Define End-State and Optimize Monitoring Program Using High-Performance Computing

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11/26/2019

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DOE-EM Sites: Progress

Approximately $6B /year

107 major sites (1995) → 16 sites (2016)

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Challenges

Remaining sites….

- **Complex contamination**
  – Multiple radionuclides, heavy metals (Hg)
  – VOC and other organic compounds
- **Hard/expensive to access**
  – Deep vadose zones
  – Increased drilling cost
- **Large volume with low contamination**
  – Not practical to remove soil (too much $$/waste)
  – Treatment/removal technologies are not effective

Environmental Monitoring

- Ensure public safety
- Prepare for liability issues

Beneficial for both residents and site operators

THE DENVER POST

OPINION

Activists ignore the science that says Rocky Flats National Wildlife Refuge is safe

By **VINCENT CARROLL** | The Denver Post
PUBLISHED: June 16, 2017 at 12:00 pm | UPDATED: June 16, 2017 at 2:36 pm

Andy Cross, Denver Post file

A herd of elk walks though a valley at the Rocky Flats National Wildlife Refuge on Sept. 25, 2015.

Good example: Monitoring data proves that the site is safe to dismiss false claims

the japan times

Reporters take photos in the basement of the planned relocation site for the Tsukiji fish market in Tokyo's Toyosu area in September. | KYODO

NATIONAL

Chemicals exceeding standards again are detected at new site of fish market in Toyosu

Bad example: Data anomaly cannot be explained → extra >$100M

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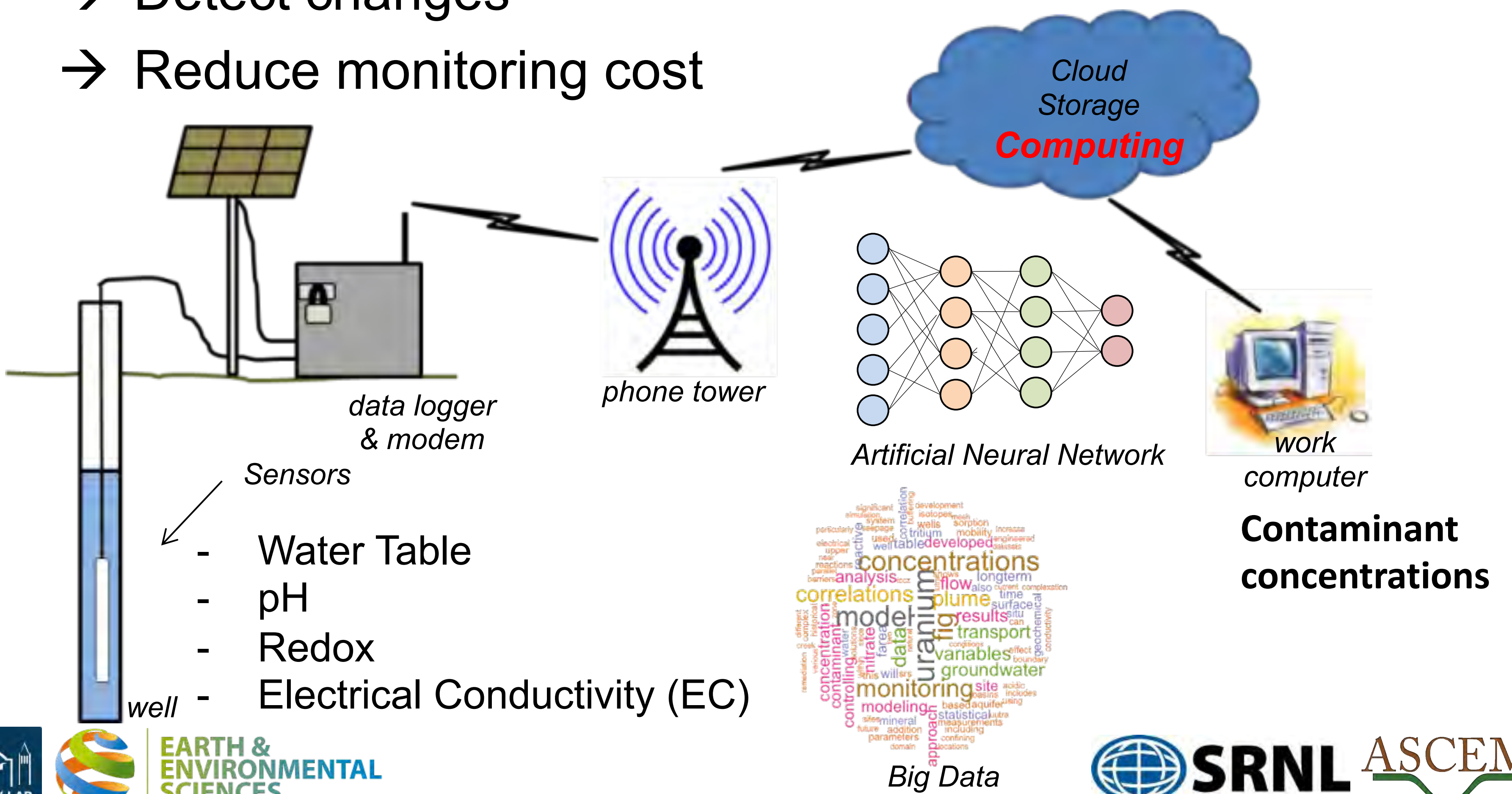
Research Goals

- Transition from **active** to **passive** remediation and **monitored natural attenuation**
  - **SRS F-Area (2004) $12M/yr → $1M/yr**
- Improve **long-term monitoring**
  - Great portion of life cycle cost (>$10M/yr)
  - Detect new leaks/migration
- Ensure **long-term stability** of plumes
  - Climate change?

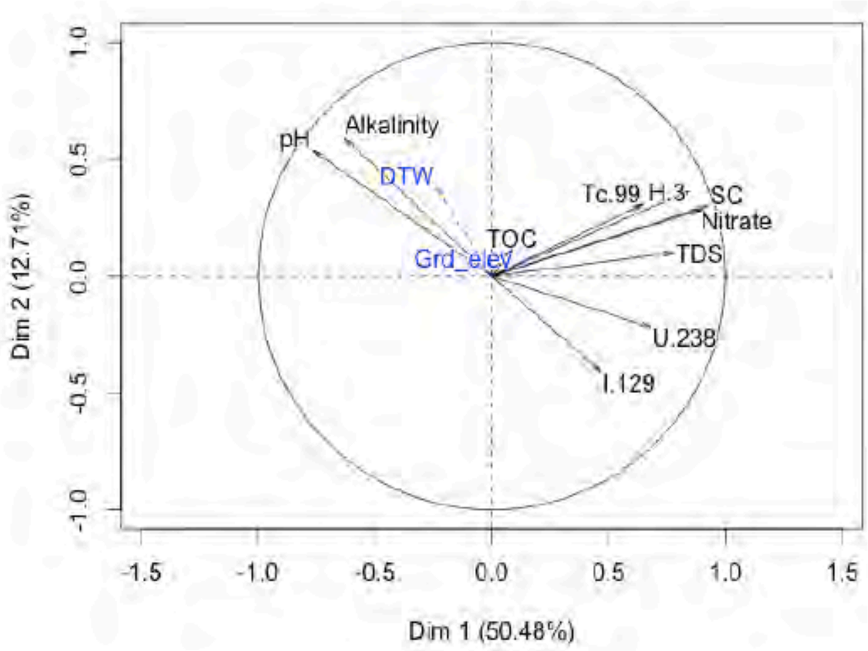
New Paradigm of Long-Term Monitoring

- In situ sensors, wireless network, cloud computing
  - → Autonomous continuous monitoring
  - → Detect changes
  - → Reduce monitoring cost

