Program Overview

ASCEM

Presented to the Hanford Advisory Board
River and Plateau Committee
August 10, 2011

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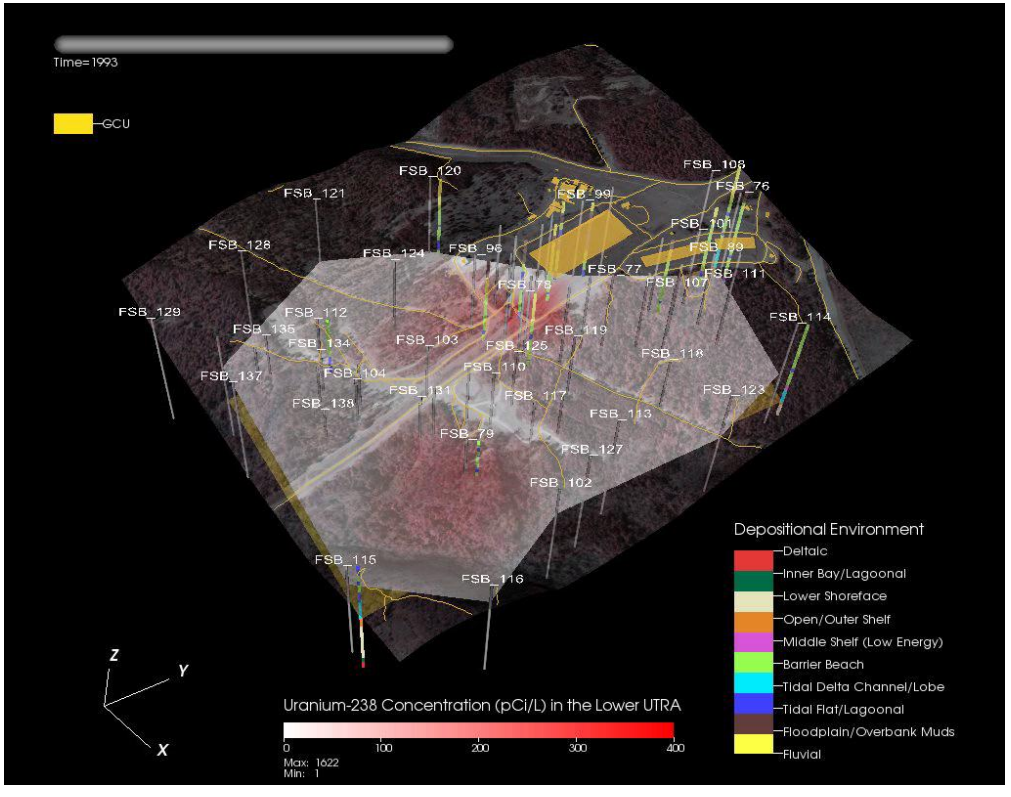
Advanced Simulation Capability for Environmental Management (ASCEM)

- A **State-of-the-art tool** for predicting contaminant fate and transport through natural and engineered systems
- The **modular and open source** design will facilitate a **new approach** for integrated modeling and site characterization
- Will enable robust and standardized future performance and risk assessments **for EM cleanup and closure**



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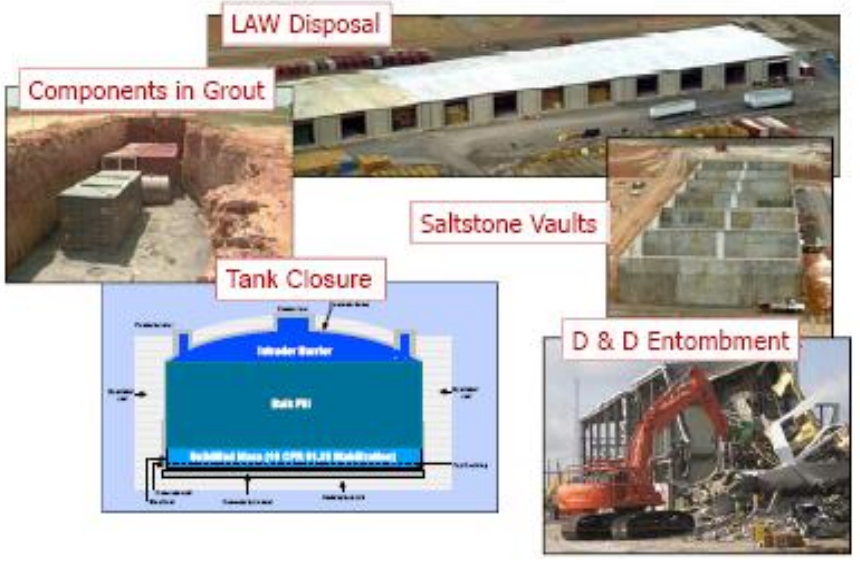
ASCEM Challenge and Impact

Challenge

- **Develop an integrated computer modeling capability** to take advantage of advances in high performance computing
- **Provide tools for decision making** including parameter estimation, visualization, uncertainty quantification, data management, risk analysis, and decision support
- **Leverage investments** made by SC, NE, RW, and FE as well as other Federal agencies to capitalize on significant investments and reduce the lifecycle development time and costs

