ASCEM Site Applications

Underground Test Area (UGTA) Site Application

Justin Marble[1]
Bill Wilborn[2], Paul Dixon[3], Zhiming Lu[3], Dylan Harp[3], Edward Kwicklis[3],
Terry Miller[3], Andrew Wolfsberg[3] and Kay Birdsell[3]

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[1]U.S. DOE, Office of Soil and Groundwater Remediation,
[2]U.S. DOE, NNSA Nevada Field Office
[3]Los Alamos National Laboratory

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ASCEM

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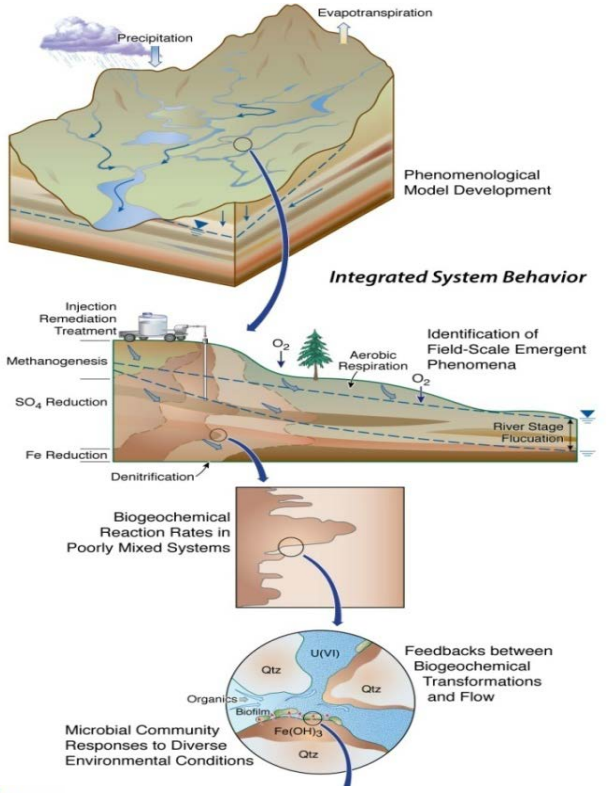
ASCEM

Advanced Simulation Capability for Environmental Management

- Purpose → Aid Sites
  - Support Performance Assessments at DOE sites
  - Simulate and Visualize Complex Systems
- Modeling toolsets for simulating contaminant fate and transport through natural and engineered systems
  - High Performance Computing (HPC) - subsurface flow and transport simulator
  - Platform – pre- and post-processing toolsets, job launching, and monitoring
  - **Site Applications – testing, demonstration, and deployment**
- Collaborative, multi-national laboratory project sponsored by DOE – EM
- Modular, extensible and open-source design



Underground Test Area (UGTA) Activity

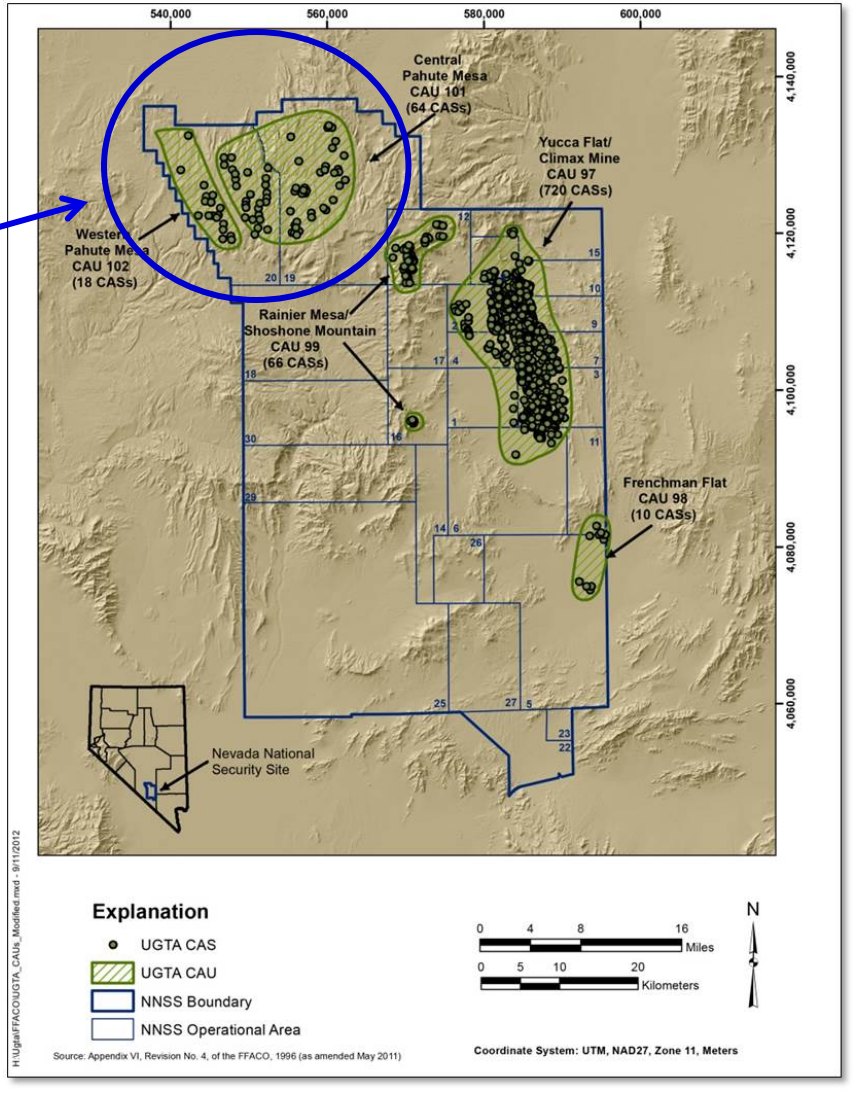
UGTA Activity – Assess groundwater contamination at NNSS (former NTS) from 828 underground nuclear tests conducted between 1957 and 1992

