Program Overview

Presented to the EM SSAB Chairs
June 16, 2011

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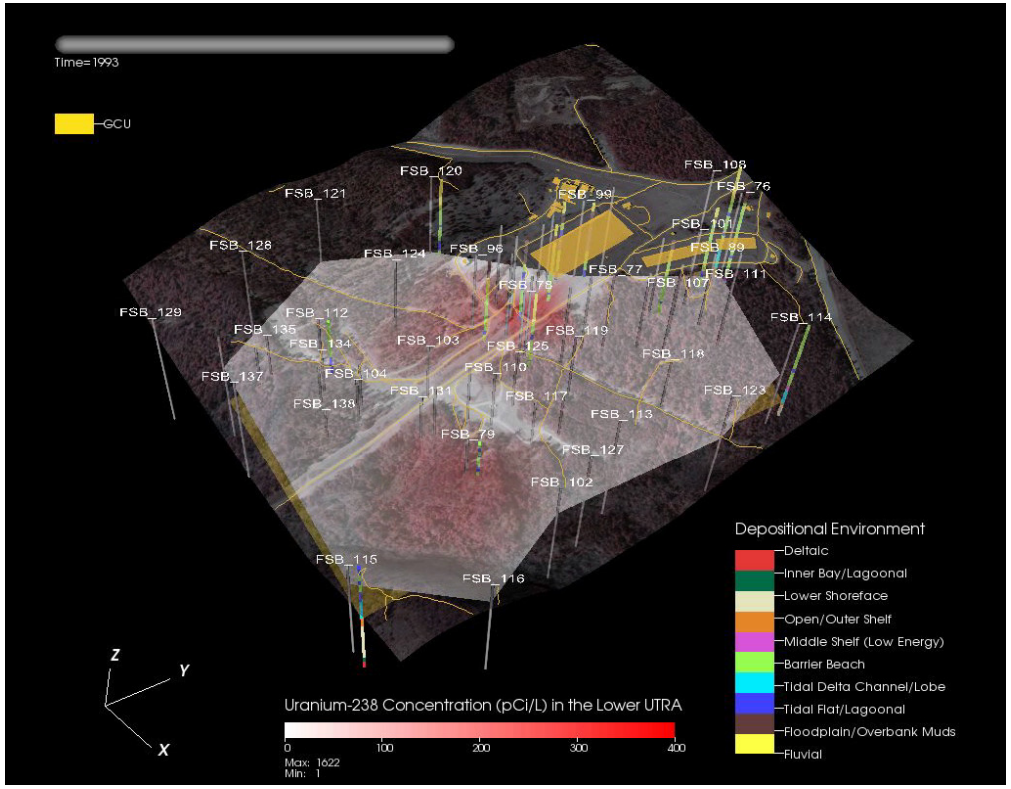
Advanced Simulation Capability for Environmental Management (ASCEM)

- 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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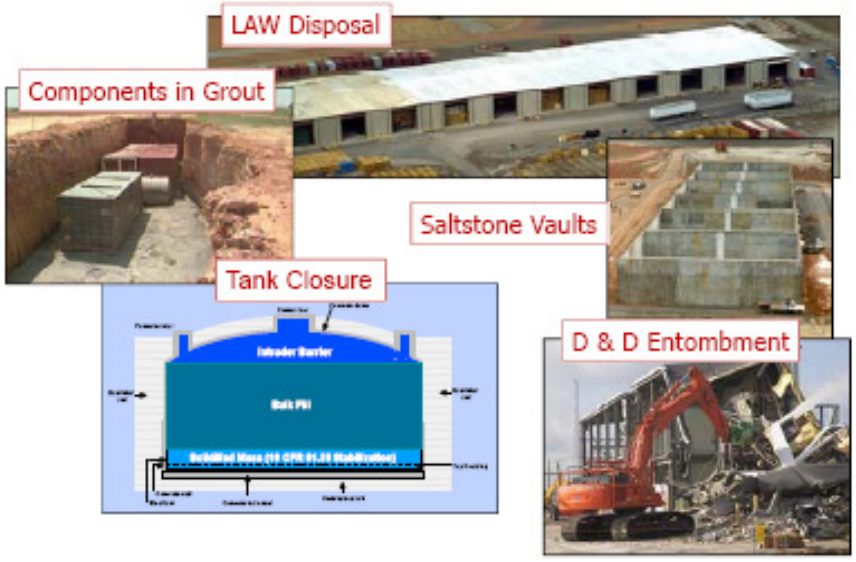
ASCEM Challenge and Impact

Challenge

- **Reduce time required and financial cost of remedial actions** at sites within EM complex by providing scientifically defensible modeling and simulation tools that accurately address complex environmental management situations
- **Develop an integrated, high-performance computer modeling capability** to simulate multiphase, multi-component, multi-scale flow and contaminant transport, waste degradation and contaminant release, including
- **Provide tools for decision making:** 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: ***technically underpin***" existing site RA's and PA's
- Inform strategic data collection for model improvement
- **Scientifically defensible and standardized EM** RA's and PA's



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ASCEM Is Delivered Through a National Laboratory Consortium

