Advanced Simulation Capability for Environmental Management Overview

ASCEM

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Paul Dixon (Multi-Laboratory Project Manager, LANL)
and Vicky Freedman (PNNL)

Technical Team: Tim Scheibe (PNNL), David Moulton (LANL), Mark Freshley (PNNL);
Stefan Finsterle (LBNL); Carl Steefel (LBNL); Haruko Wainwright (LBNL); Roger Seitz (SRNL)

Kurt Gerdes (Director, DOE Office of Soil and Groundwater)
Patricia Lee (DOE-EM)

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E M Environmental Management
safety ❖ performance ❖ cleanup ❖ closure

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Presentation outline

1. Motivation for Development of ASCEM

2. Project Development and Quality Assurance Program

3. Description of ASCEM's Platform "Akuna" and HPC toolsets "Amanzi"

4. Accomplishments to Date and Path Forward

5. ASCEM Deployment Across the DOE Complex

6. Demonstration of Current Capabilities

Why is ASCEM needed?

ASCEM provides a framework and technical underpinning for:

- ..making better use of **complex information**

- ..**optimizing** data collection and analysis within a **single user environment**

- ..creating a **standardized code** that can be used consistently across the DOE complex

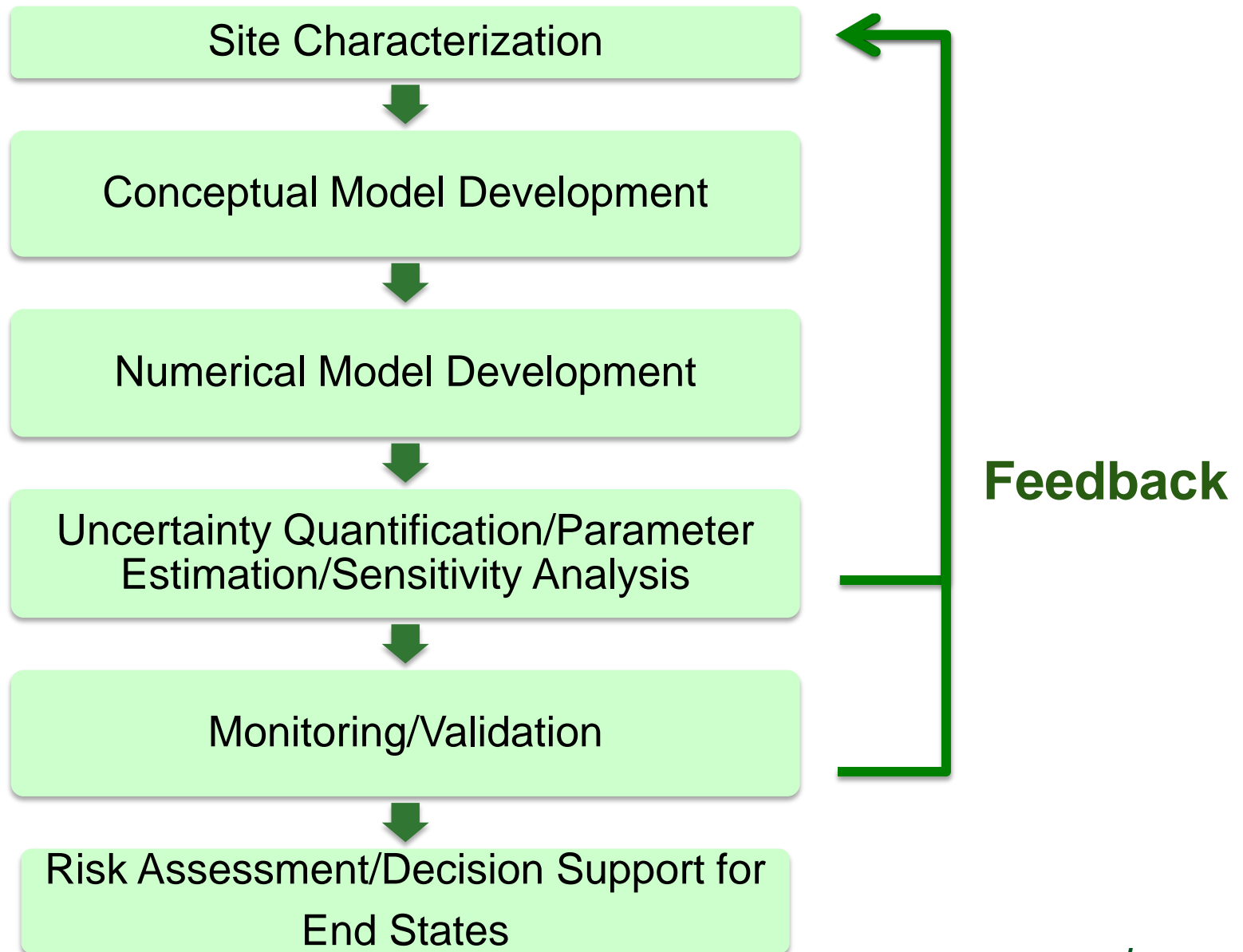- ..aiding **decision making** and answer "what if" scenarios
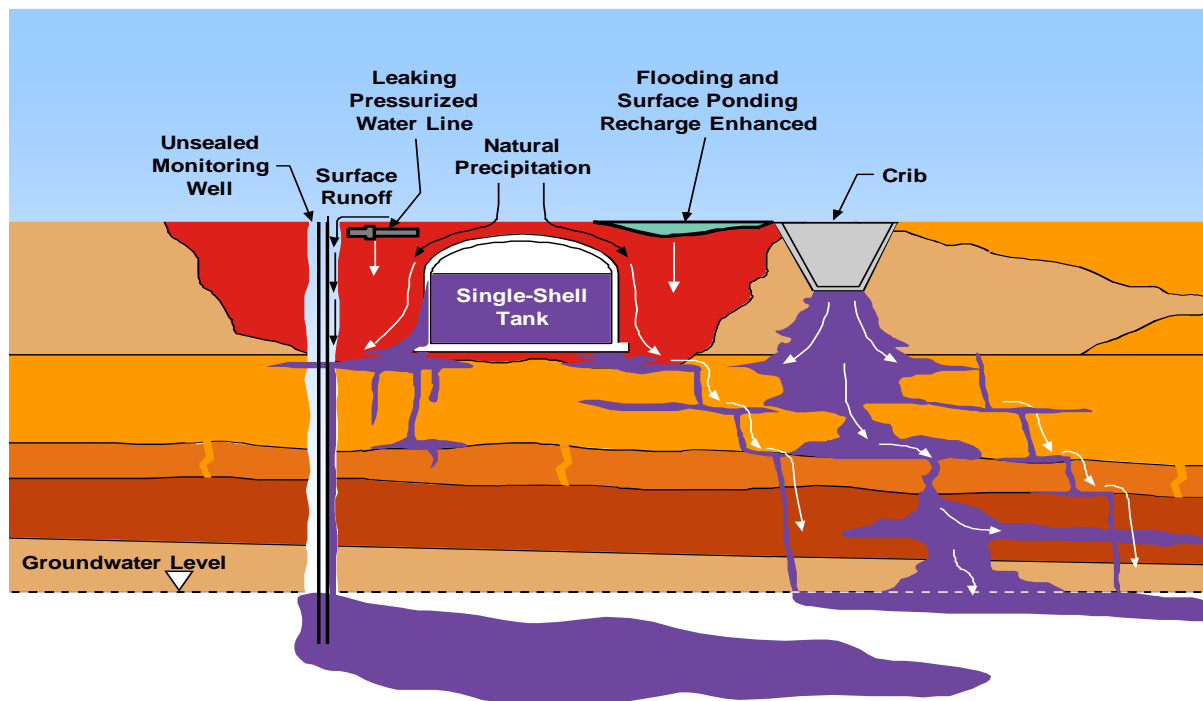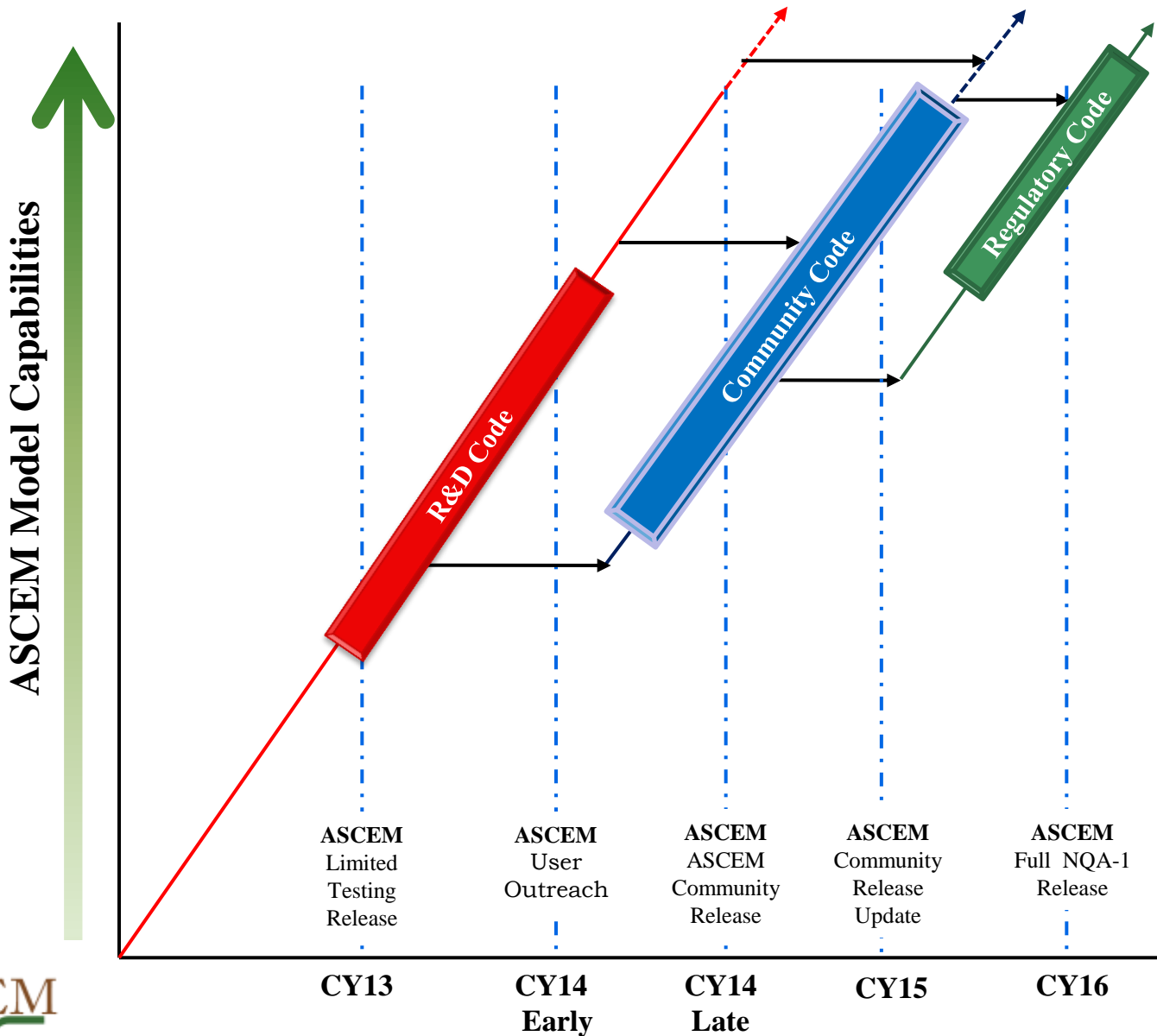
What is ASCEM?

