Advanced Simulation Capability for Environmental Management

ASCEM Program Update

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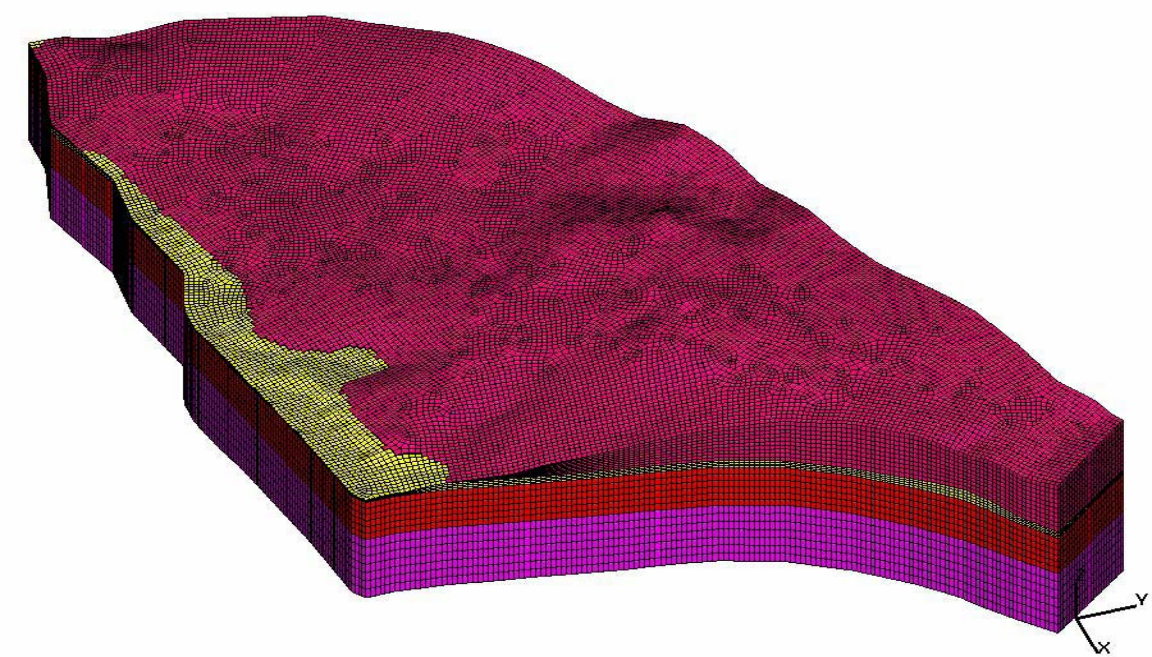
Presentation to the EM Waste Processing Technical Exchange
November 20, 2010

Presentation Outline

1) What is ASCEM?
   - Motivation
   - Who We Are
   - ASCEM Structure and Development Lifecycle
2) FY11 Phase I Demonstration Update
   - Criteria for Phase 1 Demo
   - High Level Goals of Phase 1 Demo
   - Site Selection Evaluation/Savannah River F-Basin
   - Highlights of Phase 1 Demo
3) Site Application Working Groups for FY11
4) Accomplishments Since Last LFRG Meeting
5) Conclusions and Further Discussion

What is ASCEM?

ASCEM is a state-of-the-art ***scientific tool and approach*** *for understanding and predicting contaminant fate and transport in natural and engineered systems. ASCEM is a modular and open source HPC tool that will facilitate integrated approaches to modeling and site characterization that enable robust and standardized development of performance and risk assessments for EM cleanup/closure activities*.



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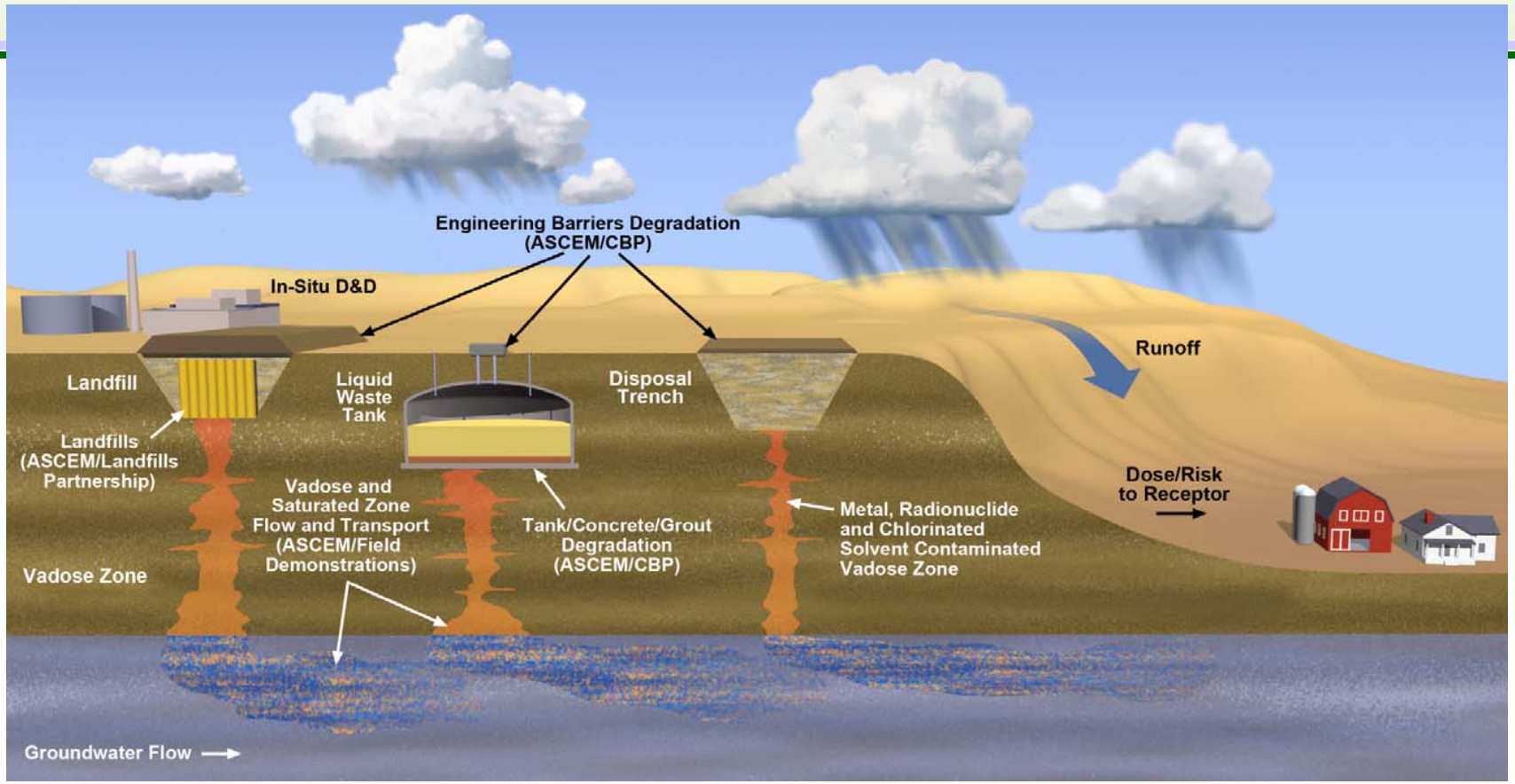
ASCEM Application Areas



- Mission is to support PA's and RA's for complex EM cleanup sites
- Early Mission**: *"technically underpin"*** existing EM RA's and PA's Modeling to support areas of greatest uncertainty in this system
- Inform strategic data collection for model improvement

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ASCEM National Laboratory Consortium

