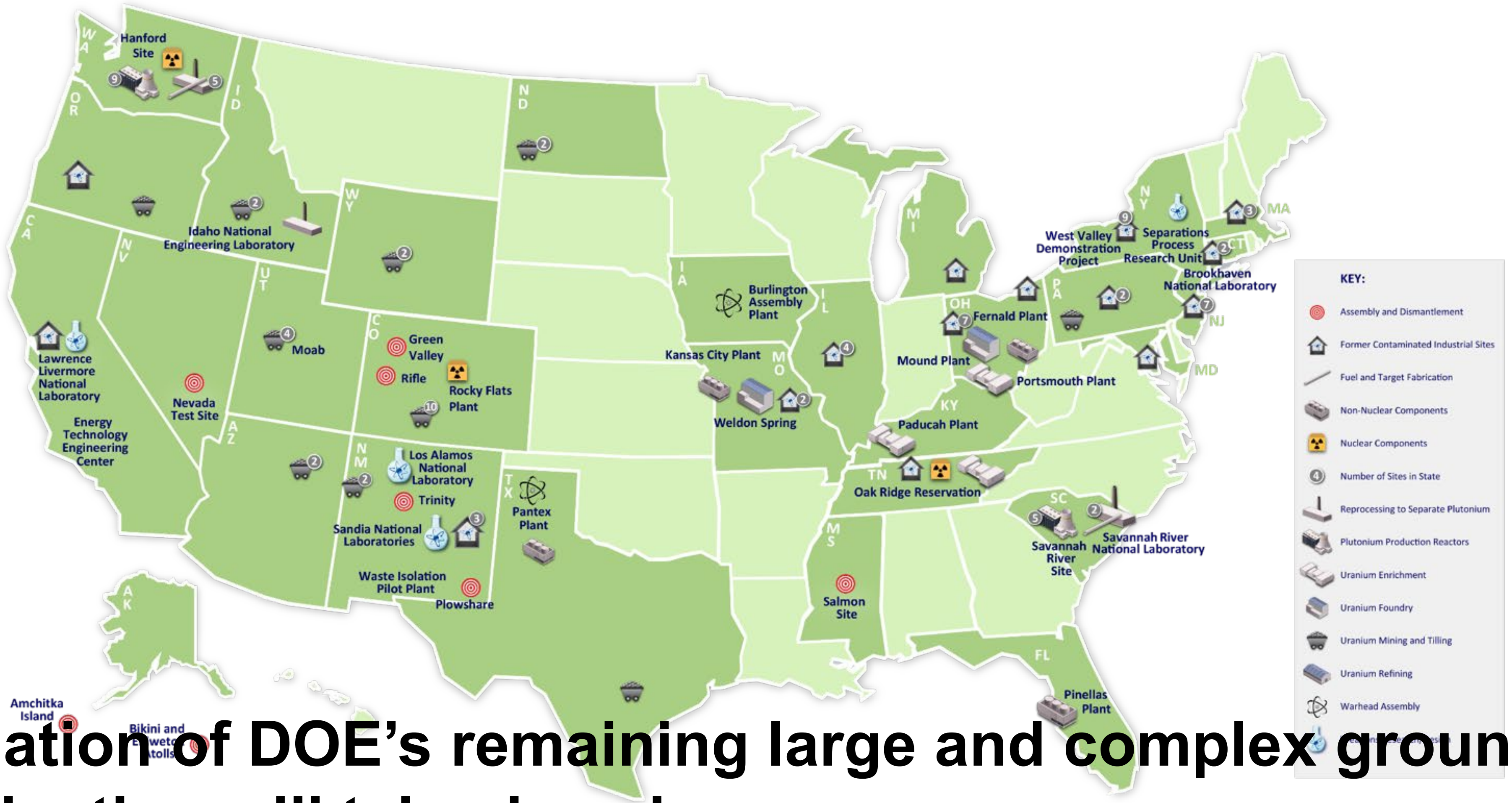
- Vivian Castillo

DOE-EM-3.21 Office of Technology Operation has sponsored a SRNL-led program since 2020

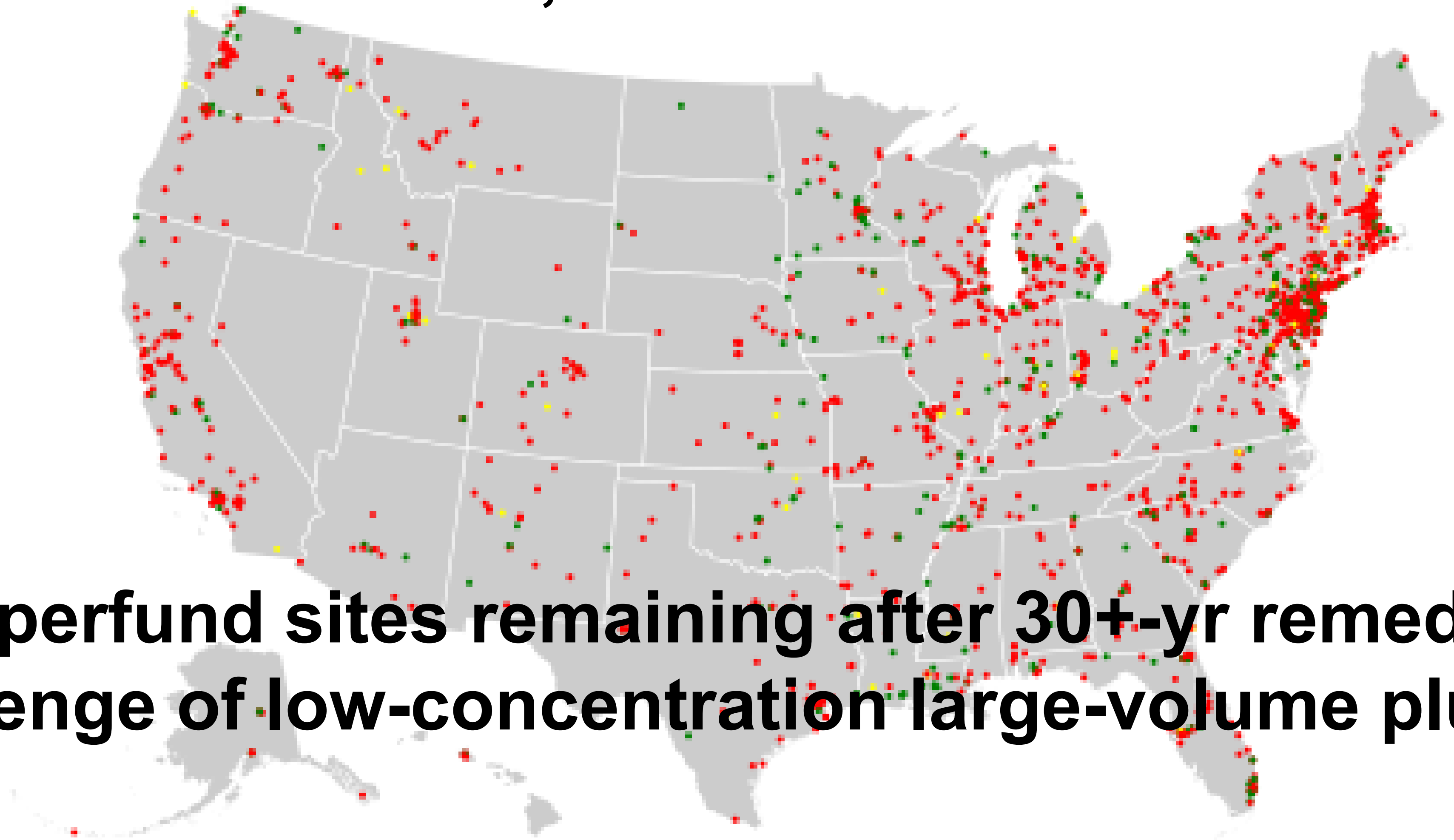
DOE's Legacy Sites



- **Remediation of DOE's remaining large and complex groundwater contamination will take decades.**
- **GAO estimates EM's liability for environmental cleanup across the country will exceed $550 billion**

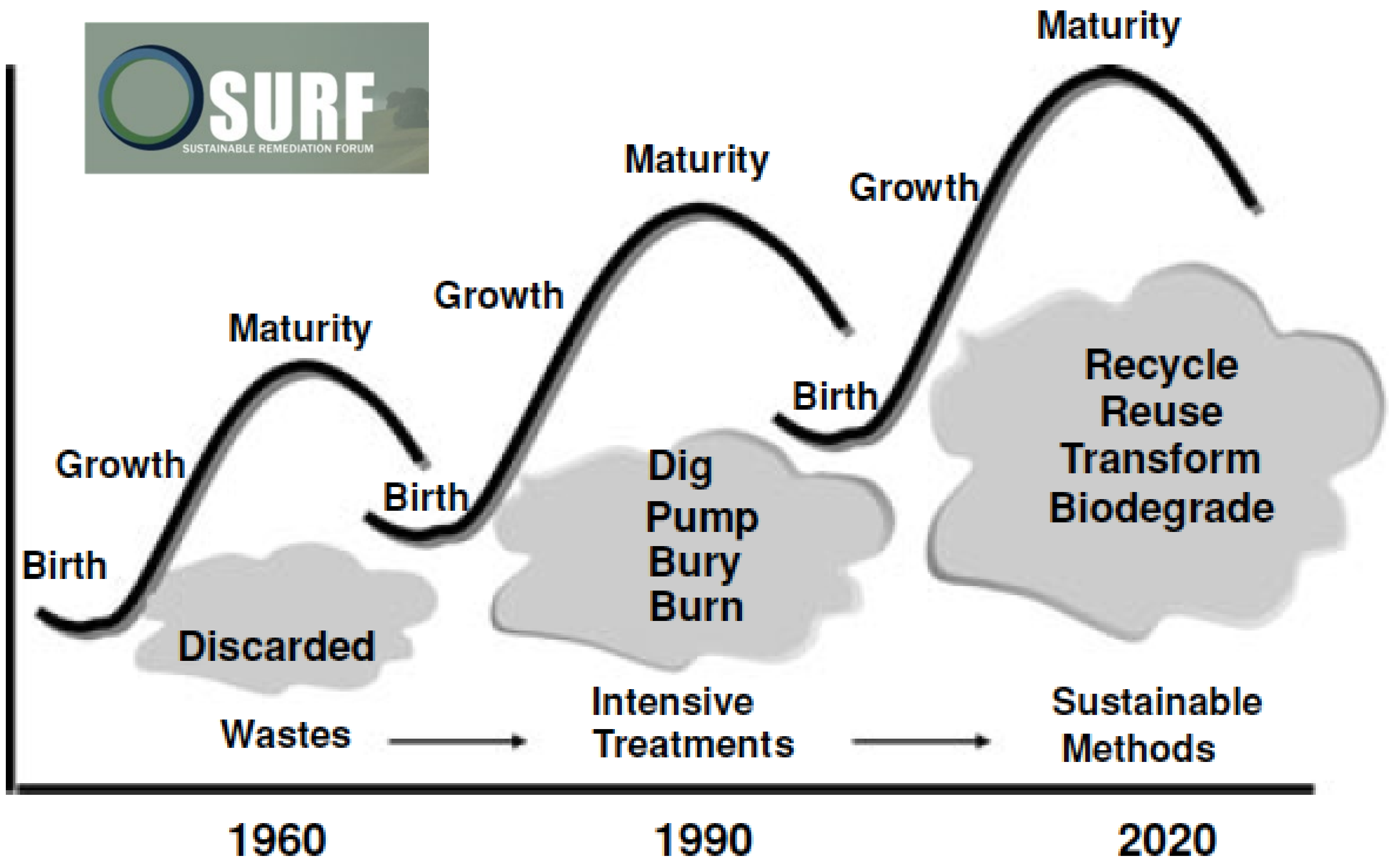
Soil and Groundwater Contamination

- Superfund Sites: >1300 sites (organic/metal/radioactive)
- Brownfield Sites: ~450,000