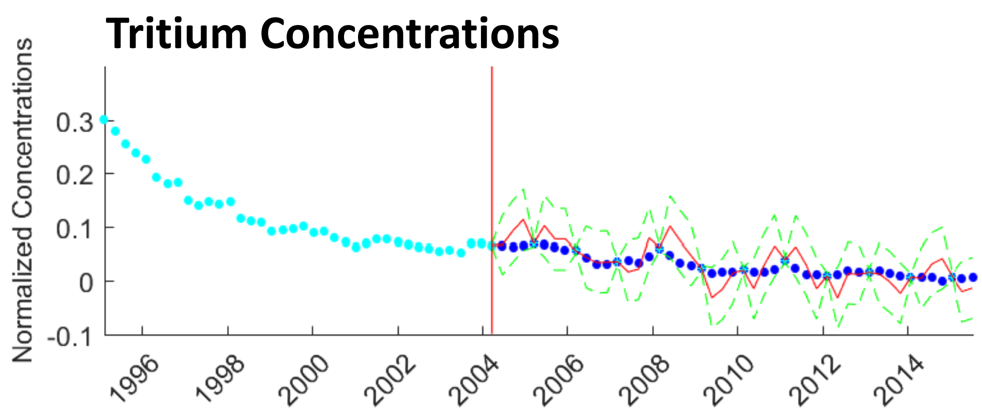


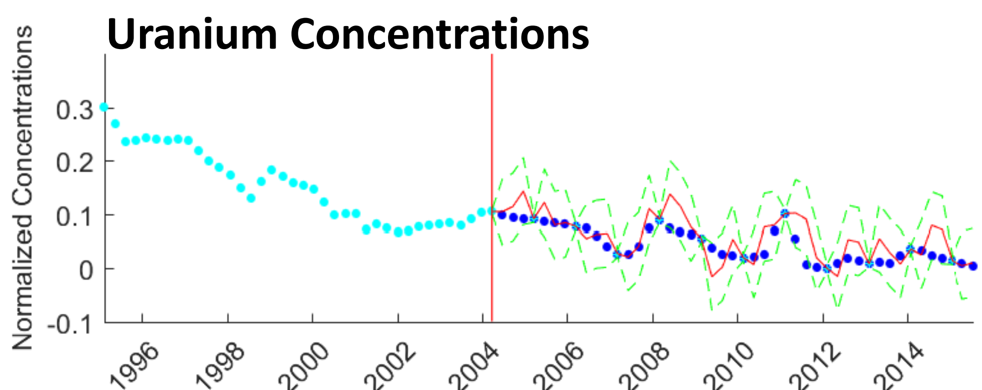
Data Analytics for Monitoring

- Big Data analytics
  - e.g., Principle component analysis (PCA)
  - System understanding
  - Master variables vs contaminant conc.



- Kalman filtering
  - In situ real-time estimation of contaminant concentration





Schmidt et al. (2018, EST)

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Big Interest in Environmental Monitoring

Environmental Science & Technology

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In Situ Monitoring of Groundwater Contamination Using the Kalman Filter

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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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New Algorithm Provides Real-Time Monitoring Of Groundwater Pollutants

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Efficiency & Environment

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

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

GCN The Technology that Drives Government IT

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Machine learning improves contamination monitoring

BY MATT LEONARD | AUG 14, 2018

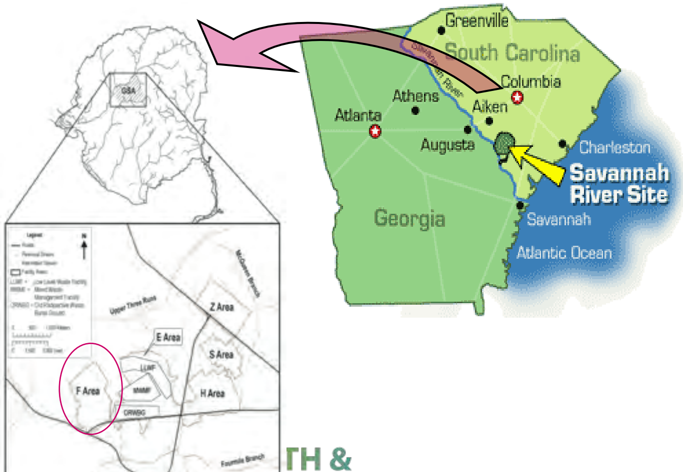
Because groundwater is susceptible to pollution from automotive fuel, fertilizer or naturally occurring substances like iron, the Environmental Protection Agency and its state-level counterparts conduct annual or quarterly sampling and analysis.

Modeling for Supporting Monitoring

- Confirm the correlations: Master variables vs contaminant concentrations
- Climate resiliency: how to place monitoring wells or what to expect in the response to climate changes
- (In development) Monitoring well placement based on simulated plume evolutions

Demonstration: SRS F-Area

- **Disposal activities**:
  - Disposal of low-level radioactive, acid waste solutions (1955–1989)
  - Acidic plume with radionuclides (pH 3–3.5, U, ^{90}Sr, ^{129}I, ^{99}Tc, ^{3}H)
- **Remediation approaches**
  - Pump & treat ($12M/yr) → Passive remediation (funnel-gate system for pH neutralization; $1M/yr)
  - Natural attenuation: long-term remediation alternative



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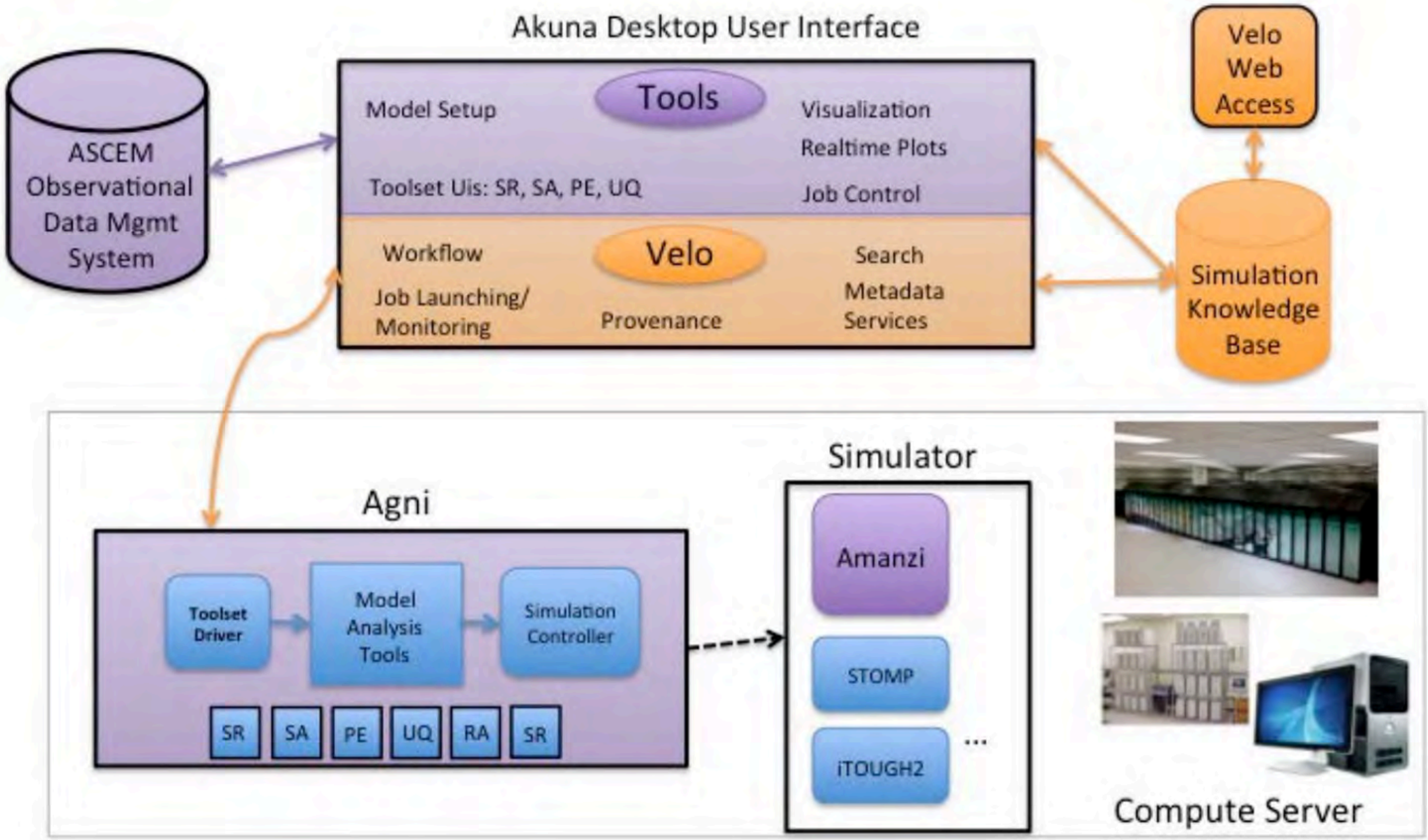
Virtual Test Bed: ASCEM Overview