Berkeley Lab

Los Alamos National Laboratory EST. 1943

Pacific Northwest National Laboratory

Oak Ridge National Laboratory

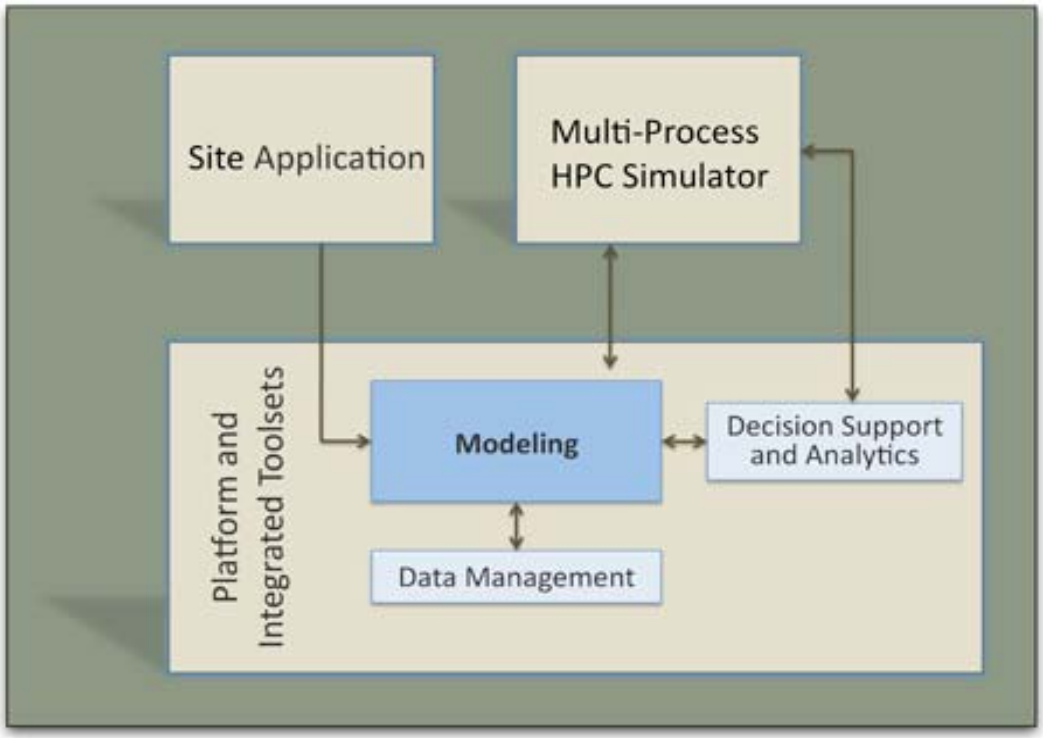
SRNL Savannah River National Laboratory

Lawrence Livermore National Laboratory
Science in the National Interest

Argonne National Laboratory

INL Idaho National Laboratory

ASCEM Overall Structure

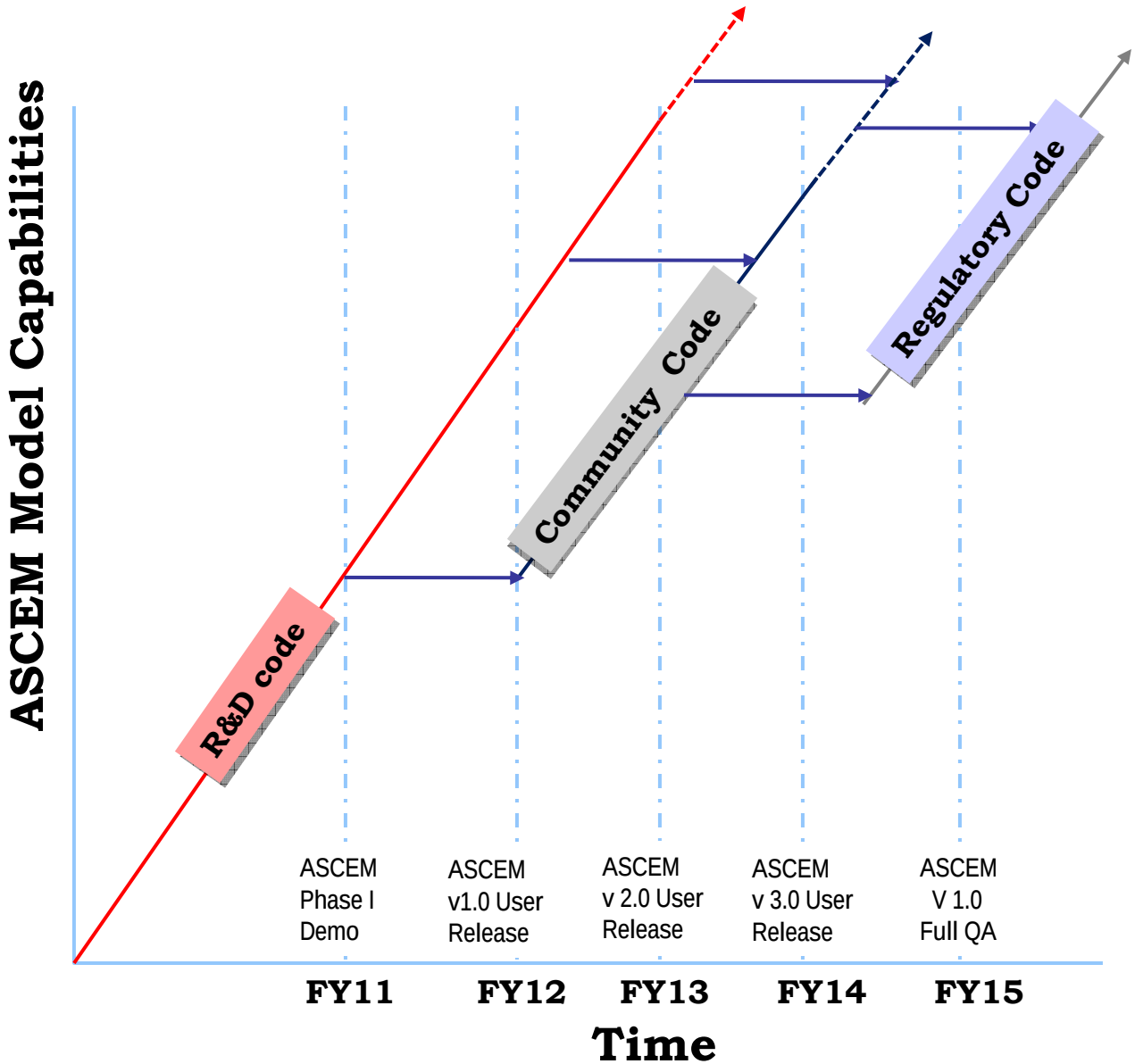


- **Site Applications**
  - Demonstration sites
  - Actively engage site user community to develop and test ASCEM tools

- **Platform and Integrated Toolsets**
  - Facilitate model development and execution, user interface, visualization, data management, parameter estimation, uncertainty quantification, decision support, and risk analysis

- **Multi-Process High Performance Computing Simulator**
  - Modular simulation capability for barrier and waste form degradation, multiphase flow and reactive transport

ASCEM Software Life Cycle



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Phase I Demo Project Criteria

The initial focus was to identify a short list of Phase I demonstration sites and associated potential projects.

- Choose a site based on best available information for Demo

- **Key criteria used to identify potential Phase 1 demonstration site:**

1. Phase 1 demo will invoke and highlight a variety of ASCEM capabilities
2. The Phase 1 demo will benefit EM / site end-user
3. Phase 1 demo is tractable within given Phase 1 timeframe **(December 17, 2010)**
4. Phase 1 demo new components tested over time (secondary)
5. Phase 1 demo will enhance engagement of site members in working team

December 2010 Phase 1 Demonstration Goals

HPC	Visualization	Data Management	Uncertainty Quantification
• 3D simulation • Richard's equation • Parallel (100 cores) • Reactive transport of uranium • Advection of non-reactive species • Aqueous speciation • Sorption • Mineral precipitation, and dissolution	• 3D navigation of concentration data • Visualization of time lapse contaminant concentrations through subsurface domain • Selectively enable several types of data	• Depositional data entered into databases • Contaminant concentrations entered into databases • Browsing and query interface with tabled output	• Initial Monte Carlo sampling capability • Automatic creation of forward simulation runs • Visualization of relationships between key parameters and model outputs

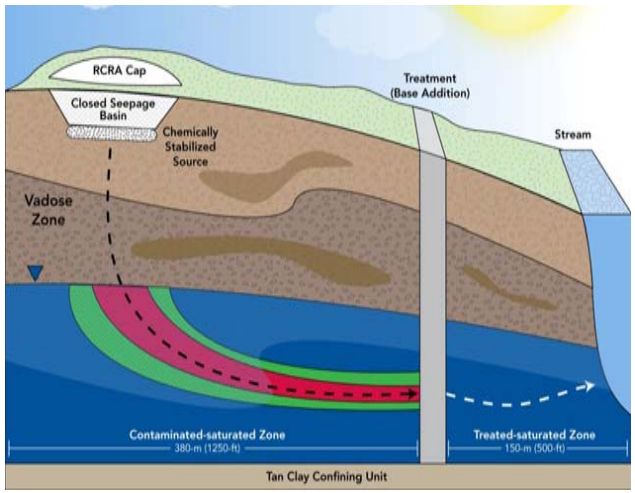
Sites Evaluated for Phase I Demonstration

ASCEM Site Selection Task Phase 1 Demo Report (In DOE review)

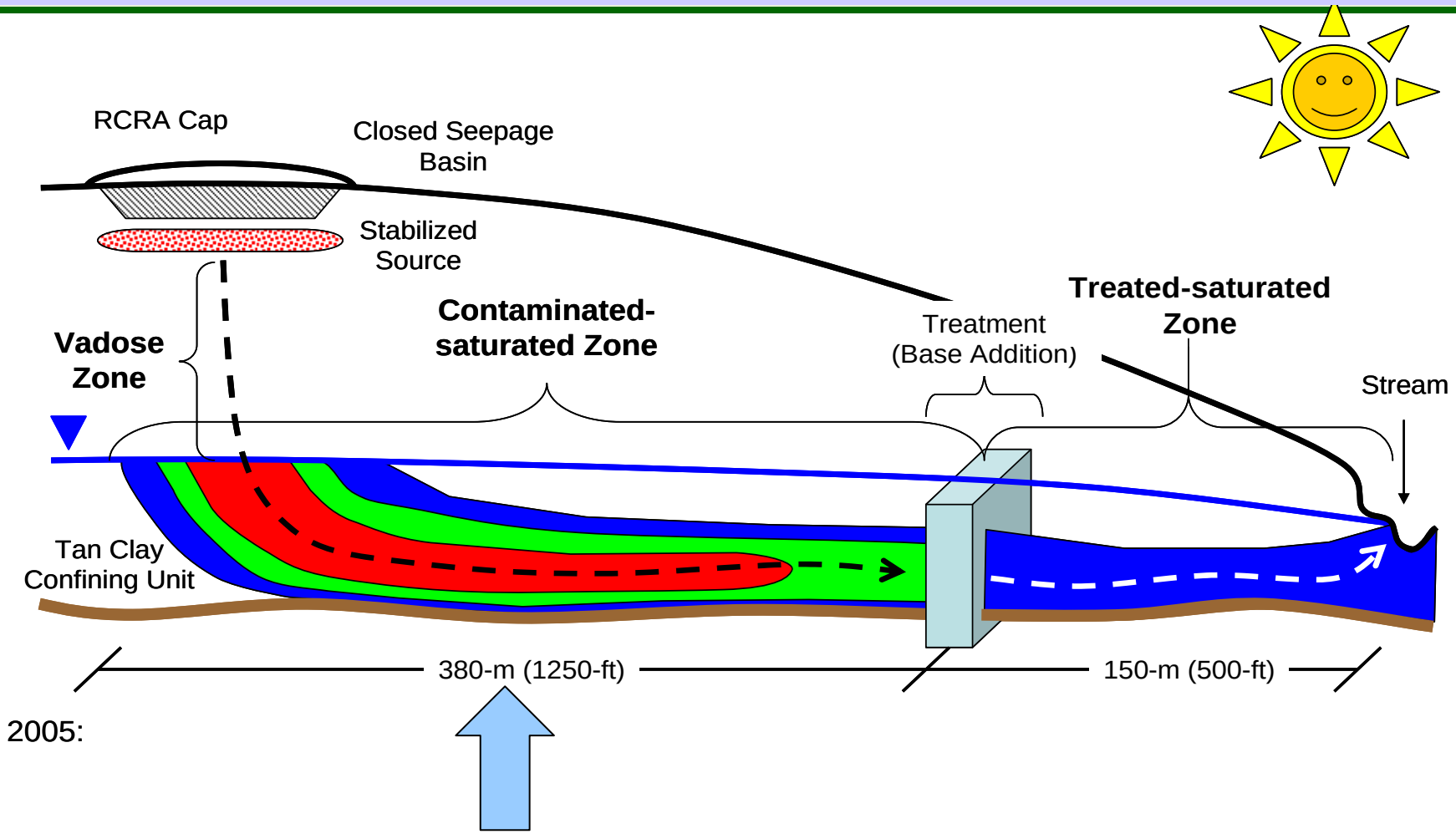
1. Savannah F-Area EM, SFA, and IFRC Sites
2. Hanford Deep Vadose Zone EM and IFRC Sites
3. ORNL EM and IFRC Sites
4. Rifle Colorado IFRC
5. PA: Tank Closure Demo (SRS example)