➢ Project goals

- 5 Corrective Action Units
  - 3 in advanced state of analysis
  - **Central and Western Pahute Mesa CAUs in Corrective Action Investigation Phase**
- Forecast extent of contaminated groundwater for 1000 years
- Define groundwater use-restriction boundaries
- Design groundwater monitoring networks

➢ Site characteristics

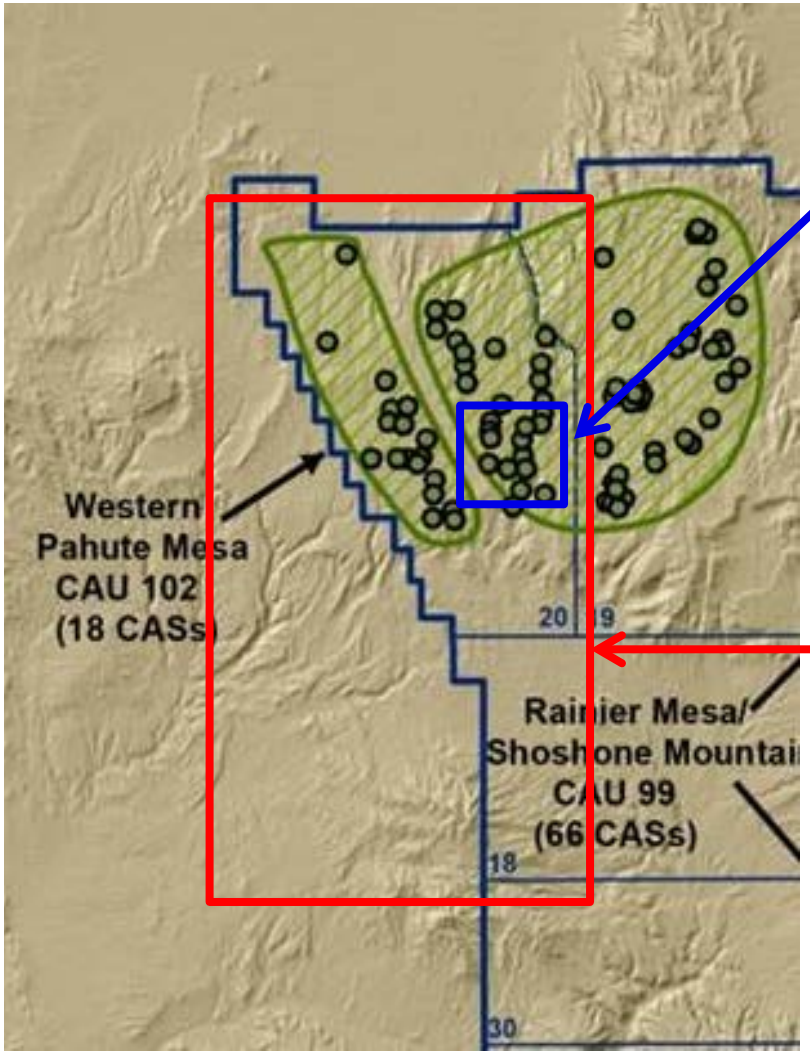
- Complex geologic setting
- Fractured and faulted volcanic and carbonate aquifers
- Deep water tables
- Multiple contaminant sources



UGTA Site Application – Pahute Mesa Focus

- Leveraging UGTA and ASCEM support to optimize project success
- Exploring high-resolution models for assessing conceptual model uncertainty
  - Realistic flow and transport runs on a large-scale, faulted, complex hydrostratigraphic domain
  - Simultaneous inversion of multiple pump tests for parameter estimation (PE) requires HPC
  - Provides justification for model simplification for Monte Carlo regulatory calculations
- FY14 – UGTA Demonstration – Single well pump test (U20-WW)
  - Amanzi verification of 3 pumping solutions (compare to analytical and FEHM solutions)
  - Testing of ASCEM Uncertainty Quantification (UQ) and PE tools using UGTA pump test data
  - Walkabout/Plumecalc (particle tracking) implementation, verification, and demonstration for UGTA test case
- FY15 – UGTA Demonstration – Large domain, multiple well pump tests
  - Amanzi flow solution
  - Parameter estimation using steady-state heads and transient pump test data from a dozen wells
  - Particle tracking solution from 49 detonations

Pahute Mesa – Model Domains



FY14 Model Domain

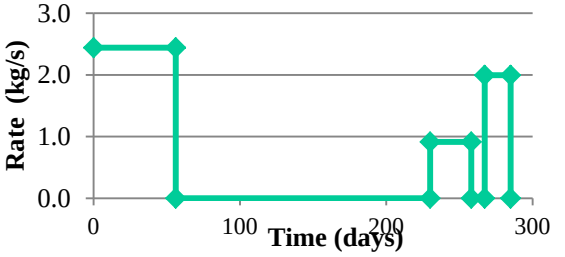
- U20-WW Pump Test Domain
- 5 km x 5 km x 1.4 km
- 15k and 125k nodes

