ZEM: Integrated Framework for Real-Time Data and Model Analyses for Robust Environmental Management Decision Making

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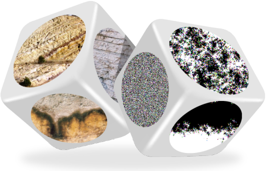


ZEM framework

- **ZEM** provides automated and reproducible workflow interconnecting Data $\Leftrightarrow$ Models $\Leftrightarrow$ Decisions
- **ZEM** is designed for **high-performance computing** and **big-data** analysis
- **ZEM** employs community software (**git**/**gitlab**) for **version control**, **team collaboration** and **project management** using cloud-based repositories (**gitlab.com** / **git.lanl.gov**) $\Rightarrow$ all past model inputs and obtained outputs are stored and can be reproduced
- **ZEM** provides quality assurance of the performance assessment process
- **ZEM** is written predominantly in julia
- julia: novel high-performance/dynamic language for technical computing (developed at MIT)

ZEM components

- **MADS** (Model Analysis & Decision Support): actively developed open-source high-performance computational framework for data- & model-based analyses in julia (madsjulia.lanl.gov)
- **MySQL** (www.mysql.com): open-source relational database management system stores all the site data (more than 10^7 entries)
- Web interfaces (for data queries and exploratory model analyses)
- Various simulators
- Visualization tools (matplotlib, gnuplot, Gadfly, Paraview, VisIt)
- julia/Python scripts to couple all the **ZEM** components
- For example, a single julia script can:
  - perform automated data query from the **ZEM** database
  - place the data in the model input files
  - initiate the simulations on HPC clusters
  - generate plots and movies with the final results

ZEM: Analytical simulators

- Analytical solutions for **groundwater flow** (implemented in **MADS** and **Wells**)
- Analytical solutions for Fickian (classical) and non-Fickian (anomalous) **contaminant transport** (implemented in **MADS**)
- Analytical simulator of groundwater flow and contaminant transport associated with infiltration recharge and perched horizons in the **vadose zone** (a fast screening tool) (implemented in **MADS**)
- Semi-analytical simulator for **capture zone** estimation and **tracer test** interpretation (push-and-pull and cross-well tracer tests; **MADS**)
- Analytical method for removal of **barometric pressure** and **tidal effects** in the water-level data (**CHipBeta**):

ZEM: Numerical simulators

- **FEHM**: groundwater flow and contaminant transport; geochemical reactions (LANL developed code)
- **PFloTran**: groundwater flow and contaminant transport; biogeochemical reactions (LANL developed open-source code)
- **LaGriT**: grid generation (LANL developed open-source code)
- **Ashley**: particle-based geochemical reactions (LANL developed code in julia)
- **FEniCS**: automated and efficient differential-equation solver (open-source community code)
- **libMesh**: advanced parallel partial-differential-equation solver (open-source community code)
- **Amanzi**: groundwater flow and contaminant transport; geochemical reactions (LANL developed code; future work)

- **Drawdown estimator**: tool for data- and model-based analysis for identification and deconstruction of pumping drawdowns (typically, drawdowns are smaller than the barometric pressure fluctuations and caused by overlapping pumping events)
- **RMF** (**R**obust **M**atrix **F**actorization): novel methodology for model-free inversion and data analysis
- Unsupervised objective **machine-learning methods** for data, model and decision analyses
- **Surrogate modeling** using state-of-the-art and newly developed methods (SVR, Bayesian)
- **Various data-analysis tools** such as principle and independent component analysis, trend analysis, spatial interpolation, etc.

(utilizing third-party julia community modules).