EM Saturated Zone Priority Site
Savannah River F-Area

- Disposal of low-level radioactive, acid waste solutions (1955–1989)
- Acidic plume has developed in groundwater beneath the basins (pH 3–3.5, NO_3, U isotopes, ^{90}Sr, ^{129}I, ^{99}Tc, tritium)
- About 100 monitoring wells, some with 25 years of monitoring records
- Remediation History & Plan:
  - Basins capped ~ 1989, pump & treat ~ 1997–2003
  - pH manipulation system installed since 2004
  - ***Natural attenuation is desired as a long-term remediation strategy***



Conceptual Plume Model
And ASCEM demonstration topic



Assess impact of uncertainty in U sorption models & acidity conditions on groundwater U plume mobility (and thus MNA viability)

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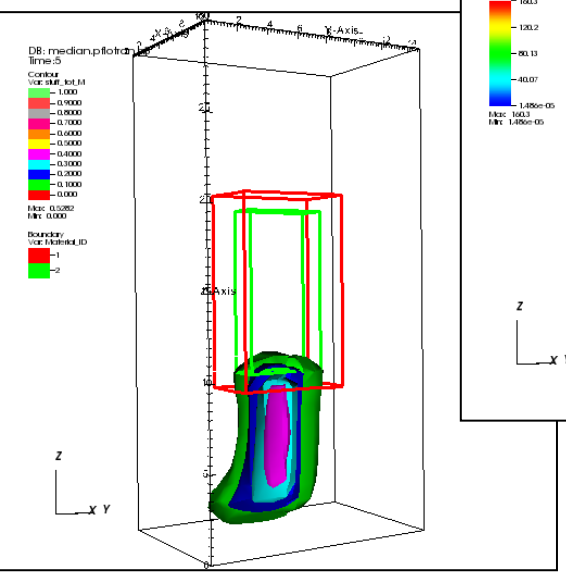
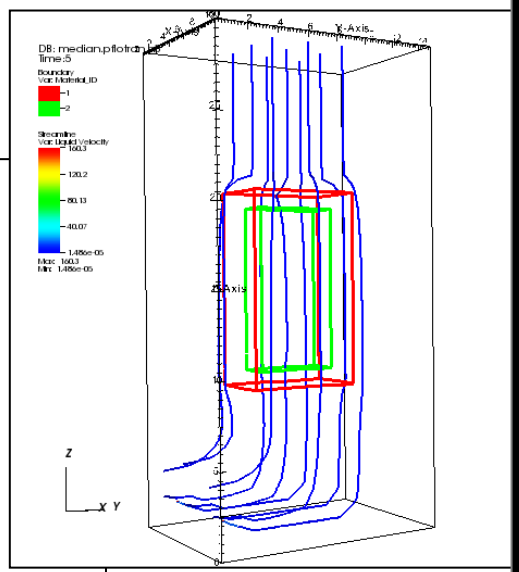
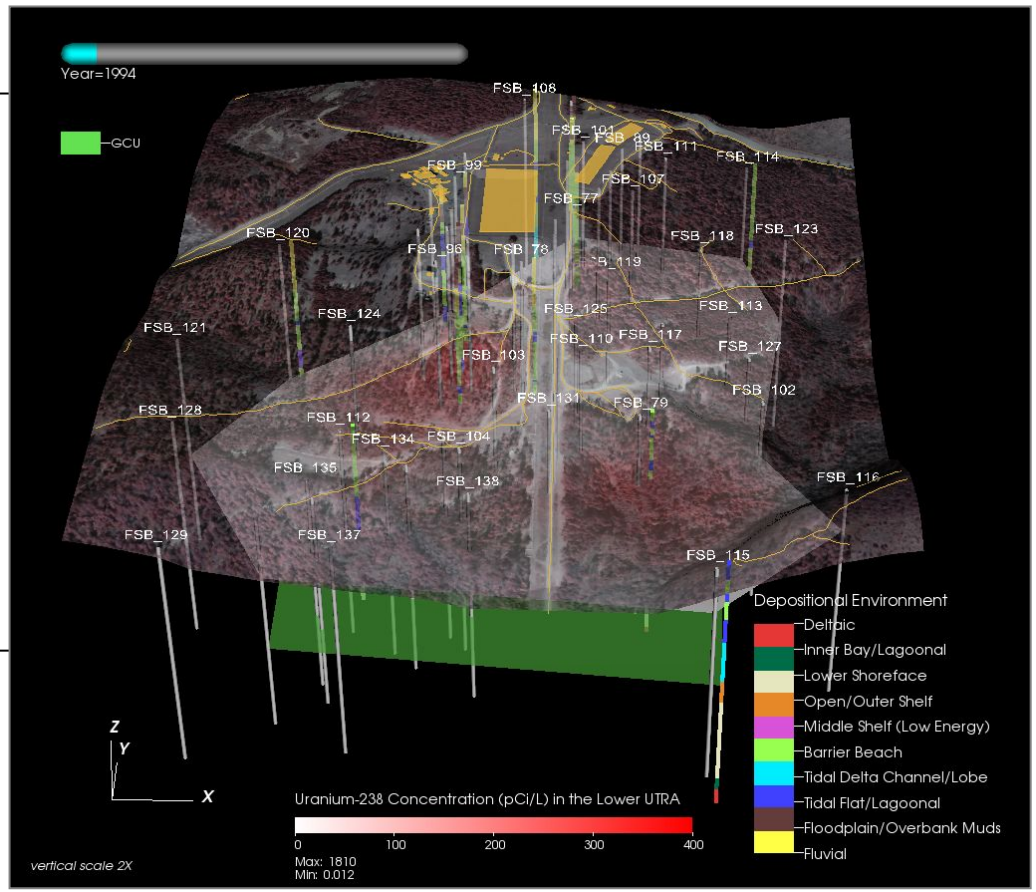
Advanced Visualization

Advanced visualization of the modeling and decision making process, with 3D navigation of information such as:

- Temporal concentration data (time evolution)
- Geospatially registered surface topography
- GIS data, and observation wells