>900 Superfund sites remaining after 30+-yr remediation
→ Challenge of low-concentration large-volume plume

Environmental Remediation: Evolution



Trade offs: Contaminant removal vs

- Waste
- CO2 emission
- Energy Use
- Ecological Impacts
- Noise, Air pollution

Sustainable Remediation Forum (SURF), "Integrating sustainable principles, practices, and metrics into remediation projects", Remediation Journal, 19(3), pp 5 - 114, editors P. Hadley and D. Ellis, Summer 2009

Sustainable Remediation

- Minimize waste/pollution/energy-use/water-use/ecological damages
- Biodegradation, immobilization
- Monitored natural attenuation
- Longer institutional control with alternative/attractive end-use

→ Long-term monitoring

Former Reilly Tar & Chemical Corporation Plant

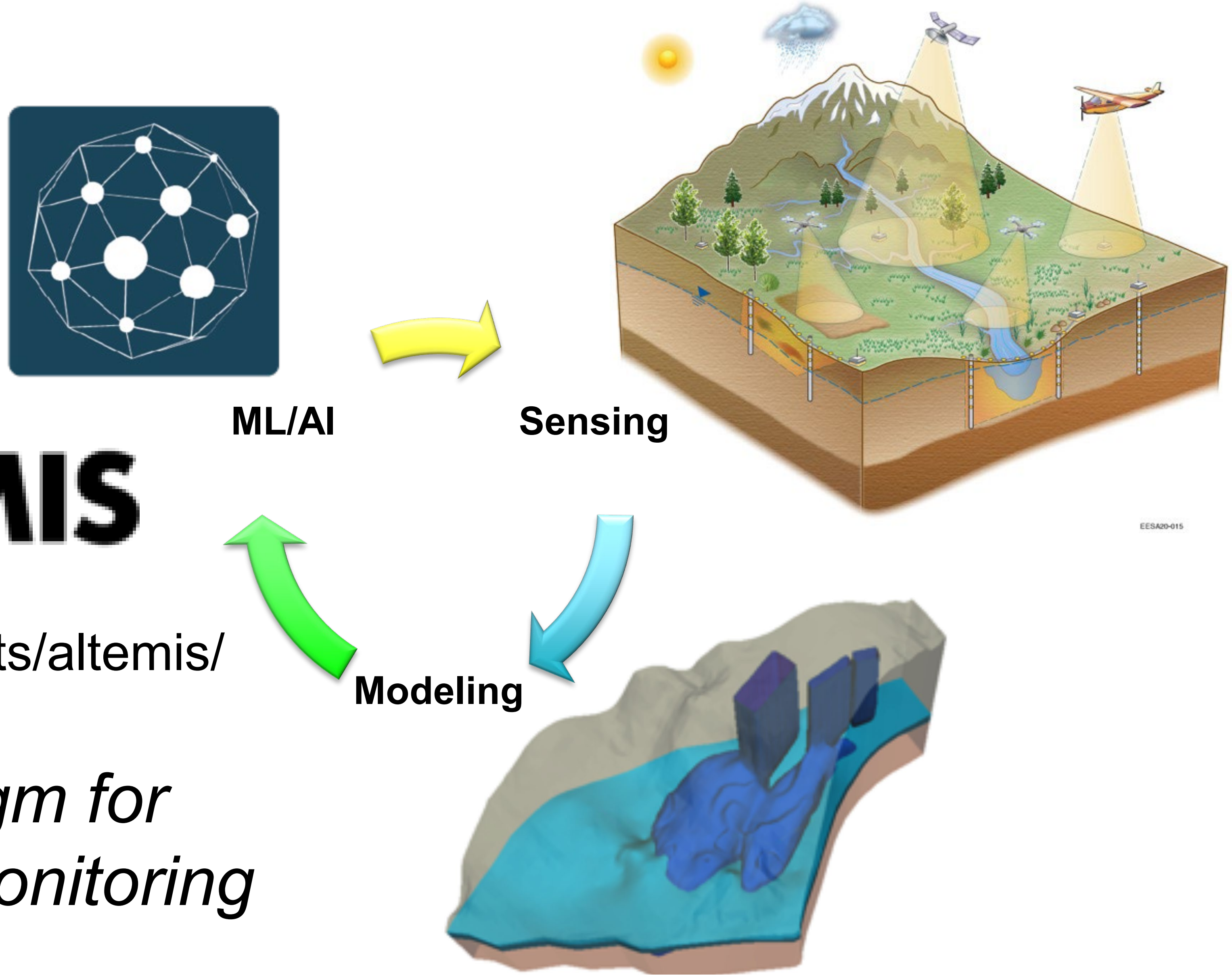
Rocky Flats National Wildlife Refuge

Environmental Monitoring

- Data/evidence provides assurance to local communities
- Detection of anomalies if they happen
- Critical ways to keep operators accountable/responsible
- Tackle misinformation and fake news

(People are skeptical of modeling results)

Advanced Long-term Environmental Monitoring Systems



ALTEMIS

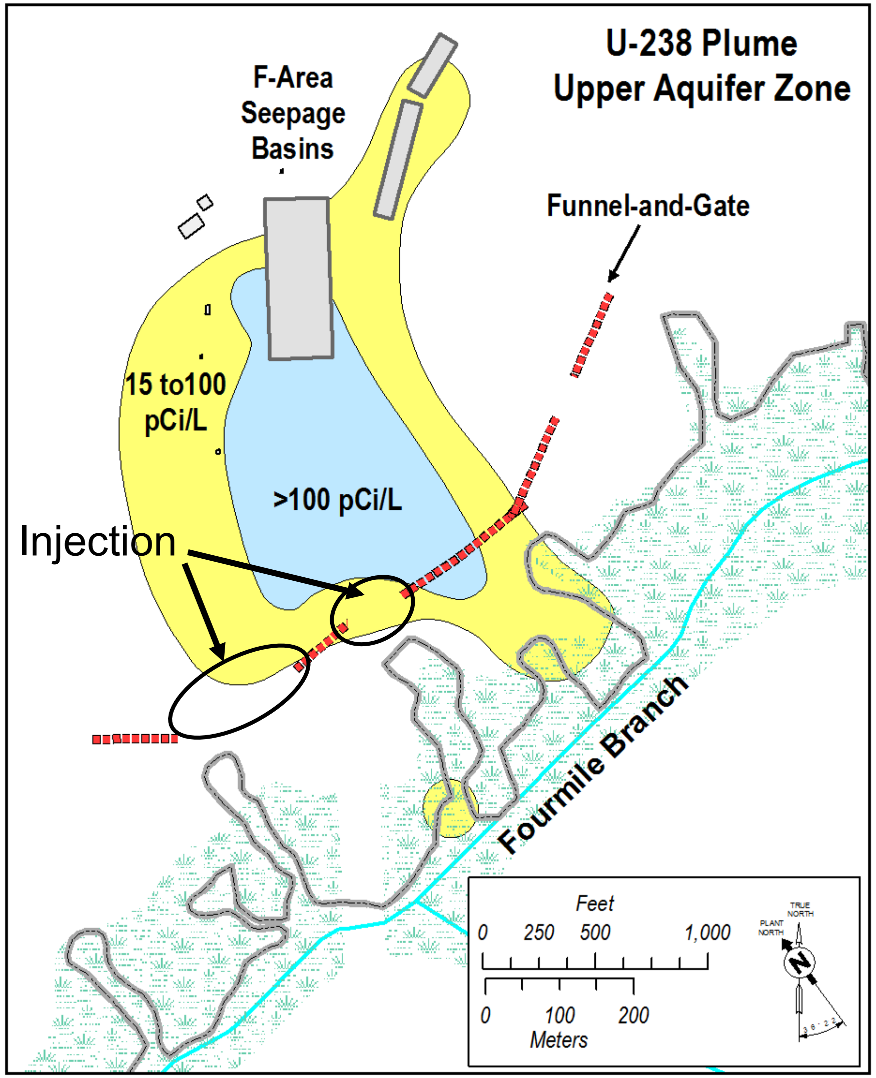
www.srnl.gov/fact-sheets/altemis/

New paradigm for long-term monitoring

Savannah River Site F-Area: Testbed

- **Disposal activities**:
  - Low-level radioactive waste from PUREX process (1955–1989)
  - Nitric acid plume: pH 3–3.5, U, ^{90}Sr, ^{129}I, ^{99}Tc, ^{3}H
- **Remediation approaches**
  - Pump & treat (the filters became highly radioactive; not sustainable)

  → Immobilization of U and ^{129}I



Guided by Real-world Observations

DOE Mound Site

- Dewatering for construction nearby

→ Shift in the groundwater table and plume direction

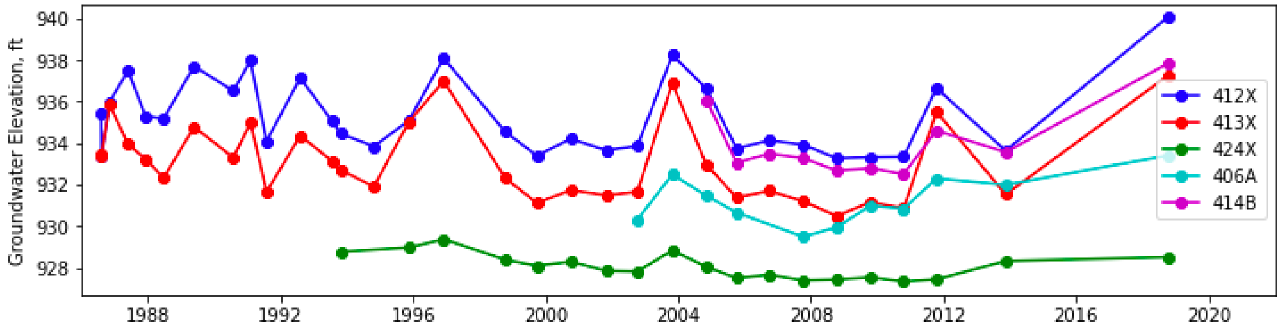
DOE Canonsburg Site

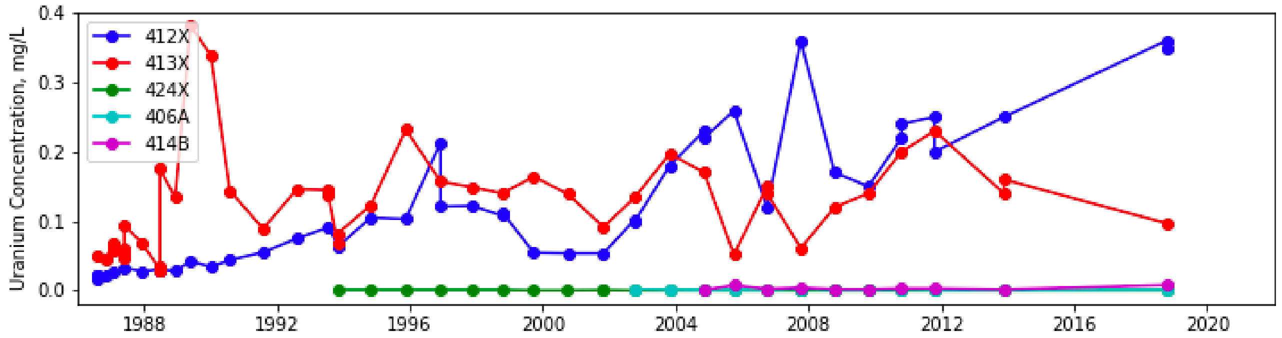
- Groundwater fluctuation associated with river stages

→ Contaminant concentration changes (hard to explain with sparse measurements)

→ Extreme weathers?