ZEM utilizes state-of-the-art and novel advanced methods for characterization of aquifer heterogeneity

- **Pilot-point**-based methods
- **Fourier**-based stochastic methods
- **Regularization**-based methods
- **Level-set** tomography (geologic facies reconstruction)
- **"Honest"** tomography (accounting for uncertainties and unknowns)
- **P**rincipal **C**omponent **G**eostatistical **A**analysis (**PCGA**; Kitanidis et al., 2014)
- **R**andom **G**eostatistical **A**analysis (**RGA**) for **big-data** tomography (Le et al., 2016)

ZEM: Analyses

ZEM have been successfully applied to support development of the site conceptual model representing hydrogeological and biogeochemical processes in the subsurface

- Contaminant source identification
- Contaminant source characterization (based on geochemical data and model-free inversion using unsupervised objective machine learning)
- Monitoring network design
- Evaluation of remediation scenarios
- Sensitivity and uncertainty quantification analyses
- Decision analyses
- In the last **3** years, **ZEM** analyses have accumulated more than **350** CPU-years of wall-clock computational time utilizing simultaneously up to **4096** processors on the LANL HPC clusters
- ... so far, all the **ZEM** blind predictions have been consistent with the new observations

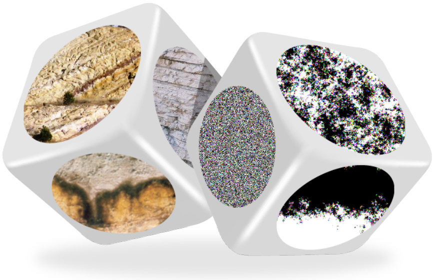
ZEM ⇔ MADS (Model Analysis & Decision Support)

- open-source, version-controlled, high-performance computing framework implementing state-of-the-art and novel adaptive computational techniques for:
  - sensitivity analysis (local / global)
  - uncertainty quantification (local / global)
  - optimization / calibration / parameter estimation (local / global) parallel Krylov-space methods for **big-data** analyses
  - model ranking & selection
  - decision analysis (GLUE, information gap, Bayesian, **B**ayesian - **I**nformation **G**ap **D**ecision **T**heory (**BIG-DT**), **Measure-Theoretic**-based approaches)
  - decision-based experimental design

ZEM ⇔ MADS (Model Analysis & Decision Support)

- provides **internal** coupling with analytical groundwater flow and contaminant transport solvers
- allow **external** coupling with any existing physics simulator
- coded in julia
- source code, examples, test problems, performance comparisons, and tutorials are available at:
  - `http://madsjulia.lanl.gov`
  - `http://madsjl.readthedocs.org/`

- Probabilistic methods work very well for dice-rolling experiments



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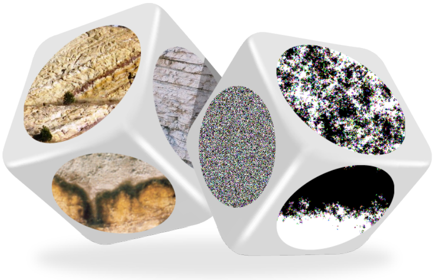
- However, many earth-science uncertainties cannot be represented probabilistically (for example, using GoldSim)



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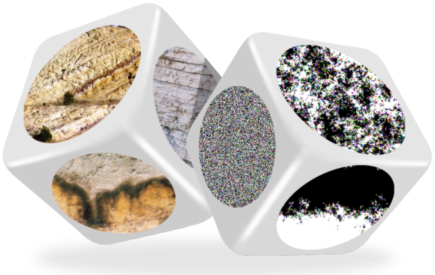
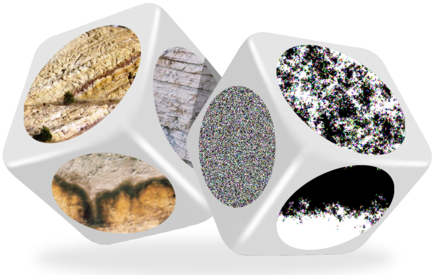
- Actual geologic heterogeneity is typically unknown (**left die**)

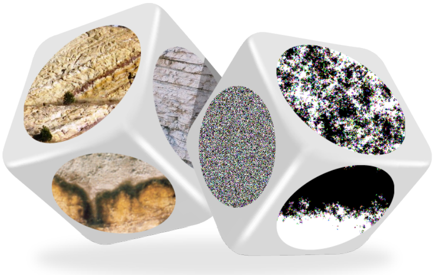
MADS: Bayesian-Information-Gap Decision Theory (BIG-DT)