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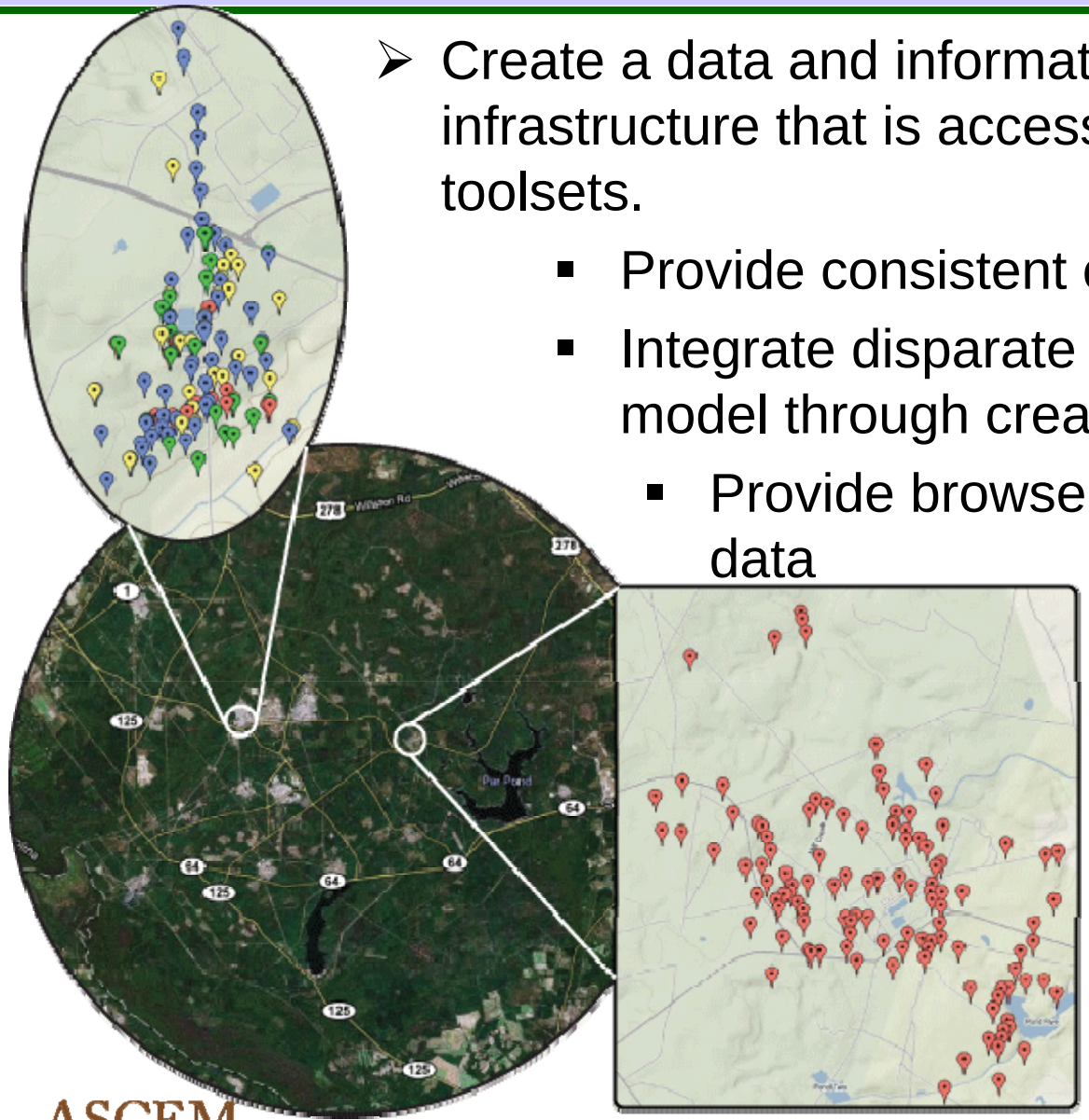
Data Management



- Create a data and information management infrastructure that is accessible to all ASCEM platform toolsets.
  - Provide consistent coordinates for all site data
  - Integrate disparate data structures into a single model through creation of data ensembles
    - Provide browse and search capabilities for data

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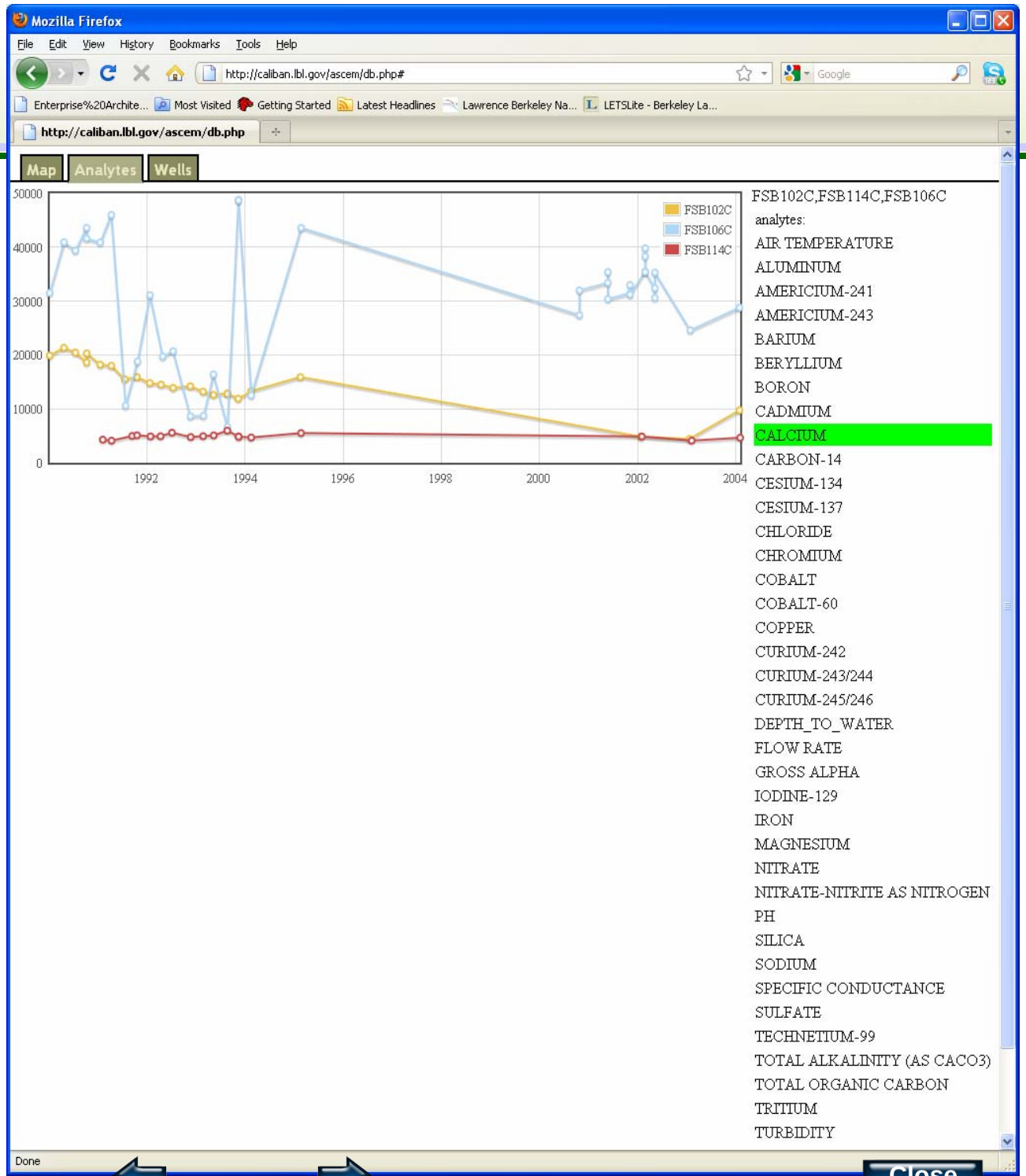
Data Example

Selecting a well from Aquifer 2.

- It provides summary information and a List of all analytes measured at that well over time.

- Selecting an analyte Generates a graph of The analyte of at that Well over time.

- Comparing same analyte from 3 wells over time



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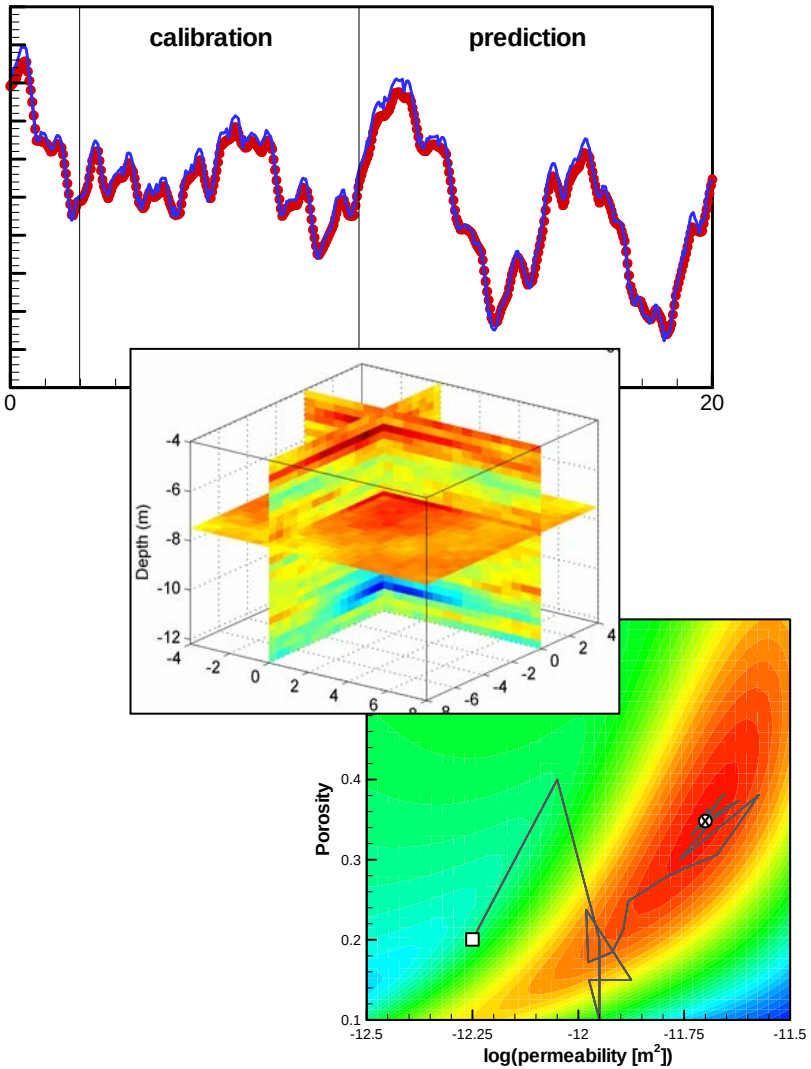
Print

Close

Parameter Estimation Toolset

- Determination of model related, process dependent, and site specific parameter values that can not be reliably obtained from independent sources.
  - Examine the ability of the model to represent the system of interest.
  - Point toward aspects of the model that require refinement.
  - Helps quantify and reduce the uncertainty of model predictions.
- Model based data inversion, (inferred from measured data.
- Analysis approaches that combine multiple sources of information for Bayesian parameter estimation.



