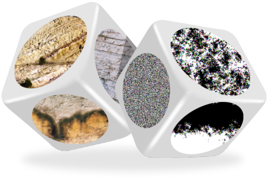
Decision Analyses for Groundwater Remediation

Velimir V. Vesselinov, Daniel O'Malley, Danny Katzman

Los Alamos National Laboratory

Waste Management Symposium, March 7, 2017
LA-UR-17-21909



Decision analyses for Groundwater Remediation

- Robust and scientifically defensible decision analyses are critical for groundwater remediation
- Groundwater contamination is a significant national and international problem
- US National Research Council (NRC) recently estimated the liabilities associated with groundwater contamination in the US at over **$100 billion**
- US NRC also reports that over “90% of court mandated groundwater remediations fail”
  - **We must perform better modeling and make better decisions**
- Frequently these failures are due to “unanticipated complexities”
  - **We must perform robust quantification of uncertainties impacting the remedial decisions**

Challenges

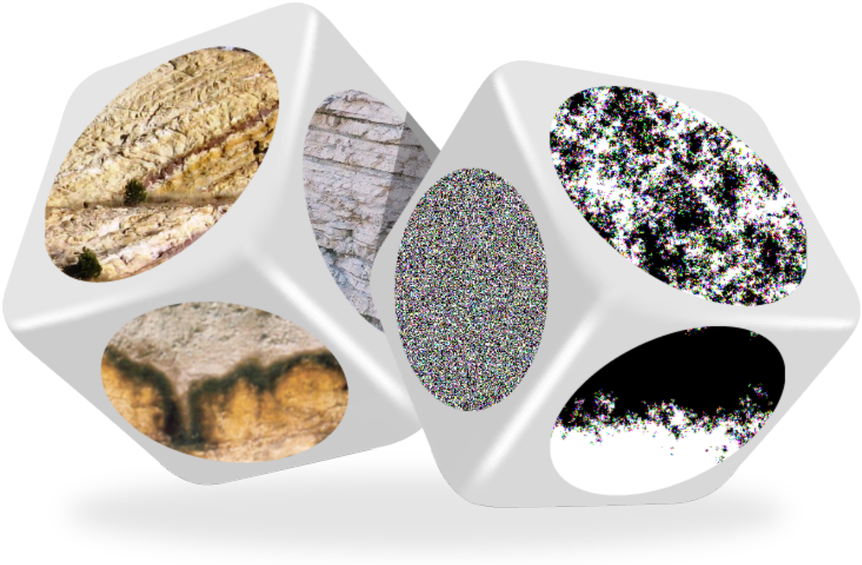
- **Scales**
- **Uncertainties**

Challenges: scales

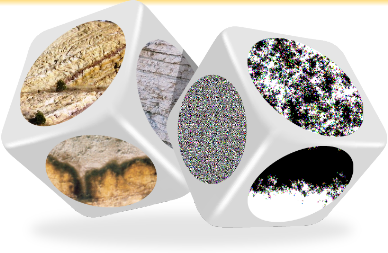
- Subsurface contaminant plumes are spread over the kilometer scale
  - **Models must predict contaminant behavior at field scales**
- Contaminant behavior is driven by processes at pore scales
  - **Models must account for processes at pore scales**
- We cannot perform even a single model run that accounts for all processes at the field and pore scales
  - **Models must be capable to capture the most important processes: *e.g.*, pore-scale mixing and field-scale spreading (dispersion)**
- Uncertainties are present at different scales
  - **Robust decision analyses tools are needed that would need to perform numerous model runs (high-performance computing)**

Challenges: Probabilistic Uncertainties

Challenges: Non-probabilistic Uncertainties

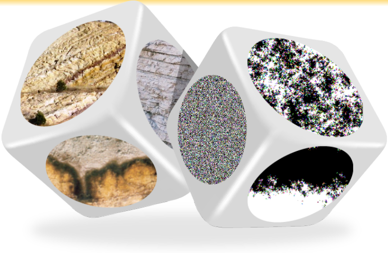


Challenges: Uncertainties



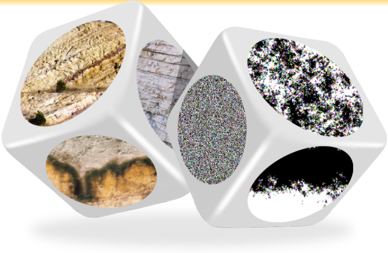
- Probabilistic methods work very well for dice-rolling predictions