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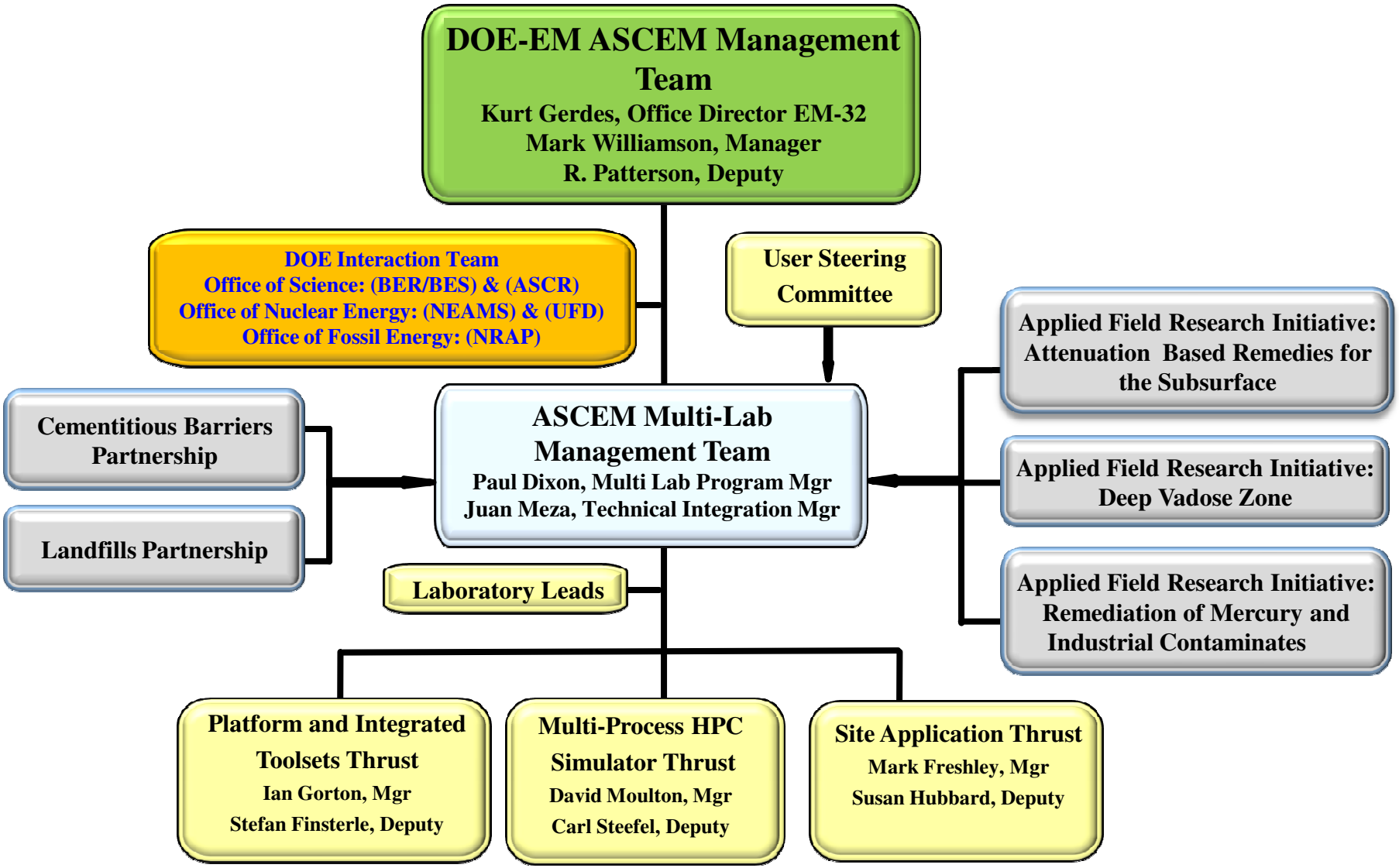
Advanced Simulation Capability for Environmental Management (ASCEM)



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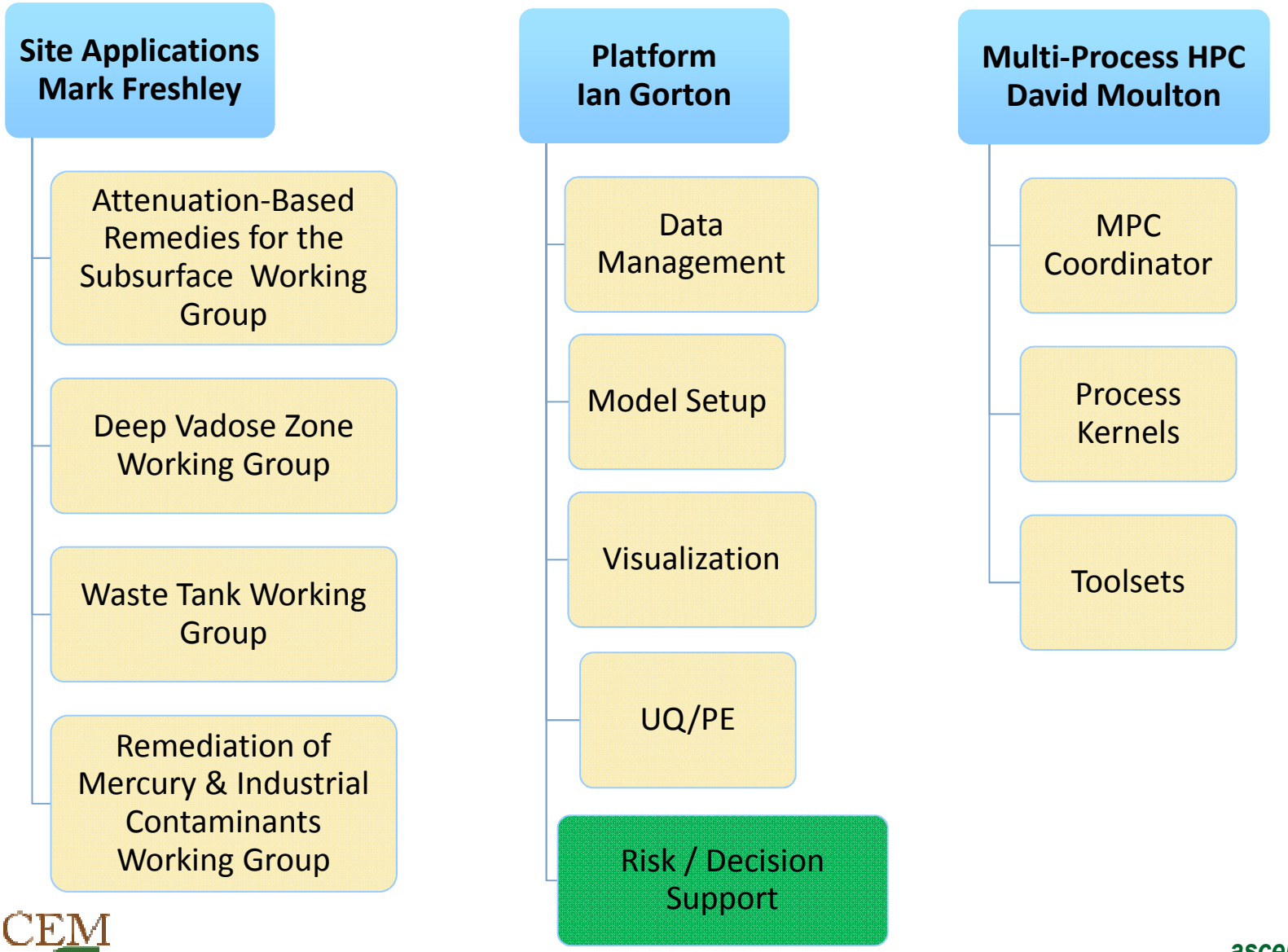
ASCEM website: http://ascemdoe.org/