- Probabilistic methods work very well for dice-rolling experiments
- However, many earth-science uncertainties cannot be represented probabilistically (for example, using GoldSim)
- Actual geologic heterogeneity is typically unknown (**left die**)
- We also do not know which of the possible models of geologic heterogeneity is representative (**right die**), but probabilistic methods require to choose a single representative model conditioned on the available data



- We also do not know what all the sides of the dice look like, and how many sides there are



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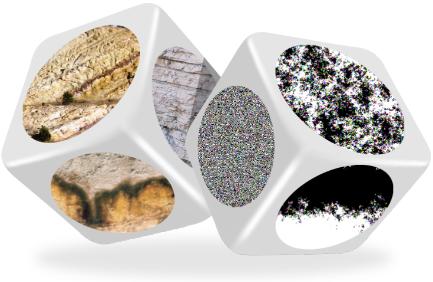

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- All these issues make purely probabilistic analyses **flawed** for many earth-science problems

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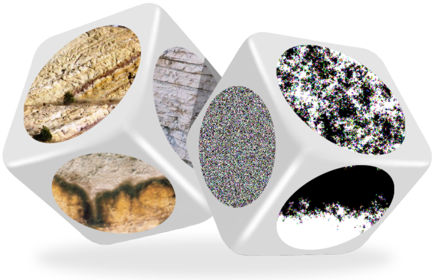
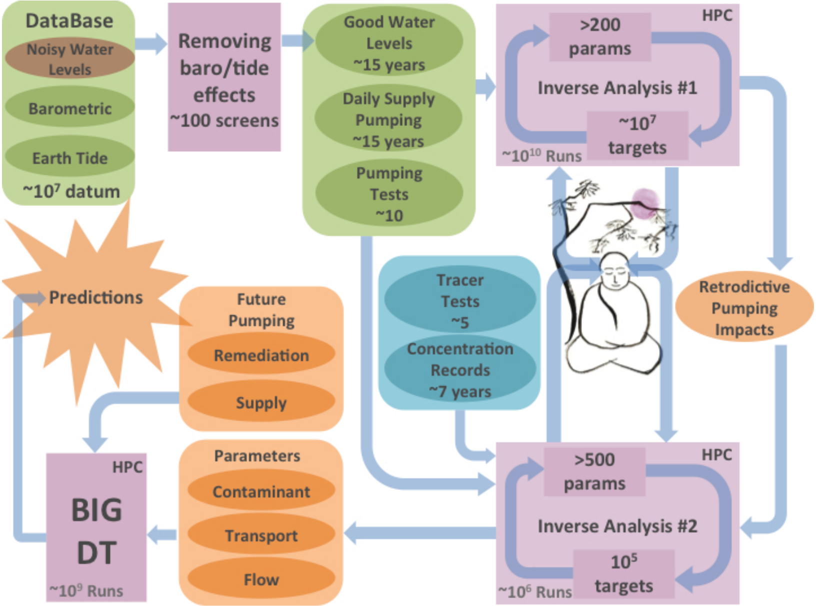


- We also do not know what all the sides of the dice look like, and how many sides there are
- Therefore, we cannot **enumerate all possible outcomes**
- All these issues make purely probabilistic analyses **flawed** for many earth-science problems
- **B**ayesian - **I**nformation **G**ap **D**ecision **T**heory (BIG-DT) for Uncertainty Quantification & Decision Analysis has been developed to address these issues (O'Malley & Vesselinov 2014 SIAM UQ)