Challenges: Uncertainties



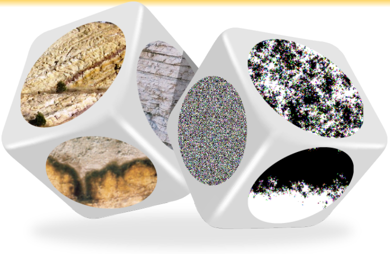
- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically

Challenges: Uncertainties



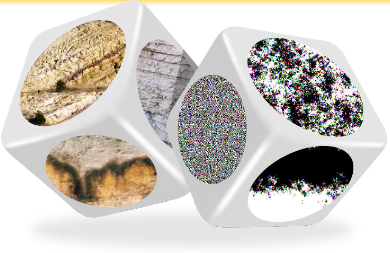
- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically
- For example, geologic heterogeneity is typically unknown (**left die**)

Challenges: Uncertainties



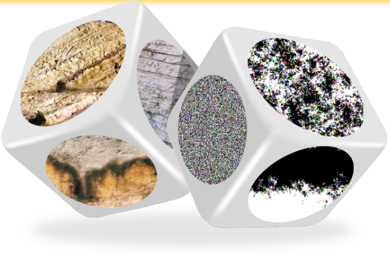
- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically
- For example, geologic heterogeneity is typically unknown (**left die**)
- We also do not know which model of heterogeneity is representative (**right die**), but we must choose a single representative model

Challenges: Uncertainties



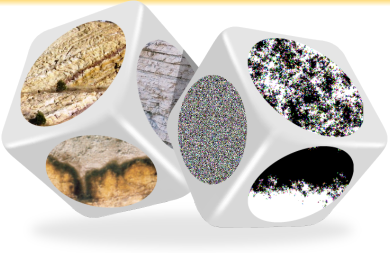
- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically
- For example, geologic heterogeneity is typically unknown (**left die**)
- We also do not know which model of heterogeneity is representative (**right die**), but we must choose a single representative model conditioned on the available site data
- We also do not know what all the sides of the dice look like, and how many sides there are

Challenges: Uncertainties



- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically
- For example, geologic heterogeneity is typically unknown (**left die**)
- We also do not know which model of heterogeneity is representative (**right die**), but we must choose a single representative model conditioned on the available site data
- We also do not know what all the sides of the dice look like, and how many sides there are
- Therefore, we cannot **enumerate all possible outcomes**

Challenges: Uncertainties



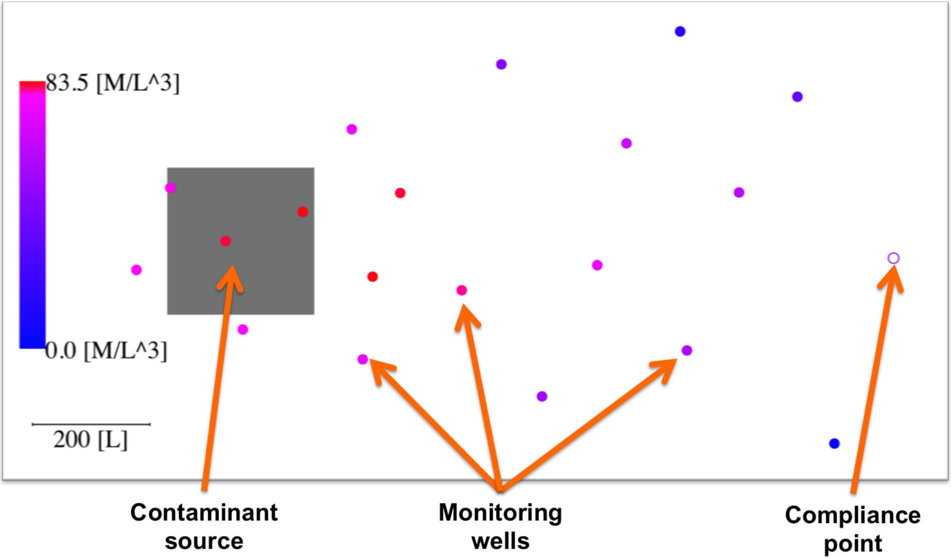
- Probabilistic methods work very well for dice-rolling predictions
- However, many environmental management uncertainties cannot be represented probabilistically
- For example, geologic heterogeneity is typically unknown (**left die**)
- We also do not know which model of heterogeneity is representative (**right die**), but we must choose a single representative model conditioned on the available site data
- We also do not know what all the sides of the dice look like, and how many sides there are
- Therefore, we cannot **enumerate all possible outcomes**
- All these issues make purely probabilistic (Bayesian) analyses **flawed** for many environmental-management problems (for example, using GoldSim)