➢ **A State-of-the-art approach for simulating contaminant fate and transport through natural and engineered systems**

➢ **A modular, extensible and open-source design:**

- Integrated toolset to address entire modeling process

- Graded and iterative approach: designed to take advantage of current and future computing architectures

- Freely available and expandable to incorporate existing modeling tools

- Provides a **community platform** for testing and integrating new process models as they evolve

- Leverages DOE investments
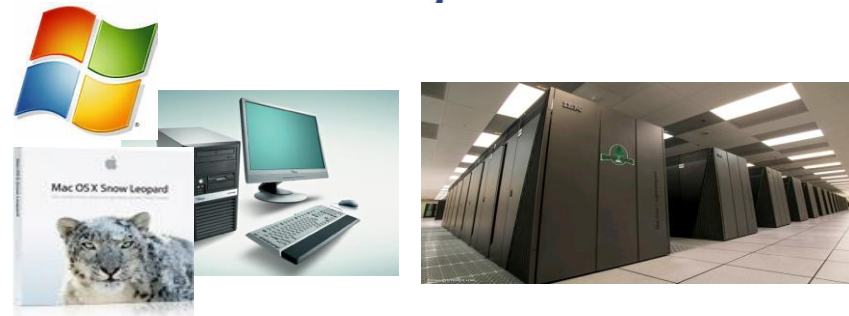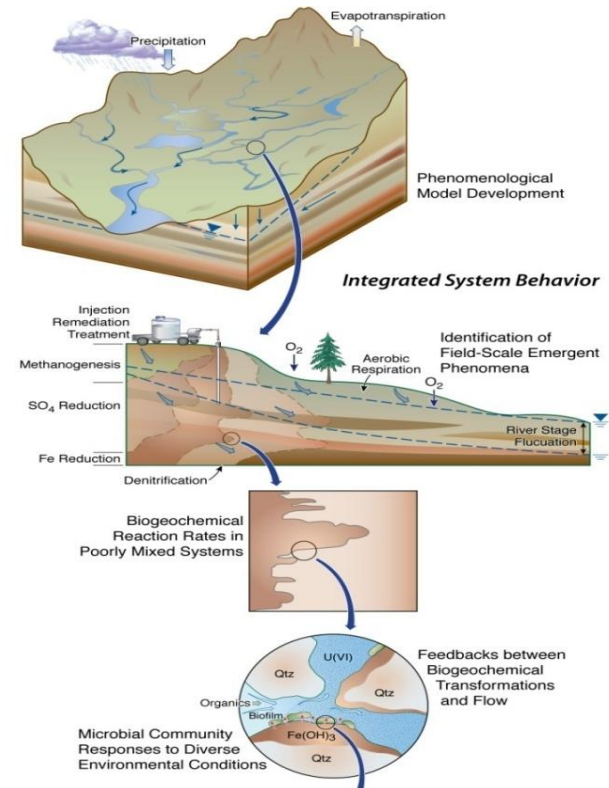
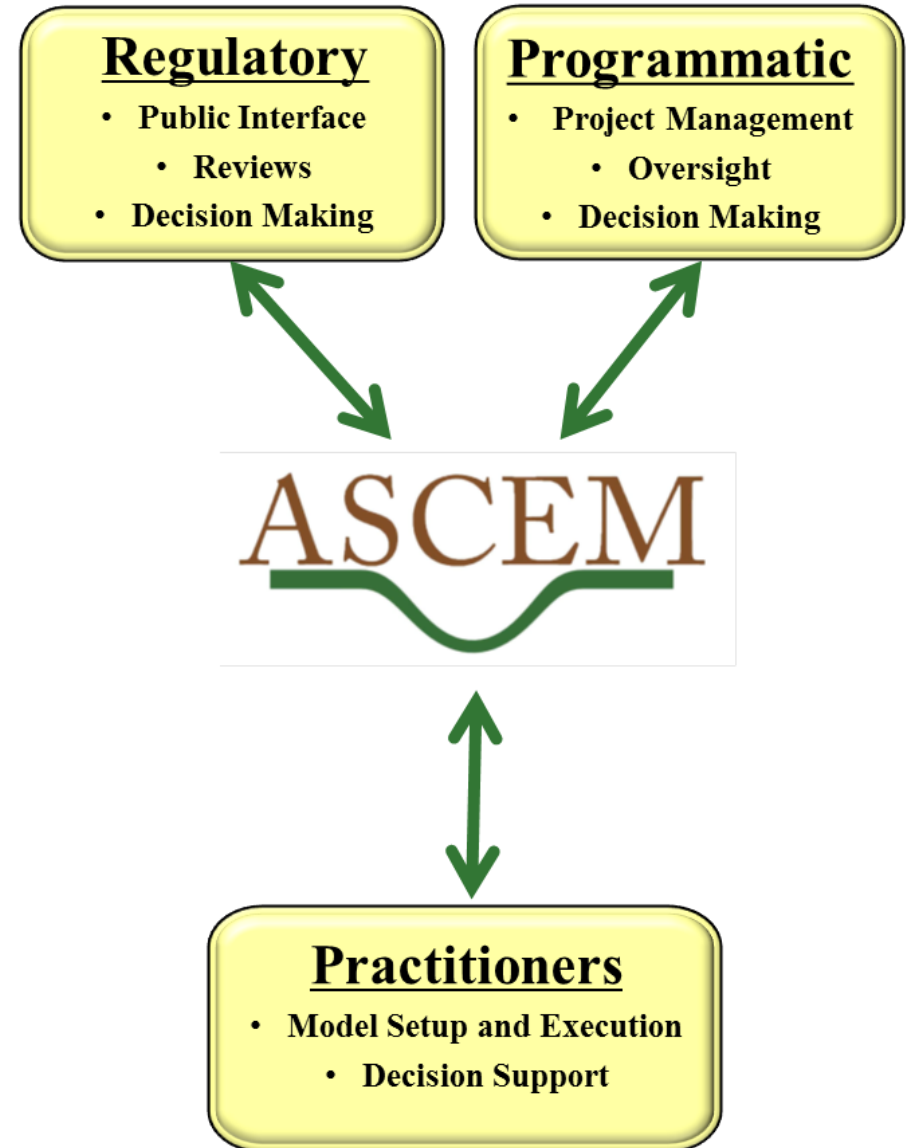**ASCEM**