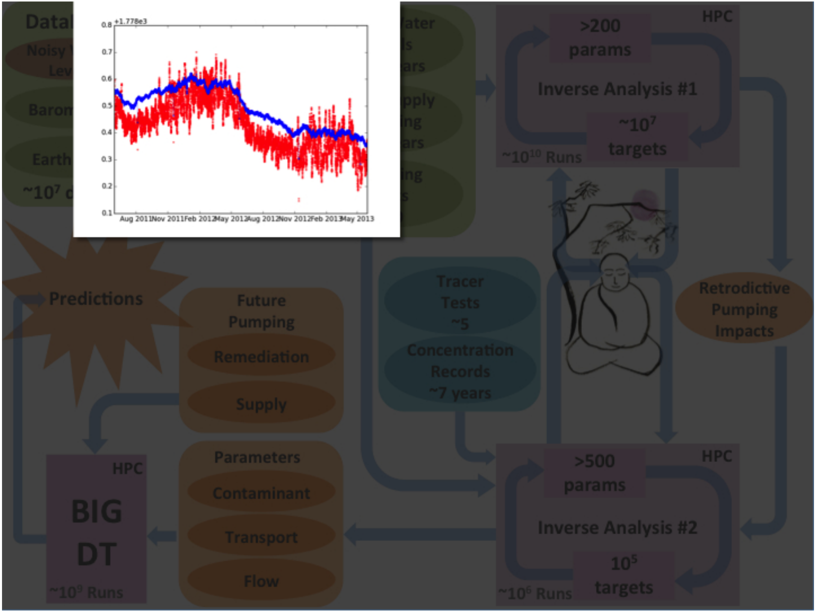
ZEM development support

- **LANL Environmental Projects**
- **DiaMonD Project**:
  - DiaMonD: Integrated Multifaceted Approach to Mathematics at the Interfaces of Data, Models, and Decisions
    - University of Texas at Austin
    - Massachusetts Institute of Technology (MIT)
    - Stanford University
    - Colorado State University
    - Florida State University
    - Los Alamos National Laboratory
    - Oak Ridge National Laboratory
  - Funded by DOE Office of Science
  - `http://dmd.mit.edu`