Impact

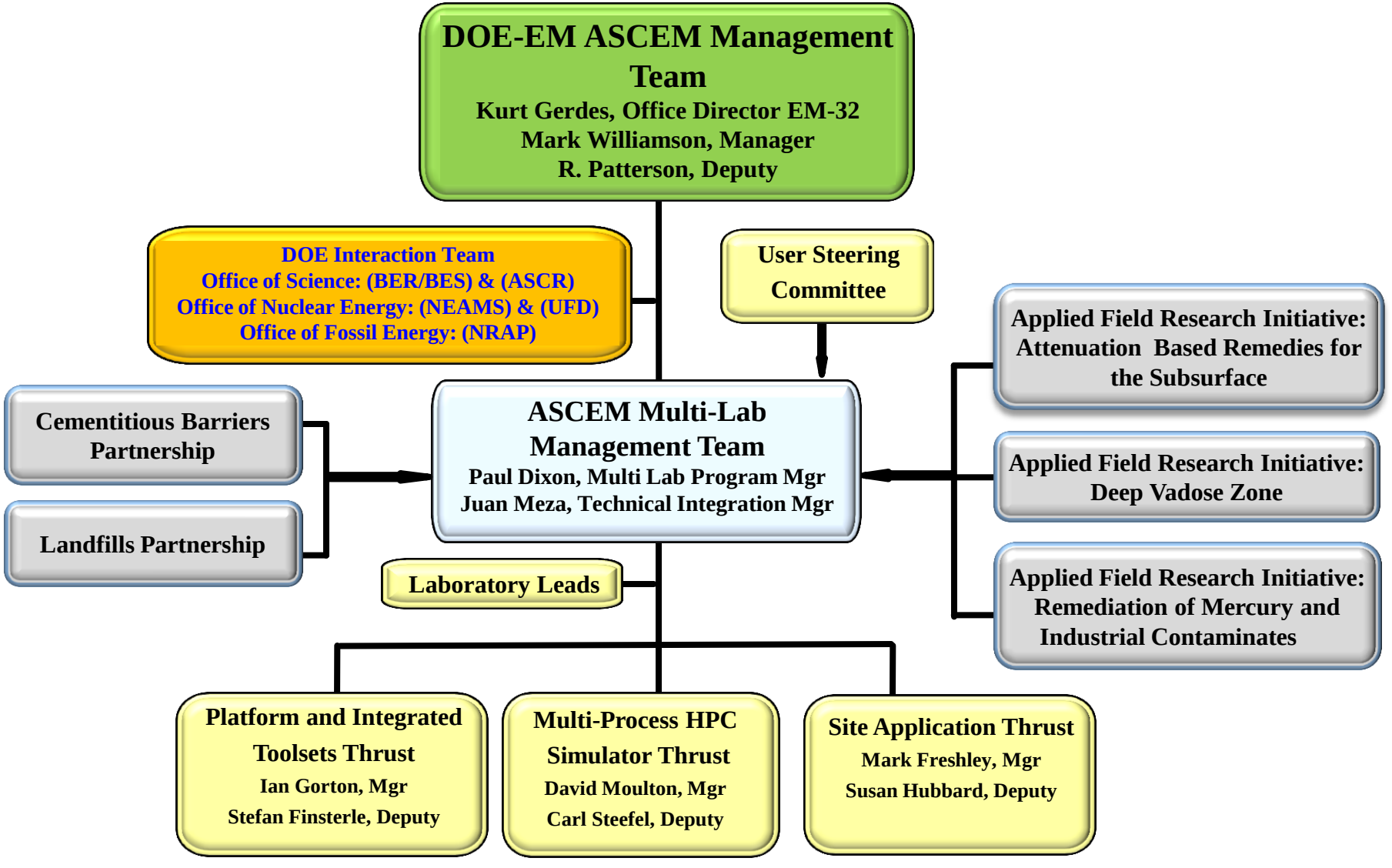
- Near-term: provide **technical underpinning for** current risk and performance assessments
- Inform strategic data collection for model improvement
- **Strengthen and standardize EM** risk and performance assessment approach



ASCEM Is Delivered Through a National Laboratory Consortium

Lawrence Livermore National Laboratory

Advanced Simulation Capability for Environmental Management (ASCEM)



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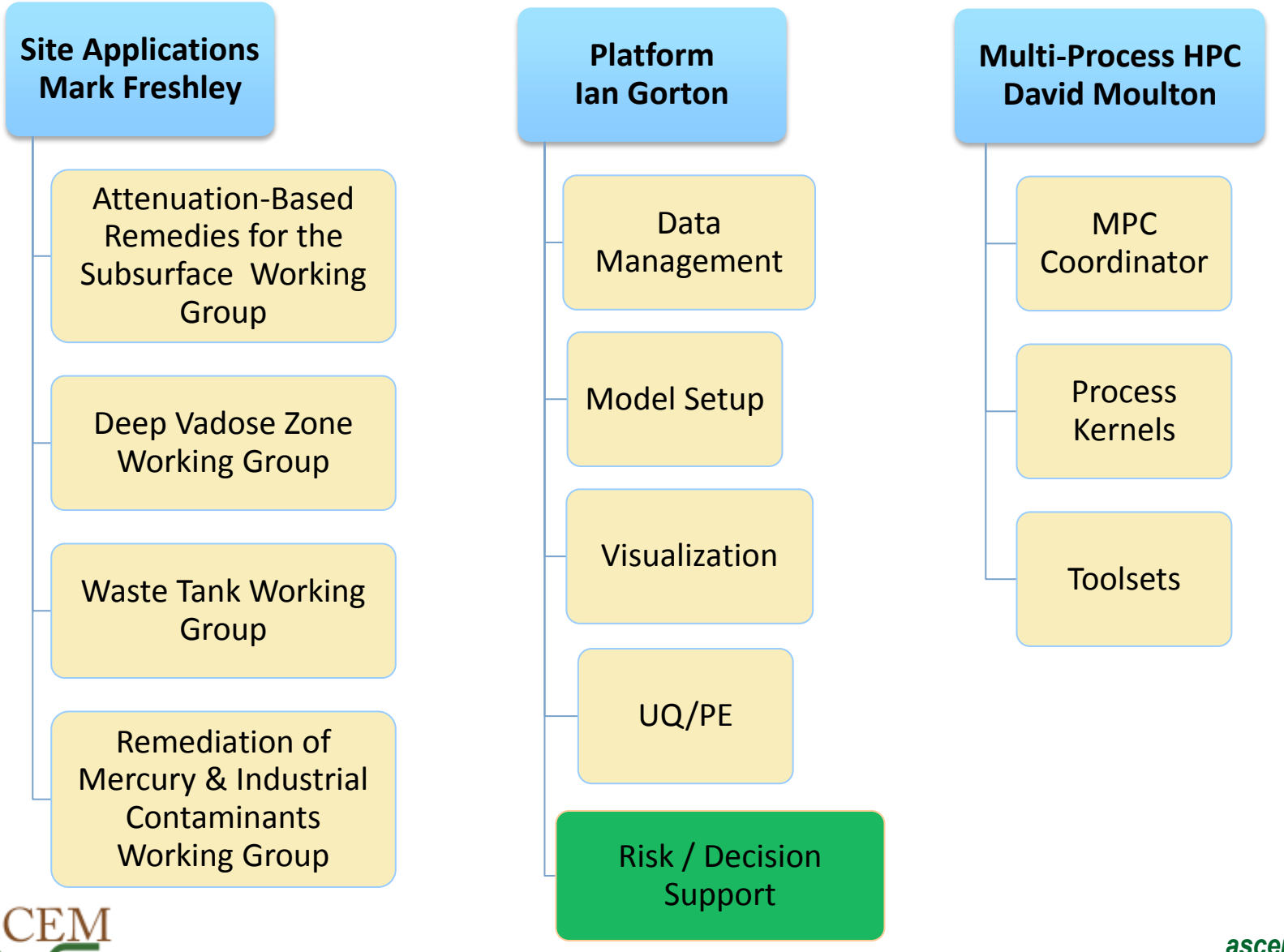
ASCEM website: http://ascemdoe.org/