ASCEM Organized Around Three Thrust Areas



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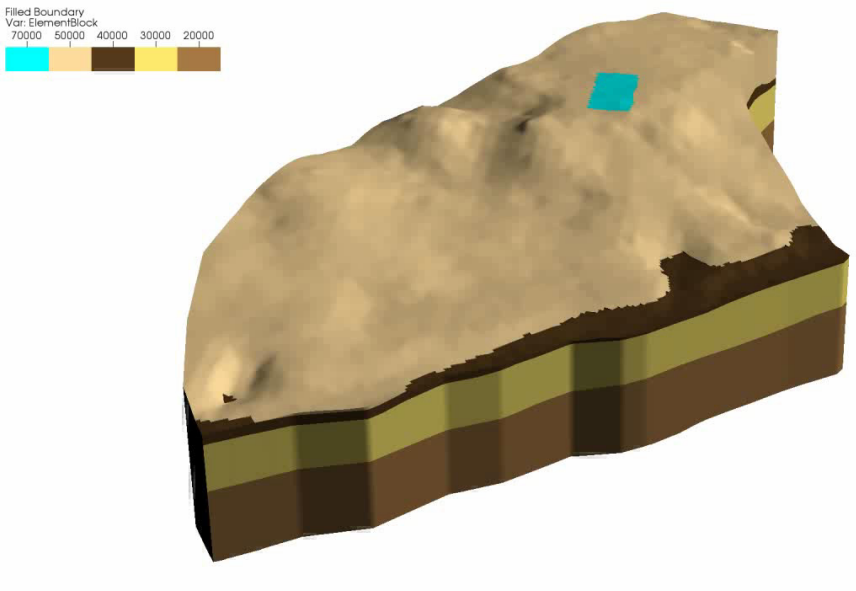
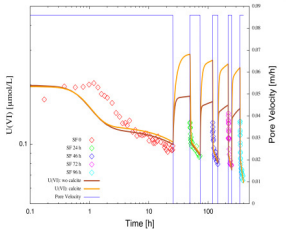
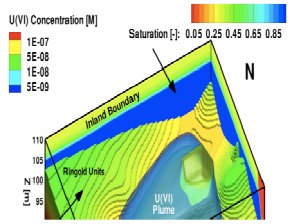
High Performance Computing

- **The ASCEM HPC simulator, Amanzi, will allow for flow and reactive transport on both structured and unstructured grids, and include physical processes such as:**

  - Biochemical Reaction Processes
  - Thermal Effects
  - Radioactive decay
  - Mechanical Effects
  - Source Term Degradation
    - Cementitious waste and structures
    - Waste tanks and metal wastes
  - Transport of Colloids (*future work*)







Wide Range of Complexity

Wide Range of Platforms

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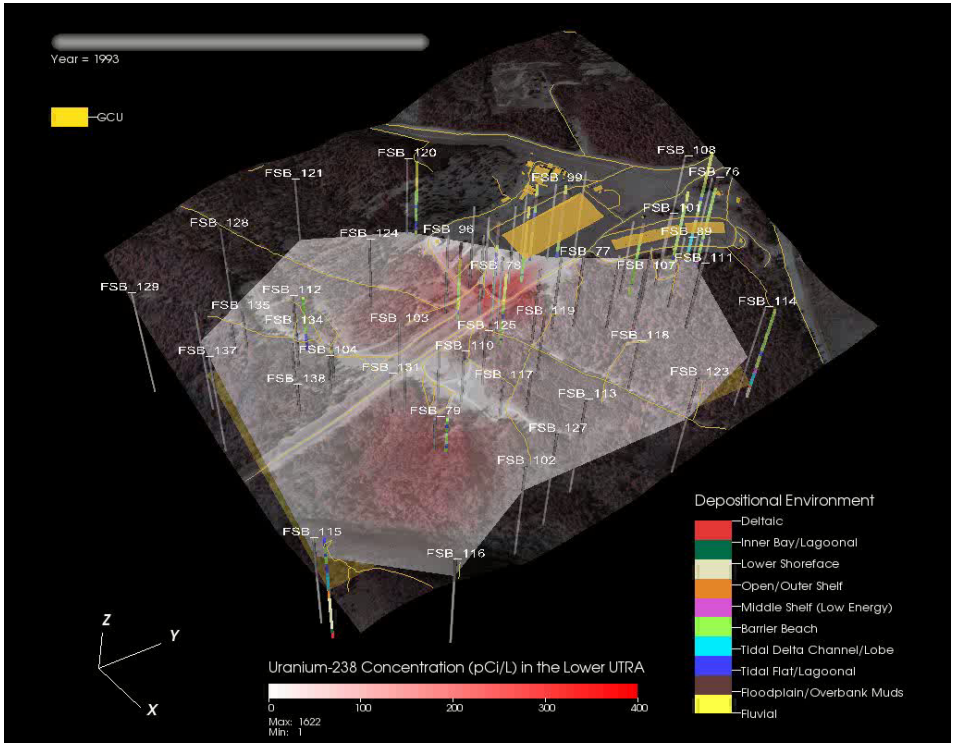
Platform and Integrated Toolsets