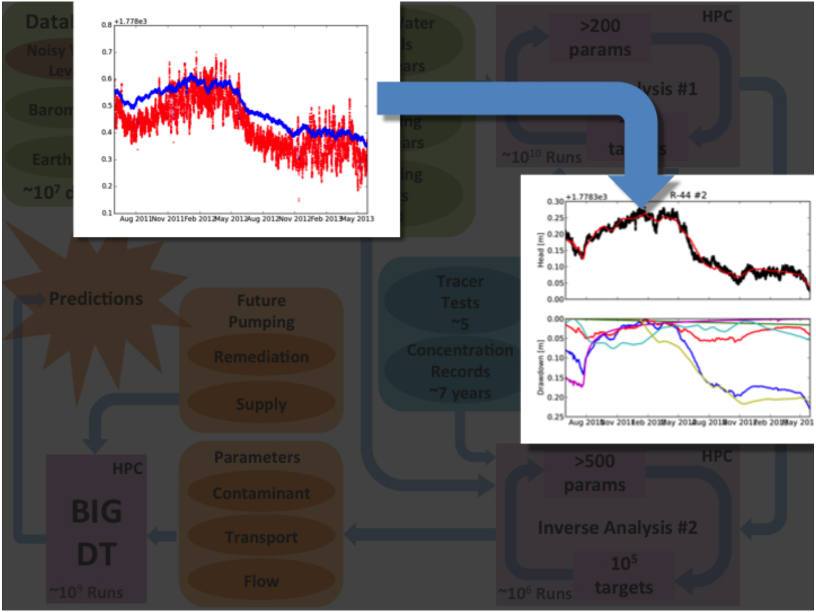
ZEM workflow: Data ⇔ Models ⇔ Decisions



ZEM workflow: Data ⇔ Models ⇔ Decisions



ZEM workflow: Data ⇔ Models ⇔ Decisions



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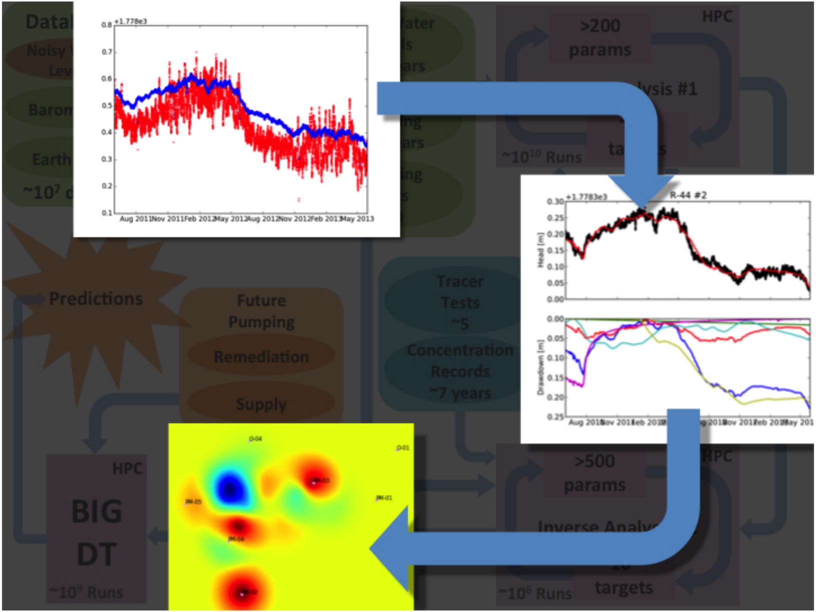

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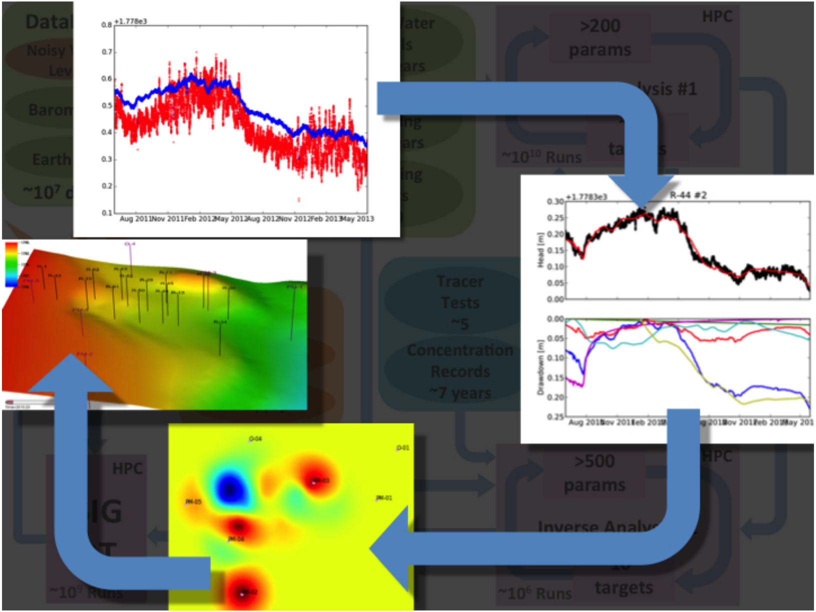