Advanced Simulation Capability for Environmental Management



Geochemistry Development

- Complex geochemistry
  - pH Dependent
  - Aqueous complexation
  - Surface complexation
  - Mineral dissolution/precipitation
  - Cation exchange
  - Decay

	$\log_{10}$ K (25° C)
[1] Equilibrium Surface Complexation	
$(>SO)UO_2^+ \leftrightarrow >SOH - H^+ + UO_2^{2+}$	-0.44

[2] Cation Exchange	K (25 C)
$NaX \leftrightarrow Na^+ + X^-$	1.0
$CaX_2 \leftrightarrow Ca^{2+} + 2X^-$	0.316
$AlX_3 \leftrightarrow Al^{3+} + 3X^-$	1.71
$HX \leftrightarrow H^+ + X^-$	0.025

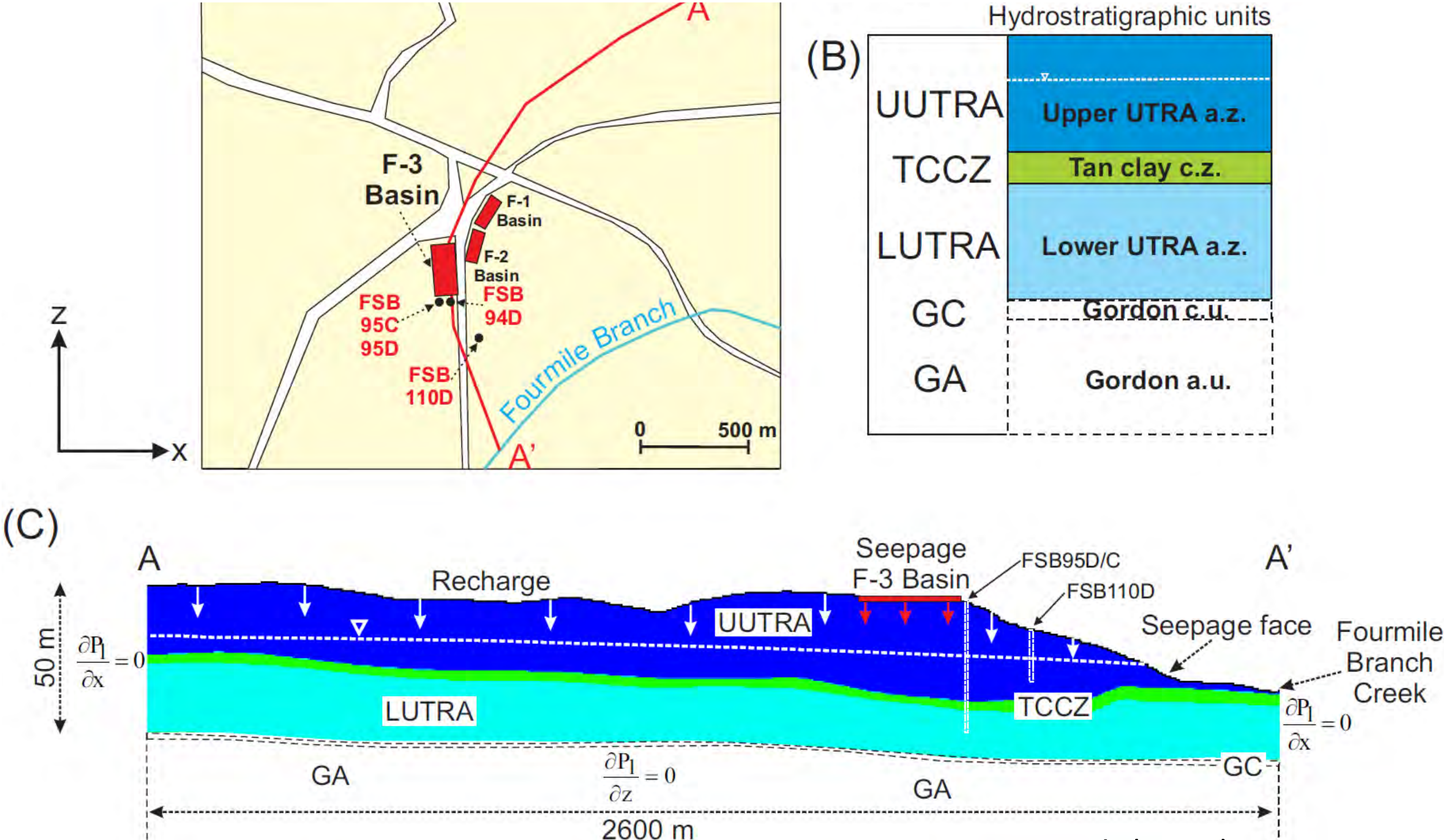
	$\log_{10}$ K (25° C)	Ref.
Quartz $\leftrightarrow SiO_2(aq)$	-3.7501	(1)
Kaolinite $\leftrightarrow 2Al^{+3} + 2SiO_2(aq) + 5H_2O - 6H^+$	7.57	(2)
Goethite $\leftrightarrow Fe^{+3} + 2H_2O - 3H^+$	0.1758	
Schoepite $\leftrightarrow UO_2^{+2} + 3H_2O - 2H^+$	4.8443	(1)
Gibbsite $\leftrightarrow Al^{+3} + 3H_2O - 3H^+$	7.738	(3)
Jurbanite $\leftrightarrow Al^{+3} + SO_4^{-2} + 6H_2O - H^+$	-3.8	(4)
Basaluminite $\leftrightarrow 4Al^{+3} + SO_4^{-2} + 15H_2O - 10H^+$	22.251	(4)
Opal $\leftrightarrow SiO_2(aq)$	-3.005	(5)

Aqueous complexiation

Reaction	$\log_{10}$ K (25° C)
$OH^- \leftrightarrow H_2O - H^+$	13.99
$AlOH^{2+} \leftrightarrow Al^{3+} + H_2O - H^+$	4.96
$Al(OH)_2^+ \leftrightarrow Al^{3+} + 2H_2O - 2H^+$	10.59
$Al(OH)_3(aq) \leftrightarrow Al^{3+} + 3H_2O - 3H^+$	16.16
$Al(OH)_4^- \leftrightarrow Al^{3+} + 4H_2O - 4H^+$	22.88

(and more)

Flow/Transport Model



Bea et al. (2013)