Challenges: Uncertainties

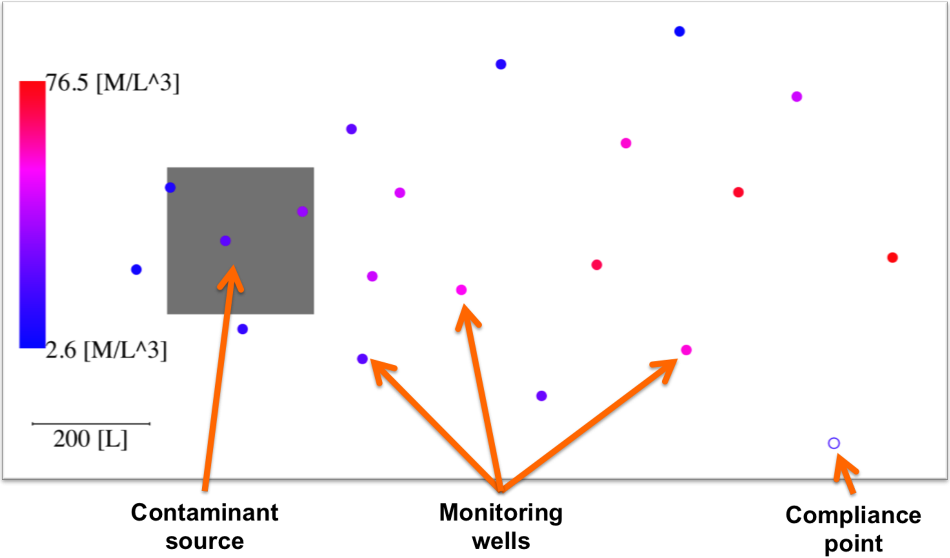
- Many uncertainties at various scales
  - Model uncertainties (conceptualization and model implementation)
  - Parameter uncertainties
  - Data uncertainties (measurement errors)
  - Uncertainties in the performance of the engineered environmental management system
- All of these uncertainties can have both:
  - **probabilistic** components, and
  - **non-probabilistic** components
- We have developed a novel methodology and advanced computational tools that can address **probabilistic** and **non-probabilistic** uncertainties
- **BIG-DT**: **B**ayesian-**I**nformation **G**ap **D**ecision **T**heory
- **MADS**: `http://mads.lanl.gov`

- **Scales**: We have developed novel modeling tools accounting for small-scale processes in large-scale models
- **Uncertainties**: We have developed novel decision analysis tools (**B**ayesian-**I**nformation **G**ap **D**ecision **T**heory/**MADS**)

BIG-DT contaminant remediation problem: Scenario 1

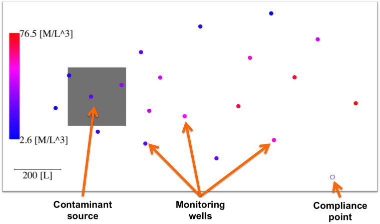


BIG-DT contaminant remediation problem: Scenario 2



BIG-DT contaminant remediation problem: knowns/unknowns

- **Known**:
  - 10 annual concentration observations at 19 wells (190 in total)
  - Location of the compliance point
- **Estimated (probabilistic uncertainties)**:
  - location, size, contaminant mass flux at the source
  - aquifer flow properties (groundwater flow direction, magnitude, etc.)
  - aquifer transport properties (porosity, dispersivity, etc.)
- **Unknown (non-probabilistic uncertainties)**:
  - geochemical reaction rate (natural/enhanced)
  - contaminant dispersion mechanism: classical (Fickian) or anomalous (non-Fickian)



- To Act or Not to Act?

BIG-DT results: Scenario 1

- To Act or Not to Act? That is the Question.