Canonsburg Data





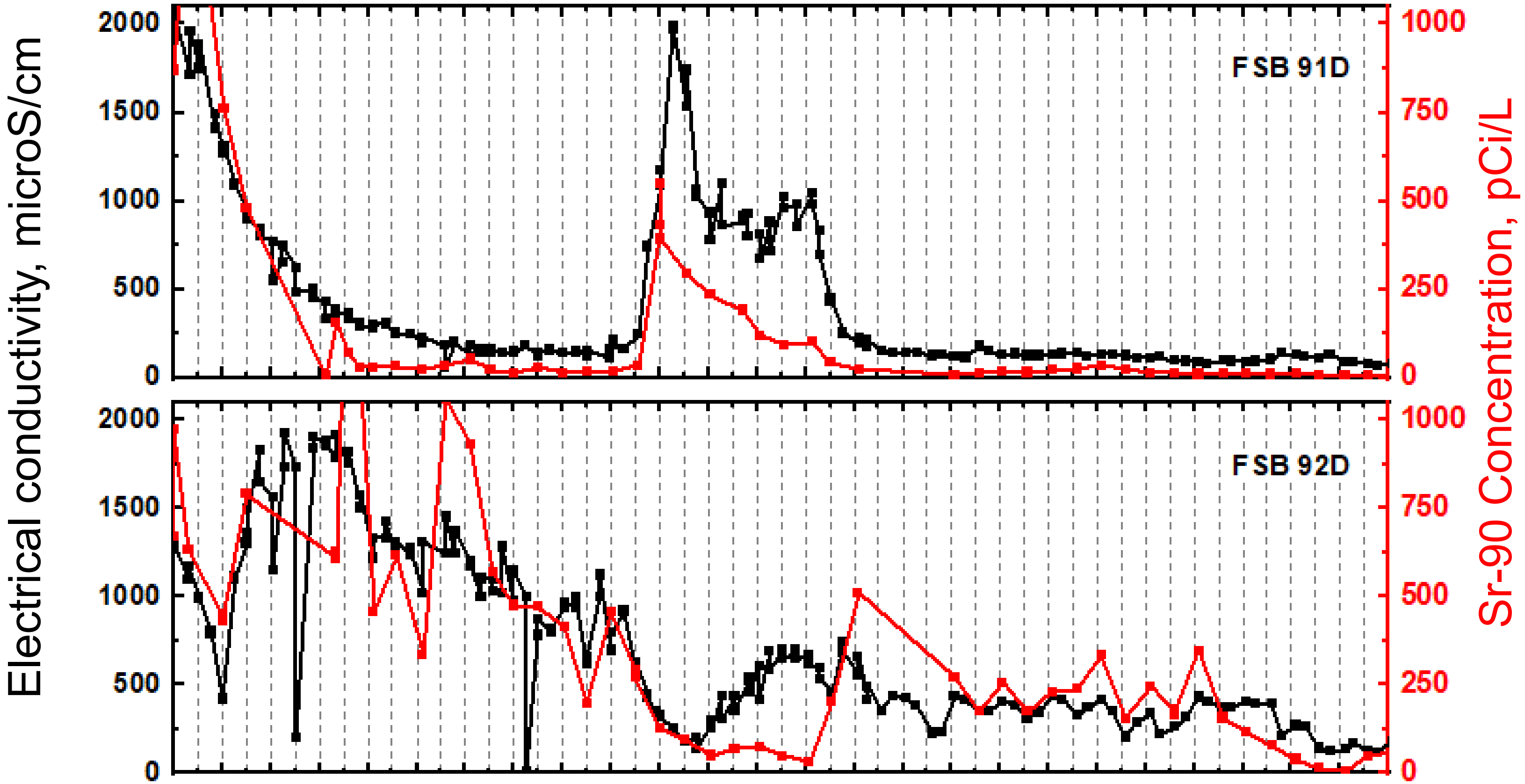
→ Importance of hydrology (e.g., water table) for contaminant mobility and plume migration

Guided by Real-world Observations

DOE Savannah River Site F-Area

- Pump-and-treat system

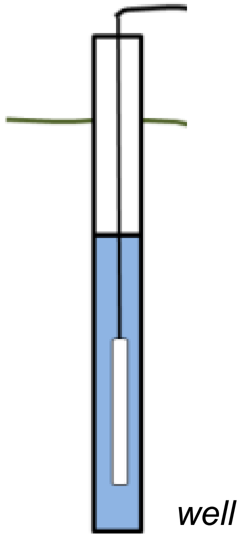
→ Re-injection increased cations → Sr-90 concentrations increased



→ Importance of in situ measurable proxies (e.g., electrical conductivity)

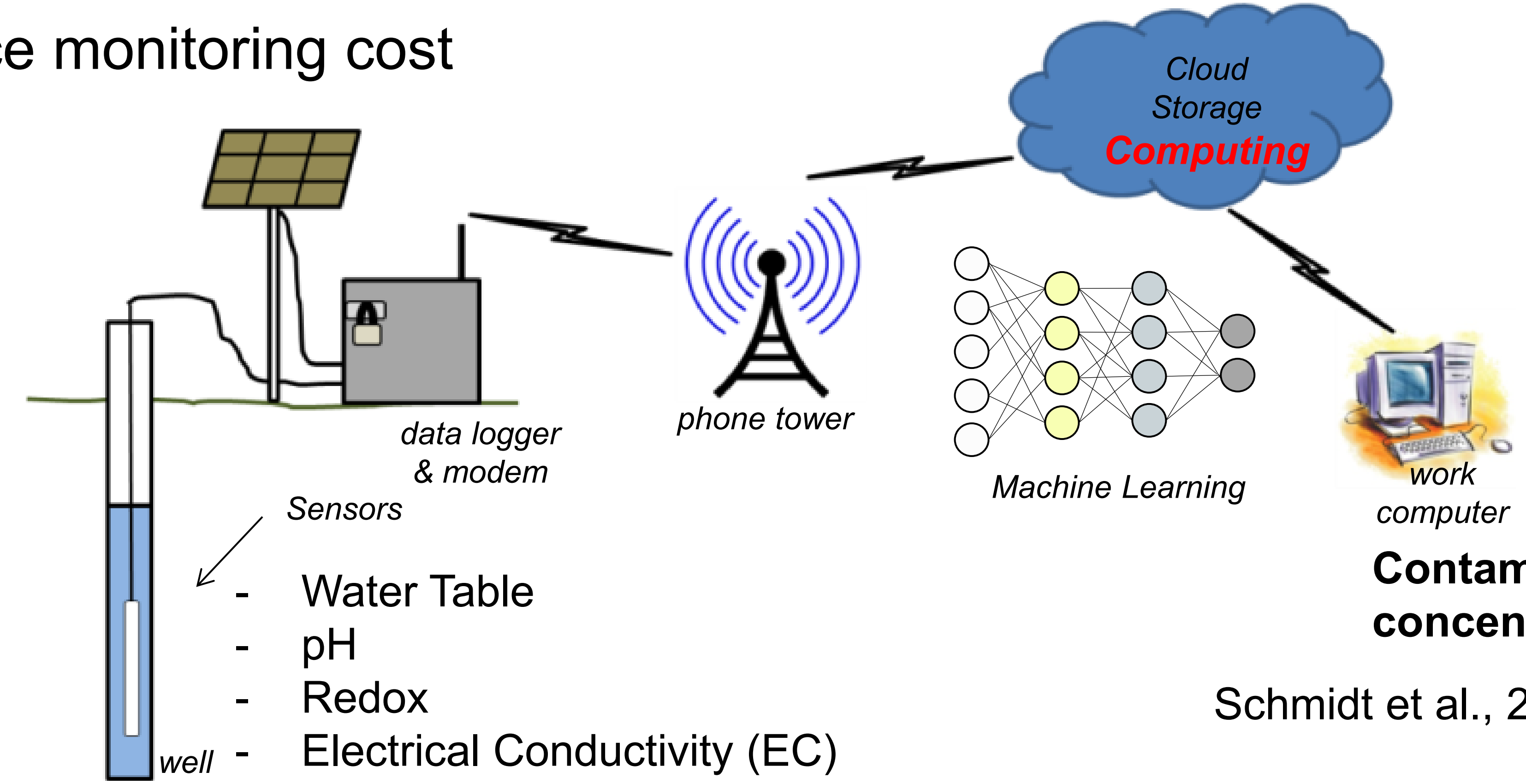
Current Groundwater Monitoring

- **Groundwater Sampling → Laboratory Measurements**
  - Expensive: 10s – 100s of wells
  - Contamination issues (requires training, equipment)
  - Temporally sparse: every quarterly, annually → Miss anomalies
  - Compliance only (no analytics)



In situ Real-time Monitoring Strategies

- **Low-cost in situ sensors, wireless network, cloud computing**
  - → Continuous monitoring of **in situ variables**
  - → Detect changes real-time = ***Reactive*** Monitoring → ***Proactive*** Monitoring
  - → Reduce monitoring cost