How is ASCEM used?
Integrated and Iterative Process

Phased Quality Assurance and Code Development

ASCEM Model Capabilities

R&D Code

Community Code

Regulatory Code

ASCEM Limited Testing Release

ASCEM User Outreach

ASCEM ASCEM Community Release

ASCEM Community Release Update

ASCEM Full NQA-1 Release

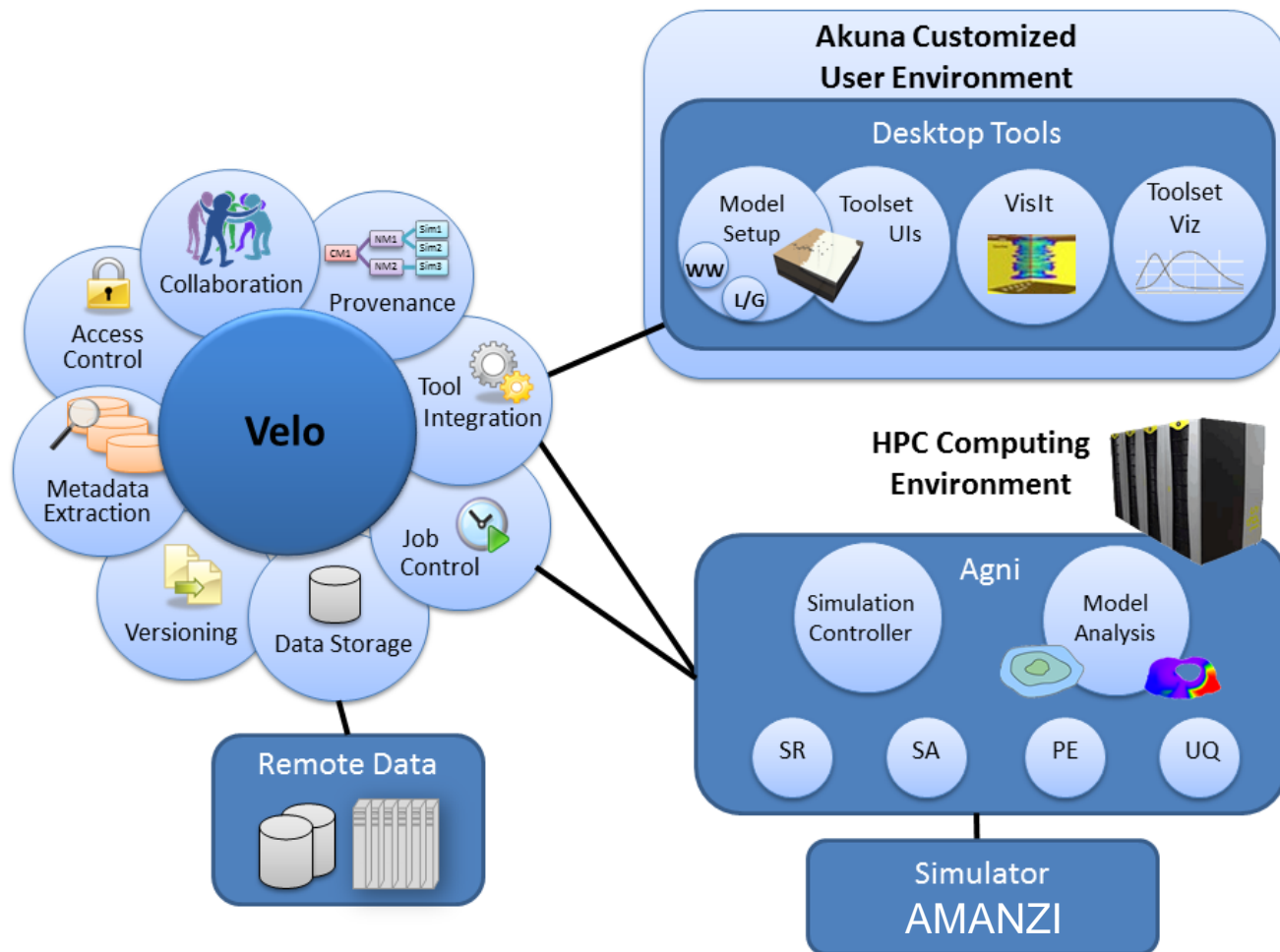CY13 — CY14 Early — CY14 Late — CY15 — CY16

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User Interactions Focus ASCEM Development

- ➢ **End users provide input for code development and applications**

- ➢ **Engagement of EM oversight groups like the Low-Level Federal Facilities Review Group (LFRG) and Performance Assessment Community of Practice**

- ➢ **User Steering Committee**

- ➢ **ITRC Team for "Remediation Management of Complex Sites"**

Regulatory
- Public Interface
- Reviews
- Decision Making

Programmatic
- Project Management
- Oversight
- Decision Making

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Practitioners
- Model Setup and Execution
- Decision Support

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Platform and Integrated Toolsets

# Savannah River F-Area: Controls on Plume migration at geochemically complex

➢ Savannah River F-Area; Disposal of low-level radioactive, acid waste solutions (1955–1989) created groundwater plume (pH 3–3.5, NO_3, U, ^{90}Sr, ^{129}I, ^{99}Tc, tritium)

➢ Ongoing remediation includes capping (1989), active pump and treat (1997-2003), and pH manipulation since 2004