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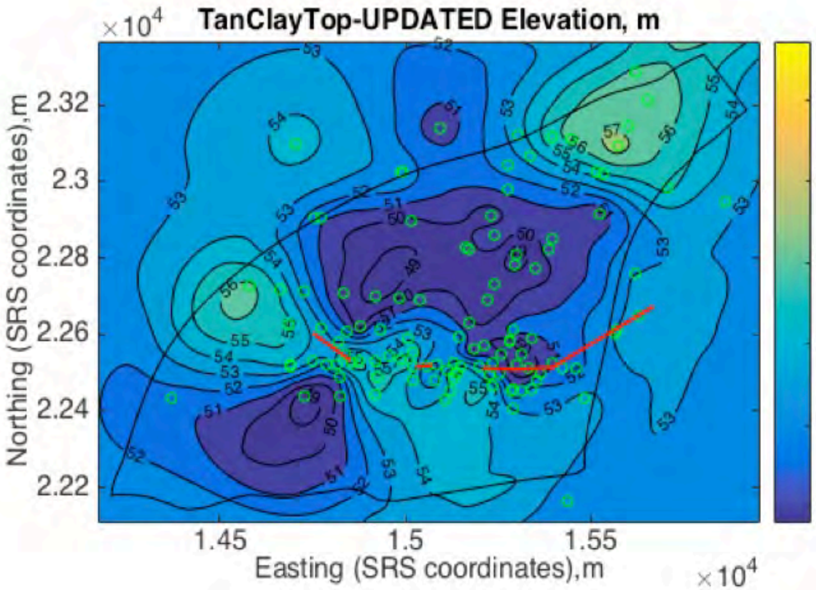
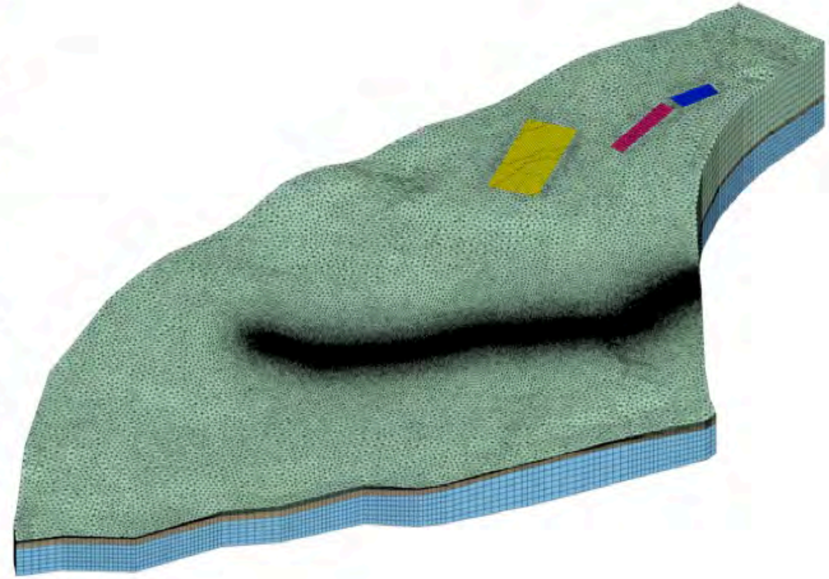
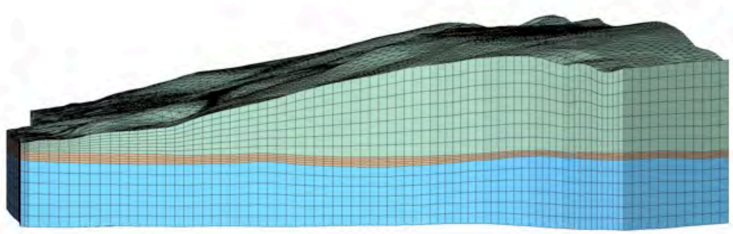
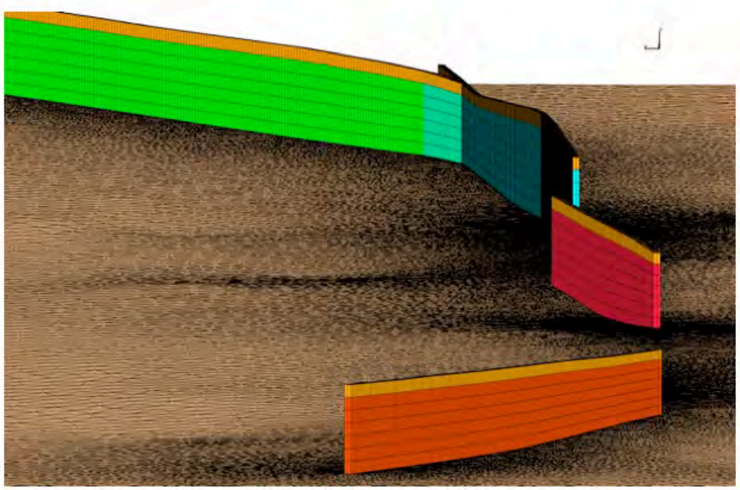
3D Mesh Development