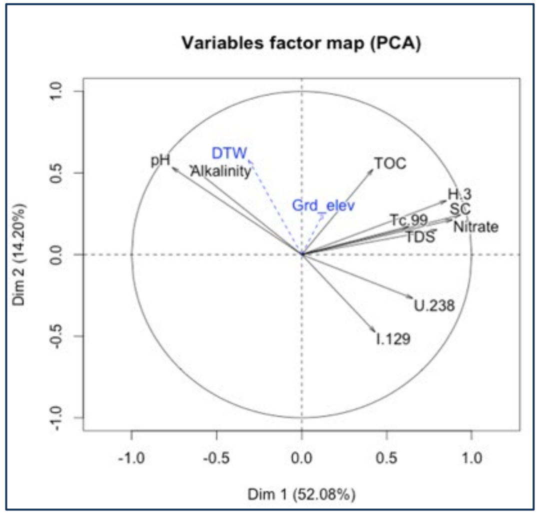


Contaminant concentrations

Schmidt et al., 2018

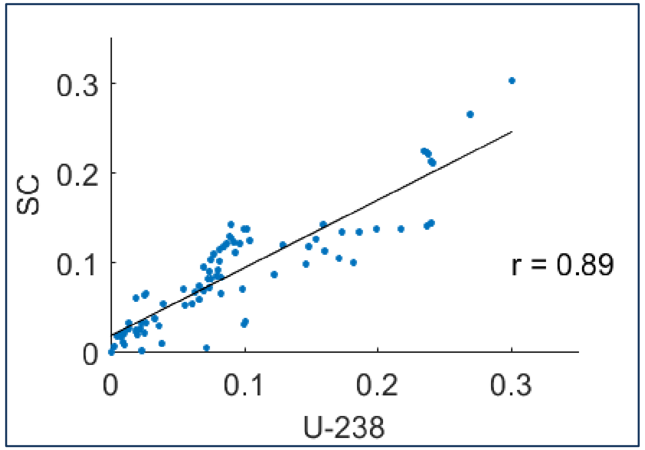
Big Data

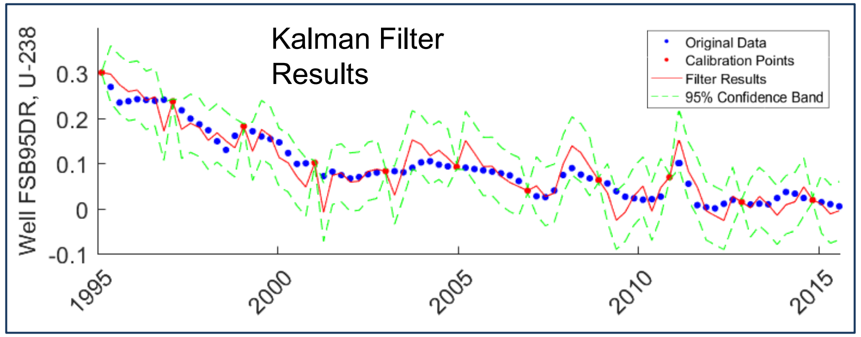
Data Analytics Workflow



Exploratory Data Analysis

Quantification of Correlations





Contaminant Concentration Estimation

Machine Learning

Schmidt et al., 2018

Environmental Science & Technology

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Article

Previous Ar

In Situ Monitoring of Groundwater Contamination Using the Kalman Filter

Franziska Schmidt[†], Haruko M. Wainwright[*,‡], Boris Faybishenko[§], Miles Denham[ǁ], and Carol Eddy-Dilek[⊥]
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Environ. Sci. Technol., **2018**, *52* (13), pp 7418–7425
DOI: 10.1021/acs.est.8b00017
Publication Date (Web): June 22, 2018
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PUBLIC RELEASE: 13-AUG-2018

Algorithm provides early warning system for tracking groundwater contamination

Berkeley Lab researchers devise system to monitor contaminant plumes

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Efficiency & Environment

Scientists develop new meth to track groundwater pollutants in real-time

It is expected to reduce the frequency of manual groundw sampling and lab analysis and therefore cut the monitorin cost

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Machine learning improves contamination monitoring

BY MATT LEONARD | AUG 14, 2018

Because groundwater is susceptible to pollution from automotive fuel, fertilizer or naturally occurring substances like iron, the Environmental Protection Agency and its state-level counterparts conduct annual or quarterly sampling and analysis.

Environmental Science & Technology

pubs.acs.org/est

Article

PyLEnM: A Machine Learning Framework for Long-Term Groundwater Contamination Monitoring Strategies

Aurelien O. Meray, Savannah Sturla, Masudur R. Siddiquee, Rebecca Serata, Sebastian Uhlemann, Hansell Gonzalez-Raymat, Miles Denham, Himanshu Upadhyay, Leonel E. Lagos, Carol Eddy-Dilek, and Haruko M. Wainwright*

Cite This: *Environ. Sci. Technol.* 2022, 56, 5973–5983

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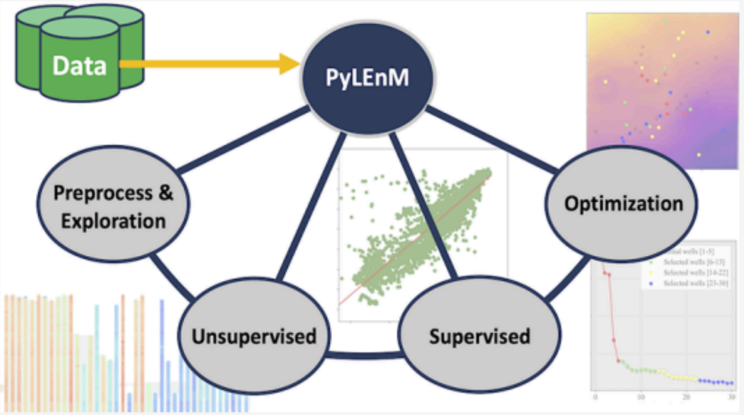
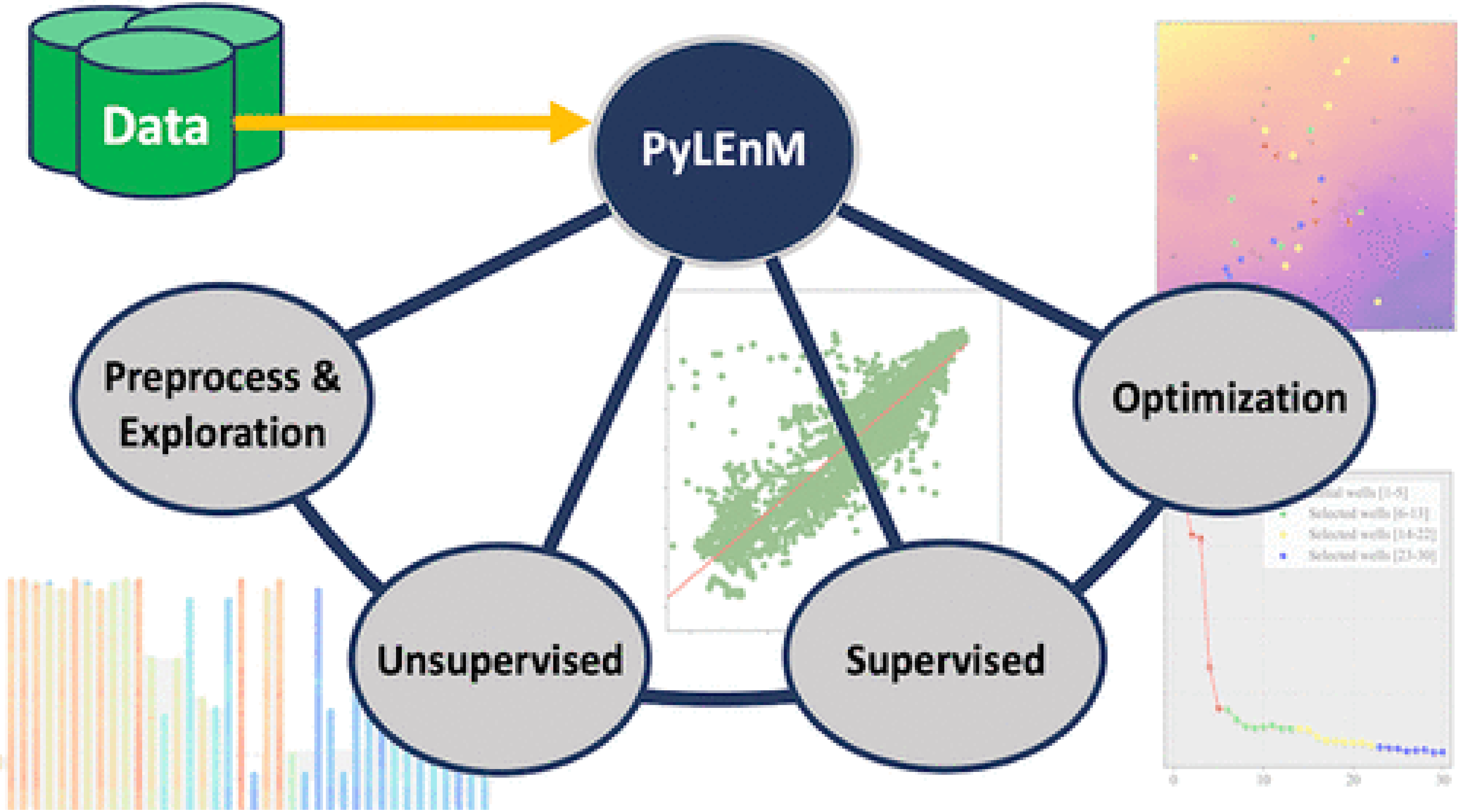


ABSTRACT: In this study, we have developed a comprehensive machine learning (ML) framework for long-term groundwater contamination monitoring as the Python package PyLEnM (Python for Long-term Environmental Monitoring). PyLEnM aims to establish the seamless data-to-ML pipeline with various utility functions, such as quality assurance and quality control (QA/QC), coincident/colocated data identification, the automated ingestion and processing of publicly available spatial data layers, and novel data summarization/visualization. The key ML innovations include (1) time series/multianalyte clustering to find the well groups that have similar groundwater dynamics and to inform spatial interpolation and well optimization, (2) the automated model selection and parameter tuning, comparing multiple regression models for spatial interpolation, (3) the proxy-based spatial interpolation method by including spatial

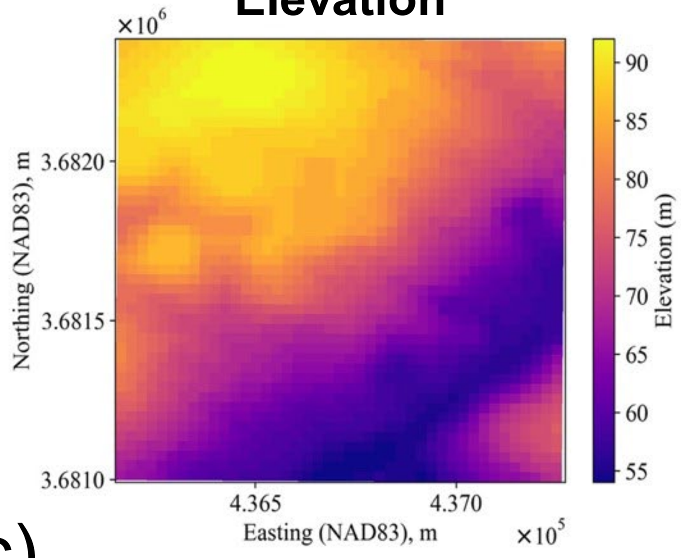
PyLenM: Python for Long-term Env. Monitoring



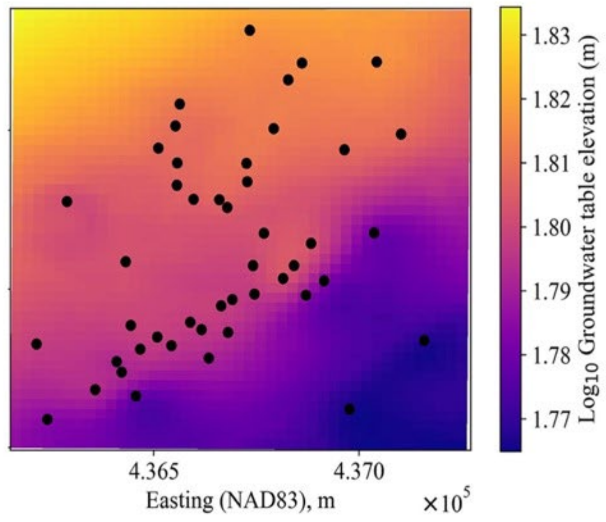
PyLenM: Supervised Learning

- **Spatiotemporal Interpolation**
  - Groundwater table
  - Contaminant concentration
- **Proxy variables**
  - LiDAR elevation data
  - Topographic metrics (slope etc)
  - Distance from the source
  - In situ measurable SC
  → tritium concentration
- **Comparison of multiple ML regression methods**