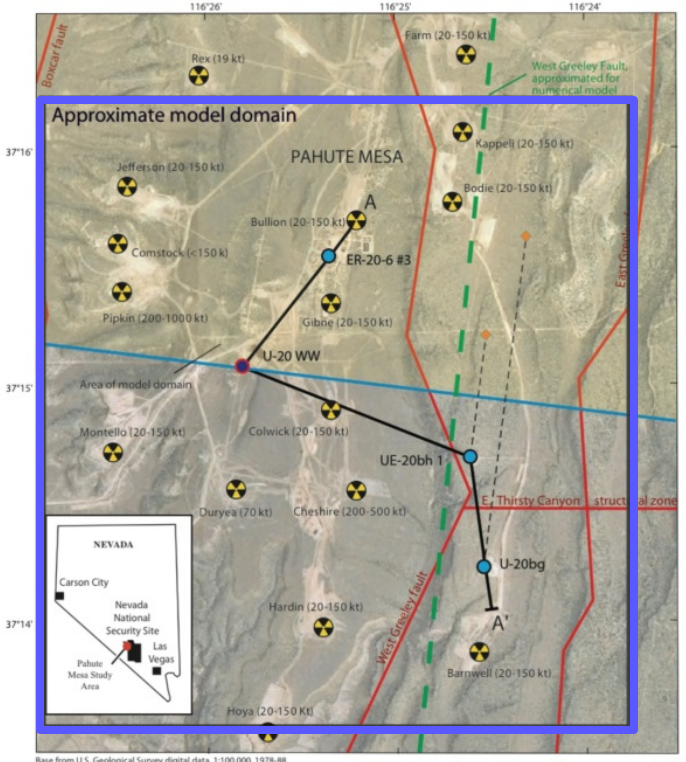
FY15 Model Domain

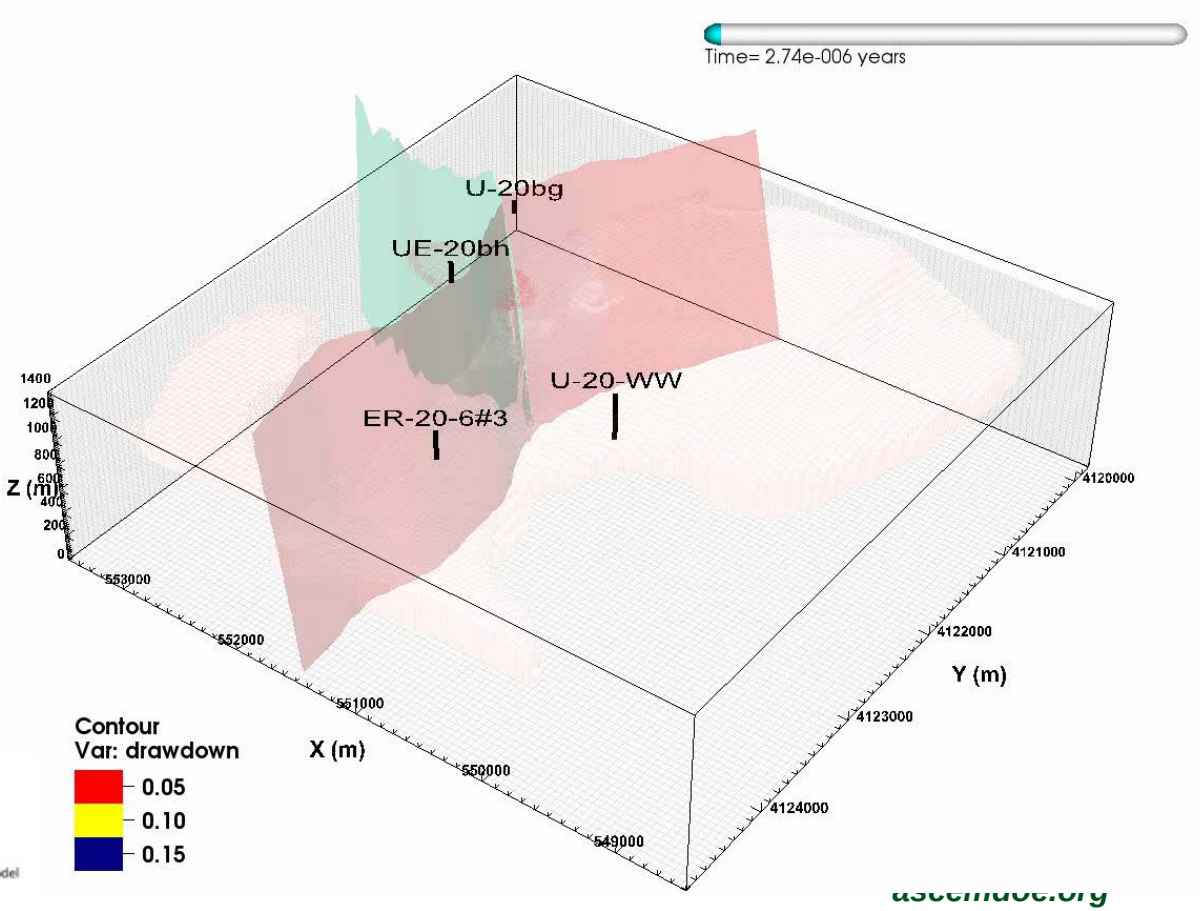
- Large-Scale Test-Bed Model
- 20 km x 35 km x 2.5 km
- 7.06 M nodes

FY14 UGTA Site Application: U-20WW Pump Test

- **U-20WW Pump Test**
  - 3 pumping periods over 285 days
  - Measured drawdown at 3 Observations wells