ASCEM Organized Around Three Thrust Areas



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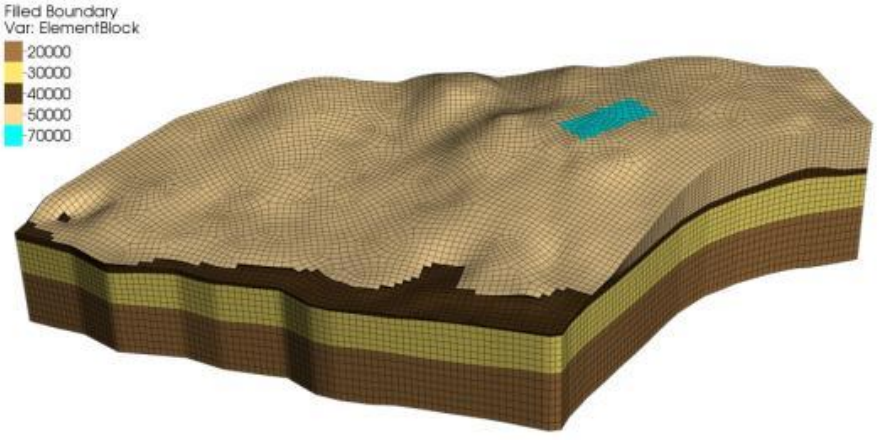
High Performance Computing

- The ASCEM HPC simulator (Amanzi) will predict flow and reactive transport on both structured and unstructured grids, including physical processes such as:
  - Biochemical reactions
  - Thermal effects
  - Radioactive decay
  - Mechanical effects
  - Source-term degradation
  - Colloid transport (*future work*)

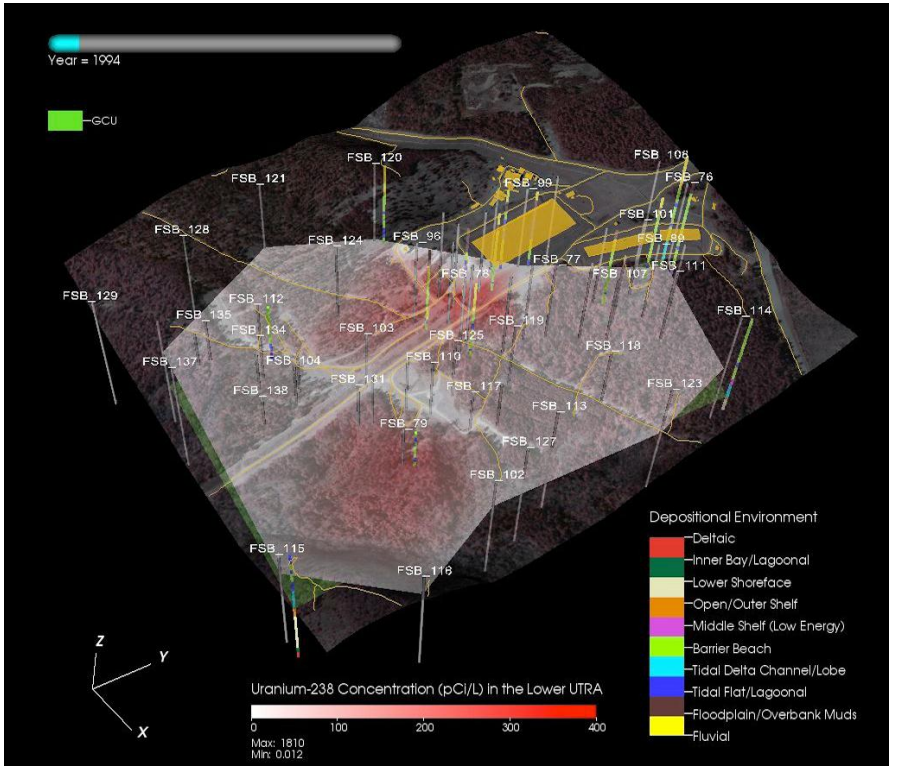


Wide Range of Complexity

Wide Range of Platforms

Platform and Integrated Toolsets

- ASCEM platform (Akuna) will include capabilities for:
  - Model Setup
  - Data Management
  - Uncertainty Quantification
  - Visualization
  - Parameter Estimation
  - Decision Support
  - Risk Analysis



- These tools will allow users to quickly and efficiently create and analyze simulation data assisting highlighting relevant processes and parameters allowing for informed decision making

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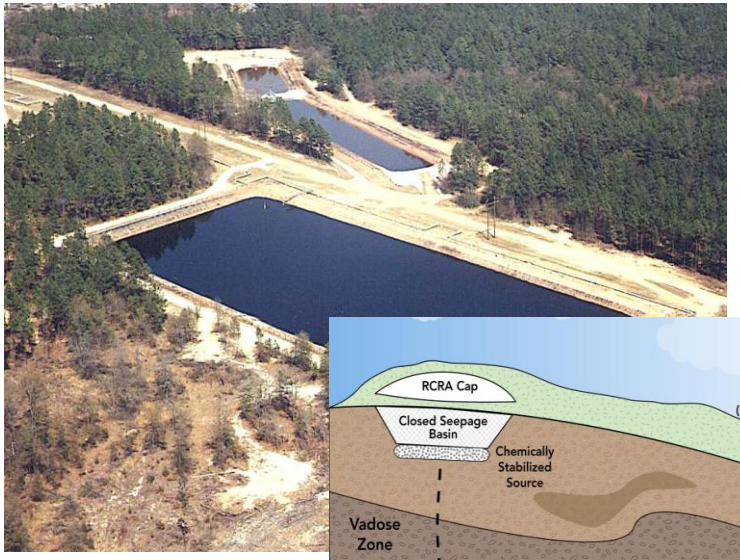
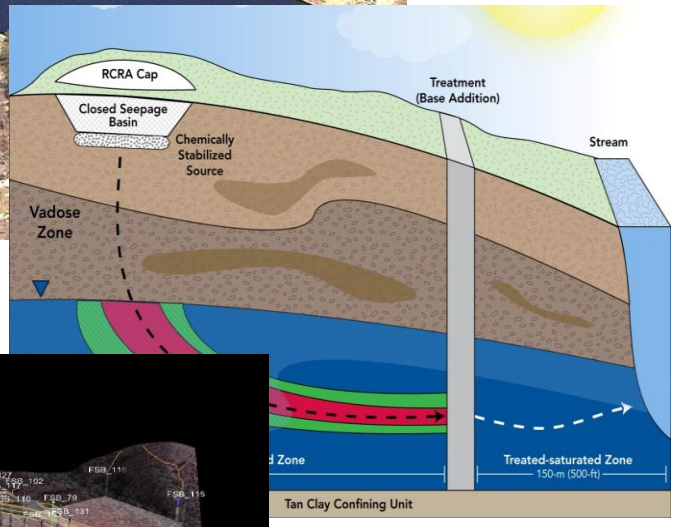
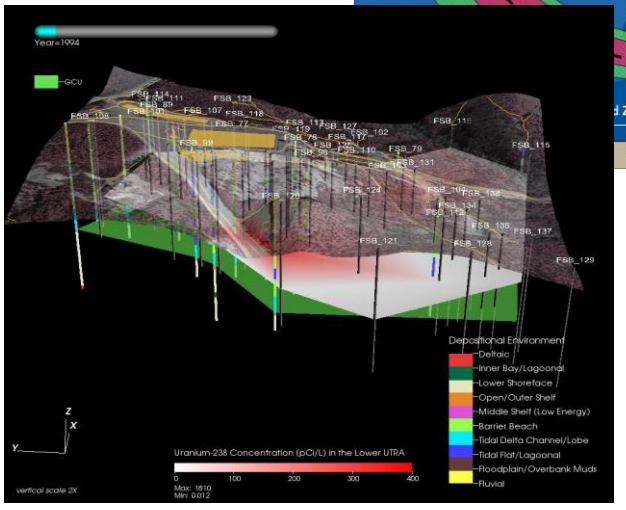
Site Applications Scope