Elevation



Groundwater table



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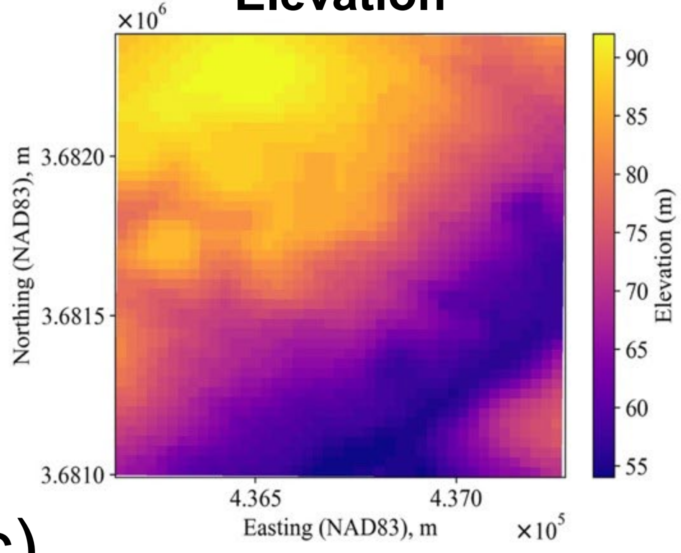
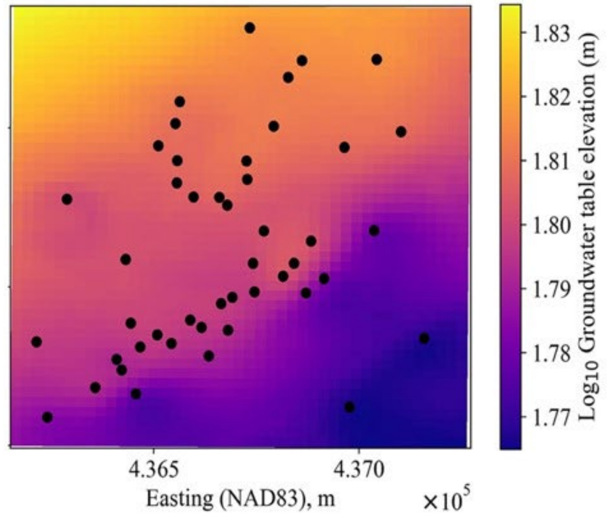
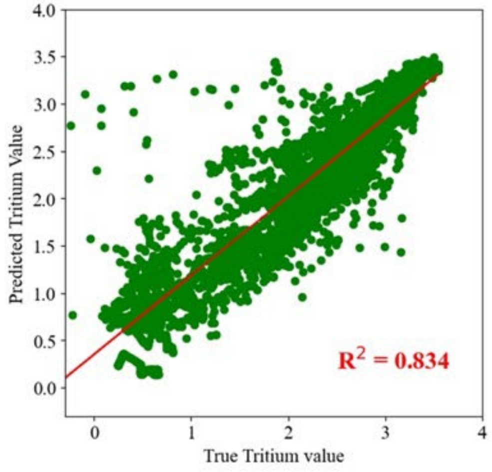
Elevation



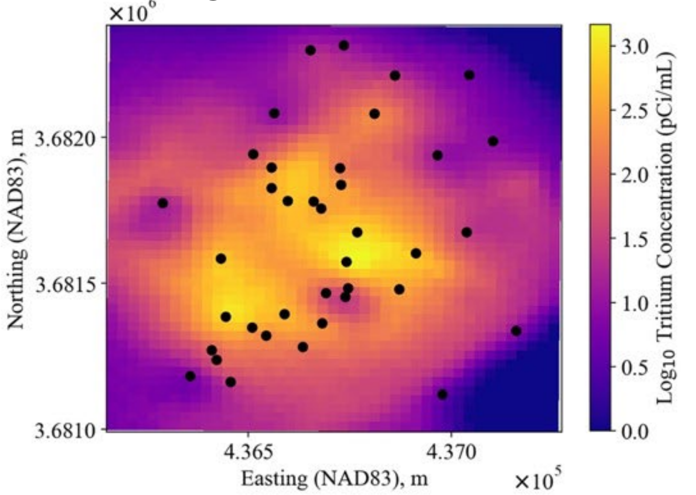
Groundwater table



SC → Tritium



Proxy-based Tritium map



PyLenM: Well Placement Optimization

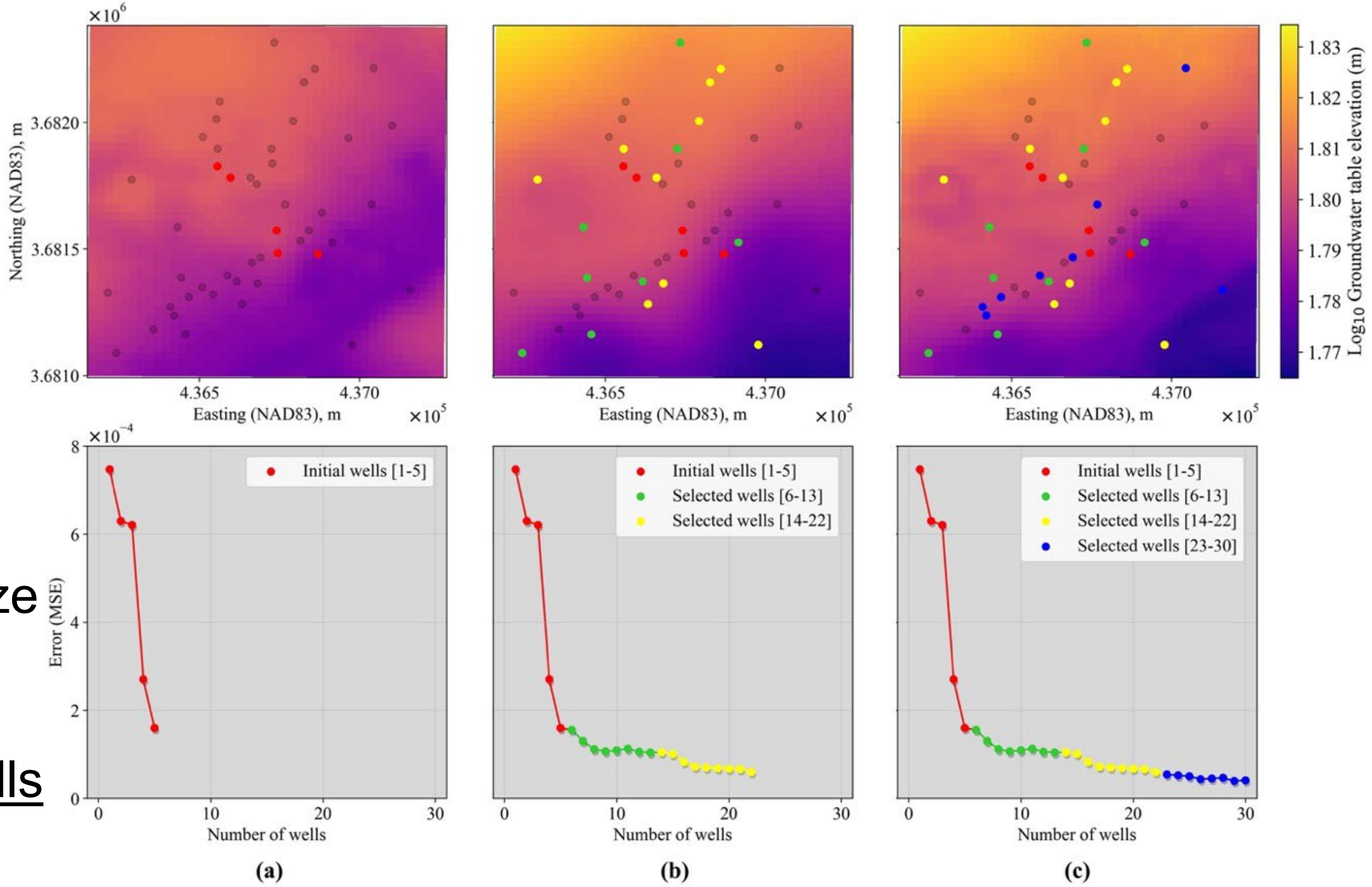
Sub-selection of wells for long-term monitoring

<u>Greedy algorithm</u>

- Reference map created using all the wells
- Interpolation with one additional well at a time
- Find the well that minimize the overall error