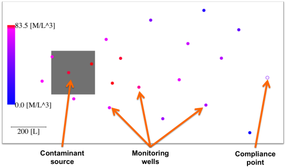
BIG-DT results: Scenario 1

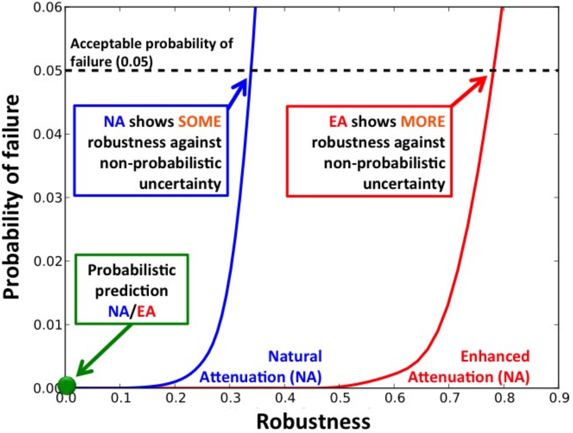
- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)

BIG-DT results: Scenario 1

- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)

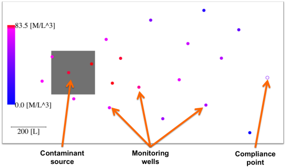
- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)
- **To Act is the Answer**

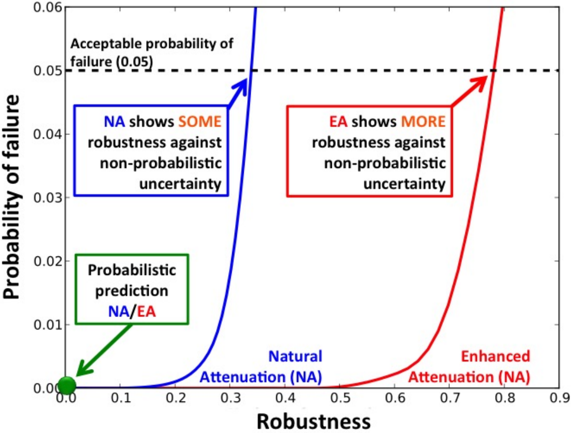




BIG-DT results: Scenario 1

- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)
- **To Act is the Answer**

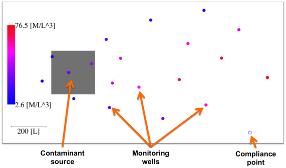


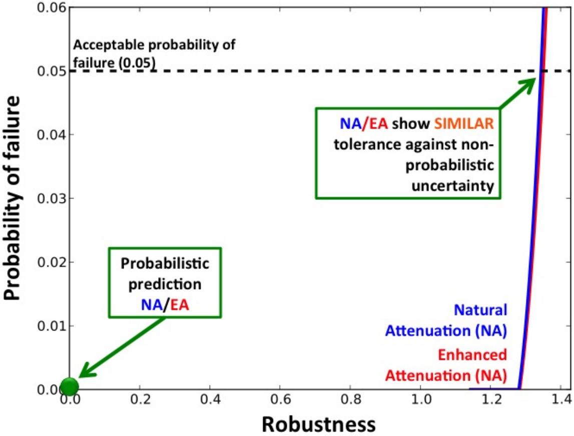


If we are very wrong about the geochemical reaction rates and the contaminant dispersion mechanisms, **EA** is the more robust option.

BIG-DT results: Scenario 2

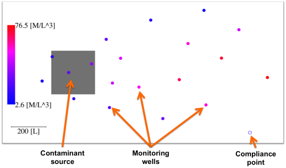
- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)
- **Not To Act is the Answer**