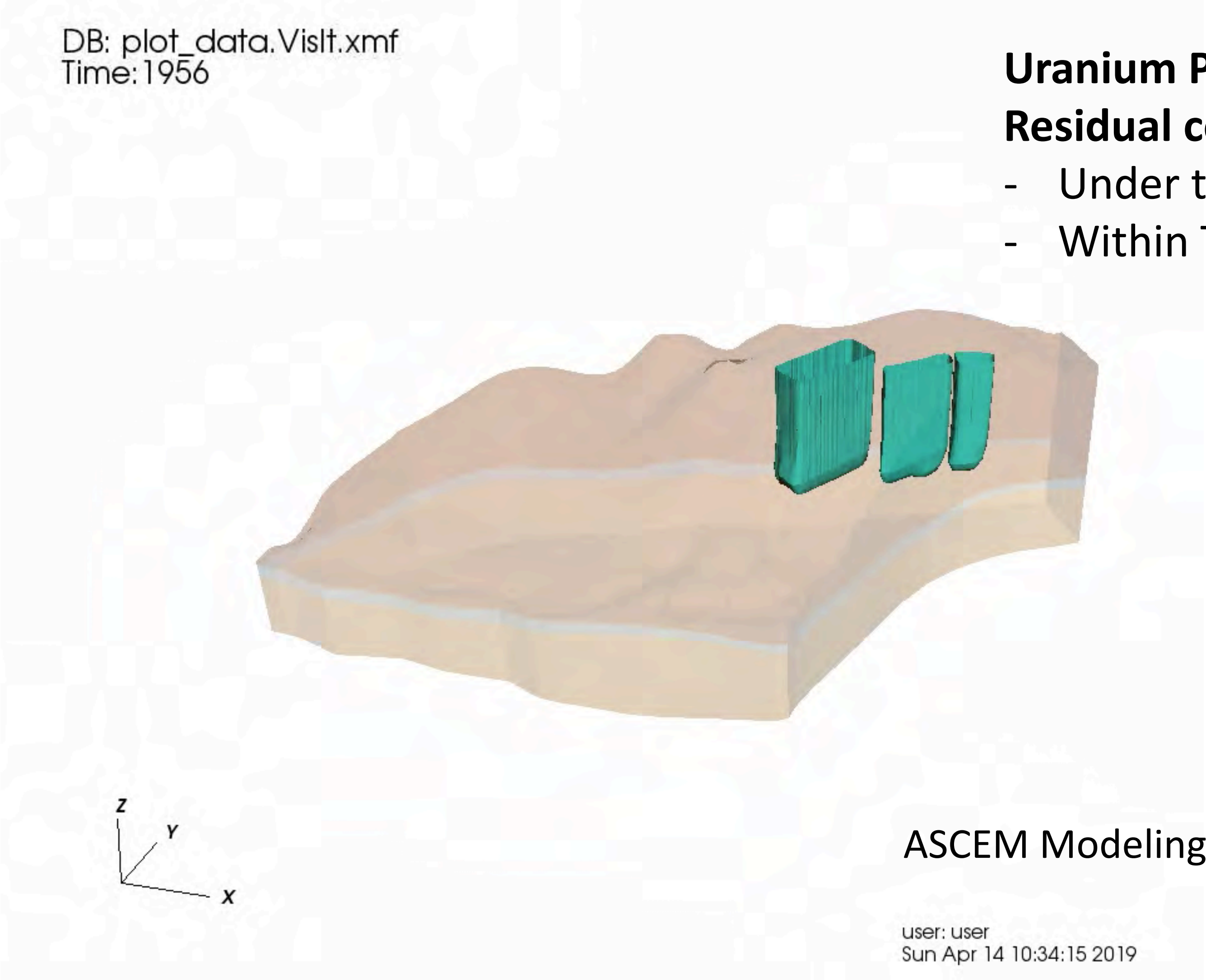








Uranium Plume Evolution



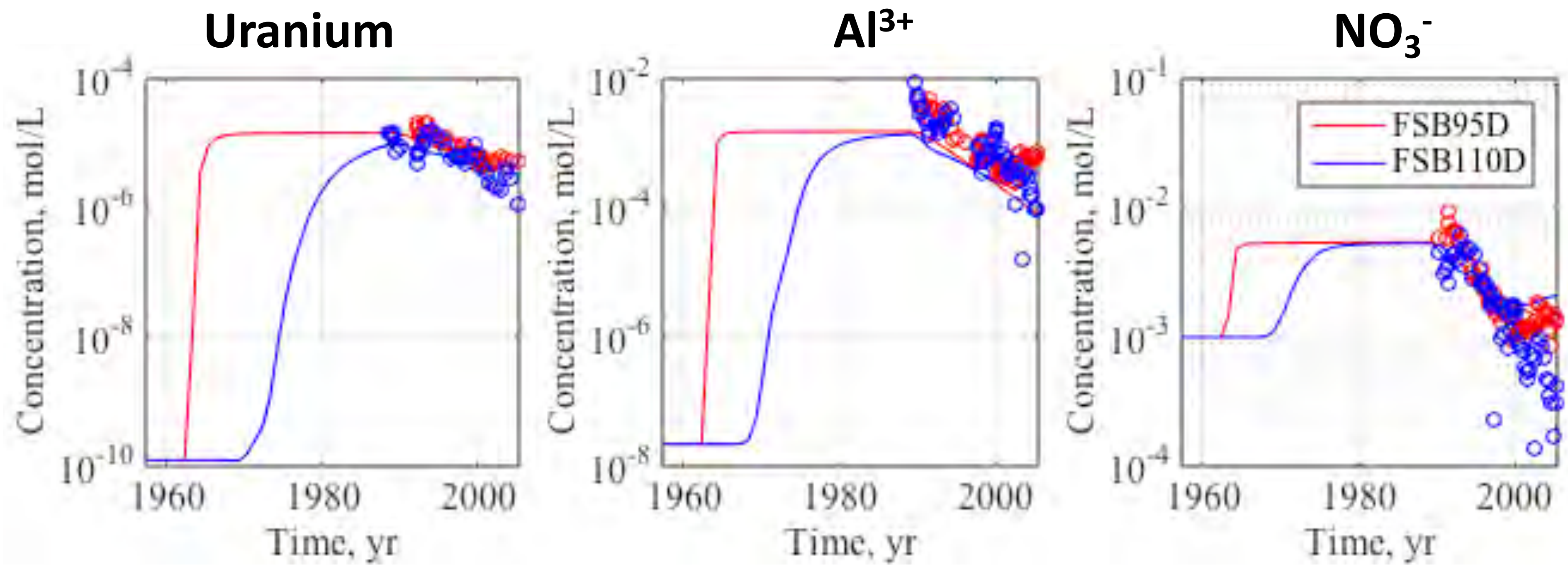
Uranium Plume:

Residual contaminants

- Under the basins
- Within Tan Clay

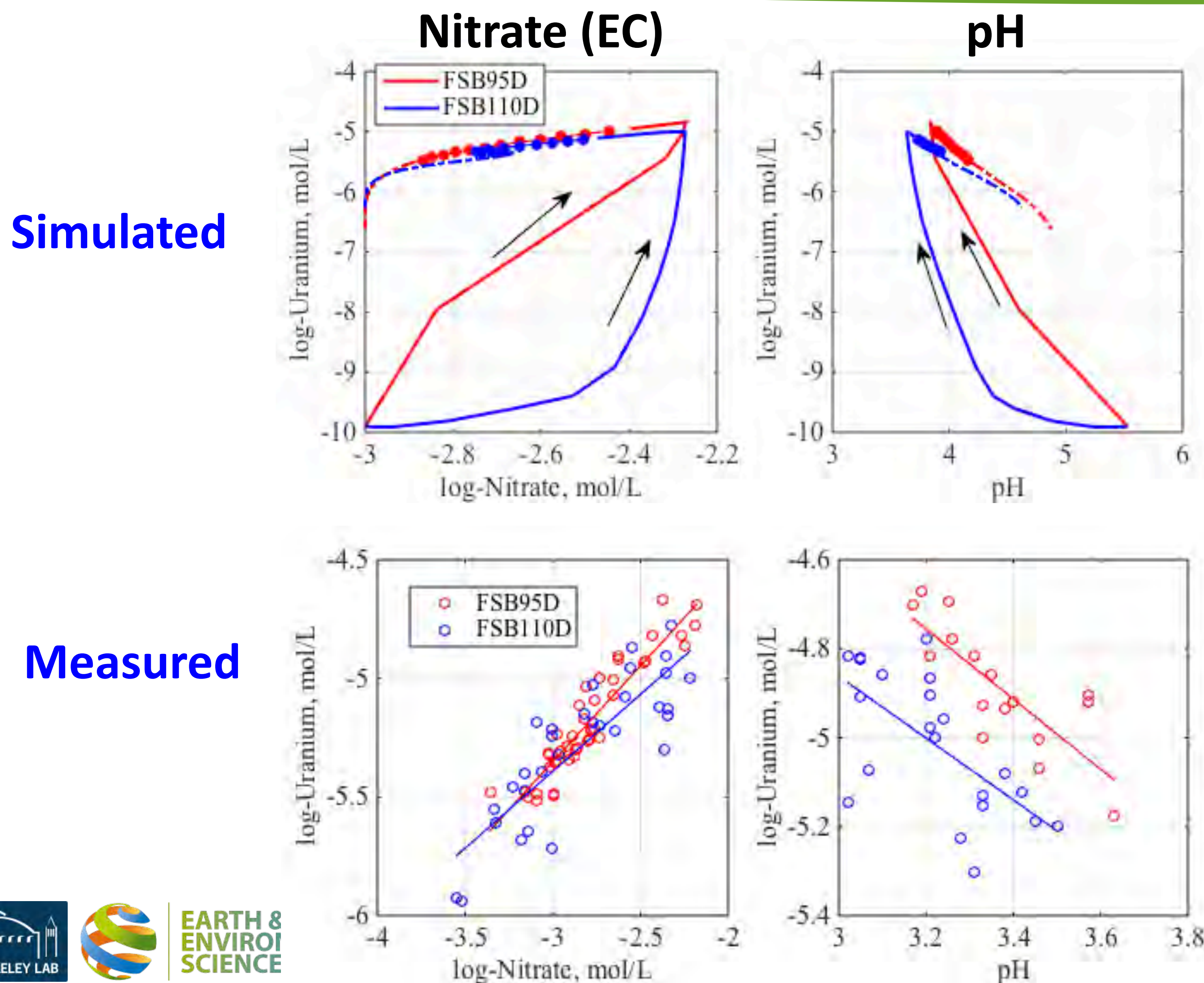
ASCEM Modeling Results

Validation with Observations



Good agreement with observations

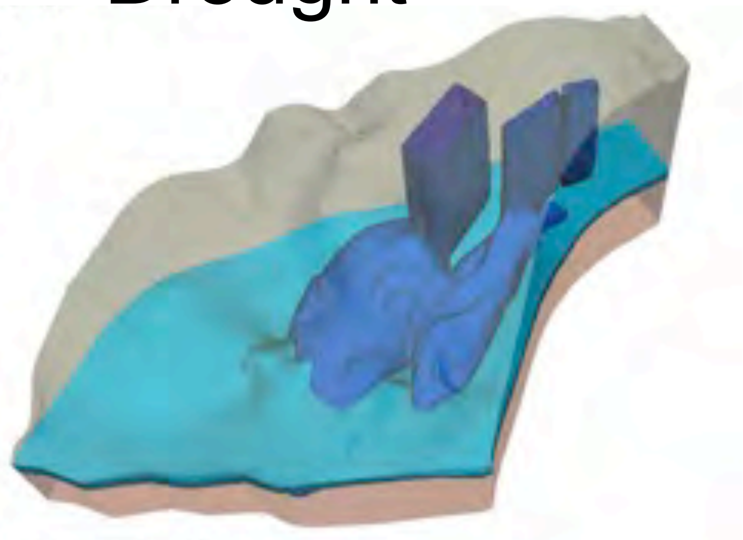
In situ Monitoring: Master Variables vs U Conc.