<u>Minimum-but-sufficient # wells</u>

- Error convergence



In situ Data Monitoring: Proxy-based Estimation

Water Table

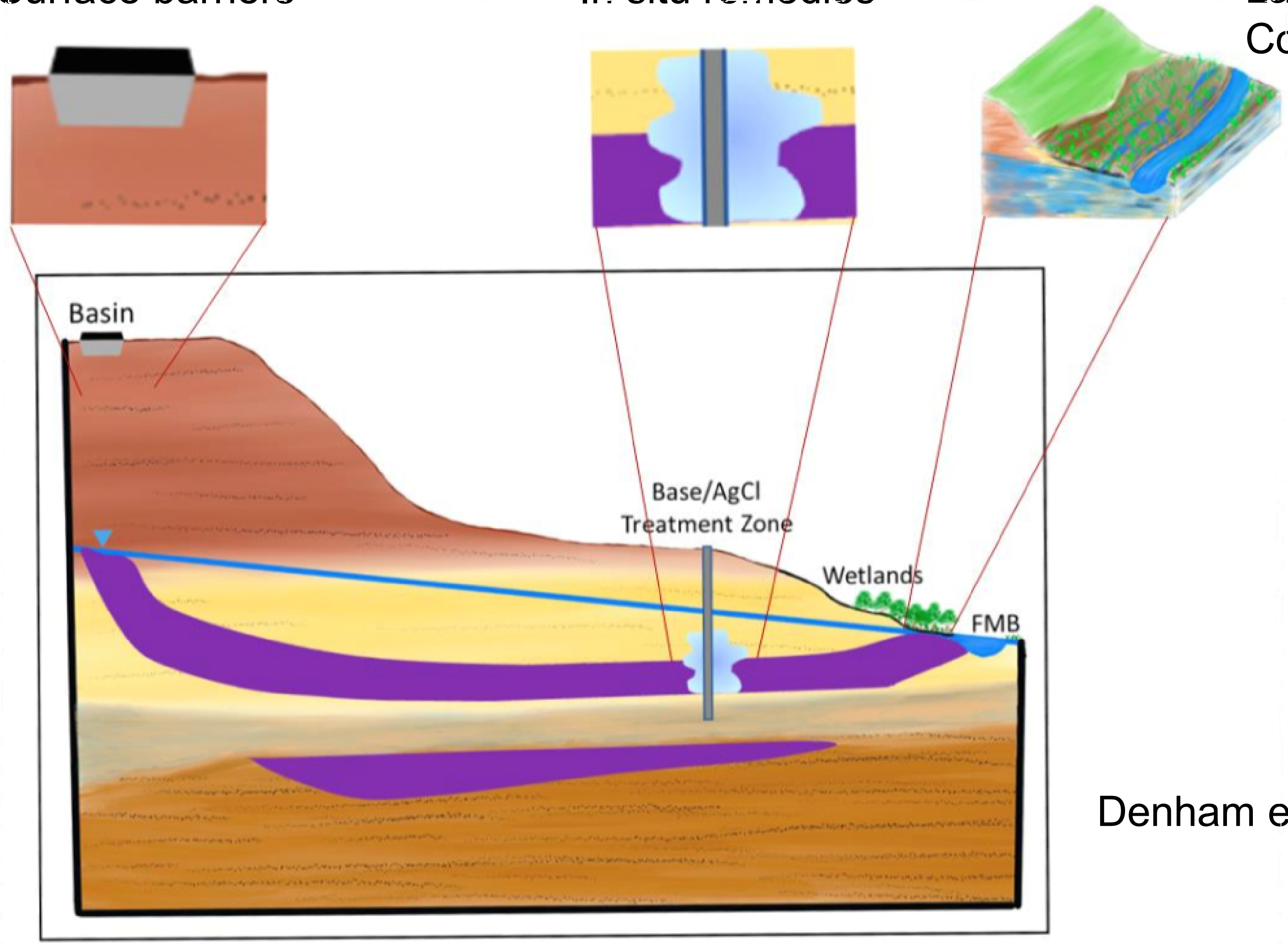
Tritium

Vulnerability Zone Concept

Source zone
Surface barriers

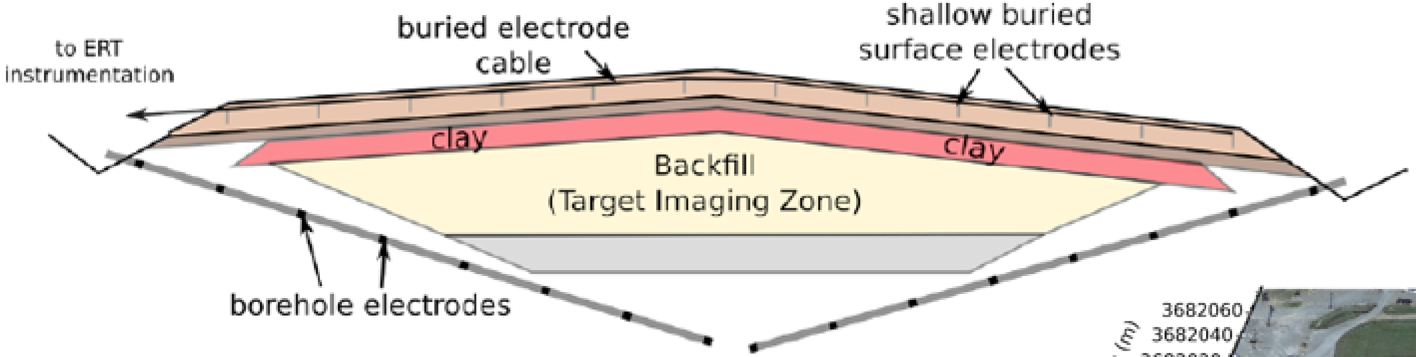
Treatment zone
In situ remedies

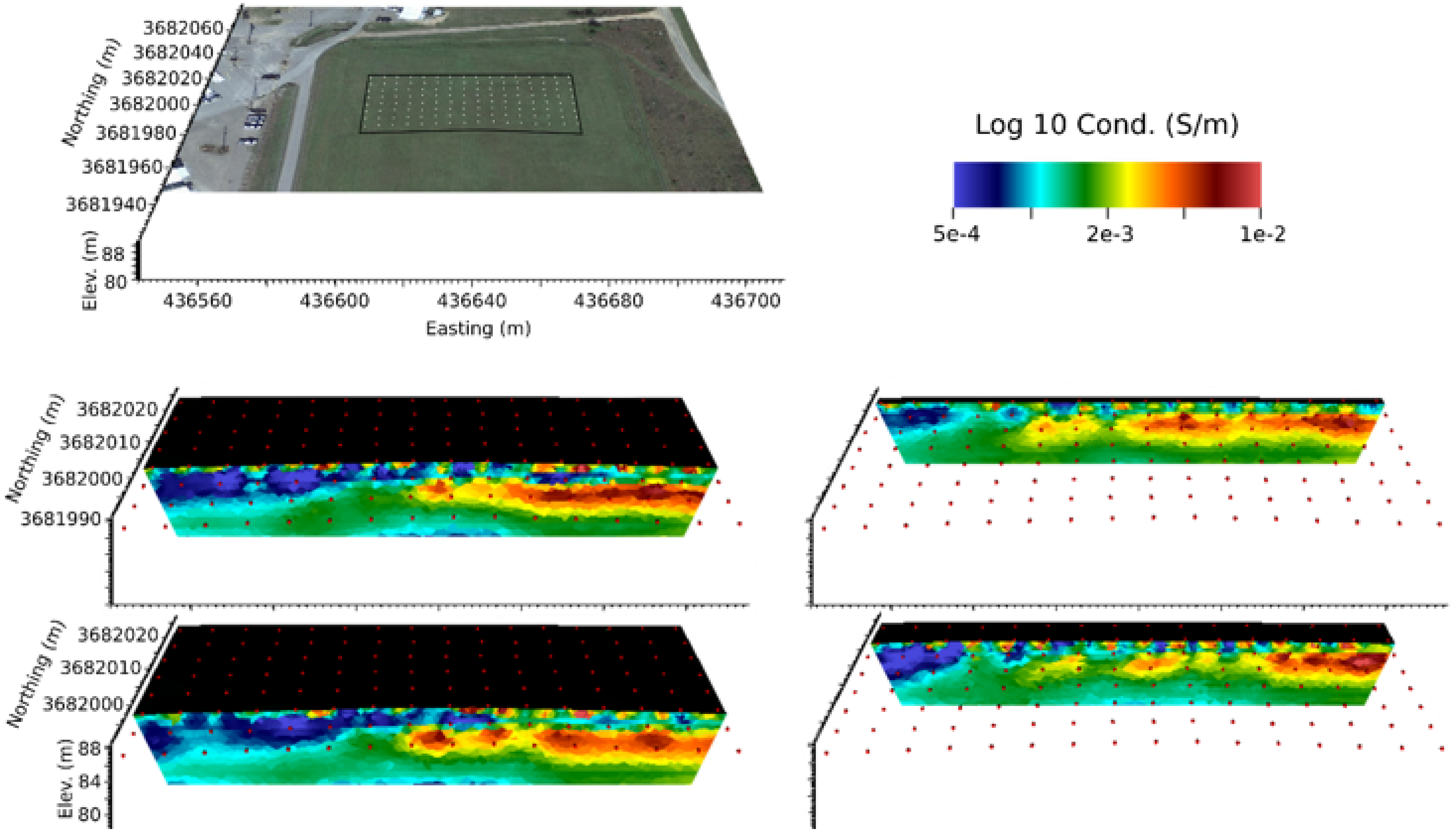
Seep zone/wetland
Last line of defense
Contaminant accumulation



Denham et al., 0220

Cap/Surface Barrier Monitoring





Cap/Surface Barrier

- Limit infiltration
- Concerns: plants, animals, erosions

Electrical Resistivity tomography monitoring

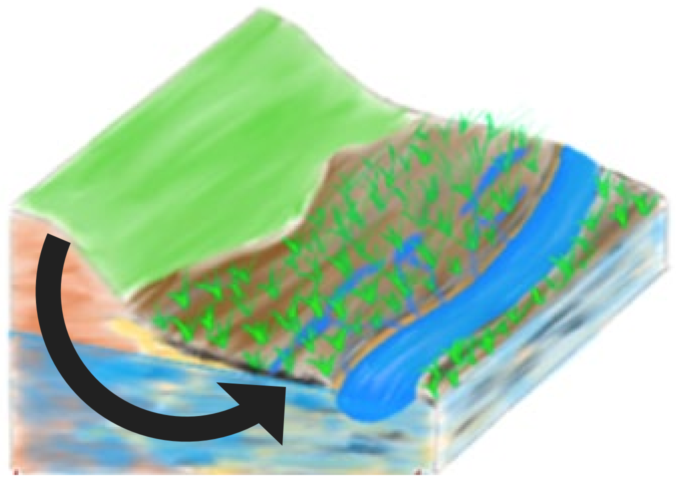
- Electrodes at and below the surface
- Image and detect anomalies continuously

Johnson et al., 2022

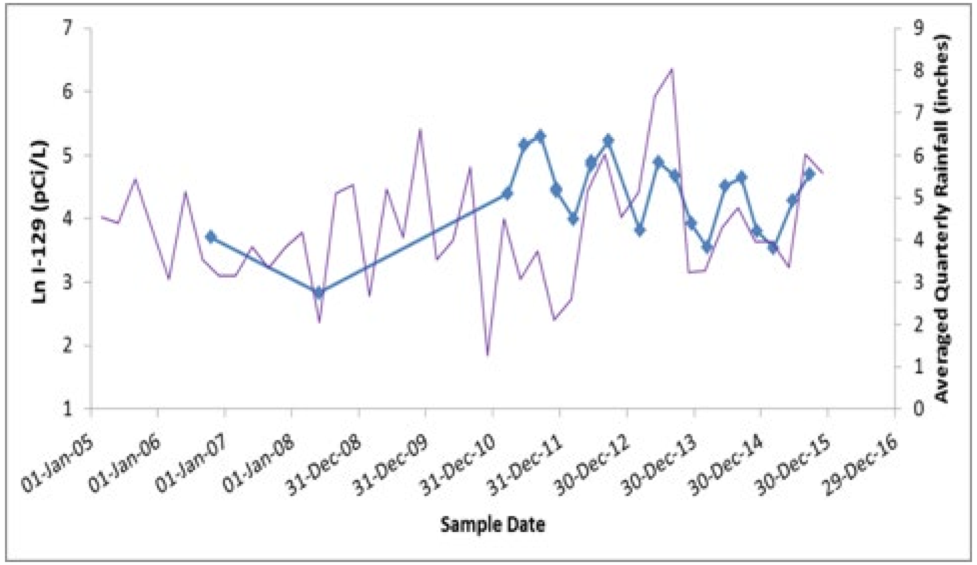
Groundwater Seep Zone Monitoring

Last line of defense
- Clay/organic-rich soil
- Sequester/accumulate contaminants

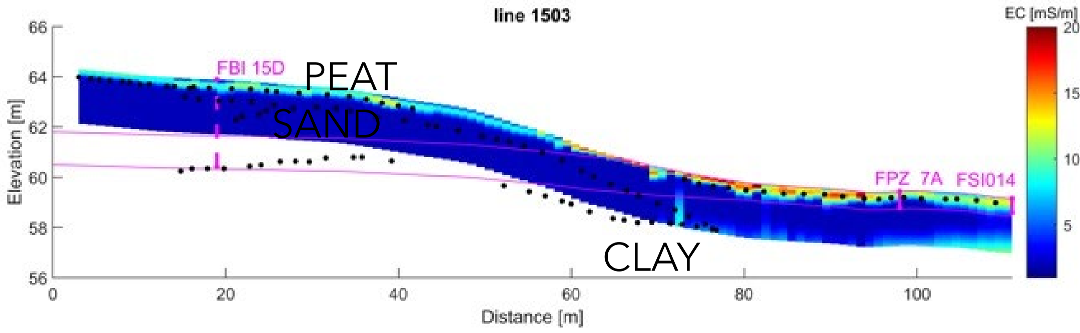
→ Vulnerability: changes in geochemistry etc