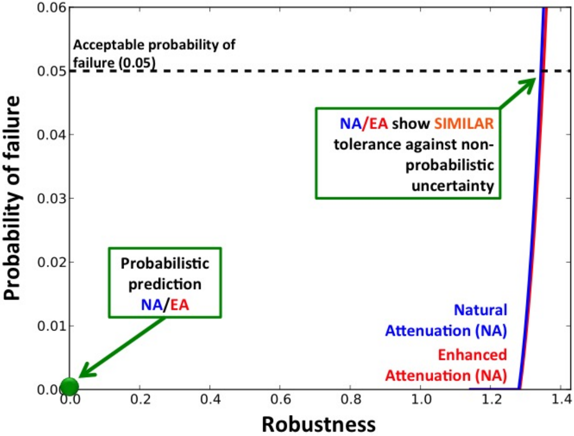




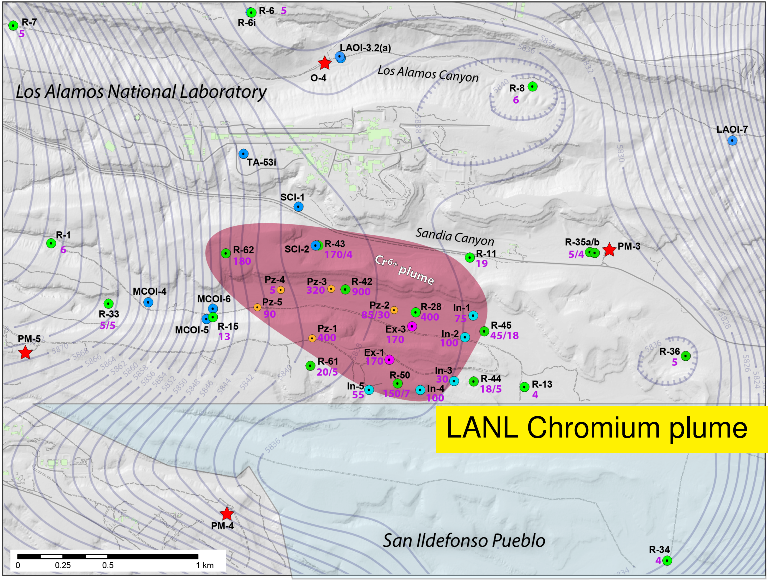
BIG-DT results: Scenario 2

- To Act or Not to Act? That is the Question.
  - Act = Perform Enhanced Attenuation (EA)
  - Not to Act = Natural Attenuation (NA)
- **Not To Act is the Answer**



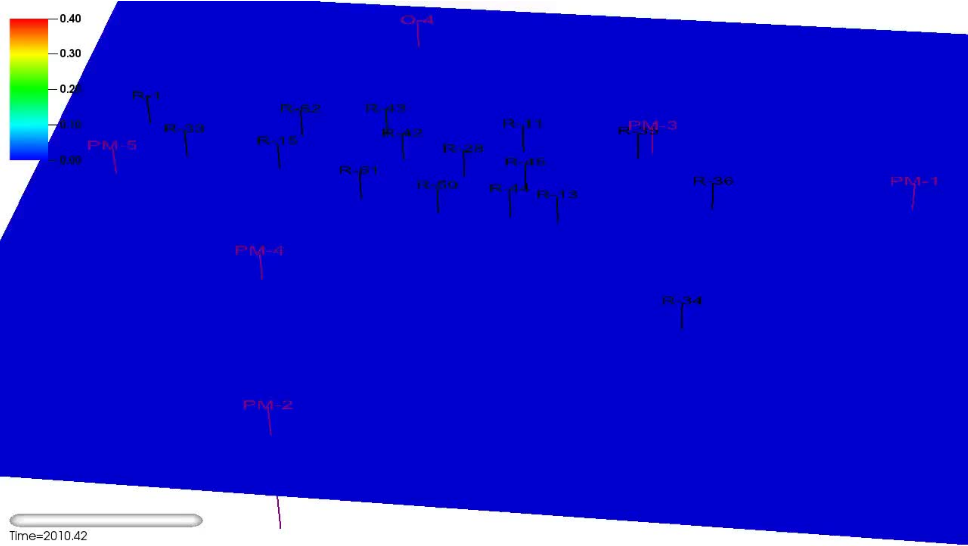


Even if we are very wrong about the geochemical reaction rates and the contaminant dispersion mechanisms, both NA and EA provide similar results.