➢ *Natural attenuation is desired as a long-term remediation strategy but technical underpinning is lacking.*
  • U sorption as function of pH variability
  • Uncertainty: Role of heterogeneity on long term plume tails, source/recharge characteristics on plume longevity, etc.
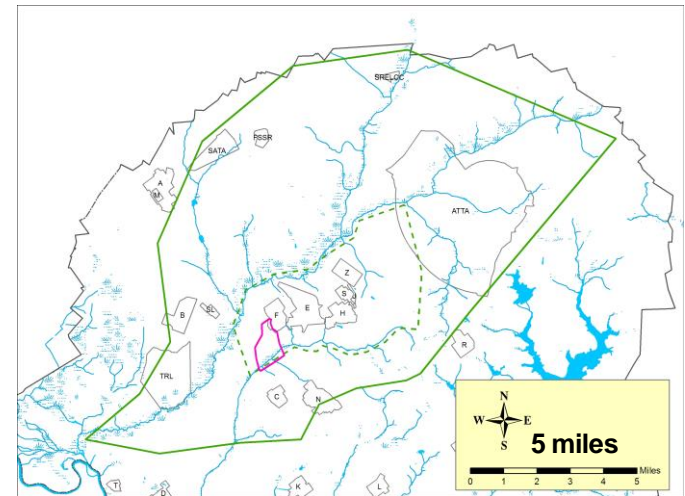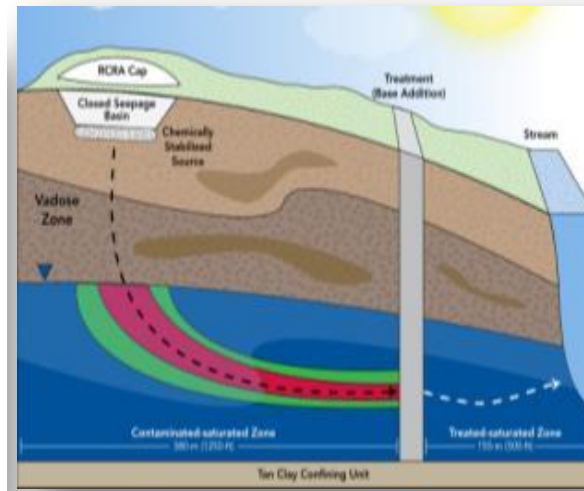
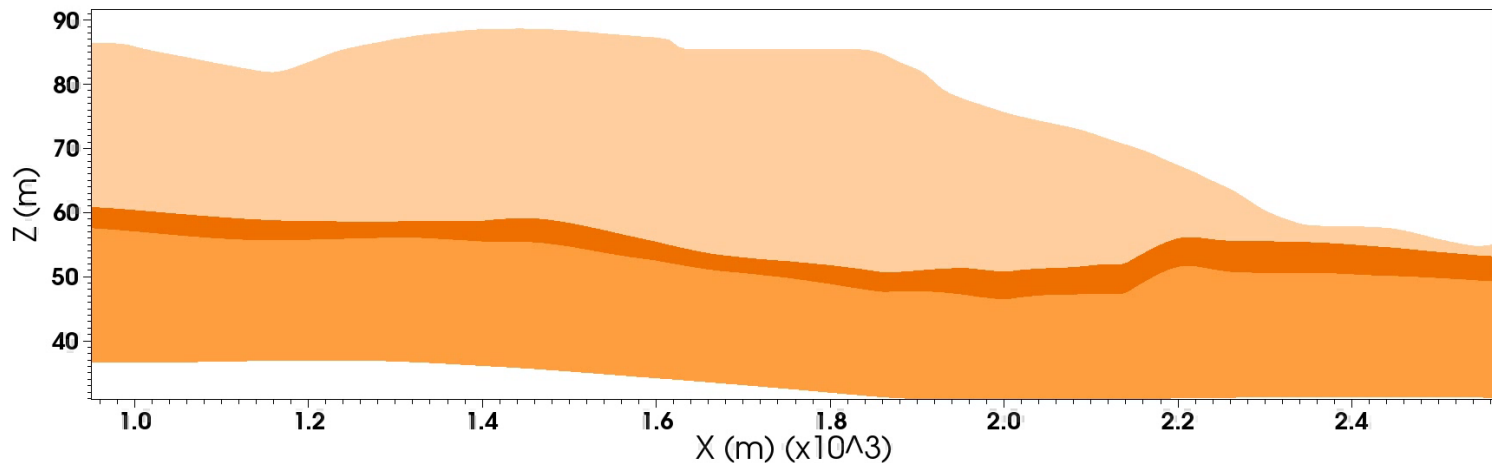# Visualization Communicates the Results of F-Area Uranium Reactive Transport
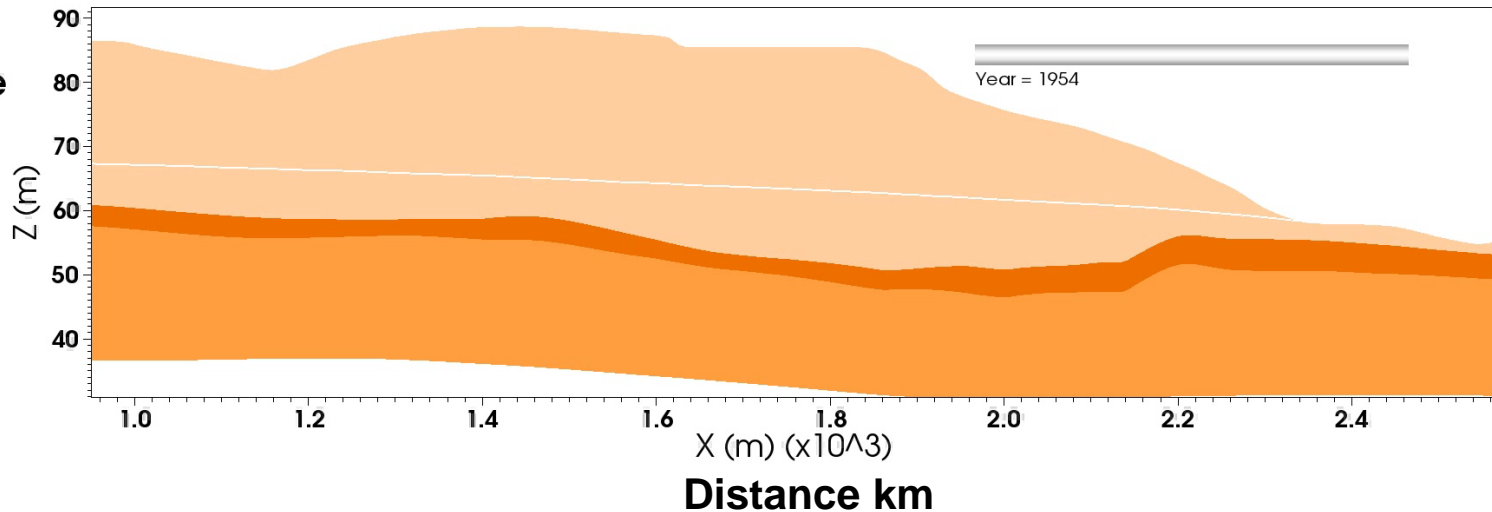
- 100s of simulations run in parallel on Hopper
- Varied 24 parameters and run on 3600 cores