I-129 Concentration seasonal dynamics



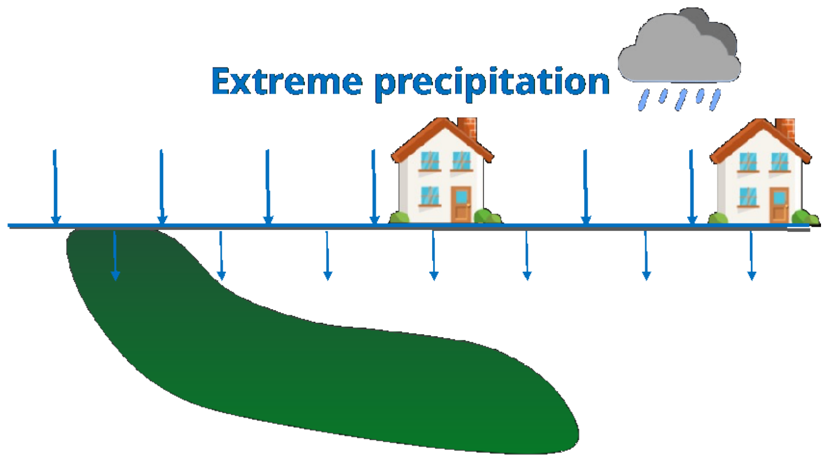
GPR/EM Subsurface Characterization



- Geochemical characterization
- Distributed sensor network
- Geophysics

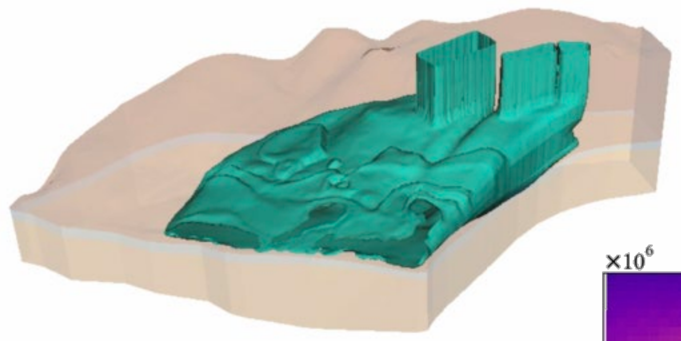
Simulation Intelligence: Simulations x ML/AI

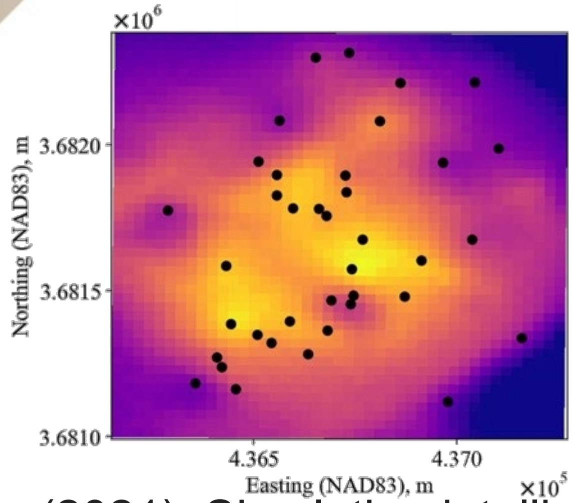
Climate Change Impact on Groundwater contamination
→ Emulator with Fourier Neural Operator



In collaboration with NASA Frontier Development Lab

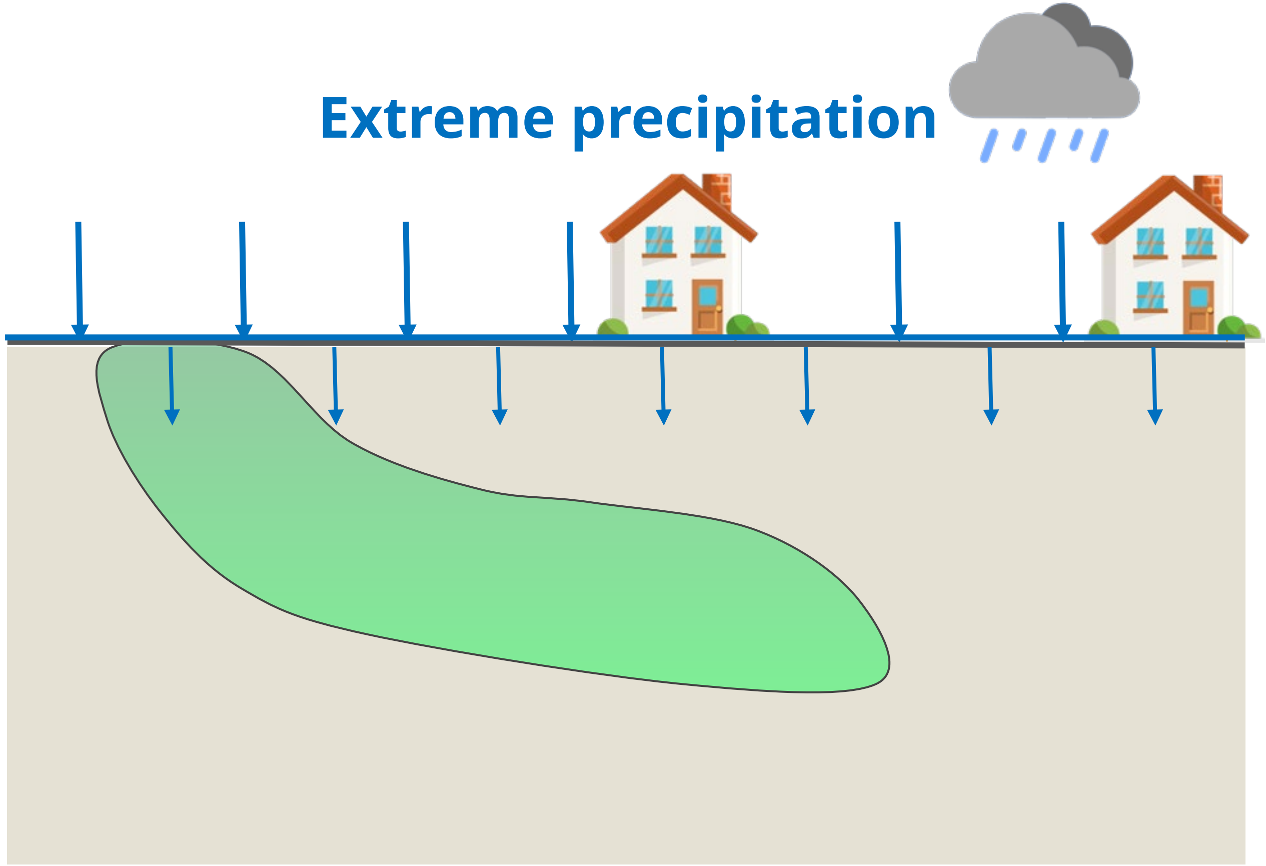
Physics-informed interpolation
→ Model-data integration with Bayesian hierarchical model





Lavin, A., Zenil, H., Paige, B., Krakauer, D., Gottschlich, J., Mattson, T., ... & Pfeffer, A. (2021). Simulation intelligence: Towards a new generation of scientific methods. *arXiv preprint arXiv:2112.03235*.

Climate Change Impacts on Contamination



Higher precipitation

- Re-mobilize residual contaminants?
- Dilute concentrations?

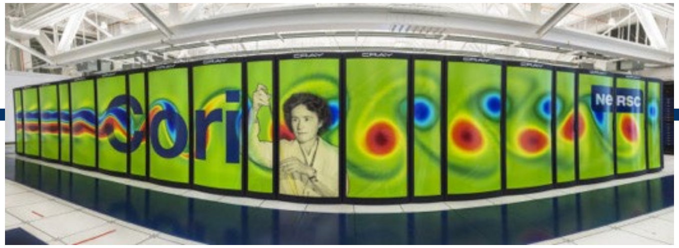
→ Change management strategies?

→ Change monitoring configuration?

- But computation is pretty heavy
- We can't run simulation on laptops

Wang, L., Kurihana, T., Meray, A., Mastilovic, I., Praveen, S., Xu, Z., ... & Wainwright, H. (2022). Multi-scale Digital Twin: Developing a fast and physics-informed surrogate model for groundwater contamination with uncertain climate models. *arXiv preprint arXiv:2211.10884*.

Deep Learning-based Emulator: Digital Twin



HPC Clusters

Parameters from PDF

$\{p_1, p_2 \ldots . p_N\}$

Simulations:

$\phi = f(p)$

$\{\phi_1, \phi_2, \ldots \phi_N\}$

Regressions:

$\phi \sim f(p)$

Emulator predictions

$\phi = f_{emulate}(p)$

Statistical representation of physical models

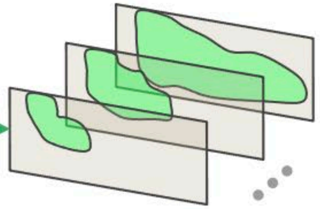
Input:

Climate + Subsurface Parameters

Emulator

Output:

Plumes



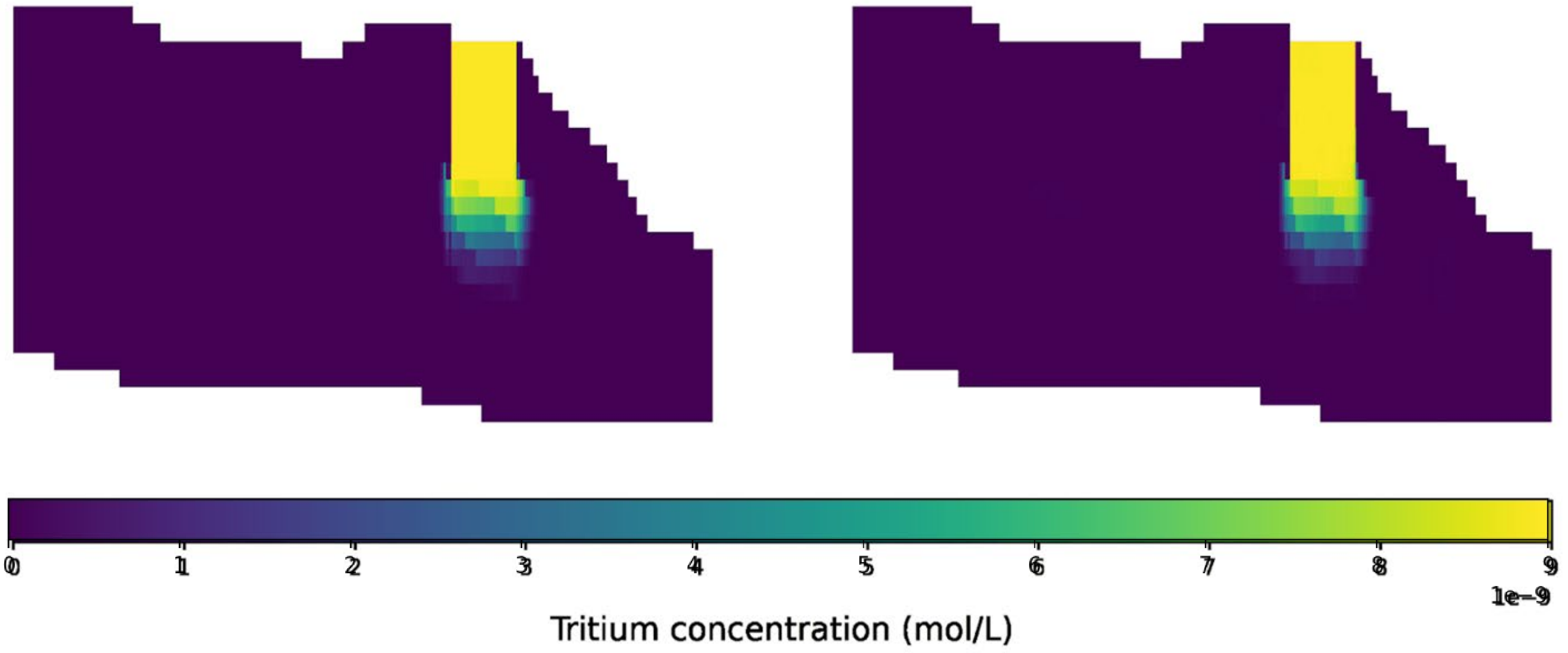
Deep Learning: Enhanced Fourier Neural Operator