ASCEM 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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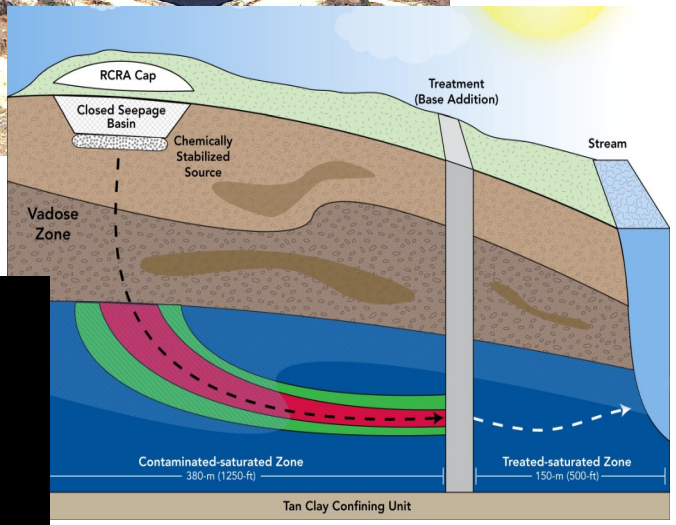
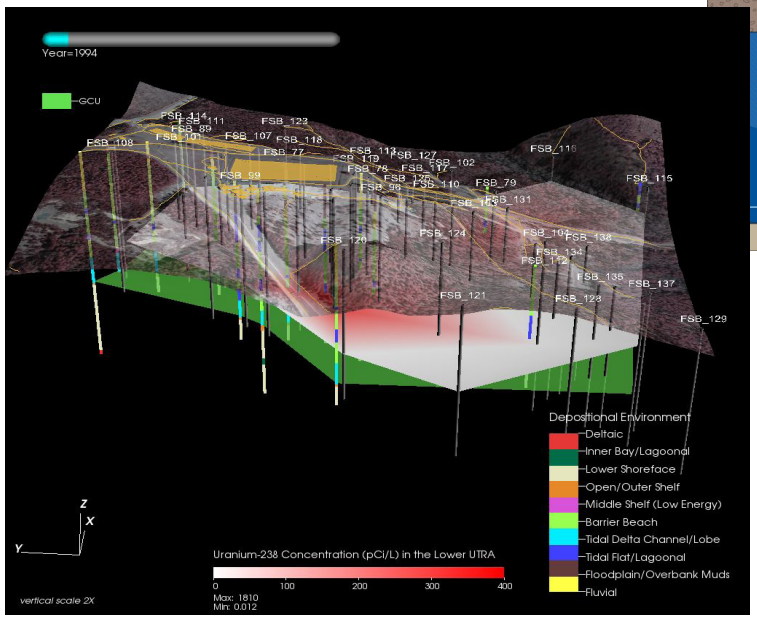
Site Applications Scope

- Provide site data for model development, testing and validation
- 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

- **Engaged 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
  - Consulted National Laboratories

- **Used recommendations as 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 the potential for 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 fit-for-purpose 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 Sites, Science Focus Areas and Integrated Field Research Challenges. (**Dae Chung Memo to Sites**)

ASCEM Leveraging

- In addition to primary ASCEM code development, significant leveraging of investments by Advanced Simulation and Computing (ASC /DOE NNSA) and Advanced Scientific Computing Research (ASCR/DOE SC)
- **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

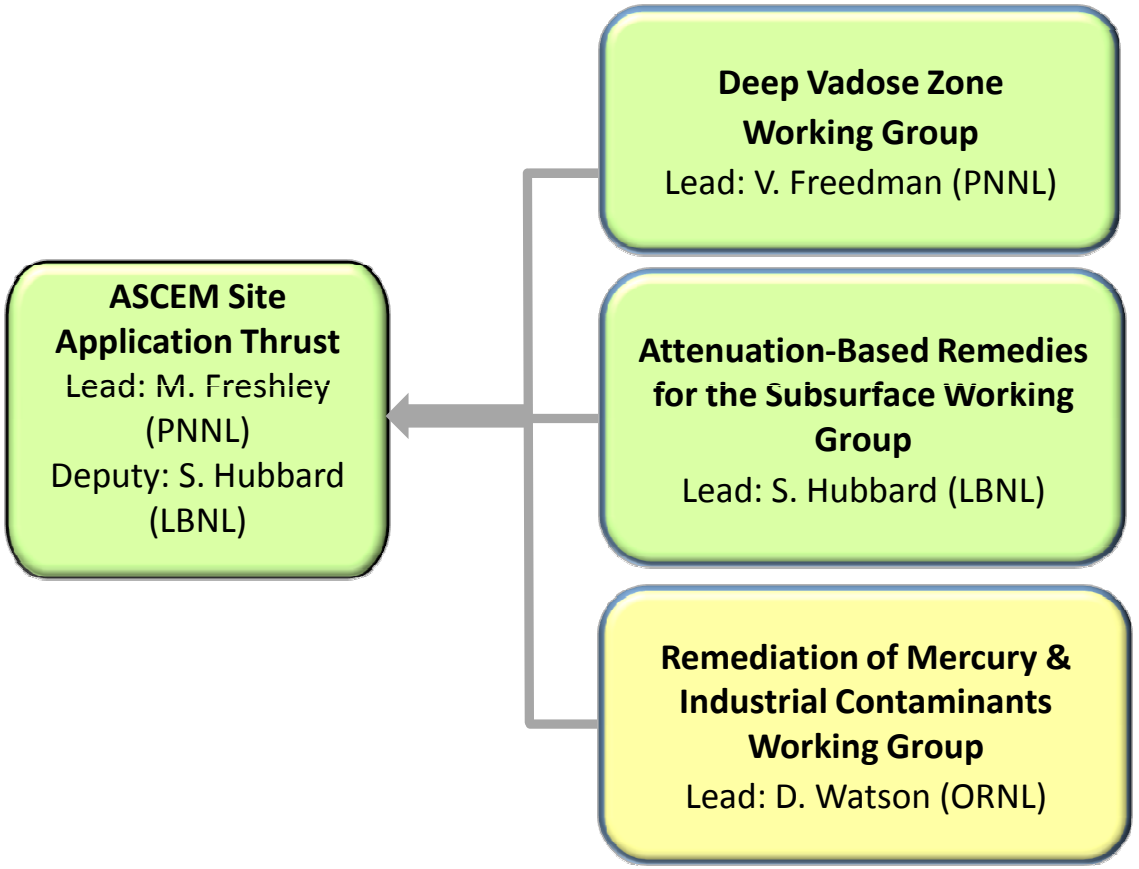
- As the request of Under Secretary Christina Johnson a workshop was held in September 2010 to investigate possible leveraging with **Fossil Energy's NRAP** program. (Report available on ASCEM website)

- 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)