Resiliency to Climate Disturbances

Extreme Events

- Flooding
- Drought



(f) 2050

Savannah River Flooding, 2016

What will happen to residual contaminants?

Technical Initiative in SURF and ITRC

- How to prepare for climate change in sustainable remediation

Resiliency to Climate Disturbances

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journal homepage: www.elsevier.com/locate/jconhyd

Climate change impact on residual contaminants under sustainable remediation

Arianna Libera[a,*], Felipe P.J. de Barros[a], Boris Faybishenko[b], Carol Eddy-Dilek[c], Miles Denham[d], Konstantin Lipnikov[e], David Moulton[e], Barbara Maco[f], Haruko Wainwright[b]

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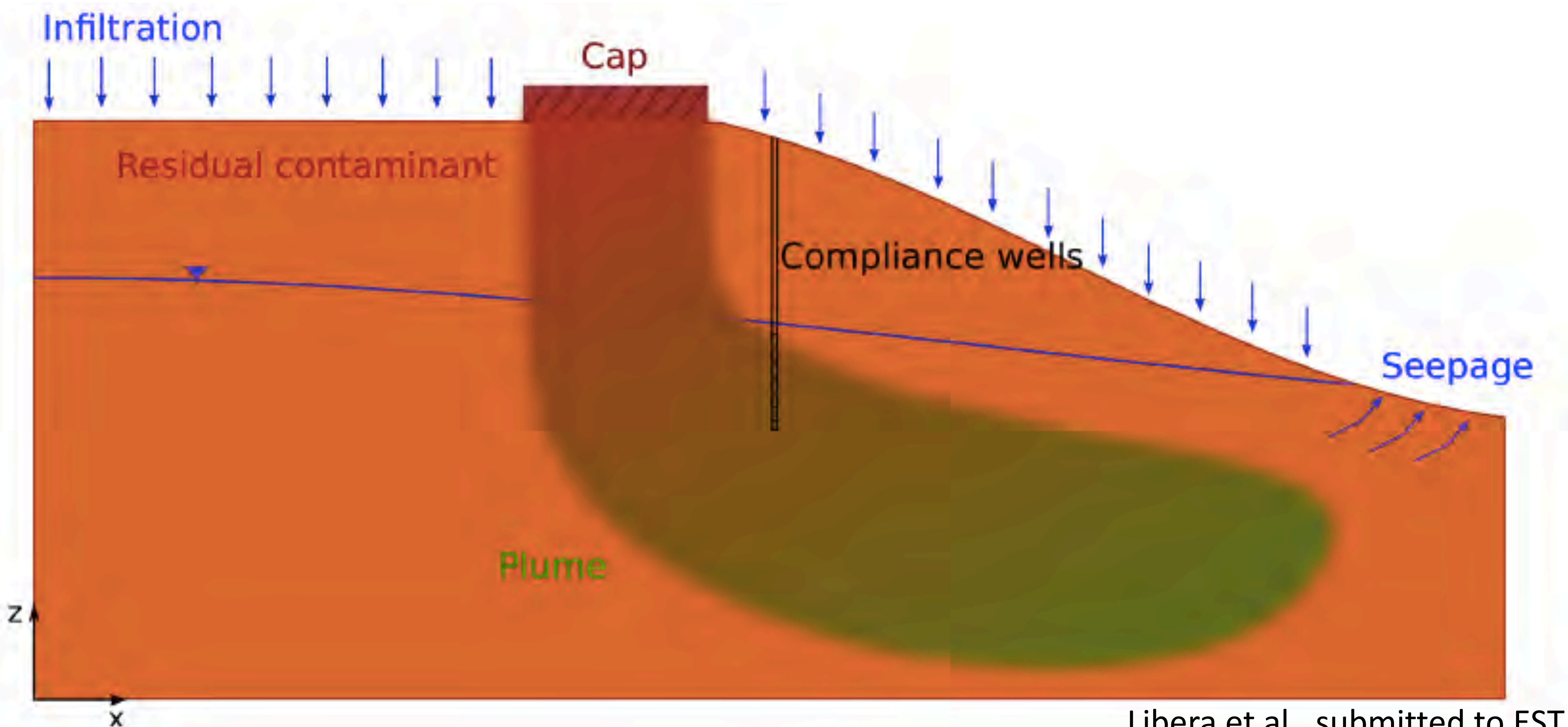
Flooding, Drought Impact