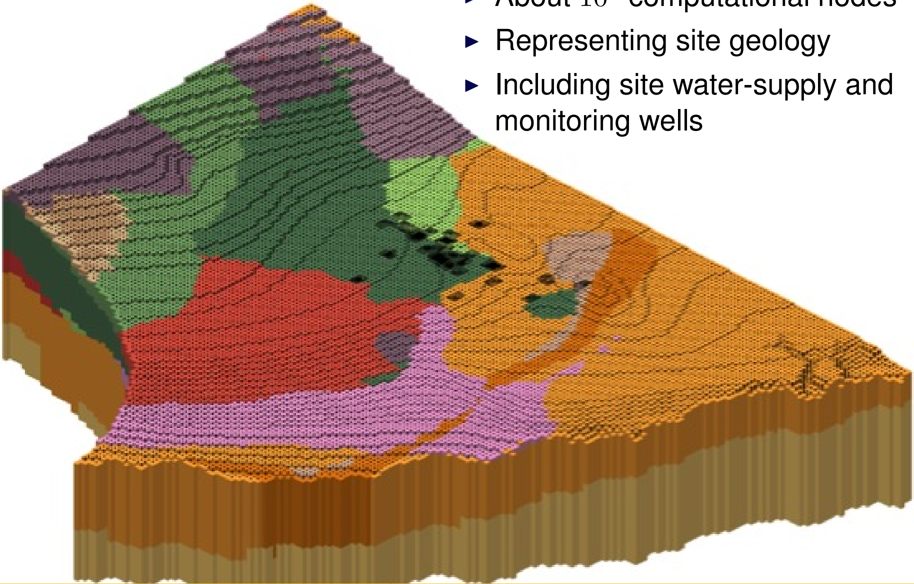
Chromium site high-level summary

- High visibility project
- ~54,000 kg of Cr^{6+} released in Sandia Canyon between 1956 and 1972 (with substantial **uncertainties** and **unknowns**)
- Cr^{6+} detected above MCL (50 ppb; NM standard) at 6 monitoring wells in the regional aquifer beneath LANL
- Cr^{6+} plume size is about 2 km^2 (region above MCL)
- Cr^{6+} plume is located near LANL site **boundary**
- Series of **water-supply wells** are located nearby (less than km)
- Contaminant mass distribution in the subsurface in **unknown**
- Contaminant source location and mass flux at the top of the regional aquifer are **unknown** due to **complex** 3D pathways through the vadose zone
- **Limited remedial options** due to aquifer depth (~300 m below the ground surface) and **complexities** in the subsurface processes
- Current conceptual model for chromium transport in the subsurface is supported by **multiple lines of evidence**

Chromium project goals

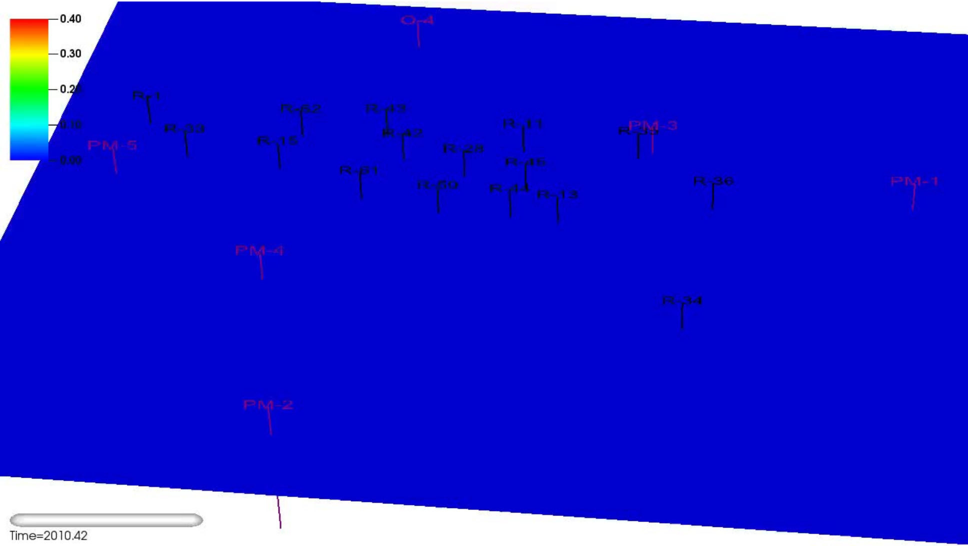
- **GOAL #1**: apply modeling to support **conceptualization** of the site geologic, hydrologic and biogeochemical conditions
- **GOAL #2**: perform data- and model-based **decision analyses** for chromium remediation taking into account existing processes and **uncertainties**/**unknowns**
- **Remedial scenarios**:
  - Natural attenuation (**NA**)
  - Enhanced attenuation (**EA**; biogeochemical processes)
  - Active remediation including mass removal in the vadose zone and the aquifer (**pump-and-treat**, etc.)
  - **Combinations** of all above at different times/locations

Chromium site model



- About 10^6 computational nodes
- Representing site geology
- Including site water-supply and monitoring wells