- Provide site data for model development, testing, and model confidence
- Conduct demonstrations of the Platform and HPC simulator
- Establish and maintain interfaces with end users
- Solicit input to requirements specification and development activities







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User Interactions Helped Shape ASCEM Development

- **DOE EM end users**
  - Performance Assessment Community of Practice and Low Level Waste Disposal Facility Federal Review Group meetings
  - Interviews at Hanford, Los Alamos, Oak Ridge, Nevada Nuclear Security Site, Portsmouth/Paducah, Savannah River and West Valley sites

- **Recommendations provided early input to requirements**
  - A graded approach is needed
  - Consider role of modeling as input for regulatory decision making
  - Take advantage of HPC to reduce need for simplifications
  - Recognize data needs as model complexity increases

User Steering Committee

- Chartered in October 2010, first formal meeting on January 24, 2011
- Objective to enhance successful implementation of ASCEM tools by encouraging input from management and key staff at contractors, regulators and DOE oversight organizations
- Membership:

Michael Graham, Chair	LANL, Environmental Programs	Bruce Crowe	NNSS, EM Science Advisor
Chris McKenney	US NRC, PA Branch Chief	Elizabeth Phillips	DOE Oak Ridge
Marty Letourneau	EM-41, LFRG Chair	Tom Gaughan/Cathy Lewis	SRNS, Area Closure Projects
Andrew Wallo III	DOE HS-20	Mark Layton	SRR, Tank Closure PA
Pat Nakagawa	LANL, Environmental Programs	Karthik Subramanian	URS
Cheryl Whalen	Washington Dept. of Ecology	Rich Bonczek	DOE PPPO, LFRG Representative
Alaa Aly/Moses Jaraysi	CHPRC, Modeling Integration	Frank DiSanza	DOE NNSS, LFRG Representative
Susan Eberlein	WRPS, Tank Closure PA	Roger Seitz, Coordinator	SRNL, Performance Assessment

User Steering Committee Recommendations

- Clearly articulate near-and longer-term objectives and establish metrics for success
- Focus on identifying a set of near-term positive impacts (e.g., targeted applications, visualization tools, guidance on uncertainty quantification)
- Maintain focus on toolset designed to support EM-related decision-making during and at the end of the modeling process
- Enhance sustainability by engaging in an annual work planning process that considers contractor and regulatory schedules for modeling and supporting activities around the DOE Complex
- Look for opportunities for demonstrations at small and large DOE sites beyond Applied Field Research Initiatives, Science Focus Areas and Integrated Field Research Challenges. (**Dae Chung Memo to Sites**)

ASCEM Leveraging

- In addition to primary ASCEM code development, we take advantage of significant leveraging of investments by several DOE Office of Science and National Nuclear Security Administration programs
- Early examples include:
  - VisIt – visualization and graphic analysis tool developed by ASC and ASCR SciDAC Program
  - Velo: Data Management
  - PSUADE – uncertainty analysis tool developed by ASC
  - Trilinos Framework – services for parallel programming and integrated software packages developed by ASC and ASCR SciDAC program
  - PETSc – Portable, Extensible Toolkit for Scientific Computation developed by ASCR SciDAC Program
  - BoxLib – parallel AMR framework developed by ASCR Base Math and SciDAC
  - MFD – Mimetic Finite Difference discretization methods developed by ASCR Applied Mathematics Program
  - Geochemistry Toolset – Use algorithms developed by computational scientists funded through DOE SC

ASCEM Coordination with other DOE offices

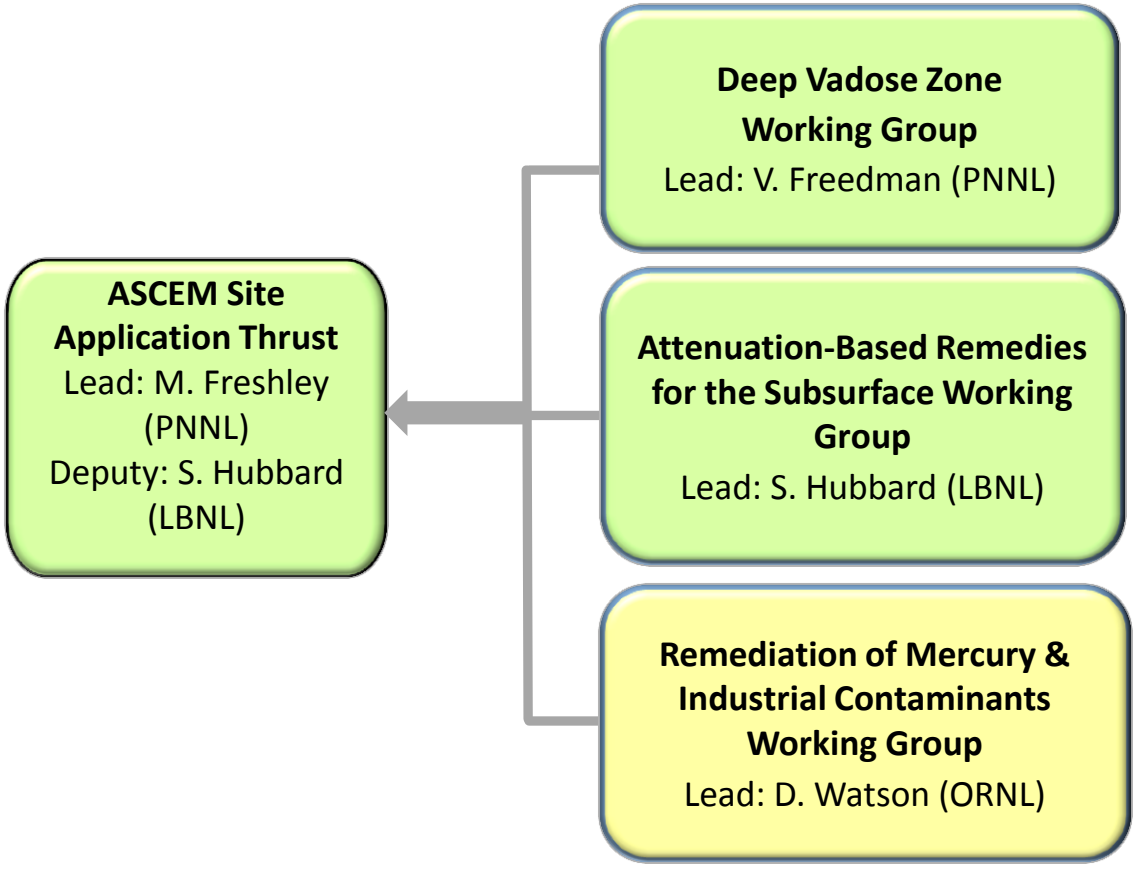
- As the request of Under Secretary Christina Johnson a workshop was held in September 2010 to investigate possible leveraging with **Fossil Energy's NRAP** program. (Report available on ASCEM website)