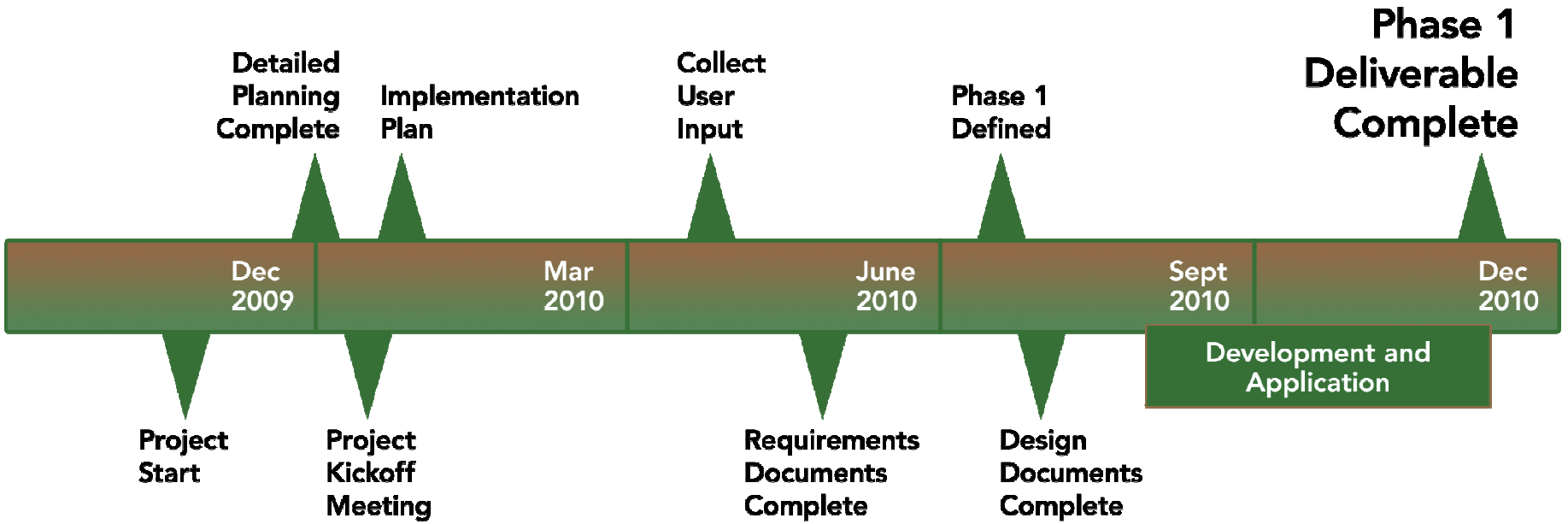
- Continue to work with the **Office of Science** to insure maximum leveraging between the two programs. Science is requiring all SFA, IFRC and SciDAC proposal renewals and new proposal include a strong tie to ASCEM. Started joint data management initiative between SC and EM.

ASCEM Relationship to the AFRIs

- ASCEM Site Applications engages AFRIs through Working Groups (**Leads Shown**)
- 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 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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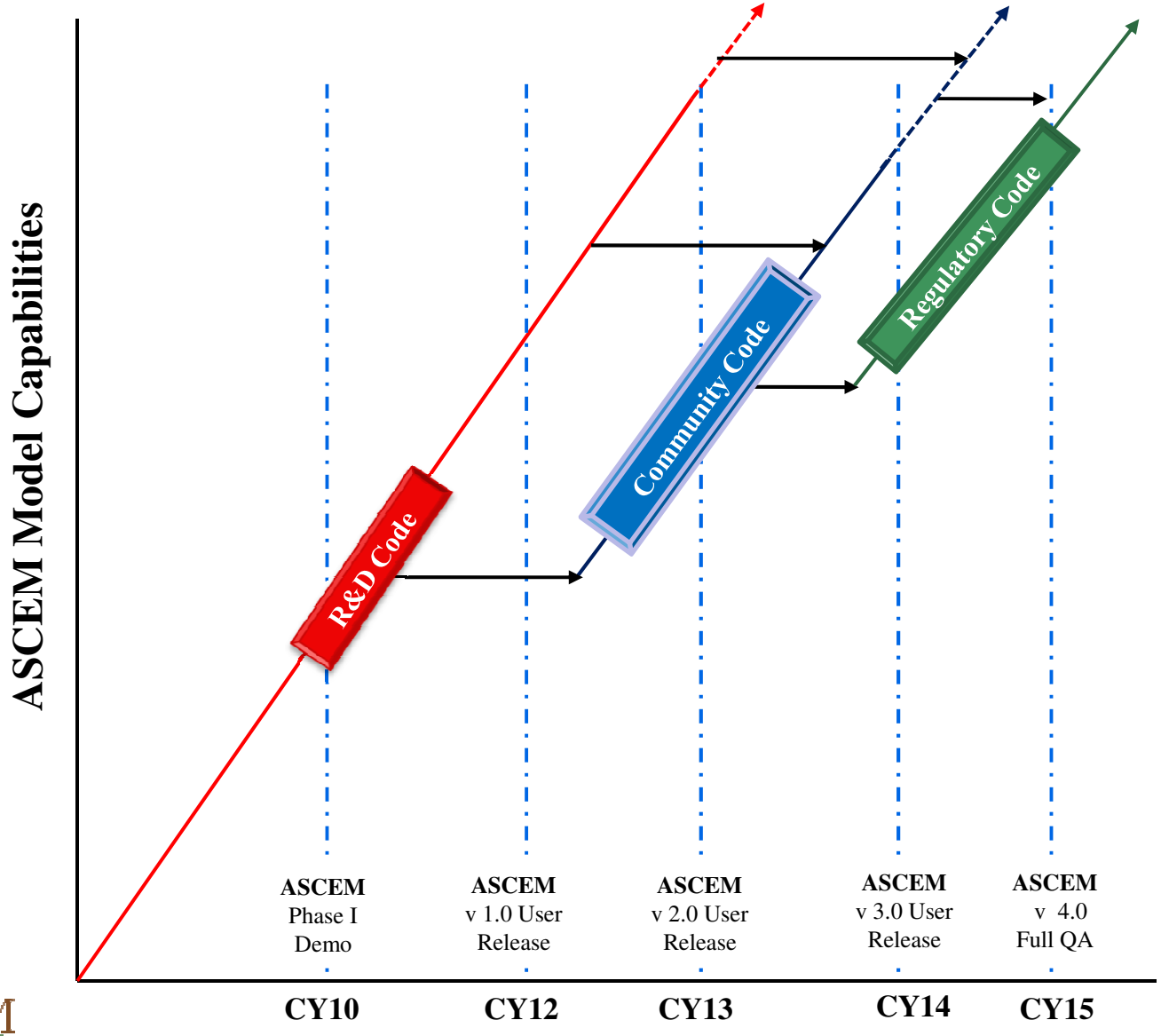
Quality Assurance Graded Approach with Code Development