Drawdowns from the existing supply wells



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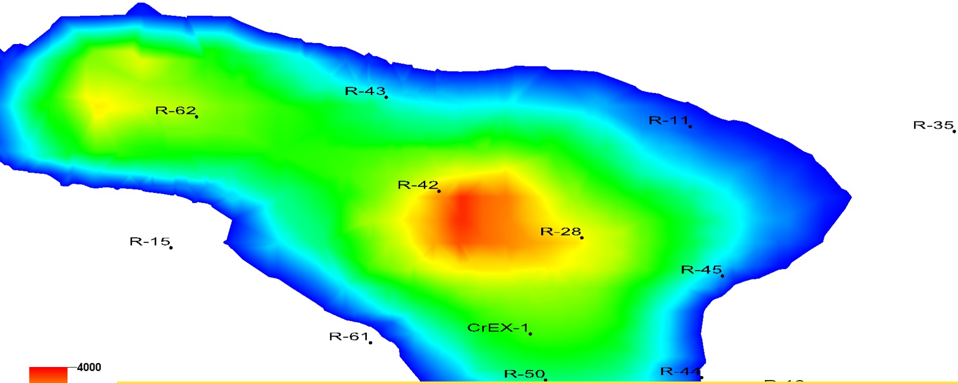
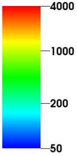
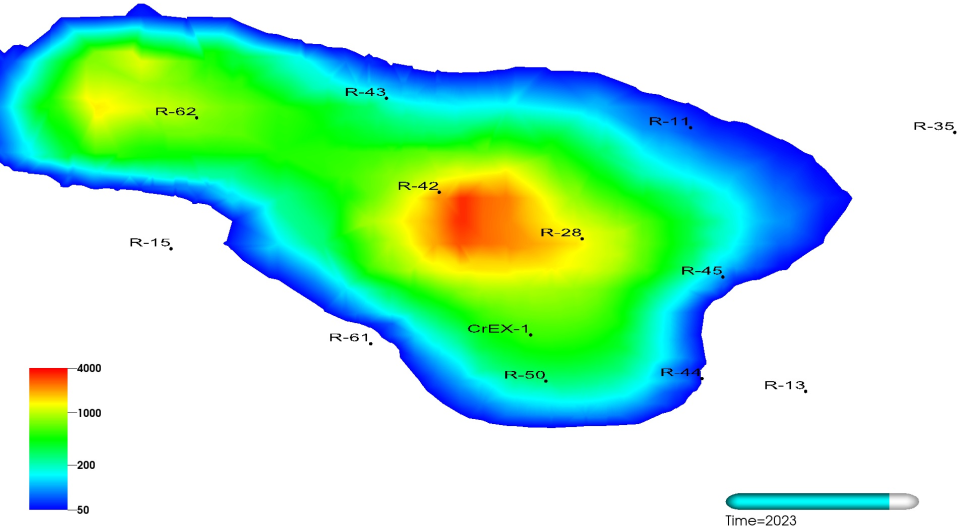
Chromium plume transients



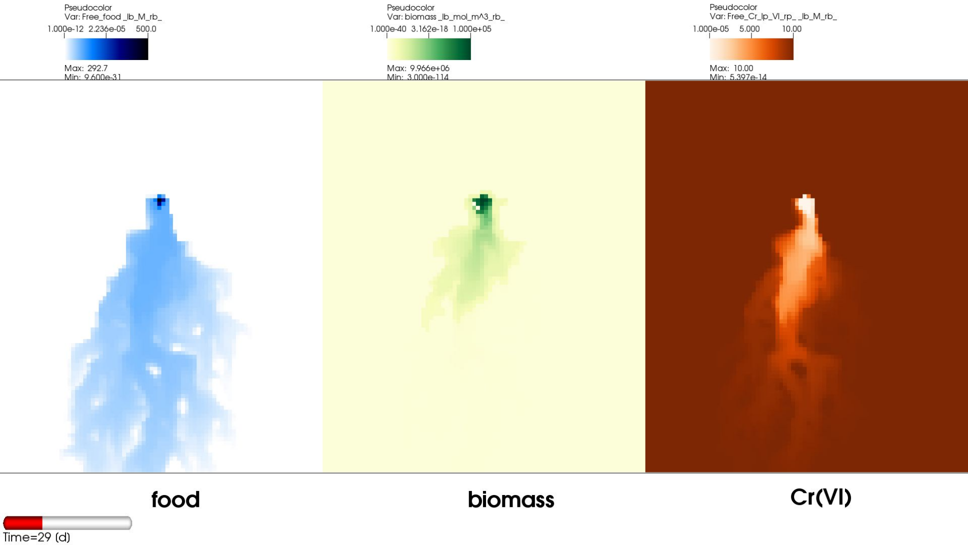


- Model is calibrated against all the pressure and concentration transients
- ... so far, ~20 CPU-years of wall-clock computational time are accumulated
- ... additional model improvements are still needed