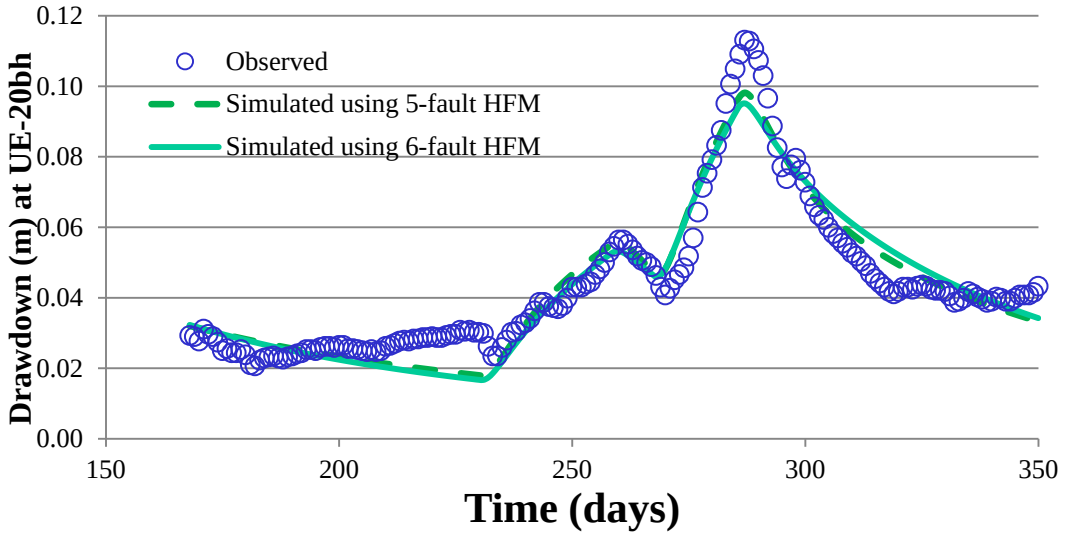




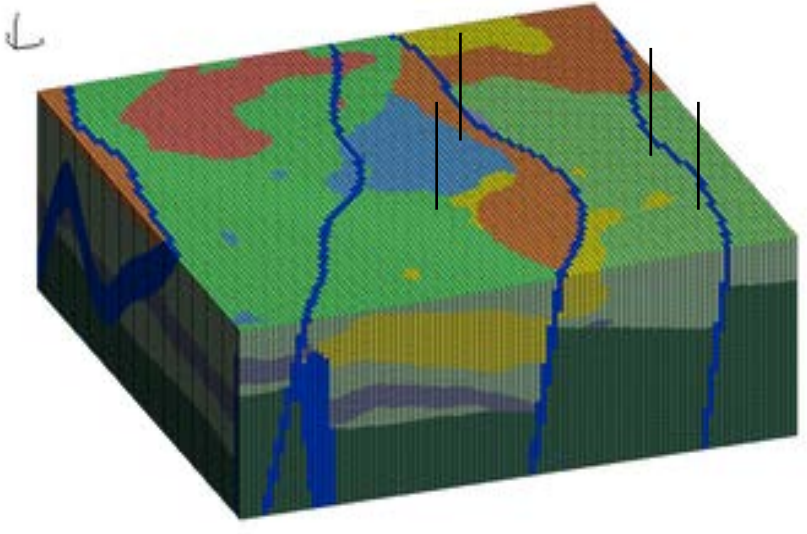
UGTA Site Application
Parameter Estimation Tool

U-20WW Pump Test

Drawdown at UE-20bh with best-fit parameters



2014 model with 6 faults

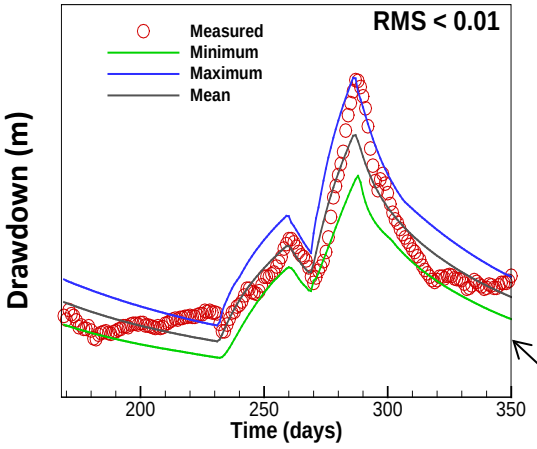


- 2 other observations wells- negligible drawdown matched
- 10 parameters estimated
- 4 rock units and the fault system
  - Permeability
  - Specific storage

UGTA Site Application
Uncertainty Quantification Tool

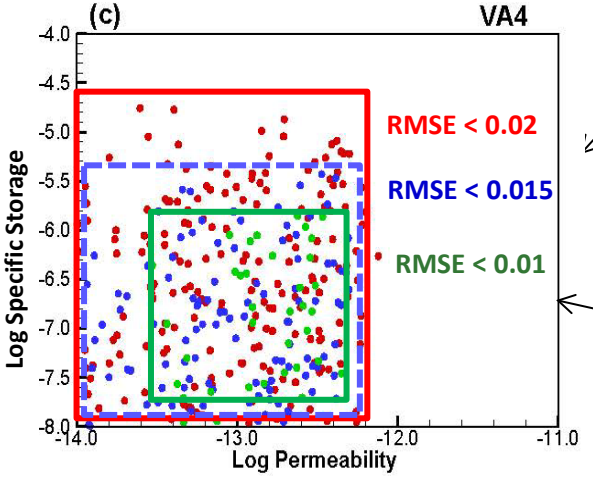
U-20WW Pump Test

- 5000 simulations run
- 10 parameters sampled with Latin Hypercube Sampling
- k, Ss for 4 units and faults
- UQ narrowed parameter ranges for:
- 2 of 4 hydrologic units (between pumping well and observation well with greatest drawdown)
- the fault zones



Root Mean Square Error
Defines best fit PDFs
RMSE < 0.02, 332 Simulations
RMSE < 0.015, 142 Simulations
RMSE < 0.01, 36 Simulations