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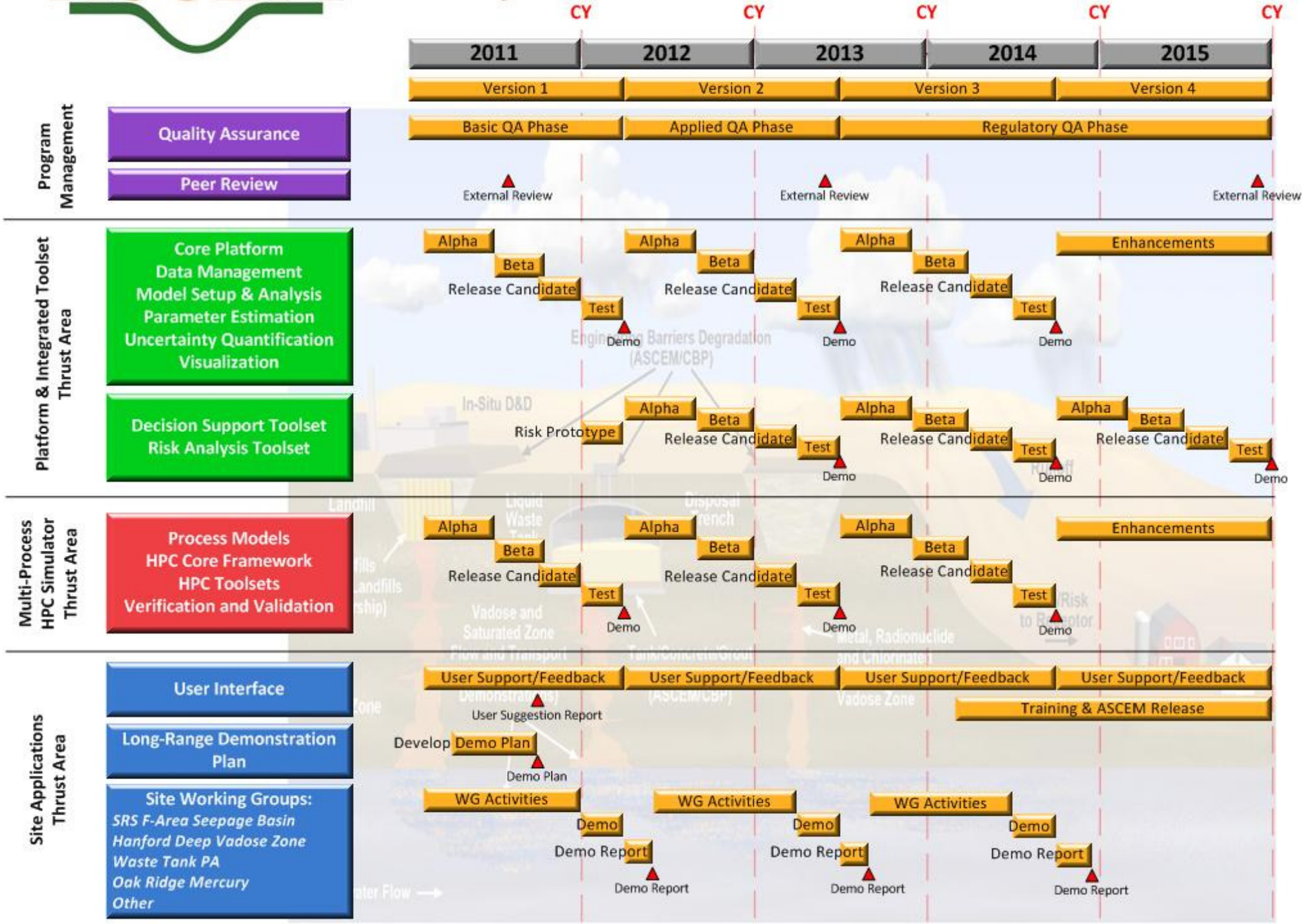
ASCEM Lifecycle Plan



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*

Looking forward: FY 2011 Work Scope Details

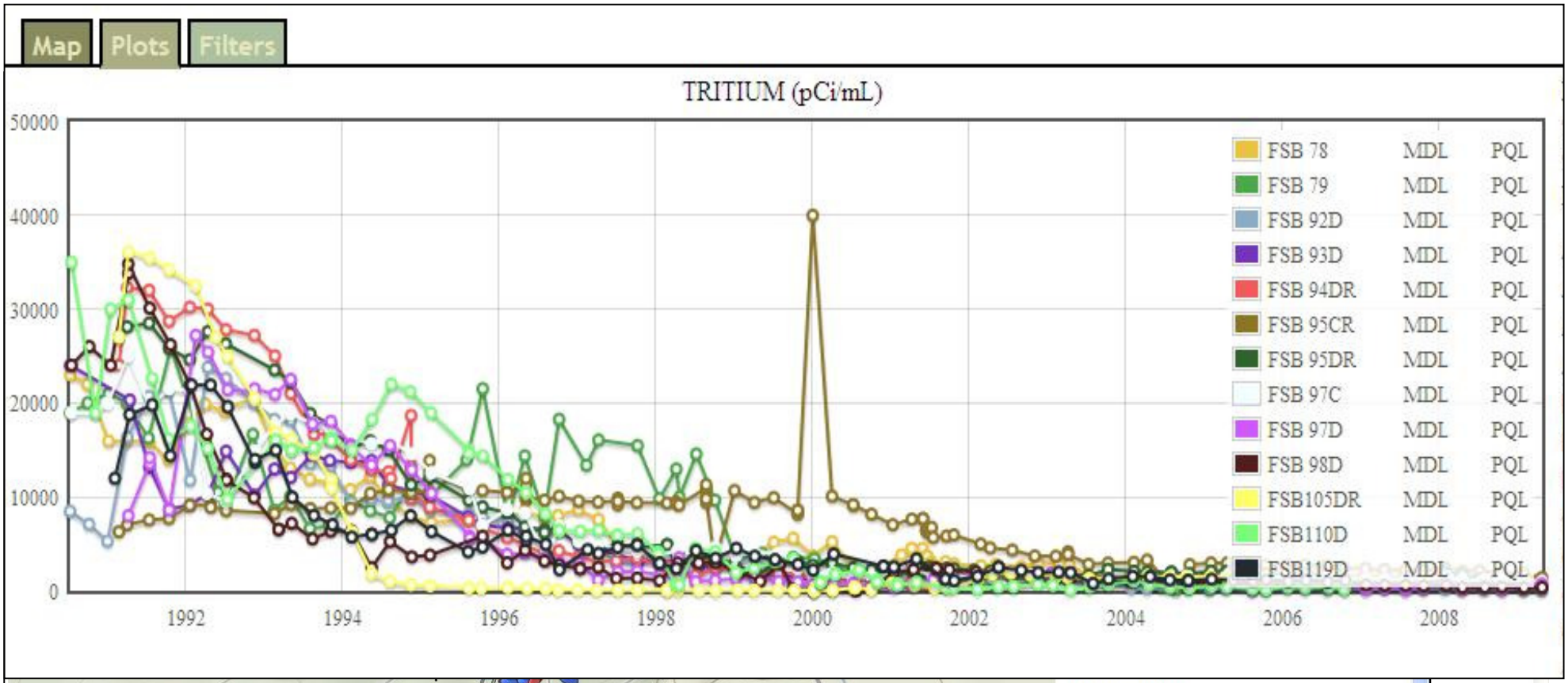
- Focus on product development and integration of components for ASCEM User Release 1.0 and Phase II Demonstration
- Conduct technical peer review in FY11
- Continue working groups for SRS F Area, Hanford Deep Vadose Zone, and Waste Tank Performance Assessment
- Continue interactions with EM Performance Assessment Community, DOE SC SBR, FE-NRAP, and NE-NEAMS/Repository Programs
- Strengthen linkages with DOE EM small sites (LANL established; West Valley, Paducah/Portsmouth, Grand Junction, Nevada Test Site and Brookhaven)
- Strengthen integration of ASCEM with the EM-32 Applied Field Research Centers