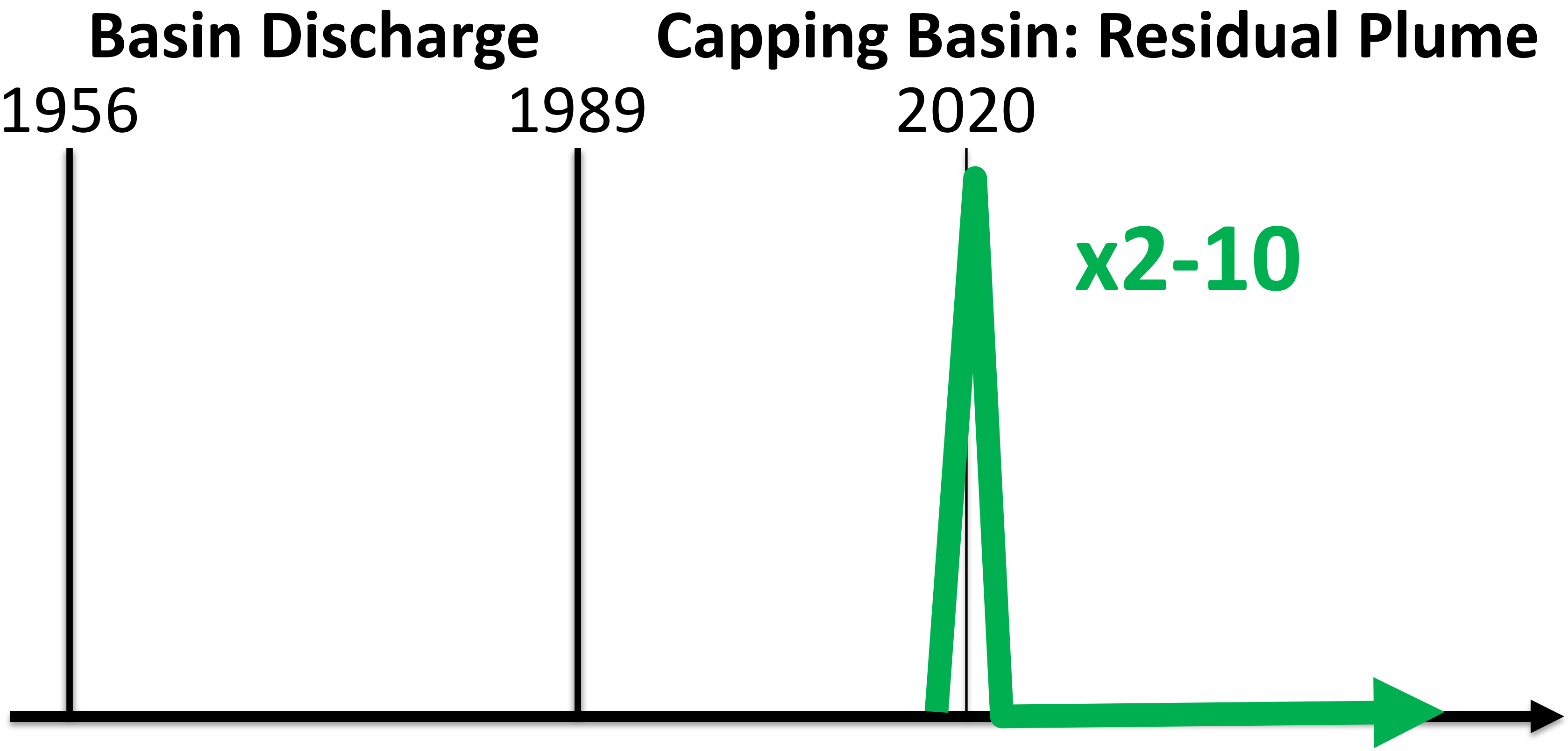


Libera et al., submitted to EST

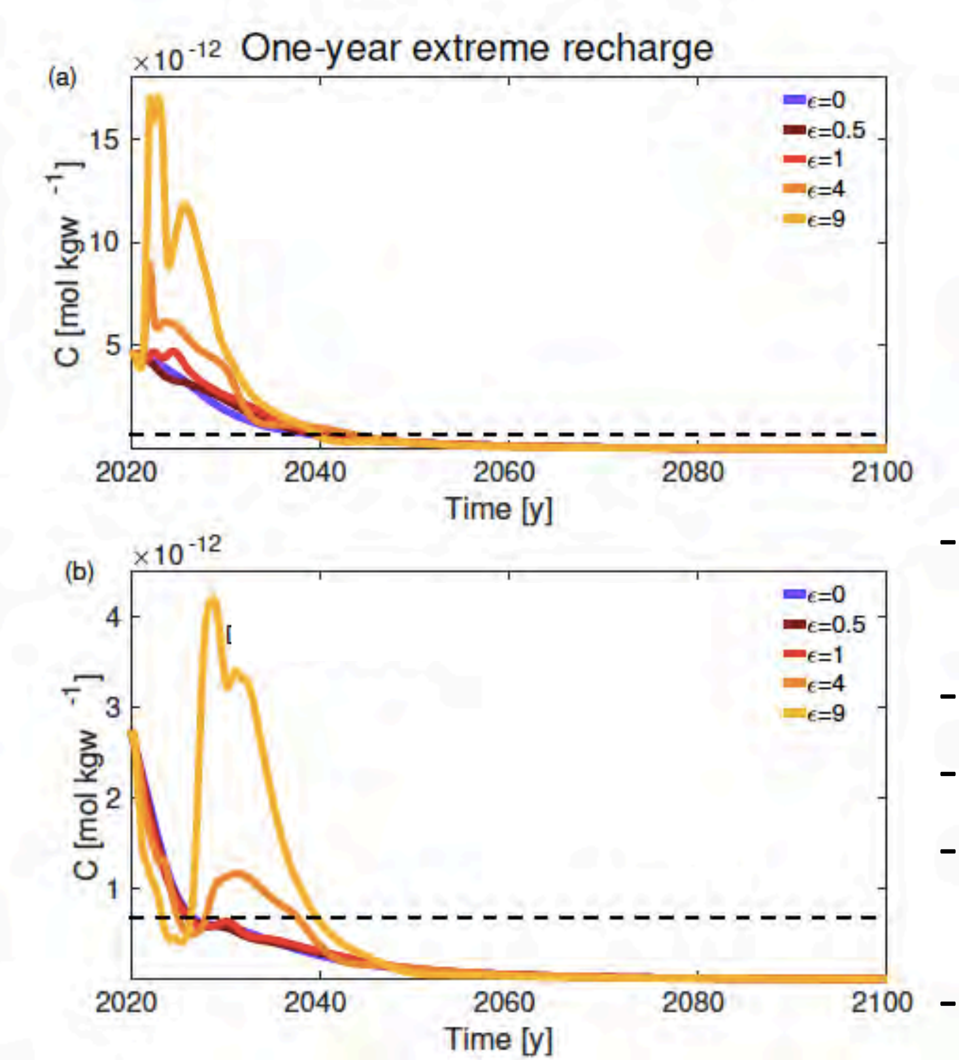
+/- Precipitation/Temperature → Infiltration, ET

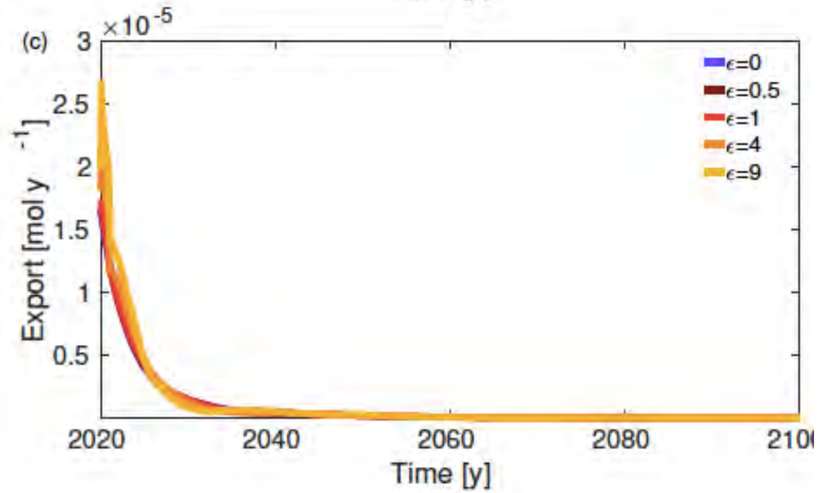
Trade off: Mobility vs Dilution

Climate Scenarios: Flooding



Flooding Event Effect





- Increase in precipitation of ONE year: x1.5 – x 10 in 2020
- Dilution then Increase
- Effect can linger for two decades
- Source zone wells important to detect remobilization
- Export to the river doesn’t change significantly

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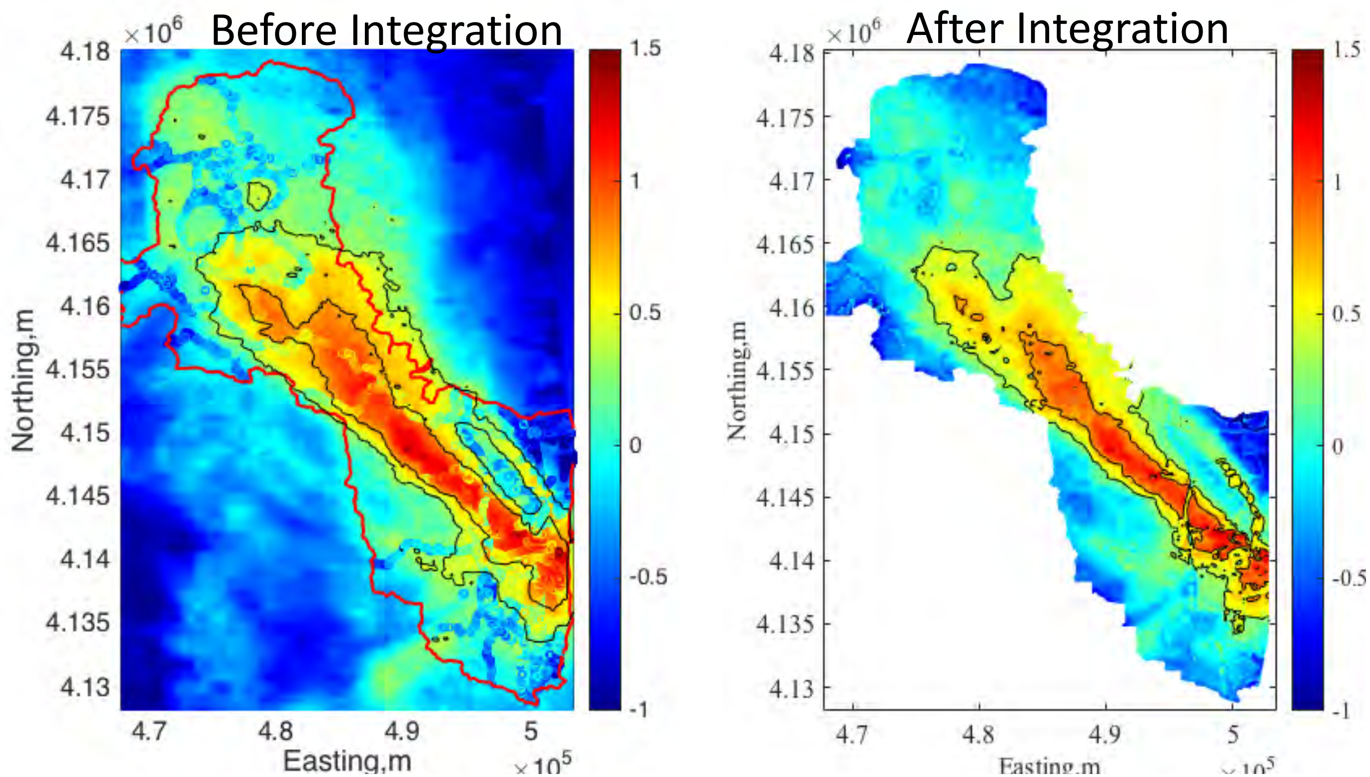
Monitoring Optimization