Lower RMSE
- Better fits observations
- Narrows parameter ranges



Original parameter ranges for 5000 simulations

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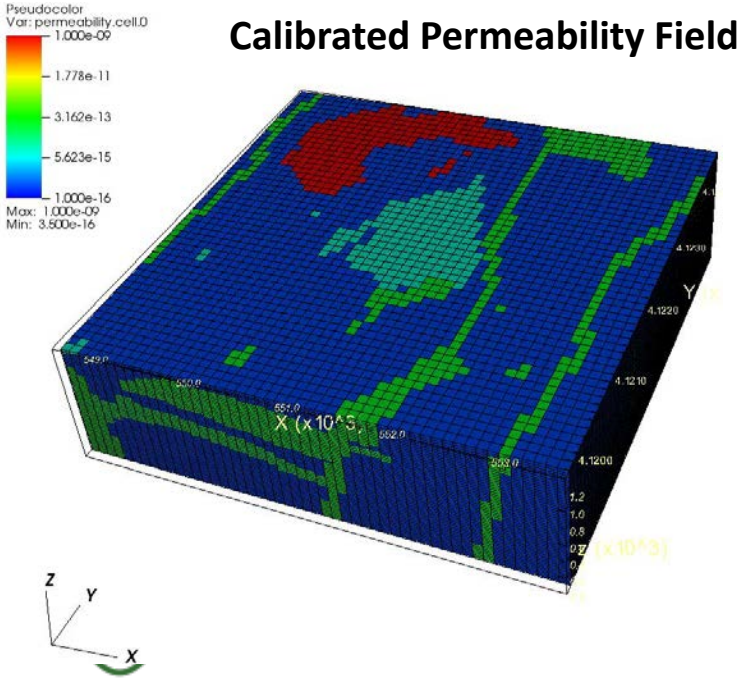
UGTA Site Application
Set Up for Particle Tracking Simulations

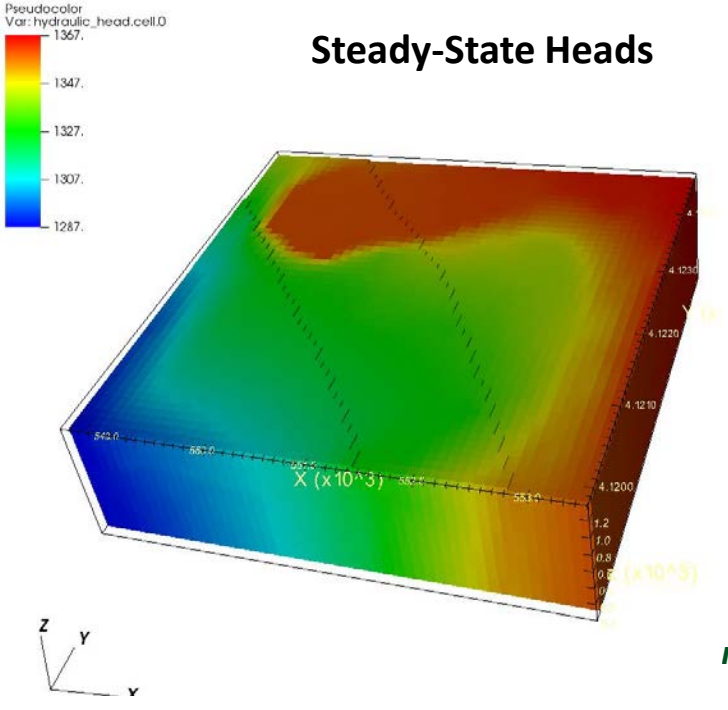
U20-WW Domain: 125k elements; 5-fault model
Grid resolution: 100m x 100m in horizontal; variable in vertical (about 25m)
Heterogeneous hydraulic properties: Derived from inversion results
Steady-flow boundary conditions: Hydrostatic conditions on side boundaries; no-flow top and bottom

Particle Tracking: (Walkabout) 125k particles instantaneously released (at internal node)
Convolution integral (PlumeCalc): Generates plume, assumes constant source in this example