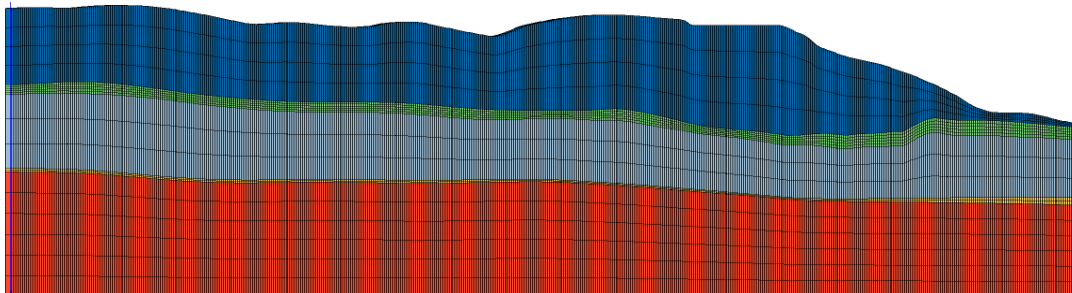*ascemdoe.org*

Amanzi: Flow and Reactive Transport Simulator
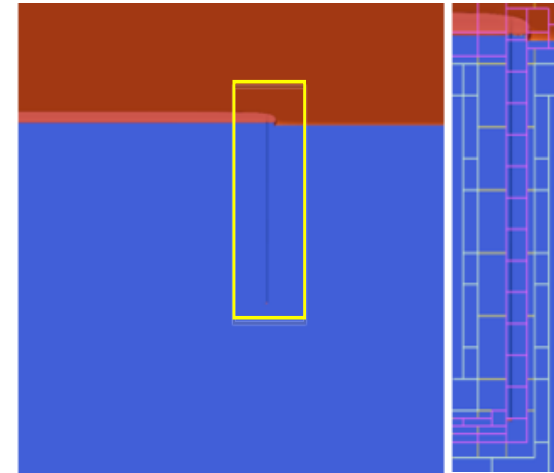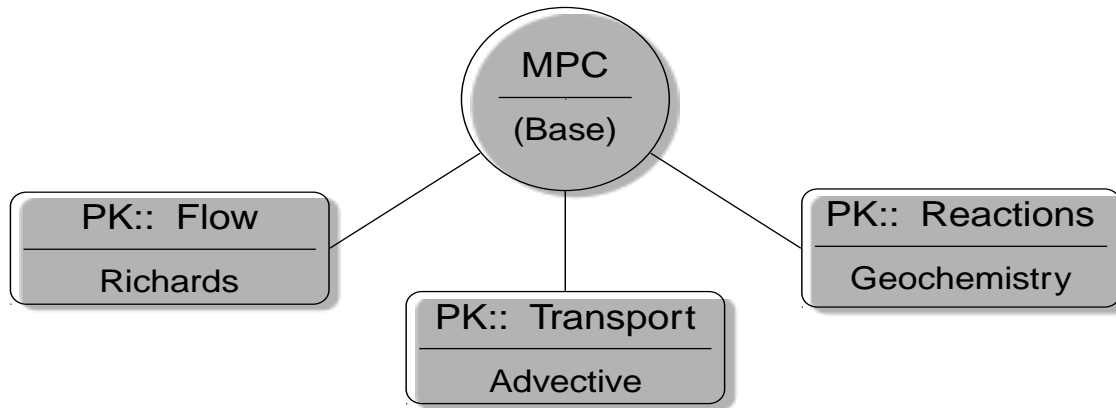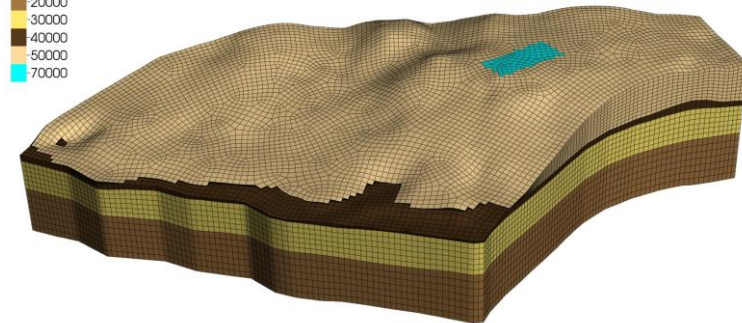
Site Applications

➢ **Provide site data for model testing and validation**

➢ **Conduct demonstrations and support deployment of the Platform and HPC simulator**