- How can we identify key monitoring locations, using increasingly available spatially extensive data?
  - Geophysical plume mapping
  - Simulated plume evolution
  - Airborne gamma mapping

Fukushima Radiation Mapping

- **Integrate various types/footprints of data**
- **Uncertainty quantification**
- **Adopted by Nuclear Regulatory Agency**



Wainwright H.M et al., (2016), A Multiscale Bayesian Data Integration Approach for Mapping Air Dose Rates around the Fukushima Daiichi NPP, J. of Env. Radioactivity

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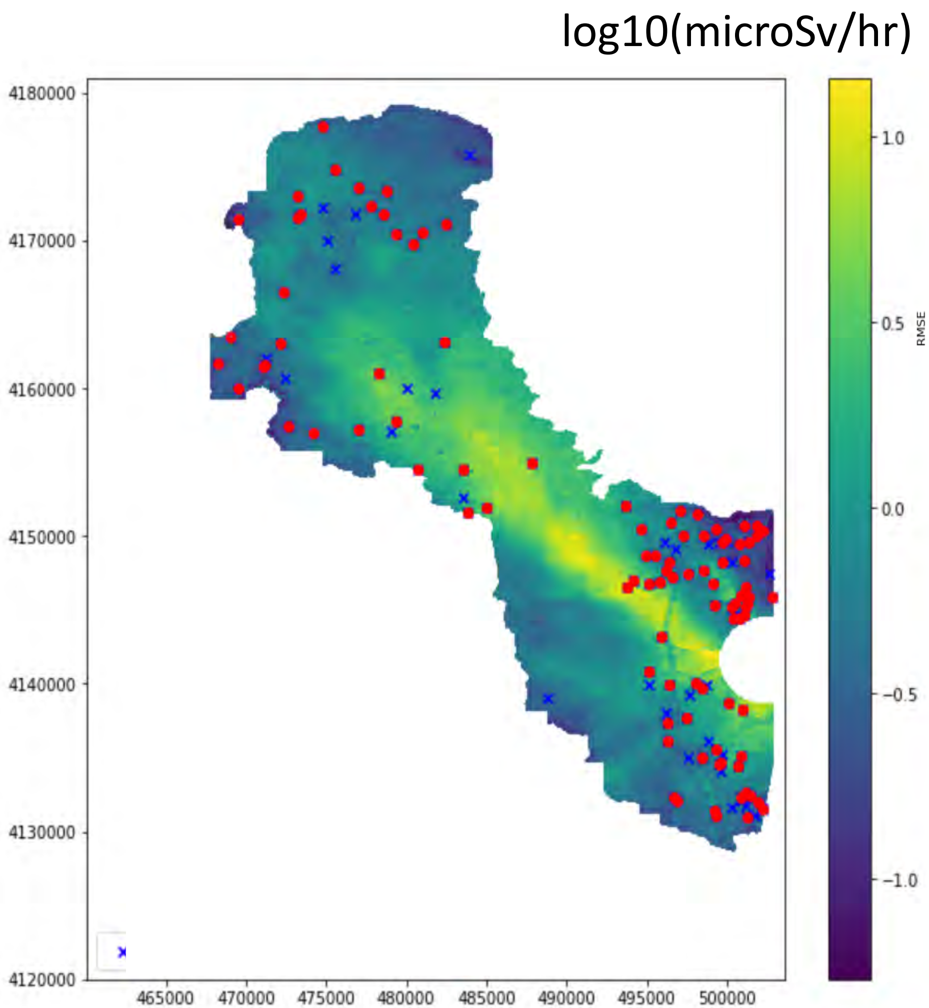
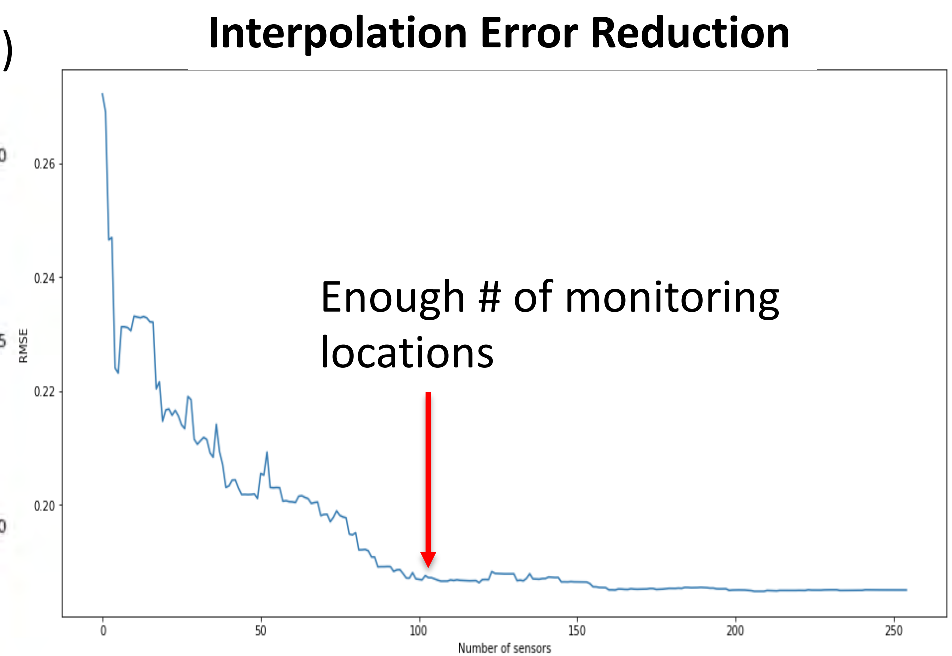
Monitoring Post Optimizations





- Identified 100 locations that capture the variability of air dose rates
- Extending to simulated plume at the F-Area

Summary

- **Cost effective strategies for long-term monitoring**
  - In situ sensors for **continuous monitoring**
  - Reduce cost while enhancing the safety
  - **Data analytics**: Kalman filter etc
- **Modeling for supporting monitoring**
  - Confirming in situ monitoring strategies
    - Correlations between master variables and contaminant concentrations: Now and future
  - Climate change: what to expect, where to monitor?
  - Optimizing monitoring locations based on spatially extensive data (mapping data or simulated data)