Calibrated Permeability Field



Steady-State Heads



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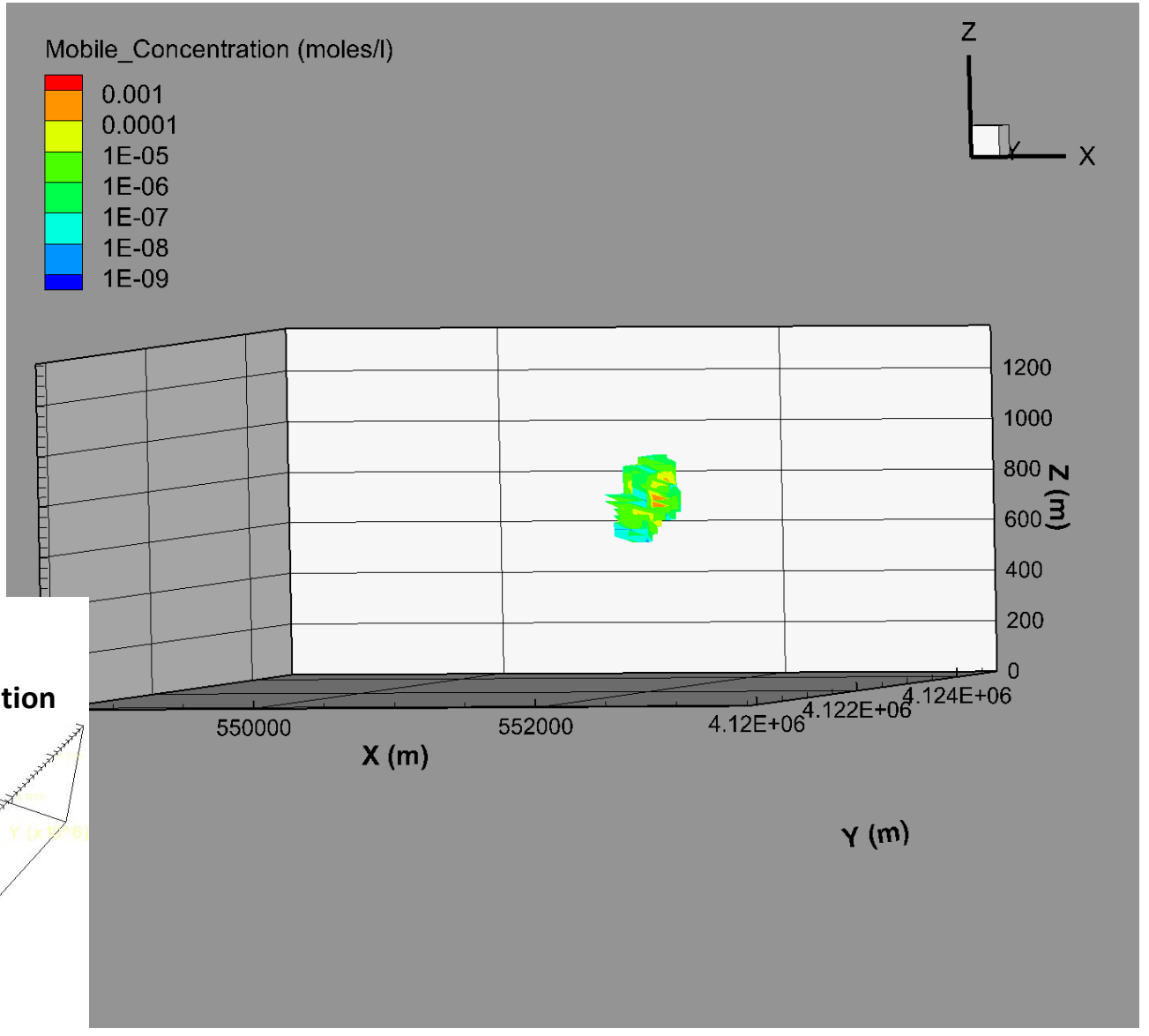
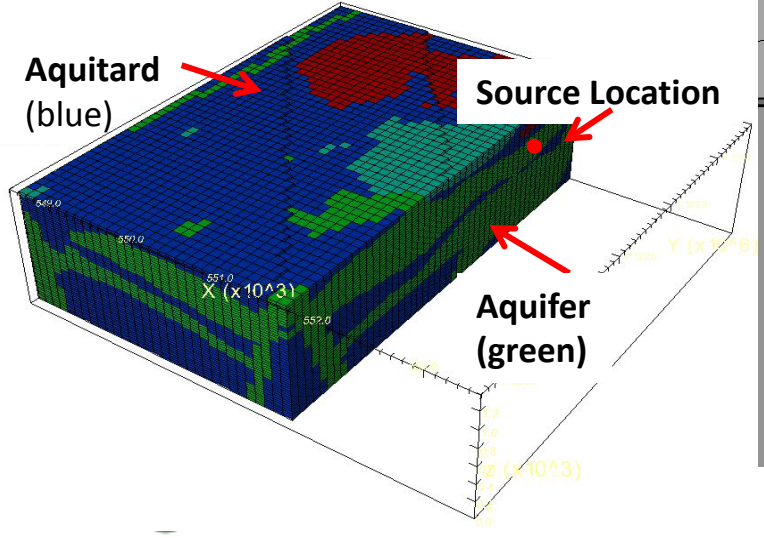
Walkabout (Particle Tracking) and PlumeCalc (Convolution Integral) transport in U20-WW Domain

3-D Transport

- Plume bifurcation around low permeability features
- Highlights need for including detailed hydrostratigraphy

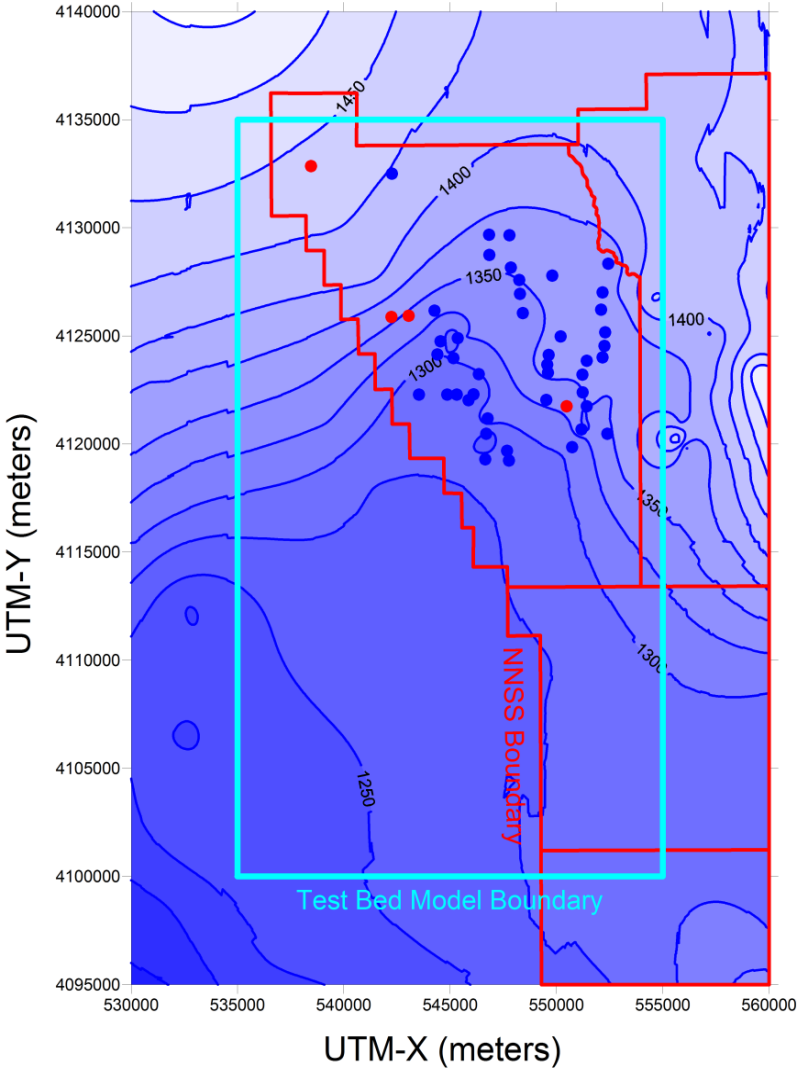




FY15 - Preliminary Model Set-up

- Model domain includes 49 deep nuclear detonations
  - 45 (in blue) are below or within 2 cavity radii of the water table
  - 4 others (in red)
- Active model domain extends from water table to 1,000 m below sea level
- Measured hydraulic heads indicate flow exits the southwest quadrant of model domain
- Model grid is ΔX=ΔY=100 m and ΔZ = 25 m
  - 7.06 M nodes beneath water table
- Model Boundary Conditions
  - Observed hydraulic heads applied to sides of model
  - Top and bottom are assumed no-flow boundaries (no recharge in preliminary runs)