- At the request of EM-1 and acting NE-1, a workshop was held in February 2011 to investigate possible leveraging with **Nuclear Energy's NEAMS program**. (The workshop available on ASCEM website)

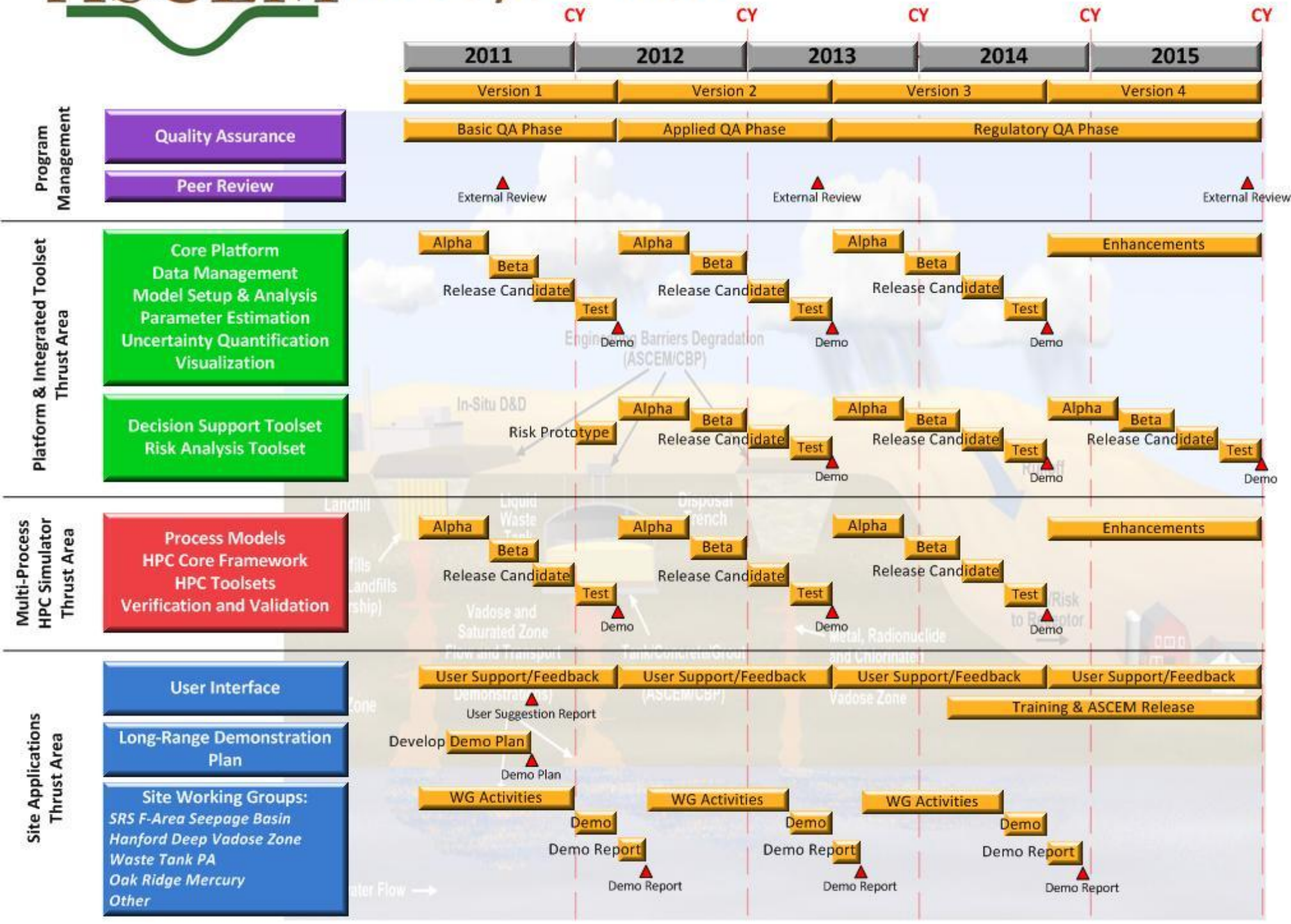
- Continue to work with the **Office of Science** to insure maximum leveraging between the two programs. Science is considering that all SFA, IFRC and SciDAC proposal renewals and new proposal include a strong tie to ASCEM. Started joint data management initiative between SC and EM.