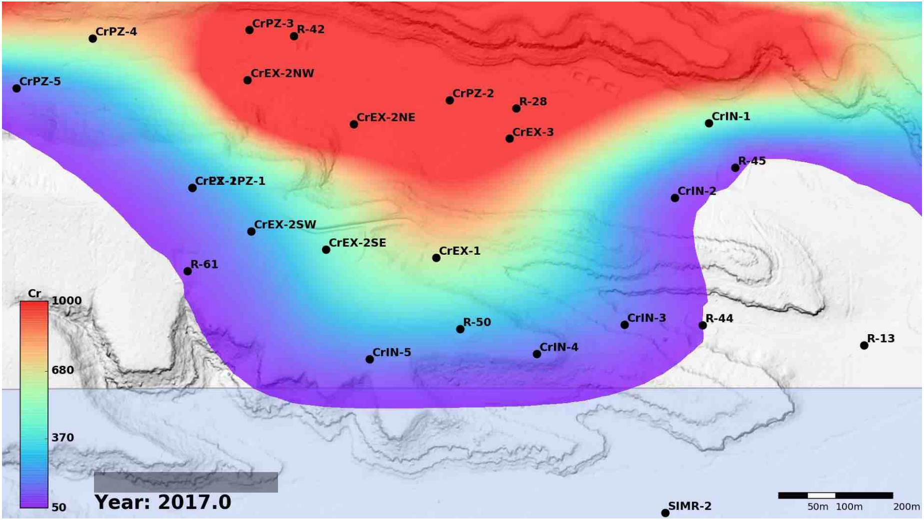


LANL Chromium plume

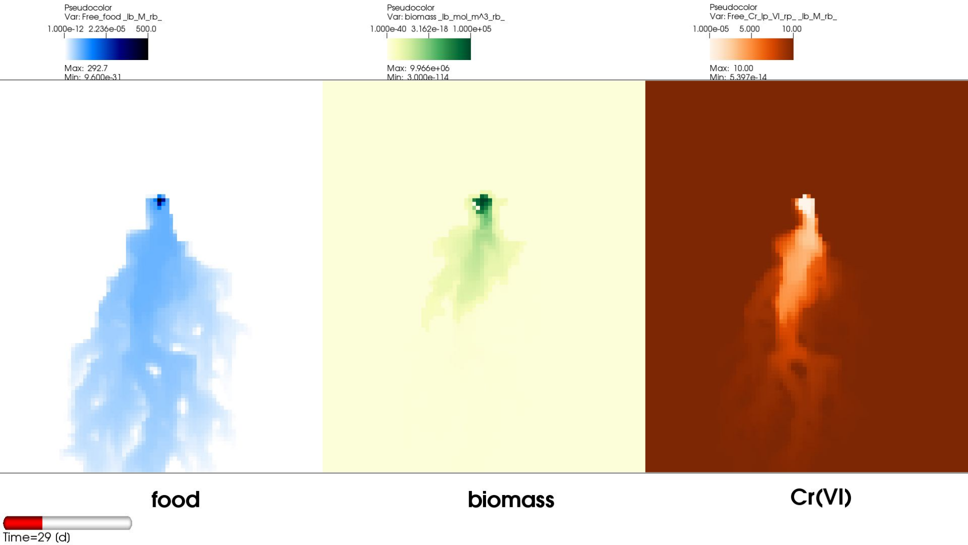
Model predicted drawdowns caused by the water-supply pumping



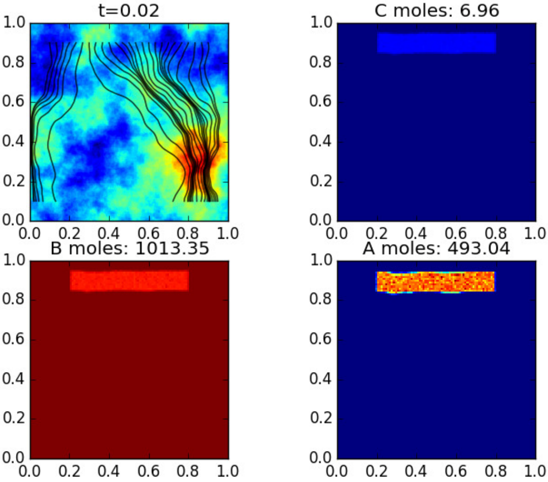
LANL Chromium plume transients



Chromium bio-remediation modeling (ChroTran)