Measured hydraulic head contours with nuclear detonations



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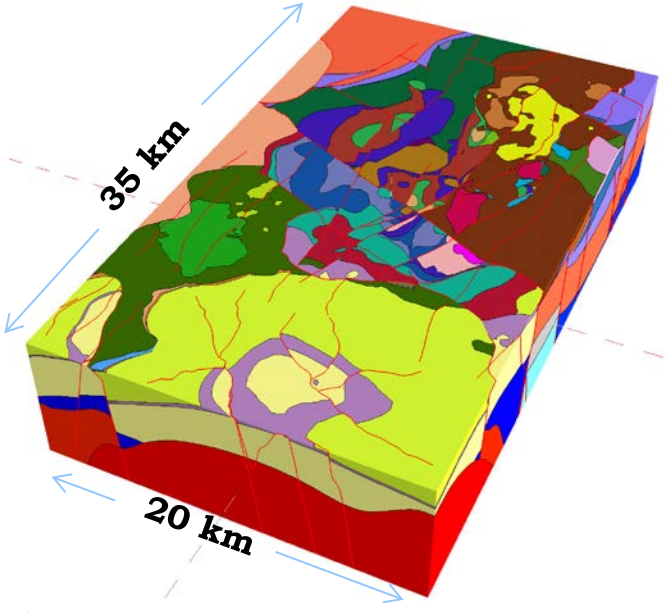
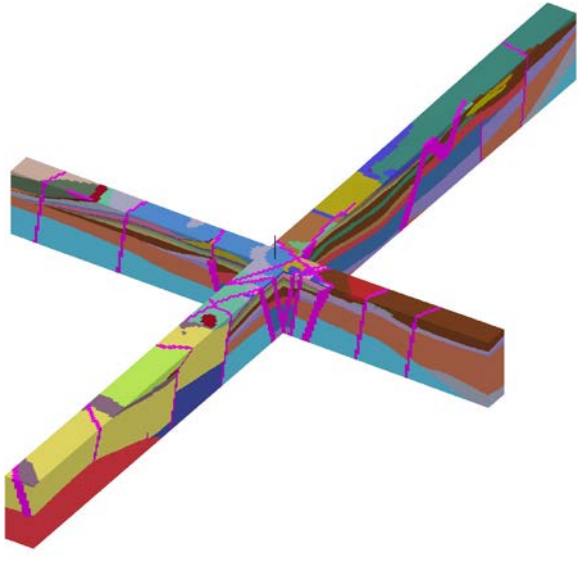
Pahute Mesa Test-Bed Model