ASCEM Within DOE EM-32 Program

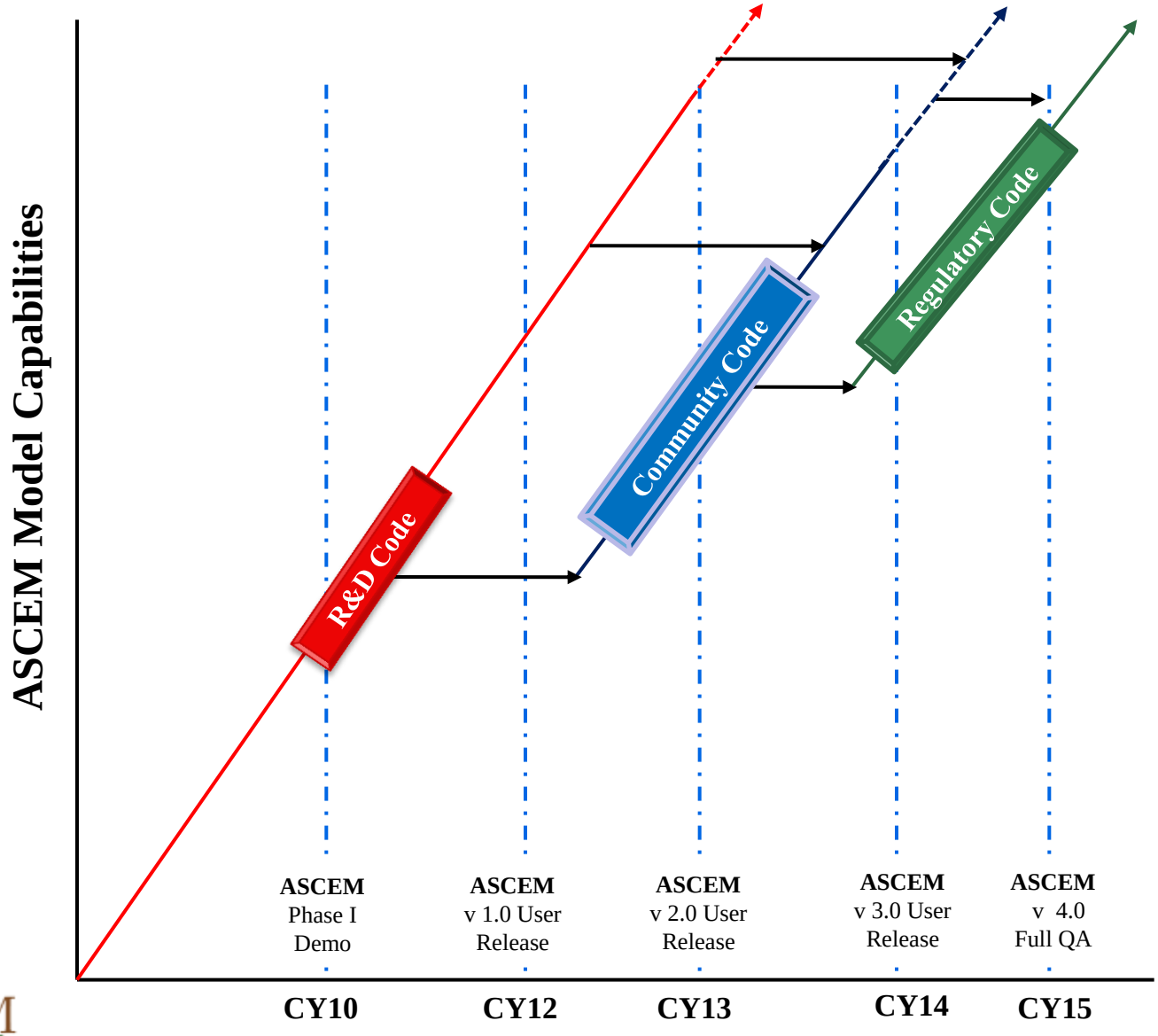
- ASCEM Site Applications engages Applied Field Research Initiatives (AFRIs) through Working Groups
- Active interfaces include Deep Vadose Zone and Attenuation-Based Remedies for the Subsurface AFRIs
- Remediation of Mercury and Industrial Contaminants Working Group in planning stage



ASCEM Lifecycle Plan



Quality Assurance Graded Approach with Code Development



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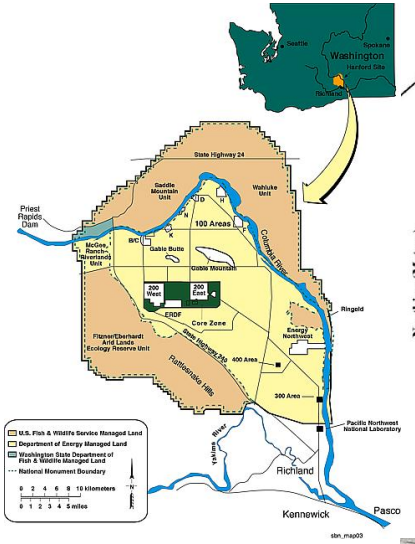
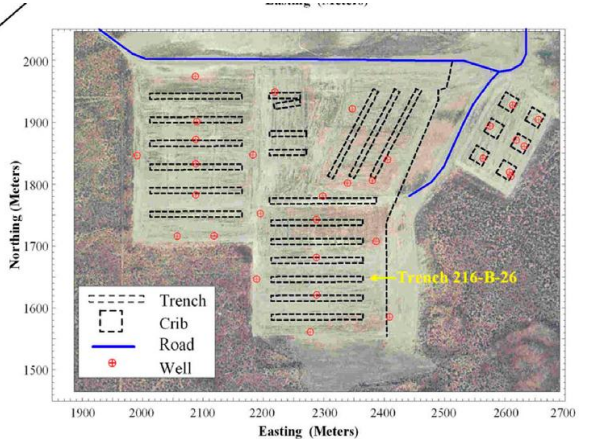
FY 2011/12 Phase II Demonstration

- Integrate across capabilities and applications to address specific, site-related questions
- Emphasize high-level integration through Platform and HPC in working groups
  - **Deep Vadose Zone (end to end demonstration)**
  - Attenuation-Based Remedies for the Subsurface (data management, HPC, and UQ)
  - Waste Tank Performance Assessment (visual analysis tools for model sensitivity and UQ as well as HPC applications)
  - Initiate activities for Oak Ridge Mercury

Deep Vadose Zone Working Group Background and Goals

- **Background:** BC Cribs and Trenches; characterized by thick heterogeneous vadose zone; soil desiccation treatability test
- **Goals of Phase II Demonstration:**
  - Demonstrate end to end integration of Platform and HPC toolsets for sparse data
  - Investigate vadose zone transport properties and impacts of soil desiccation technology





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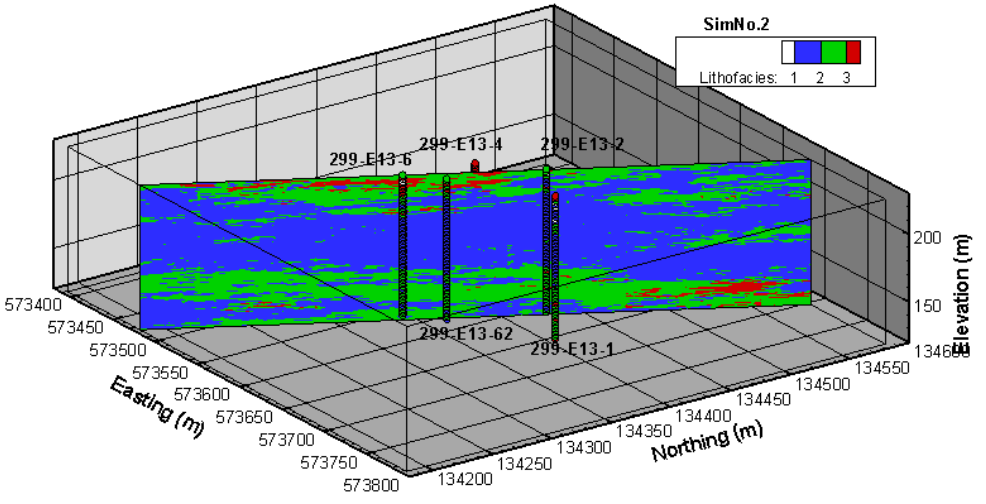
Deep Vadose Zone Working Group
Model Setup

- Generated 100 realizations of subsurface geology
- Model Setup Tool will translate conceptual model to grid and generate Amanzi input
- Evaluating temporal resolution of recharge (1956 – 2006) for model calibration
- Statistical correlation will relating grain-size distributions to hydraulic properties