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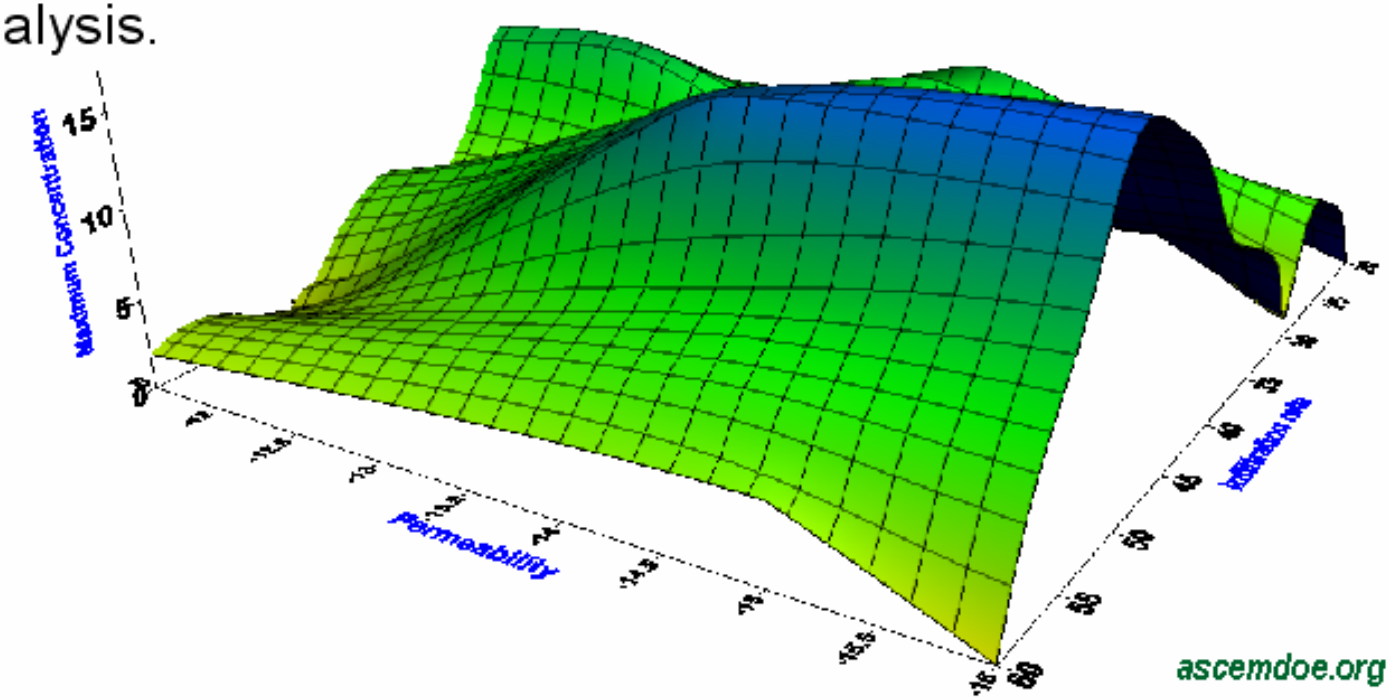
Uncertainty Quantification

- **Propagation of uncertainties through a forward model.**
  - Generate ensembles of parameter and conceptual model variations.
  - Forward error/uncertainty propagation.
    - Forward model response surface approximations.
    - Generation of relatively small ensembles of forward model runs that will approximate the performance of larger ensembles.
  - Sensitivity Analysis.



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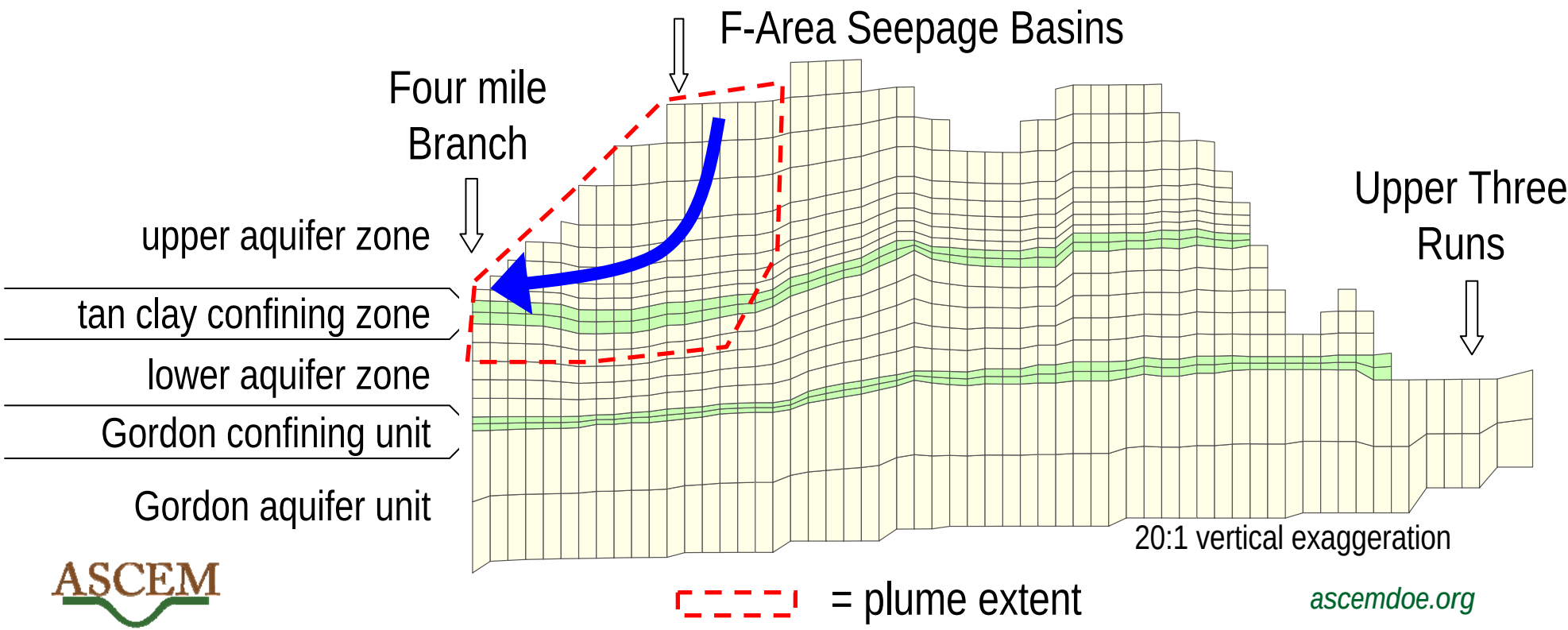
HPC Phase I Demo

The HPC Phase I demonstration will highlight our progress on developing advanced flow and reactive transport capabilities for ASCEM. Features we are highlighting include:

- Full three-dimensional simulations.
- Advanced discretizations capable of handling tensor material properties (e.g., permeability) on general grids.
- Unstructured hexahedral grids fit to stratigraphy.
- Parameters and heterogeneity based on real data and existing conceptual models.
- Designed and implemented parallel from the start, with consideration for emerging architectures.

Conceptual Layers

A conceptual model of the General Separations Area was developed by Greg Flach et al. (2004) at SRNL. Members of our team are collaborating with Greg and the F-Basin Site Working Group to establish a conceptual model of the sub-region we are focusing on in the demo. The fundamental layered structured is shown here. The elevation of Fourmile Branch motivates our sub-region focusing above the tan clay confining zone.



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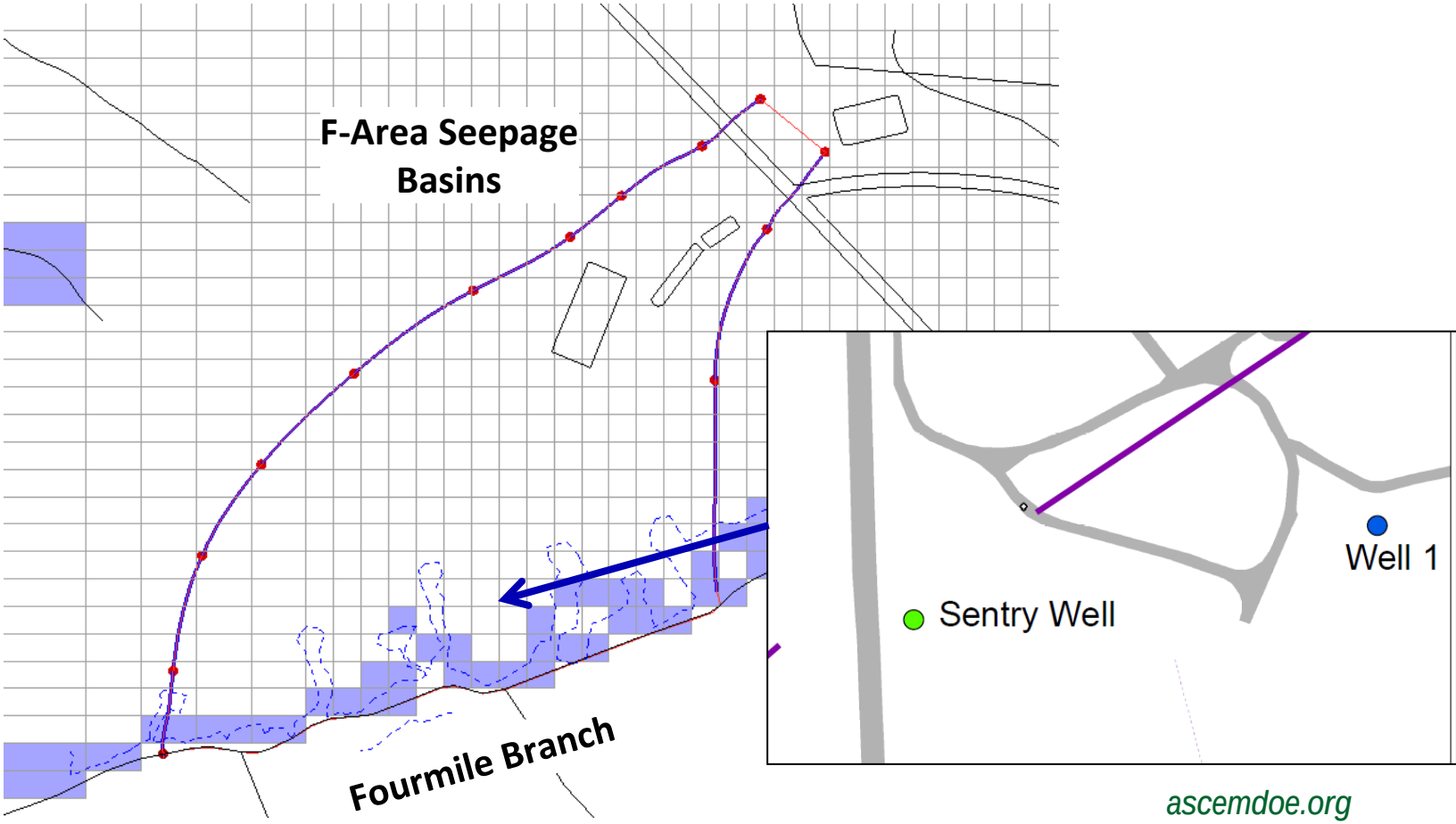
The Physical Domain