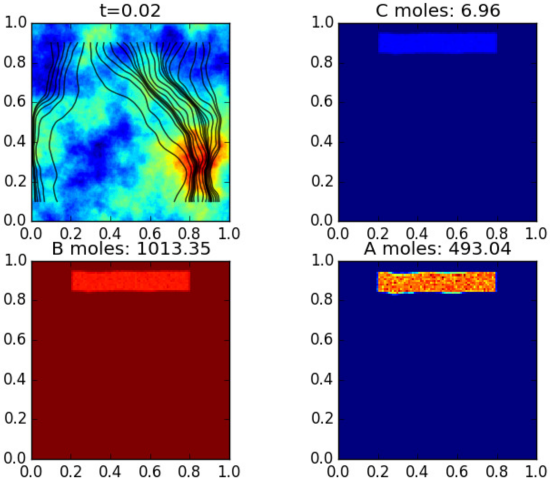


Geochemical particle-based modeling

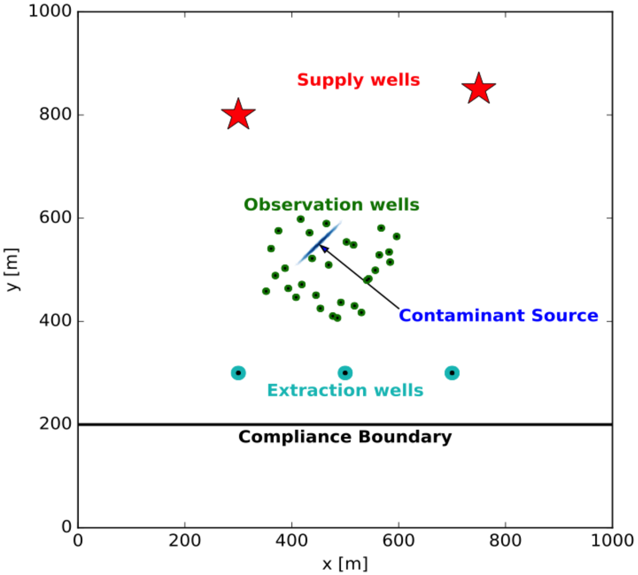


- **A** + **B** = **C**
- $X + Cr^{6+} = Cr^{3+}$
- Reduction of contaminant **B** by injecting **A**
- Reduction of contaminant **A** by interacting with **B**
- **A** instantaneously released (500 moles)
- **B** uniformly distributed in the aquifer (1000 moles)

Geochemical particle-based modeling



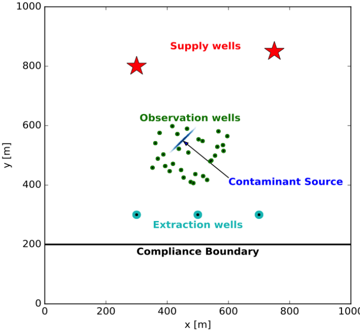
- **20%** of **A** did not react


Supply wells
Observation wells
Contaminant Source
Extraction wells
Compliance Boundary
y [m]
x [m]
0
200
400
600
800
1000

Bayesian Information Gap Decision Analysis: Setup

Unknowns:

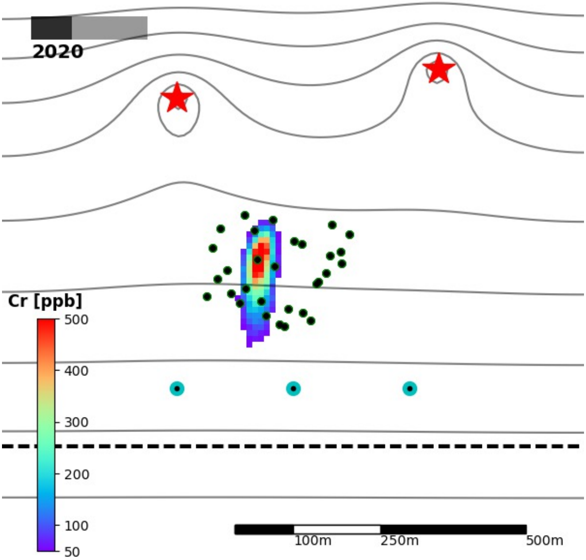
- contaminant mass release, source location (x, y) and size
- hydraulic conductivity
- porosity
- dispersivity (longitudinal and transverse)
- contaminant transport parameters (mean mobile/immobile times of pore-scale mixing)