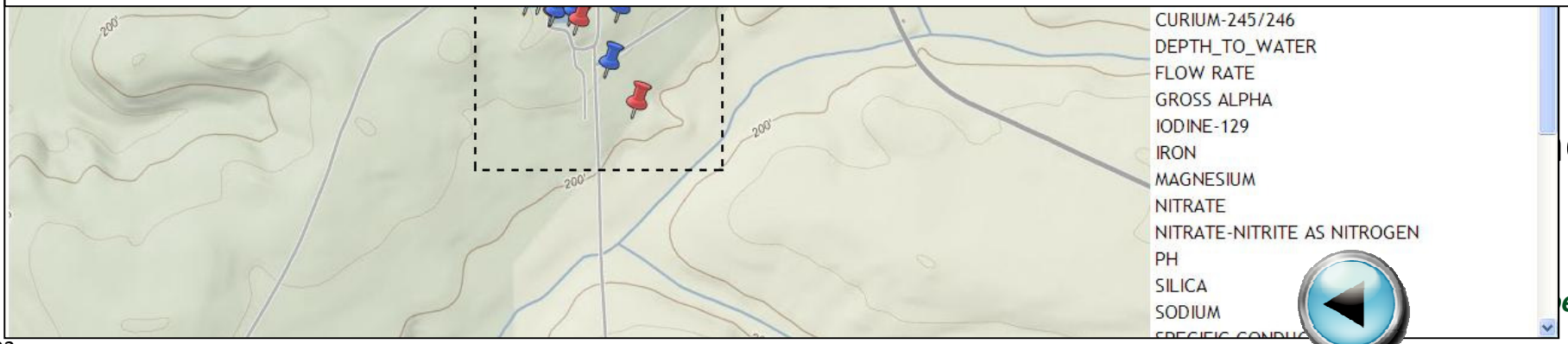
More Information about ASCEM

- *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

Data Management Phase I Accomplishments: Interactive Map of Wells for Each Aquifer





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Uncertainty Quantification Demo

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Uncertainty Quantification Phase I Accomplishments