Emulator-based Plume Prediction

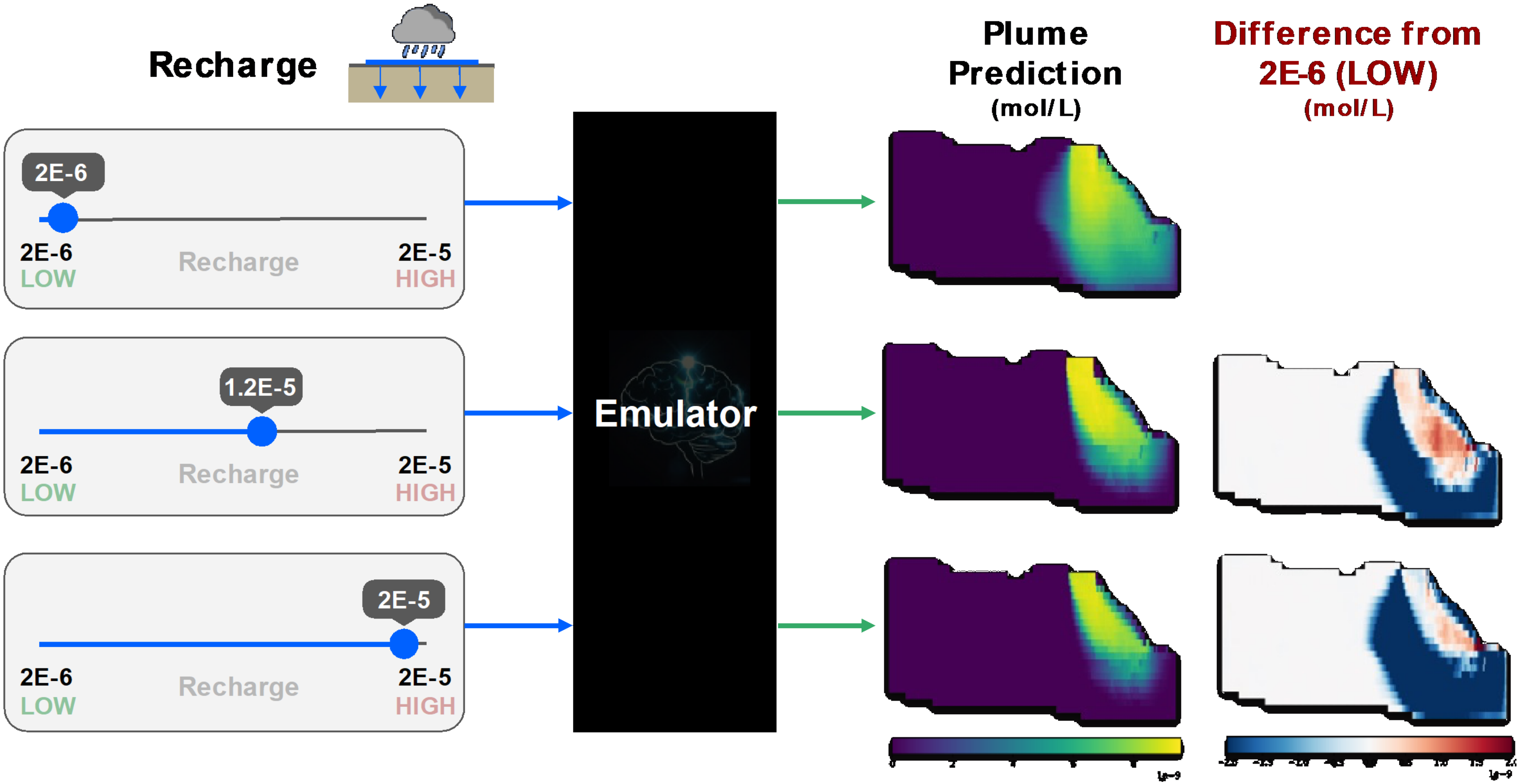
1955

Contaminant Concentration

TRUTH | **PREDICTION**

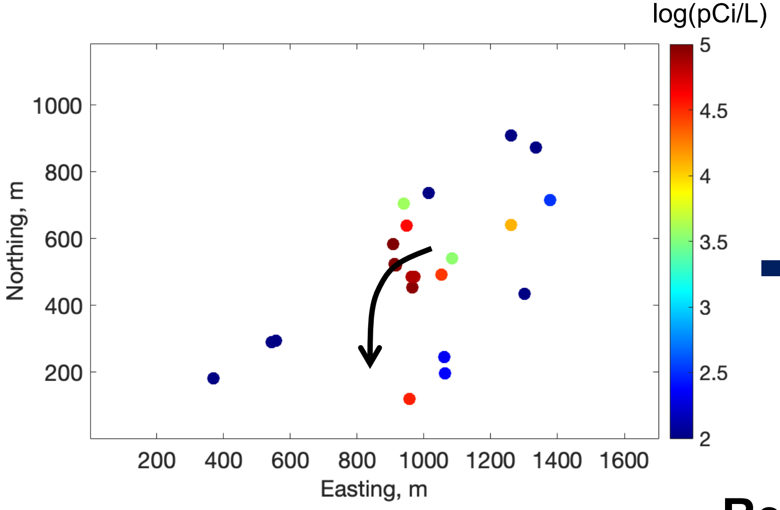


Off-Line Climate Change Assessment

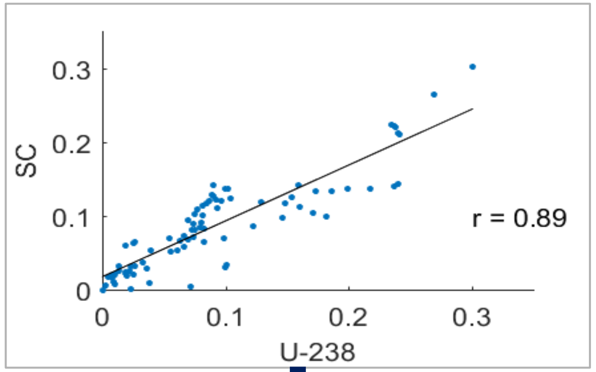


Physics-informed Spatiotemporal Interpolation

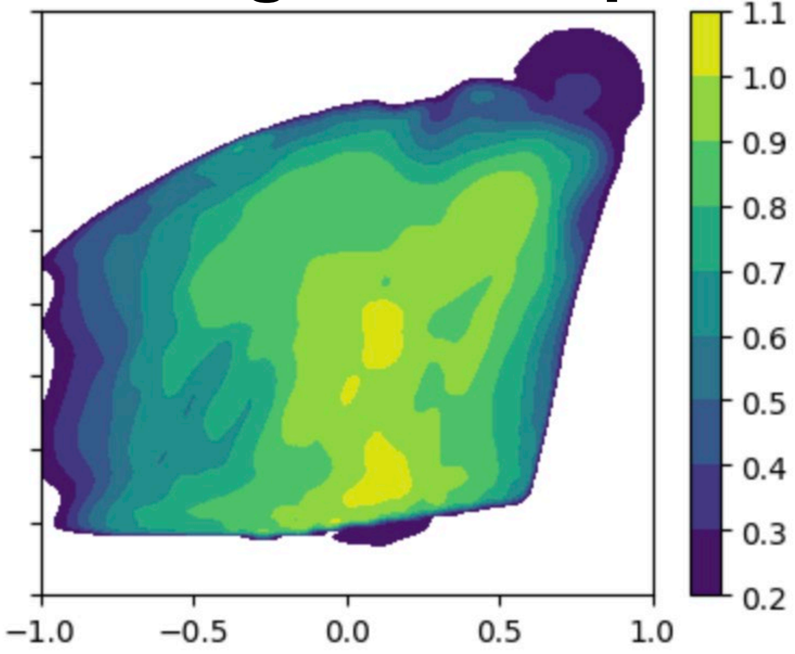
Concentrations at Wells (2015)



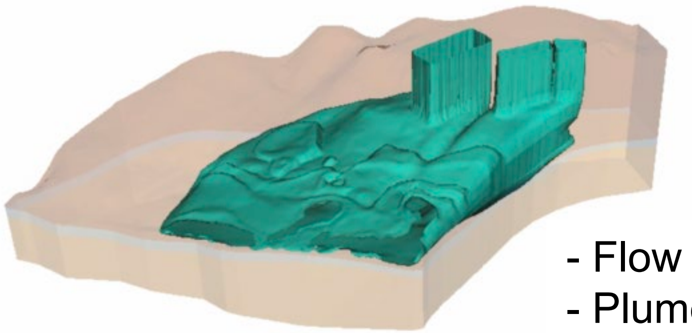
In situ Sensor Data



Integrated map



Reactive Transport Model



- Flow direction
- Plume source

Multiscale data integration using Bayesian hierarchical model with Gaussian Process Models, Wainwright et al. (2017)

Wainwright et al., 2019

Pathway to Adaptation

- **Understand regulations**
  - Stepwise implementation: in situ sensor deployment
  - Reducing sampling frequencies is easier
  - Then reducing # variables and reducing # wells
- **Emphasize additional safety assurance**
  - Continuous monitoring → early warning, explaining anomalies
  - Guide monitoring strategies (e.g., climate change)
- **Autonomous monitoring → AI-assisted monitoring**
  - Anomaly detection → instrument failure, system changes
  - Realistic plume visualization
  - Digital twin → simulate what can happen in the future

Summary

- **Motivation: Sustainable remediation**
  - Net environmental impact: contaminant removal vs other side effects
  - Long-term institutional controls with passive remediation, monitored natural attestation
- **ALTEMIS Project**
  - **Long-term monitoring with new sensor technologies**
    - In situ real-time monitoring with low-cost low-maintenance sensors
    - Vulnerable concepts to guide key technology implementation strategies
  - **PyLenM: Python for Long-term Environmental Monitoring**
    - ML framework from data exploration to mapping and well optimization
    - Open-source python package for groundwater data analytics
  - **Simulation Intelligence: Simulations x ML/A**
    - Emulators for evaluating climate change impact on residual contamination
    - Physics-informed spatial interpolation (physics-informed monitoring)
  - **Pathway to adaptation**

Thank You!

Contact

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Acknowledgment

DOE Office of Environmental Management