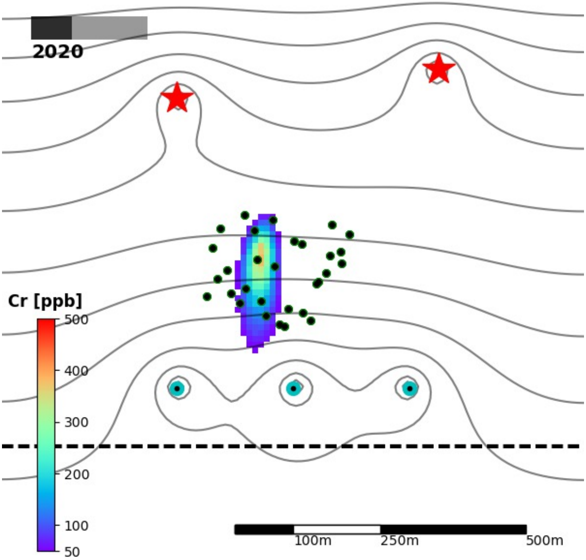
Knowns:

- well locations
- well pumping rates
- ambient hydraulic gradient
- location of compliance boundary
- hydraulic heads at the monitoring wells
- contaminant concentrations at the monitoring wells
- 30 monitoring wells
- 10 annual observations (heads/concentrations) per well (600 in total)

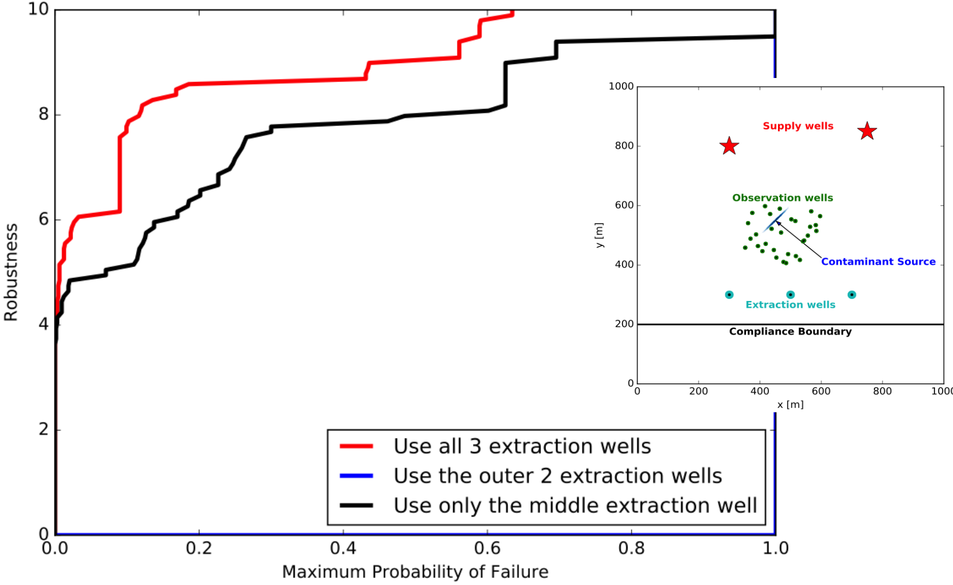
Bayesian Information Gap Decision Analysis: No action



Bayesian Information Gap Decision Analysis: Pumping



Bayesian Information Gap Decision Analysis: Results



MADS: Model Analysis & Decision Support

- **MADS** is an open-source high-performance computational framework
- **MADS** implements a wide range of state-of-the-art and novel advanced computational techniques for **big-data** and **complex** model analyses (including machine learning).
- **MADS** provides tools for coupling with any existing physics simulator (FEHM, Amanzi, PFloTran, ChroTran, etc.)
- **MADS** source code, examples, test problems, performance comparisons, and tutorials are available at:
  - `http://mads.lanl.gov`
  - `http://madsjulia.github.io/Mads.jl`

MADS has applied to perform various types of data- and model-based analyses related to the LANL chromium site:

- Contaminant source identifications
- Contaminant source characterizations (using models and **machine learning**)
- Monitoring network designs
- Optimization of injection/extraction well locations for hydraulic plume control
- Sensitivity analyses
- Uncertainty quantifications
- Evaluation of remediation scenarios
- Decision analyses

- In the last **10** years, model analyses have accumulated more than **1,000** CPU-years of computational time utilizing simultaneously up to **4,096** processors on the LANL HPC clusters
- ... so far, all the blind model predictions (estimates/uncertainties) have been generally consistent with the new site observations