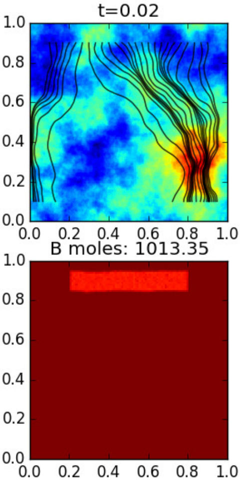
Chromium plume transients



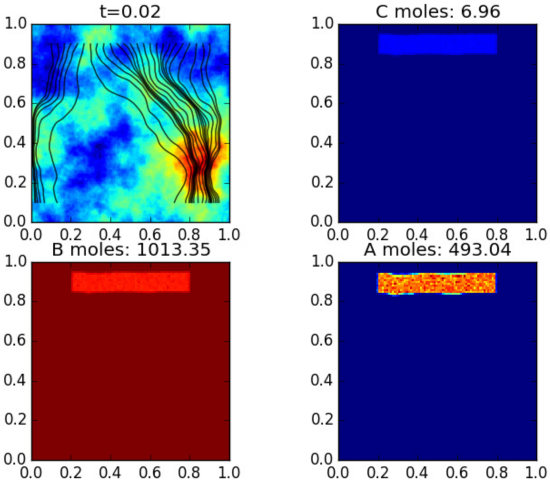
Chromium bio-remediation modeling (PFloTran)



Geochemical particle-based model (Ashley)



- A + B = C
- 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)



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

Play/Pause

Highlights

- **ZEM** provides automated and reproducible workflow interconnecting Data ⇔ Models ⇔ Decisions using **high-performance computing** and **big-data** analysis tools
- **ZEM** have been successfully applied to perform various data- and model-based analyses at the LANL Chromium site.
- In the last **3** years, **ZEM** analyses have accumulated more than **350** CPU-years of wall-clock computational time utilizing simultaneously up to **4096** processors on the LANL HPC clusters
- ... so far, all the **ZEM** blind predictions have been consistent with the new observations

Highlights

- Many uncertainties in the environmental management problems **cannot** be represented probabilistically
- Newly developed methodology **BIG-DT** (**B**ayesian-**I**nformation **G**ap **D**ecision **T**heory) is developed to address this issue (O'Malley & Vesselinov 2014 SIAM UQ)
- **BIG-DT** is applicable to any real-world engineering problems
- **BIG-DT** is available in **MADS** (open source code written in julia)
  - `http://madsjulia.lanl.gov`
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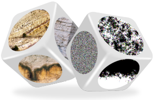

Relevant Publications

1. Grasinger, M., O'Malley, D., Vesselinov, V.V., Karra, S., Decision Analysis for Robust CO_2 Injection: Application of Bayesian-Information-Gap Decision Theory, IJGGC, doi: 10.1016/j.ijggc.2016.02.017, 2016.
2. Mattis, S.A., Butler, T.D. Dawson, C.N., Estep, D., Vesselinov, V.V., Parameter estimation and prediction for groundwater contamination based on measure theory, WRR, doi: 10.1002/2015WR017295, 2015
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4. O?Malley, D., Vesselinov, V.V., Bayesian-Information-Gap decision theory with an application to CO2 sequestration, Water Resources Research, doi: 10.1002/2015WR017413, 2015
5. Lu, Z., Vesselinov, V.V., Analytical Sensitivity Analysis of Transient Groundwater Flow in a Bounded Model Domain using Adjoint Method, WRR, doi: 10.1002/2014WR016819, 2015
6. O'Malley, D., Vesselinov, V.V., Cushman, J.H., Diffusive mixing and Tsallis entropy, Phys.Rev E, 91, 042143, 2015
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Team

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Why ZEM?

- **ZEM** $\approx$ **ZEN**
- **ZEM**: **Z**eitgeist (spirit of the time) **E**nvironmental **M**odeling
- **ZEM**: the Slavic root word for Earth