Lithofacies:
1 – clean sand
2 – sandy gravel
3 – muddy sand

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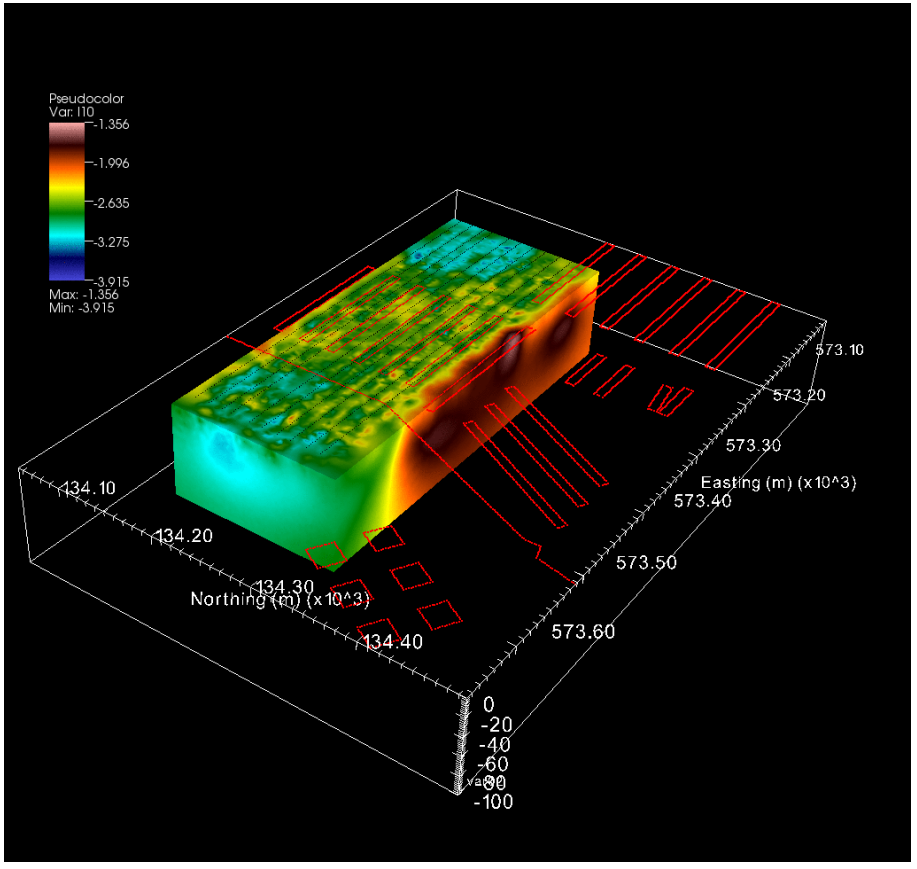
Deep Vadose Zone Working Group
Initial Concentration Distribution

- Subsurface electrical conductivity estimated by Electrical Resistance Tomography inversion
  - High conductivities caused by nitrate contamination
- Will be used as initial condition for uncertainty analysis examining variability of hydraulic parameters



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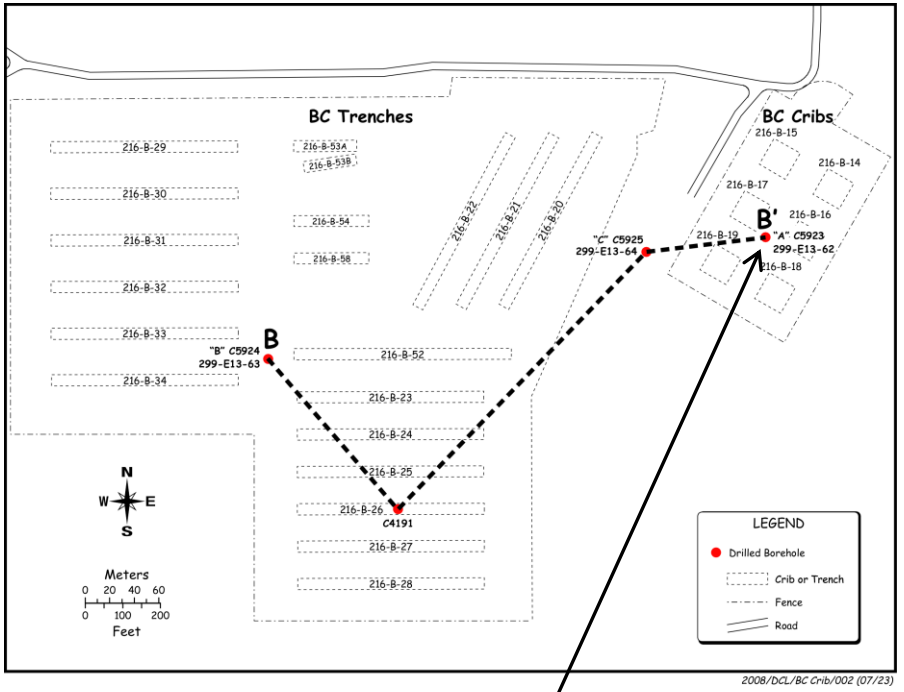
Deep Vadose Zone Working Group
Parameter Estimation



Borehole "A"

- Estimate flow and transport parameters for hydrogeologic units ($K_{sat,}$ van Genuchten α, n)
- Use data on releases to cribs in 1956
- History match 2006 data at Borehole "A"
  - Measurements of moisture content and ^{99}Tc concentration

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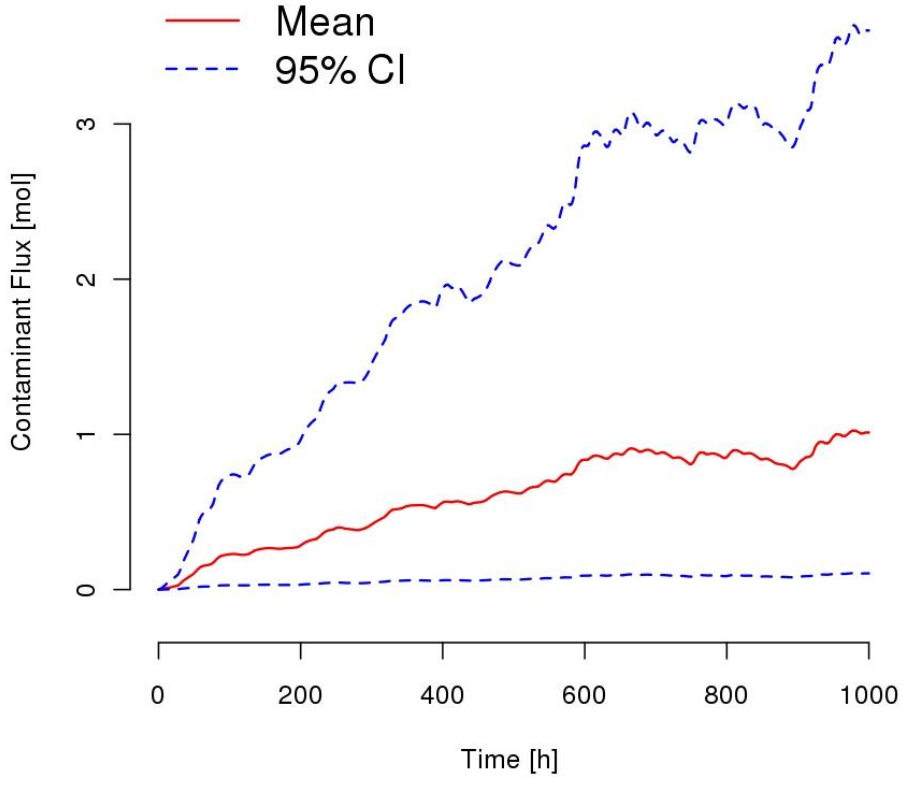
Deep Vadose Zone Working Group
Uncertainty Quantification