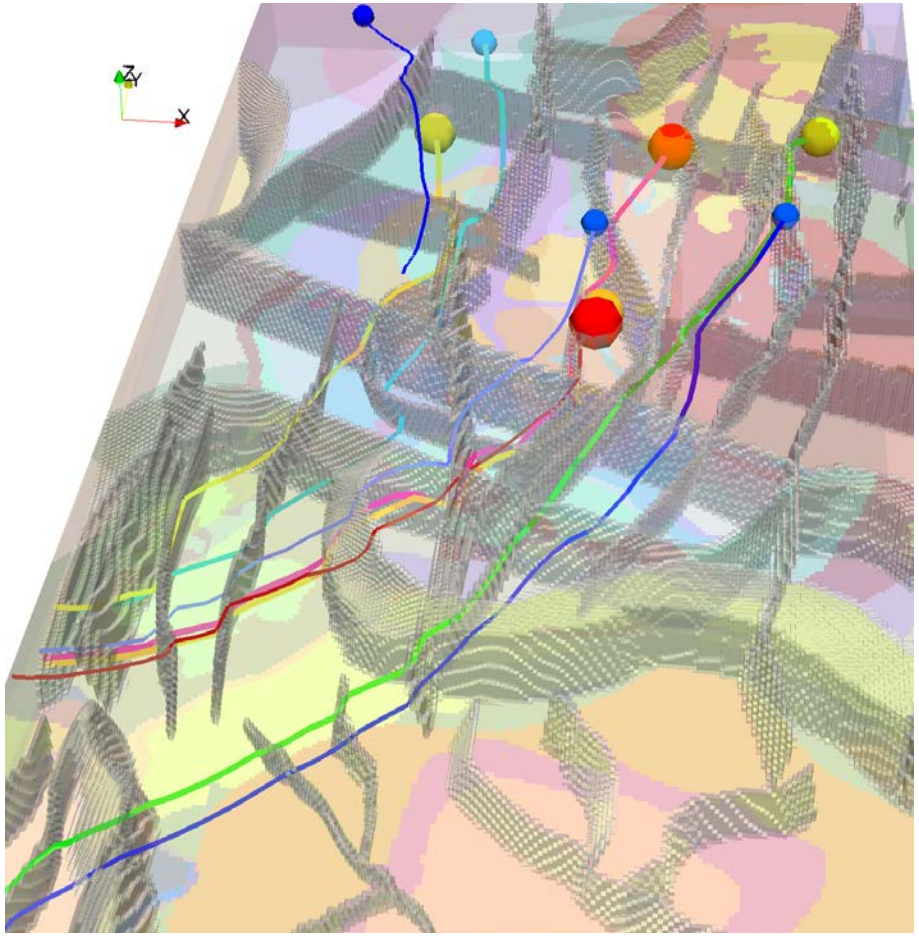


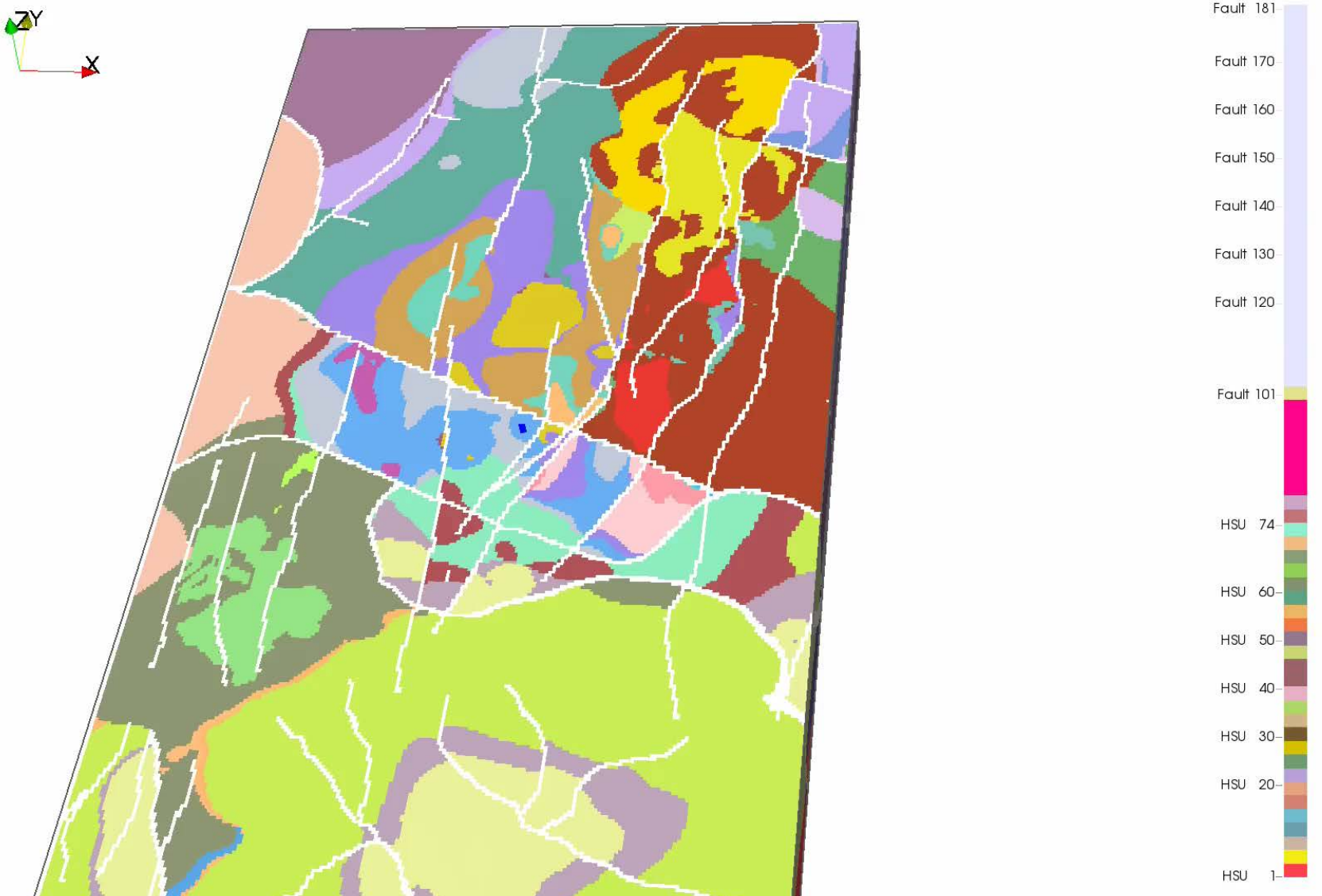
- New high-fidelity (7M+ nodes) AMANZI model for Pahute Mesa transport corridor (Area 20, Bench and NW Caldera); 95 units and 44 faults
- Goals of the Test Bed Model
  - Demonstrate HPC capability for flow and transport in a geologically complex environment
  - Test conceptual models of flow and transport in western Pahute Mesa
  - Estimate flow & transport parameters using transient hydraulic test data, steady-state heads, and observed contaminant extent
  - Provide basis for model simplification as may be appropriate for regulatory calculations and/or extensive Monte Carlo runs

Preliminary Test-Bed Model Results

- Model calibration to occur Spring 2015
- Preliminary results assume typical permeabilities for known aquifer types
  - Faults: 1.e-11 m^2
  - Lava & welded tuff aquifers: 1.e-12 m^2
  - Tuff confining & composite units: 1.e-13 m^2
  - Intrusive confining units: 1.e-14 m^2
- Preliminary flow results and particle tracks reflect prescribed permeabilities
  - With these assumptions, particles tend to follow faults along much of their travel distance

Particle Tracks from 9 sources




Z
Y
X
Materials
Fault 181
Fault 170
Fault 160
Fault 150
Fault 140
Fault 130
Fault 120
Fault 101
HSU 74
HSU 60
HSU 50
HSU 40
HSU 30
HSU 20
HSU 1

Summary

- Collaborative partnership between UGTA and ASCEM results in substantial mutual benefits to both parties
  - State-of-the-art HPC simulation capability available to UGTA
  - Provides high-resolution simulations for conceptual model testing, parameter estimation and up-scaling, and model simplification
  - Code capability testing on complex field site for ASCEM
- Previous years' (FY12-FY14) collaboration has implemented and tested new capabilities for flow and radionuclide transport relevant to UGTA, particularly for the Pahute Mesa CAUs
- FY15 collaboration will demonstrate integrated capabilities for flow and radionuclide transport in a fractured and faulted, geologically complex environment at high resolution