➢ **Establish and maintain interfaces with end users**
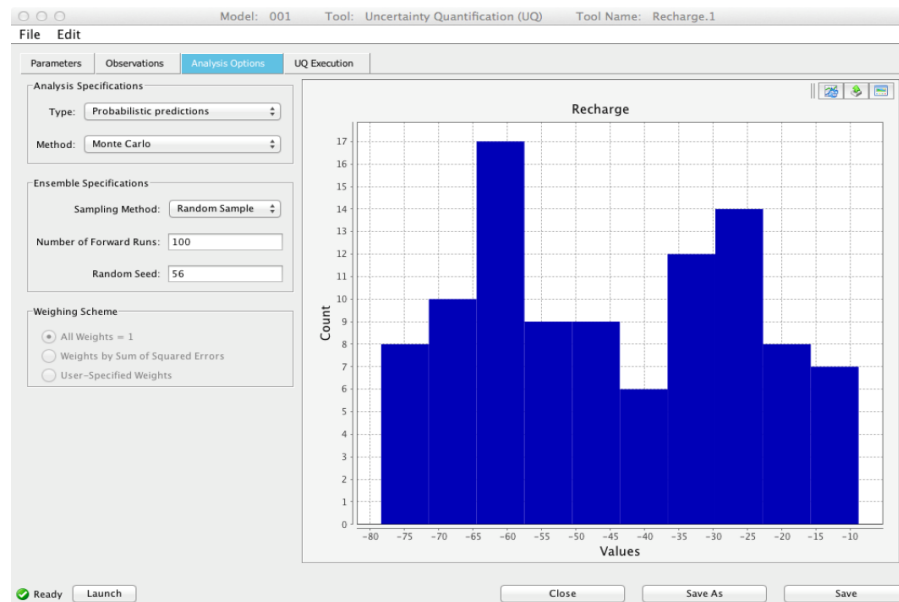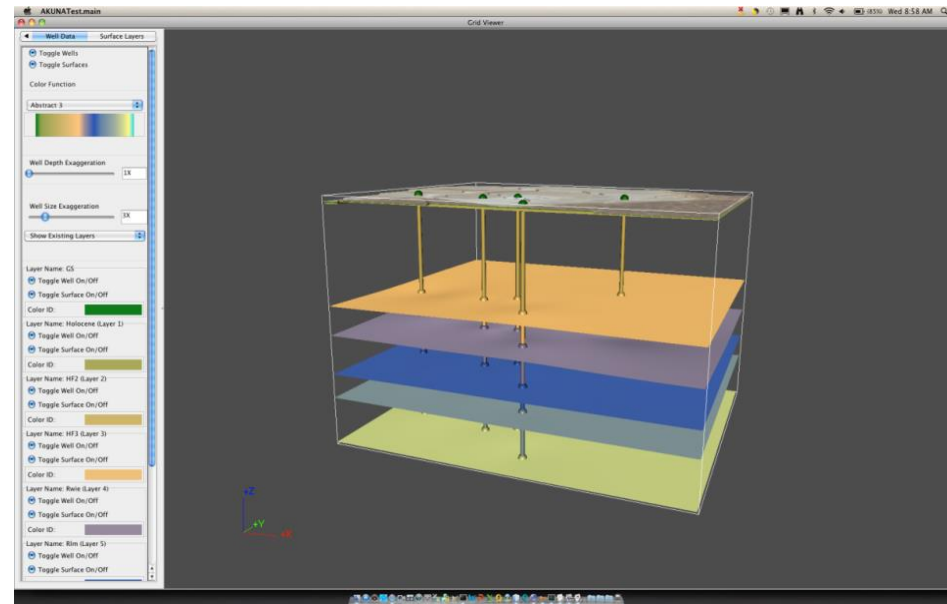

e.g. SRS Type IV tank
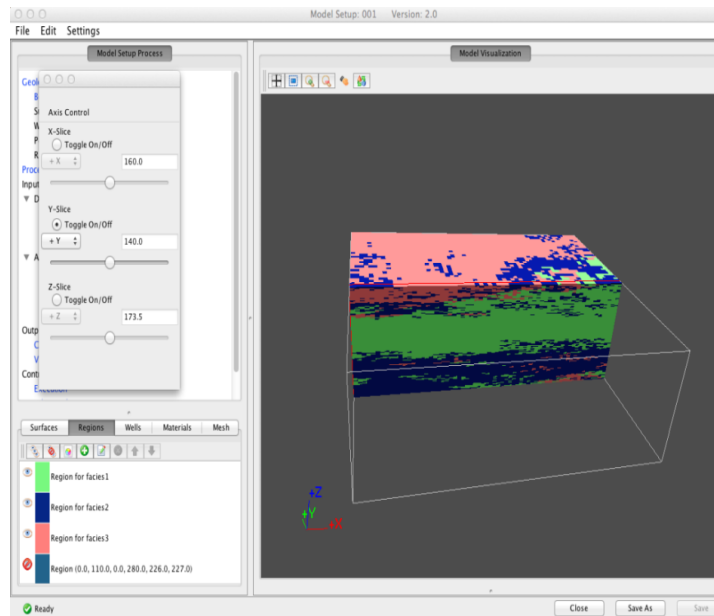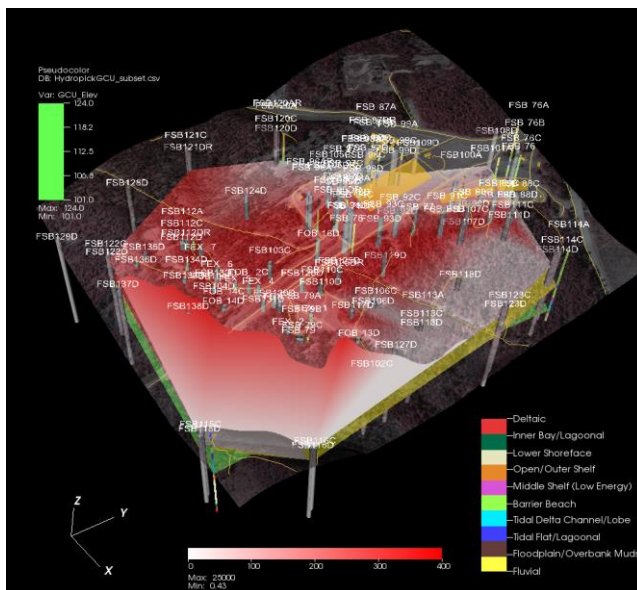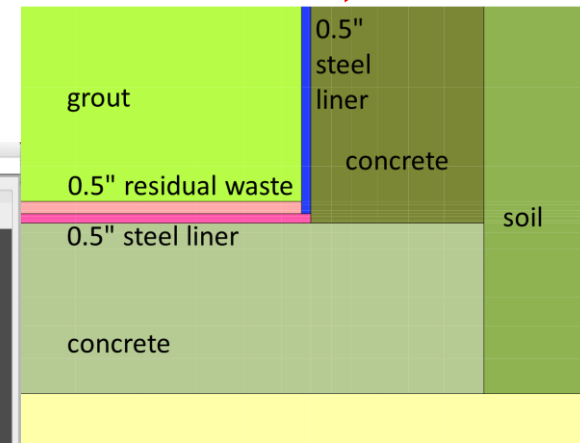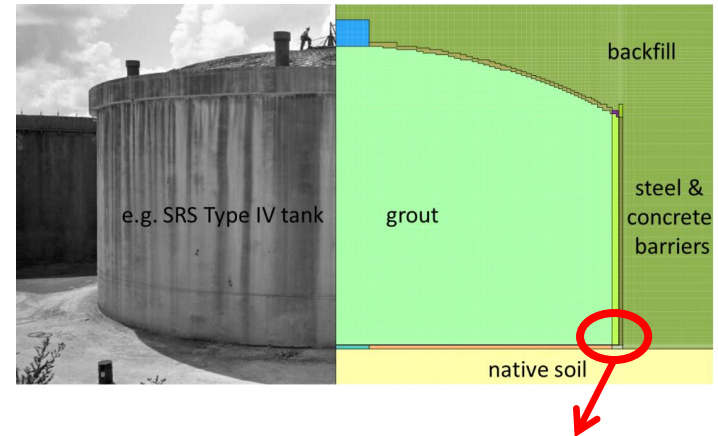
2014 Outreach Activities