The demonstration will focus on a sub-region of the General Separations Area that will include the unsaturated and saturated zones, approximately to the depth of the "tan clay" confining unit, and with an areal extent of the F-Area basin and the Fourmile Branch.



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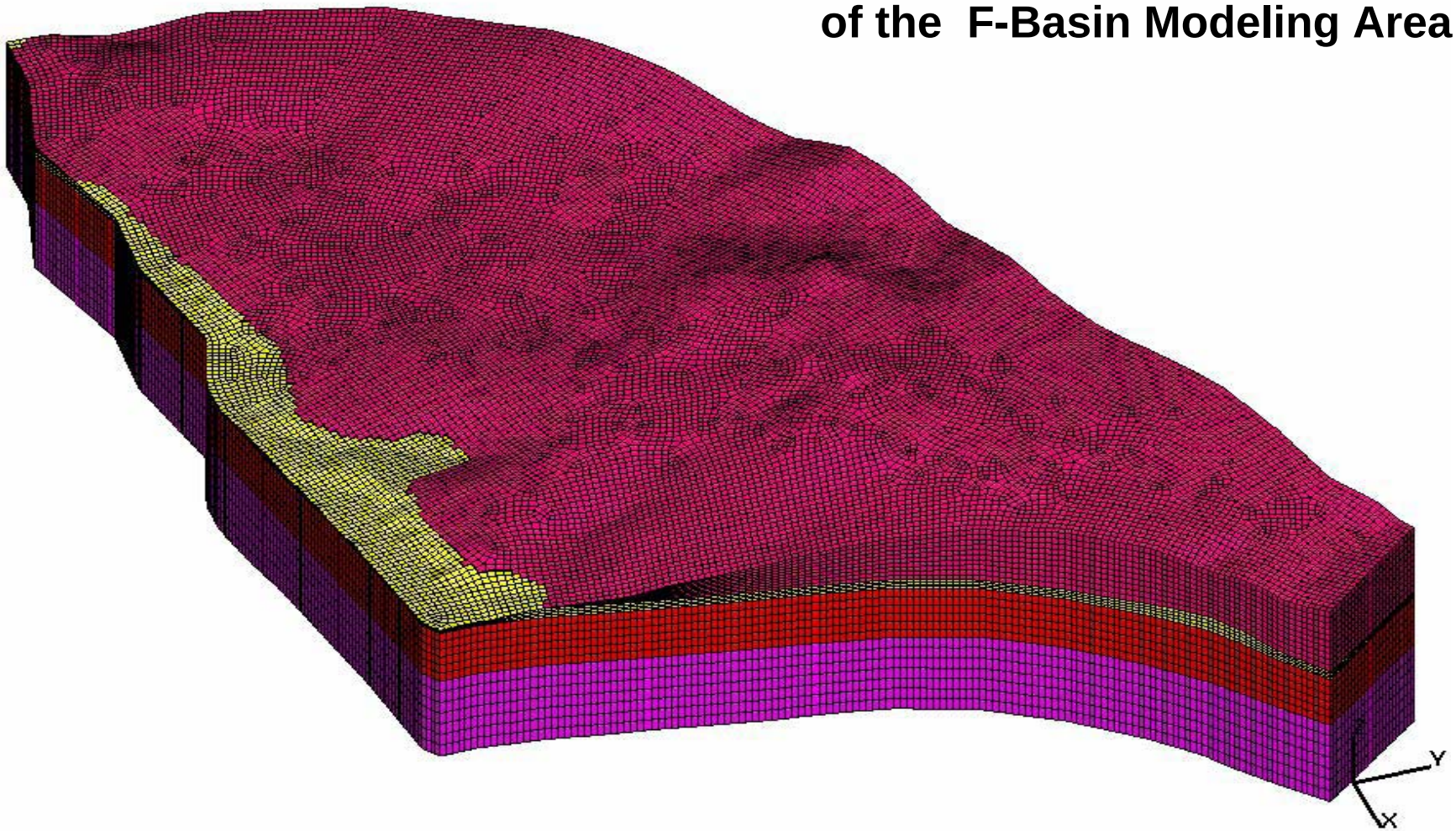
Prototype Grid

High resolution unstructured grid of the F-Basin Modeling Area



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Unsaturated/Saturated Flow

- Richards' equation with a van Genuchten relation will model unsaturated flow.
- We use the pressure as the primary variable to enable a smooth transition to the saturated zone and a single-phase Darcy model.
- A layered model is used, developed by Greg Flach (SRNL) in collaboration with Glenn Hammond (PNNL).
- Three-dimensional unstructured hexahedral grids are being developed by Carl Gable (LANL).
- We will run the simulation in parallel on at least 100 processors to obtain a steady-state flow field for passive and reactive transport simulations.

Non-reactive and Reactive Transport

The transport simulations will use the steady-state flow field generated in the parallel flow simulations.

- Evolve the concentration of a non-reactive tracer released from the source region (basins) over time.

- Geochemical processes and transport are weakly coupled through operator-splitting this year. These processes include:
  - Aqueous speciation
  - Mineral precipitation and dissolution
  - Soprtion

- Evolve the concentration of Uranium as a result of the release from the source region in the vadose zone and visualize the plume over time.

Site Applications Working Groups FY11

1) **Savannah River F-Basin**
   - Impact of uncertainty in U sorption model and acidity conditions on groundwater plume mobility and MNA viability
   - Impact of Waste degradation uncertainty on PA decisions
2) **Deep Vadose Zone Working Group**
   - Evaluation of different types/scales of conditioning data for accurate simulation of infiltration in the vadose zone (Sisson & Lu site)
   - Impact of initial contaminant distribution uncertainty on long-term vadose zone transport predictions in the deep vadose zone
   - Impact of fluctuating water table
   - Impact of geochemical uncertainty of U sorption and release
3) **PA Tank Demonstration Working Group**
   - Top-down approach from perspective of PA user needs
   - Visualization of 3-D Monte Carlo uncertainty analysis results
   - Alternative modeling approaches to improve efficiency of tank simulations
4) **Mercury Contamination Working Group**
   - Mercury release, transport, and distribution in sediments and surface water
   - PA related uncertainty and risk analysis
   - Nitrate, U, and ^{99}Tc fate and transport in groundwater and streams

FY10 Accomplishments Since May 2010

1. FY10-FY15 Implementation Plan July 1, 2010
2. Requirements Documents
   - ASCEM Platform and Integrated Toolset Requirements Document
   - ASCEM High Performance Computing Requirements
   - ASCEM Mathematical Formulation and Specifications
   - ASCEM User Suggestions Requirements
3. ASCEM User Steering Committee Charter
4. ASCEM Scientific Advisory Board Charter
5. ASCEM Quality Assurance Plan
6. ASCEM/NRAP Workshop September 1-2, 2010
7. ASCEM Peer Review September 8-9, 2010
8. Numerous ASCEM presentations given at: PACoP, LRFG, Waste Processing Technical Exchange, SESP, and SBR
9. ASCEM Phase 1 Demonstration December 17, 2010