PARAMETERS VARIED

Sour

Chem

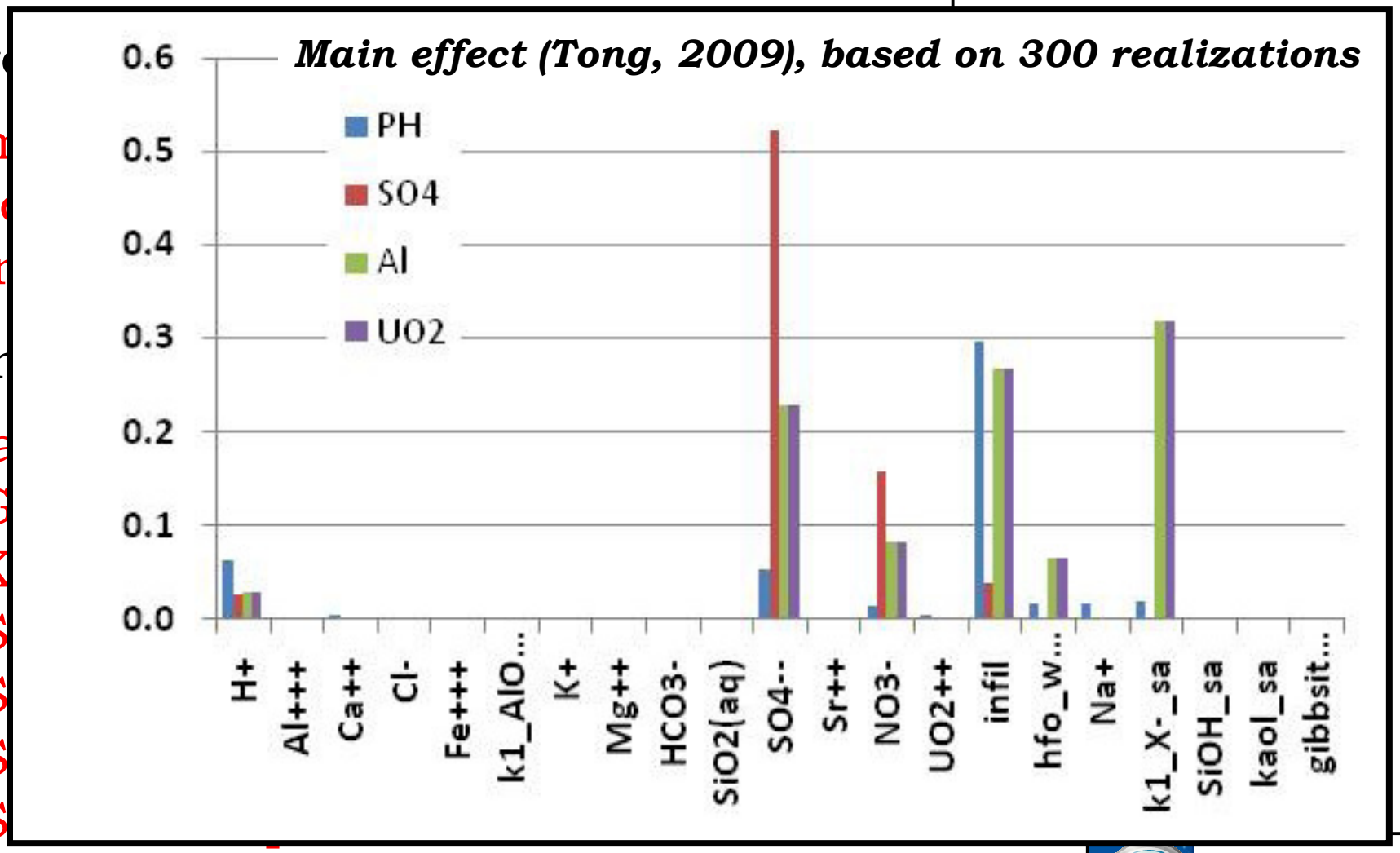
Cl, Fe

Basin

Sedim

Surfa

- G
- K
- S
- S
- S
- S



Tan Clay Confining Unit

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Visualization Demo

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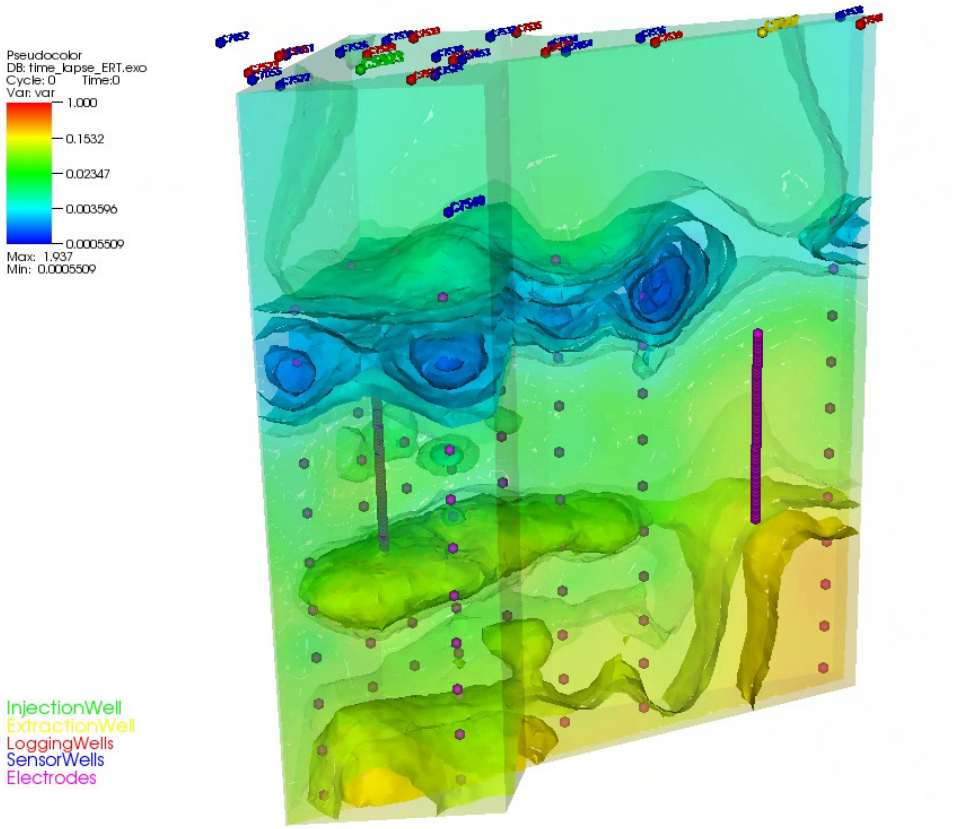
Initial Desiccation Test Geophysical Monitoring

Preliminary Electrical Resistance Tomography Characterization

- In the vadose zone, electrical resistivity is primarily governed by porosity, saturation, pore fluid conductivity, and to a lesser degree temperature.
- Pre-desiccation ERT images of the site are shown in two different views above (middle and right).
- Higher conductivity lenses (warmer colors) are diagnostic of finer grained materials with higher saturations and fluid conductivities.



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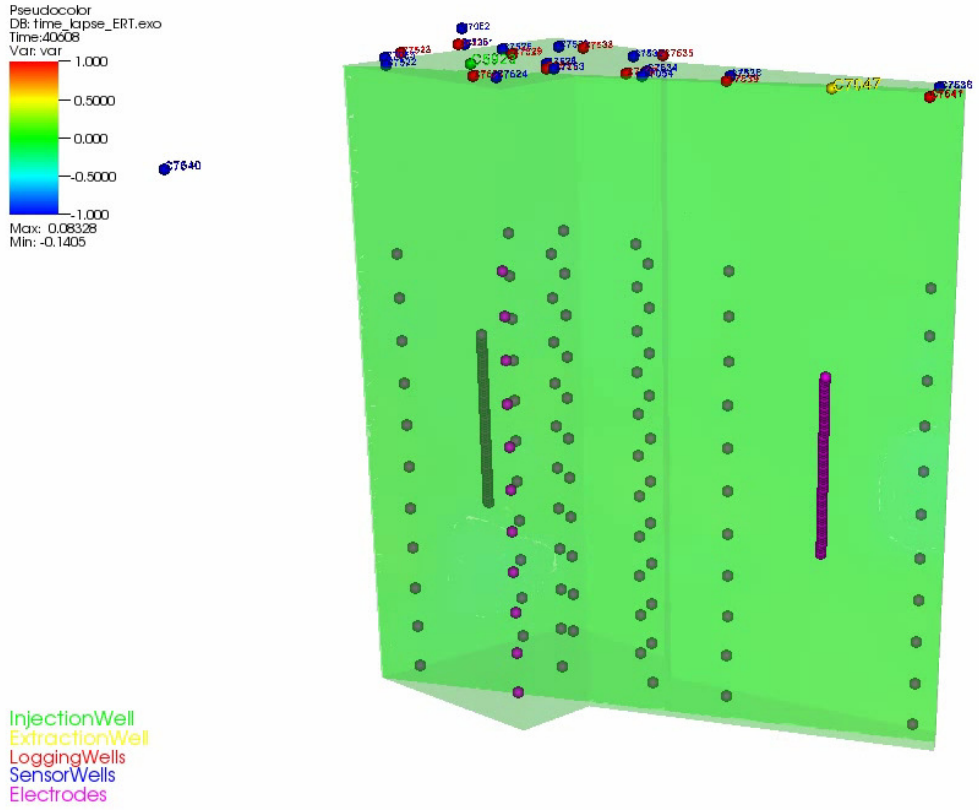
High Performance Monitoring: 3D time-lapse desiccation imaging at the BC Cribs Area

- The time-lapse images above show the change in 3D subsurface conductivity during desiccation in terms of percent change from background.
- The changes in conductivity are caused by decreases in saturation during desiccation



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