- Includes sensitivity analysis
- Assess uncertainty using Monte Carlo simulation of contaminant flux to the water table
  - Predict mean and confidence intervals
- Evaluate the contribution of data uncertainty (ERT, borehole ^{99}Tc concentrations) on uncertainty of mass flux to the water table

FY 2011 Work Scope

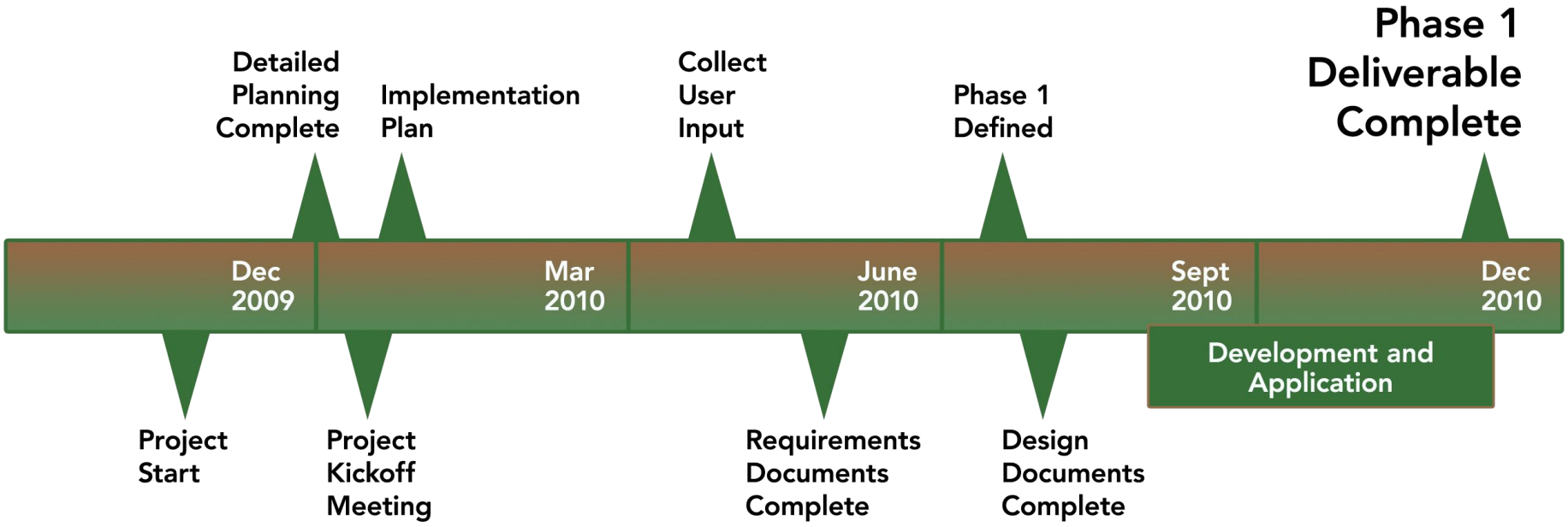
- Focus on code development and integration of components for ASCEM User Release 1.0 and Phase II Demonstration
- Conduct technical peer review in FY11
- Continue working groups for SRS F Area, Hanford Deep Vadose Zone, and Waste Tank Performance Assessment; initiate work at ORNL
- Continue interactions with EM Performance Assessment Community, DOE SC SBR, FE-NRAP, and NE-NEAMS/Repository Programs
- Strengthen linkages with DOE EM small sites (LANL; West Valley, Paducah/Portsmouth, Grand Junction, Nevada Test Site and Brookhaven)

More Information about ASCEM

- *ASCEM Site Applications Thrust Site Selection Task 'Select Phase I Demonstration' Milestone 2010, ASCEM-SITE-091310-01, 2010*
  - *Summary of salient features of candidate sites and the selection process*
- *Mathematical Formulation Requirements and Specifications for the Process Models, ASCEM-HPC-101510-01, 2010*
  - *Contains the general mathematical description for the process models envisioned for the final ASCEM product*
- *System Requirements for ASCEM Platform and Integrated Toolsets, ASCEM-PIT-102710-03, 2010*
  - *Describes use cases and requirements for the Platform toolsets*
- *ASCEM Phase 1 Demonstration, ASCEM-SITE-102010-01, 2010*
  - *Phase 1 Demonstration report describing the accomplishments from the first year*

Questions

ASCEM FY2010 A Year in Review



- ✓ Initiate technical part of Project after January 2010 kickoff meeting
- ✓ Completed assembly of team, extensive work planning, requirements definition, and design
- ✓ Engaged a broad spectrum of end users for input to requirements and design
- ✓ Performed Phase 1 demonstration at Savannah River Site F Area
- ✓ Assembled open source components over four months to support Phase I demonstration
- ✓ Developed a new open-source HPC Simulator in four months:
  - leveraged and enhanced existing open-source tools and the Trilinos framework
  - implemented several key components from scratch
- ✓ Executed simulations on supercomputers at NERSC

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ASCEM 2010 to 2015 Program

- **2010 Prototype: Demonstration of individual ASCEM modules**
  - *Impact: Engage end users in development of prototype integrated, open source PA capability*
- **2011-2012 ASCEM Version 1: Integration of ASCEM Modules**
  - *Impact: First prototype of an integrated, open source simulation capability for EM demonstrated*
- **2013 ASCEM Version 2: Applied Phase and End User Engagement**
  - *Impact: Version 2.0 of an integrated, open source simulation capability released to science and EM community for application*
- **2014 ASCEM Version 3: Applied Phase and Initiation of Regulatory Quality Assurance V&V Testing**
  - *Impact: Version 3.0 of integrated, open source simulation capability demonstrated*
- **2015 ASCEM Version 4: Regulatory Code Release and Training**
  - *Impact: Fully integrated, open source simulation capability released and maintained*