- ➢ **Sessions at Hanford and Savannah River Site**
  - ▪ Tutorials
  - ▪ Guided interactions with users
  - ▪ Questions and answers
  - ▪ On-line feedback session
- ➢ **Targeted interactions**
  - • LBNL
  - • LANL
  - • NNSS/LANL
- ➢ **User Steering Committee**

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2014 User Release Interactions

- **Hanford C Tank Farm Performance Assessment and B/C Cribs and Trenches**
  - Richland Operations - CHPRC/Intera
  - Office of River Protection - WRPS
  - Washington State Department of Health

- **Savannah River Site (SRS) H Tank Farm Performance Assessment**
  - Liquid Waste – SRR
  - Computational Sciences - SRNL

- **Nevada National Security Site (NNSS)**
  - Provide technical underpinnings for PA based compliance model's and allow rapid sensitivity and uncertainty analyses for regulators

- **LBNL Scientific Focus Area and SRS F Area Attenuation-Based Remedies for the Subsurface**
  - Modeling of groundwater treatment systems and visualization of contaminate plumes
  - Collaboration with Area Completion

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Accomplishments and Future Activities

➢ **2010 Prototype: Demonstration of individual ASCEM modules**

▪ *Impact: Engage end users in development of prototype integrated, open source PA capability*

➢ **2011-2012 ASCEM Phase 1: Integration of ASCEM Modules**

▪ *Impact: First prototype of an integrated, open source simulation capability for EM demonstrated*

➢ **2013-2014 ASCEM Phase 2: Applied Phase and End User Engagement**

▪ *Impact: Phase 2 demonstrated an integrated, open source simulation capability and led to a release to science and EM community for application.*

➢ **2014-2015 User Releases: Initial User Release (12/2013) and Community R&D Code Release (12/2014)**

▪ *Impact: End User Outreach and input on code use and development.*

➢ **~2016: Regulatory Code Release and Training**

▪ *Impact: Fully integrated, open source simulation capability released and maintained*

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FY 2015 and Beyond Projected Activities

➢ **Interim Release Upgrades to Support User Outreach (May 2014)**
  - Model calibration, sorption, proxy authentication, collaborative modeling

➢ **Community Release (December 2014)**
  - New geochemistry interface
  - Database and visualization toolset integration
  - Additional grid generation tools
  - Development of integrated test suites and user manuals

➢ **Applied Release (Projected for September 2015)**
  - Integration of the risk and decision support toolsets
  - Integration of geostatistics toolset
  - Increased testing and documentation for meeting NQA-1 requirements

➢ **Regulatory (NQA-1) Release** (FY15/FY16)
  - Site training and deployment
  - Regulatory quality assurance support

ASCEM Contact List and POC's

- **Amanzi Questions**
  - David Moulton (Moulton@LANL.gov; 505-665-4712)
- **Akuna Questions**
  - Tim Scheibe (Tim.scheibe@pnnl.gov; 509-372-6065)
- **Site Application Questions**
  - Mark Freshley (mark.freshley@pnnl.gov; 509-372-6094)
- **General Questions**
  - Paul Dixon (p_dixon@lanl.gov; 505-699-1744)
  - Justin Marble (justin.marble@em.doe.gov; 301-903-7210)
  - Patricia Lee (patricia.lee@em.doe.gov; 301-903-9639)

- Updates on schedule and additional information can be found at: http://ascemdoe.org

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Conclusions

➢ ASCEM represents the next-generation **agile, open source, and modular computing framework** that that has utility for multiple DOE missions

- ASCEM facilitates model setup, execution, analysis, and visualization

- High performance computing enables multiple simulations of complex models with reduced computational times

➢ The ASCEM development is motivated by and aligned with DOE directions of developing **advanced and flexible community tools**

➢ The main goal of ASCEM is to support the cleanup process and achieve end states that are safe

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Thank You!

http://ascemdoe.org/

Demonstration of the ASCEM Capabilities

By: Vicky Freedman

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Questions

Tc-99 (pCi/L)

Facies 1   Facies 2   Facies 3

Year = 1956

through Cribs 15,17,19 at y=162.5

through Cribs 14,16,18 at y=117.5

through Borehole A and near Cribs 17, 18