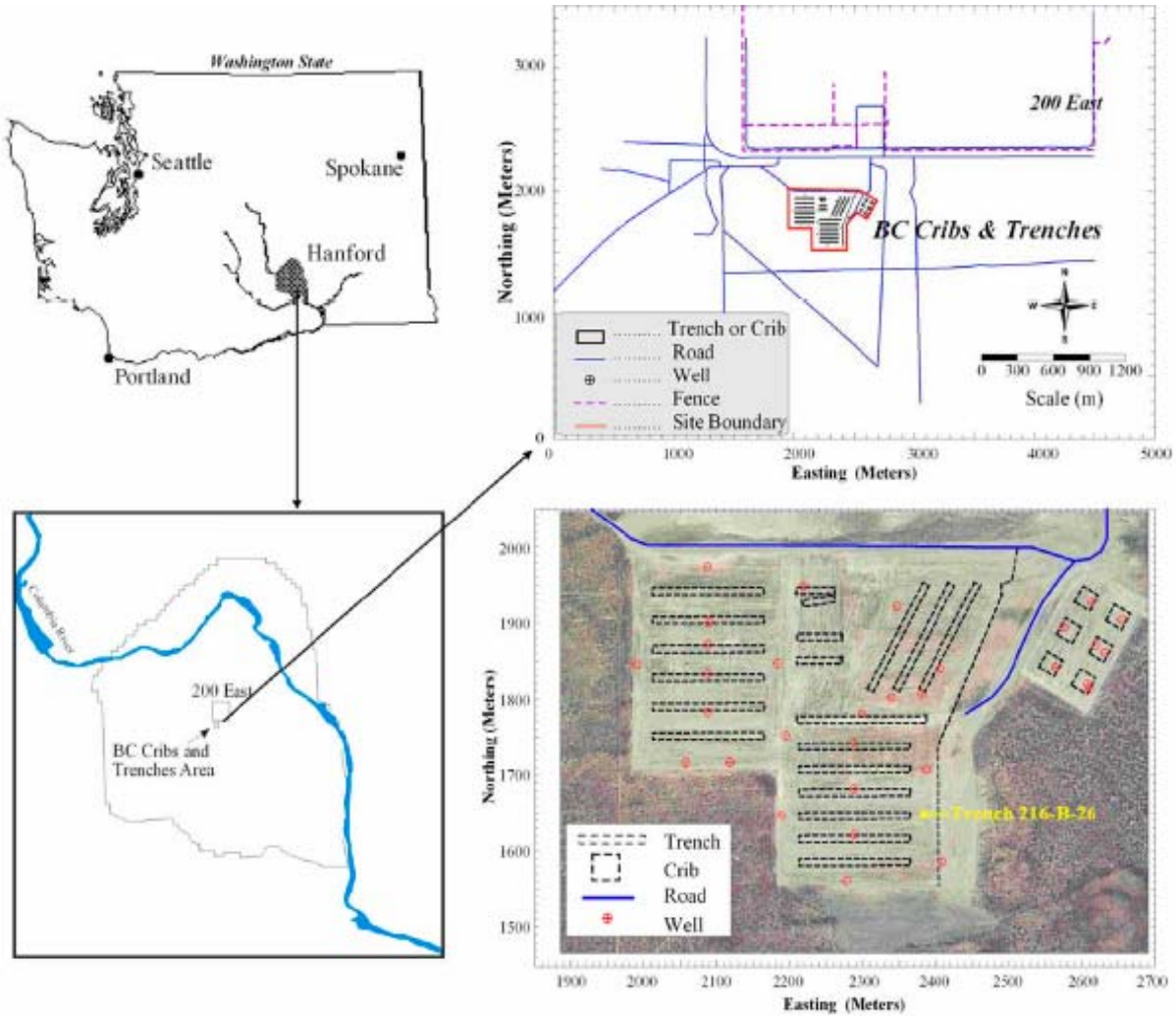
Conclusions and Thank You

- In the near-term:
  - Work on Phase 1 Demo
  - Prepare for Technical Peer Review 2nd Q FY11
- Rest of FY11: begin development of ASCEM User Release V1.0
- ASCEM will provide the technical underpinnings for DOE EM cleanup decisions through implementation of the next generation performance and risk assessment tools
- ASCEM will be used in combination with advanced remediation strategies to reduce risk, cost, and time-line for site closure
- Integration of ASCEM with field site demos and CBP will help to create a transformational, systems-based technical solution for EM
- Success will be found through active coordination with site end users, direct site involvement, and leveraging efforts in other DOE offices

Backup Slides

EM Deep Vadose Zone Priority Site
Hanford BC Cribs

- The BC cribs and trenches received in excess of 189 million liters (50 million gallons) of highly radioactive tank waste – largest Tc99 plume at Hanford
- Technetium-99 does not appear to have reached the water table.
- Release of technetium-99 from these waste sites is projected to lead to future groundwater contamination above the MCL.



Rucker and Fink, 2007

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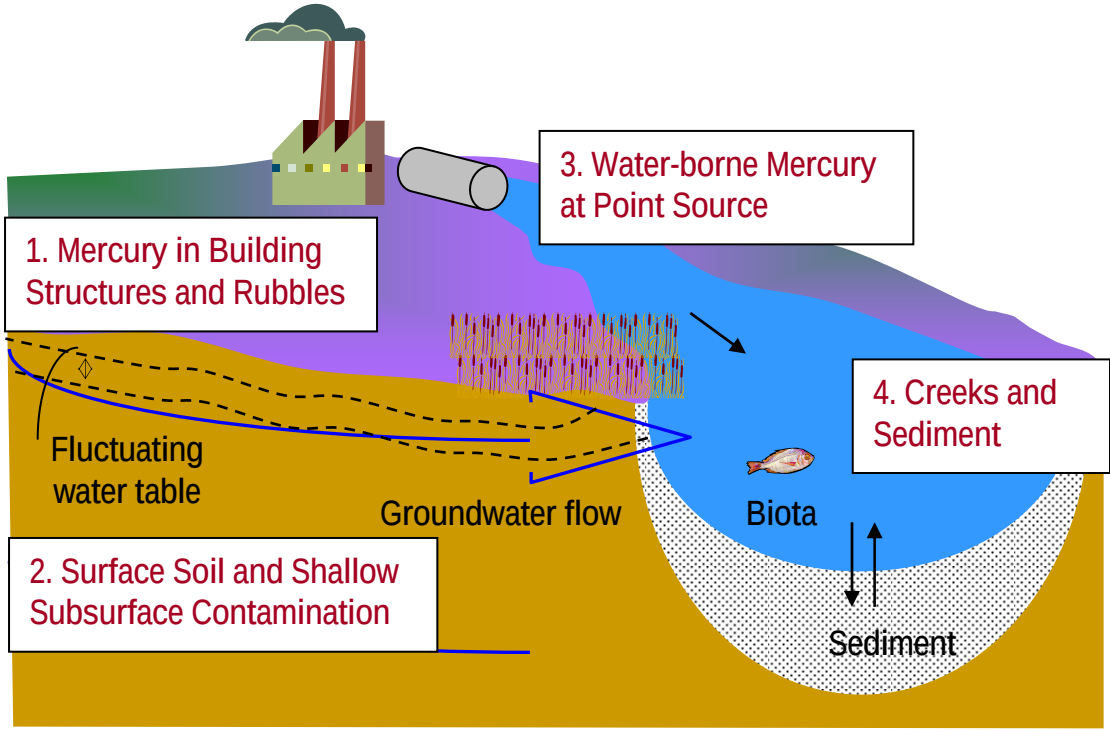
On-going Efforts for Mercury Characterization & Remediation

(Mercury accidental losses total ~194,100 kg)

- Develop and demonstrate reliable tools to detect and quantify mercury in soil, rubble, and fractured rock

- Develop and validate physical and chemical amendments to stabilize mercury in soil, sediment, and stream banks



- Demonstrate and optimize novel treatment methods for mercury in water
- Improve the understanding of biochemical and environmental controls on mercury methylation and food-chain transfer *(collaboration with Office of Science)*
- Develop and apply systems analysis and predictive tools (collaboration with ASCEM)

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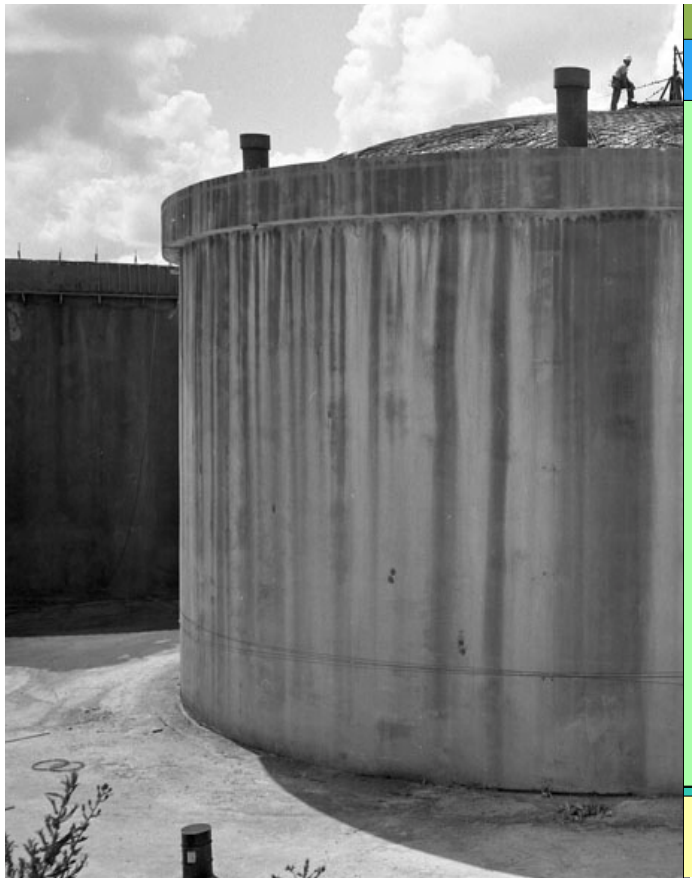
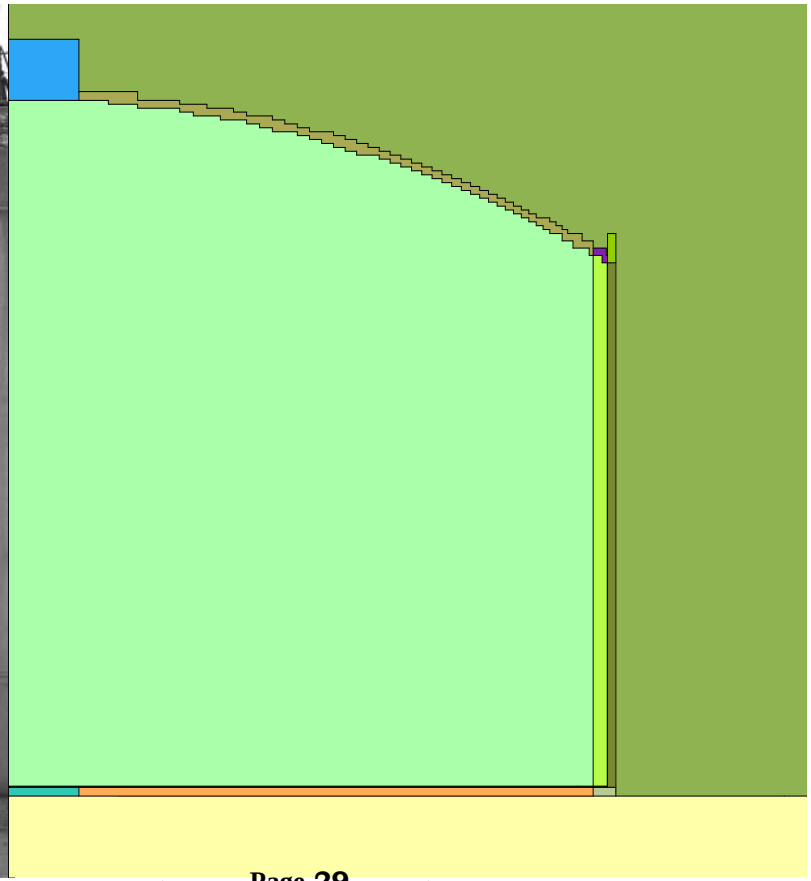
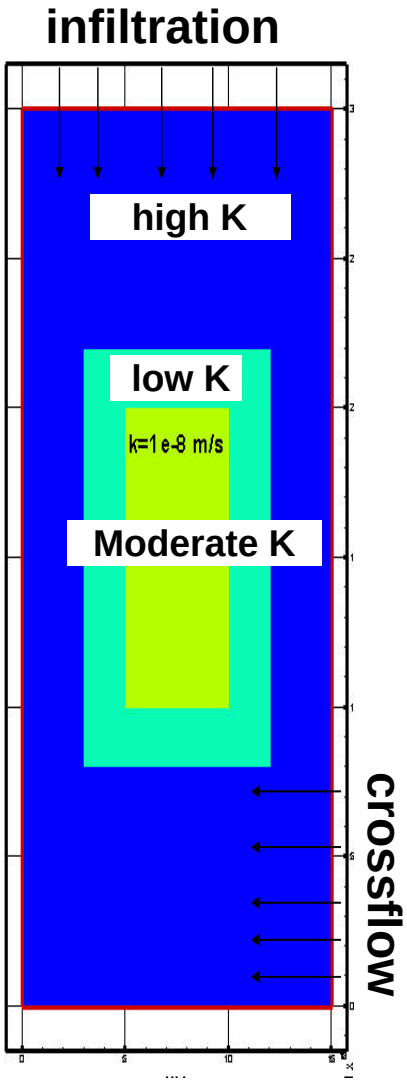
Engineered Barrier System: PA Tank Closure

- Visualization:
  - animations to show stakeholders of system evolution
  - Illustrations of uncertainty quantification







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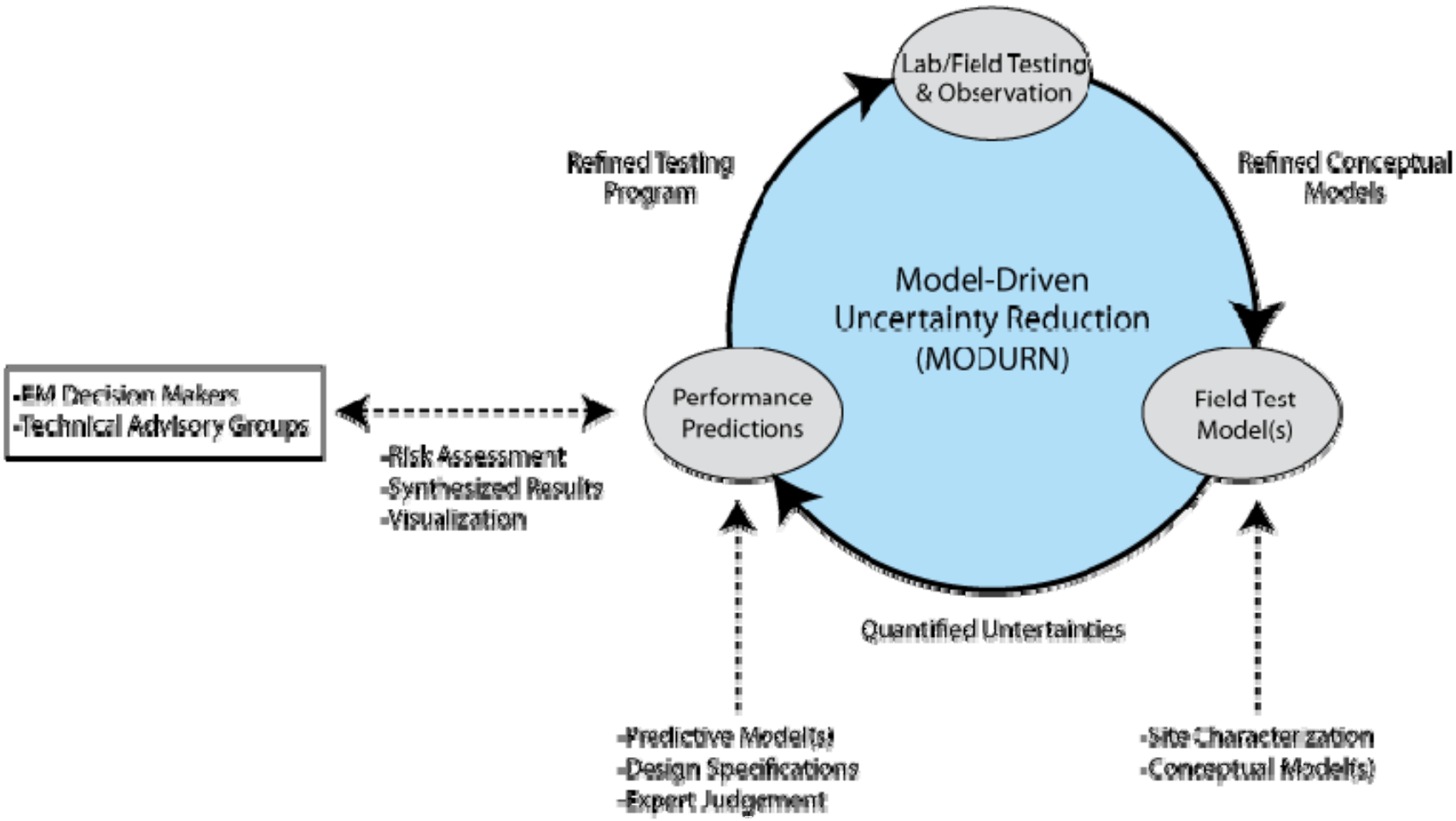
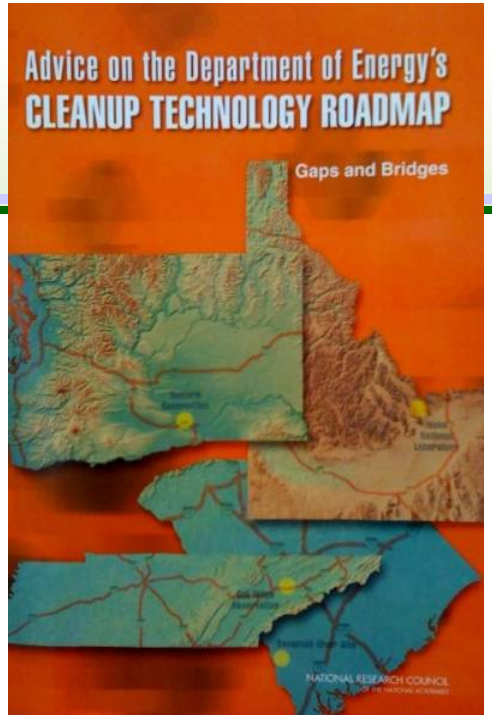
Approach


Lab/Field Testing & Observation
Refined Testing Program
Refined Conceptual Models
Model-Driven Uncertainty Reduction (MODURN)
Performance Predictions
Field Test Model(s)
-EM Decision Makers
-Technical Advisory Groups
-Risk Assessment
-Synthesized Results
-Visualization
Quantified Untertainties
-Predictive Model(s)
-Design Specifications
-Expert Judgement
-Site Characterization
-Conceptual Model(s)

EM Groundwater & Soil Program Technology Challenges



National Academies of Science reviewed and validated the EM Technology Program: *Advice on the Department of Energy's Cleanup Technology Roadmap: Gaps and Bridges* (2009)

NAS prioritization of needs for the Groundwater and Soil Remediation with ties to Waste Processing

GS#	Gap	Priority
GS-1	**Contaminant behavior in the subsurface is poorly understood.**	**high**
GS-2	Site and contaminant source characteristics may limit the usefulness of baseline subsurface remediation technologies.	medium
GS-3	Long-term performance of trench caps, liners, and reactive barriers cannot be assessed with current knowledge.	medium
GS-4	**Long-term ability of cementitious materials to isolate wastes is not demonstrated.**	**high**