# Advanced Simulation Capability for Environmental Management Overview


**Paul Dixon (Multi-Laboratory Project Manager)**
**Justin Marble (DOE EM-10 ASCEM Program Manager)**

**Ian Gorton, David Moulton, Mark Freshley , Stefan Finsterle**
**Carl Steefel, Susan Hubbard, and Roger Seitz**


**NRC Workshop on Performance Assessments of Near-Surface Disposal Facilities: FEPs Analysis, Scenario and Conceptual Model Development, and Code Selection**

**August 29 – 30, 2012**
**Rockville, MD 20852**

EM Environmental Management
safety ❖ performance ❖ cleanup ❖ closure

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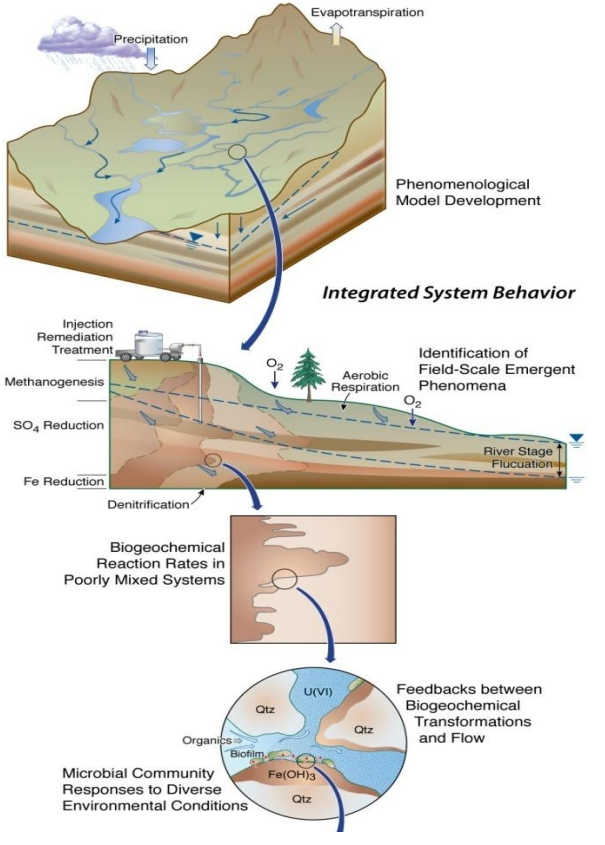
# Advanced Simulation Capability for Environmental Management (ASCEM)

- **Amanzi:**
  - **State-of-the-art simulator** for predicting contaminant fate and transport through natural and engineered systems
  - **Modular, extensible, open source** design facilitates a **new approach** for integrated modeling and site characterization
  - **'Born'** parallel for execution on emerging architectures.
- **Akuna:**
  - **User Platform** for rigorous, standardized performance and risk assessments **for EM cleanup and closure**
  - **Powerful** user interface
  - **Built** in **U**ncertainty **Q**uantification, **P**arameter **E**stimation, **S**ensitivity **A**nalysis





Wide Range of Platforms

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# User Interactions Helped Shape ASCEM Development

- **ASCEM is actively** seeking input from regulators, project management/oversight, and practitioner for their perspectives

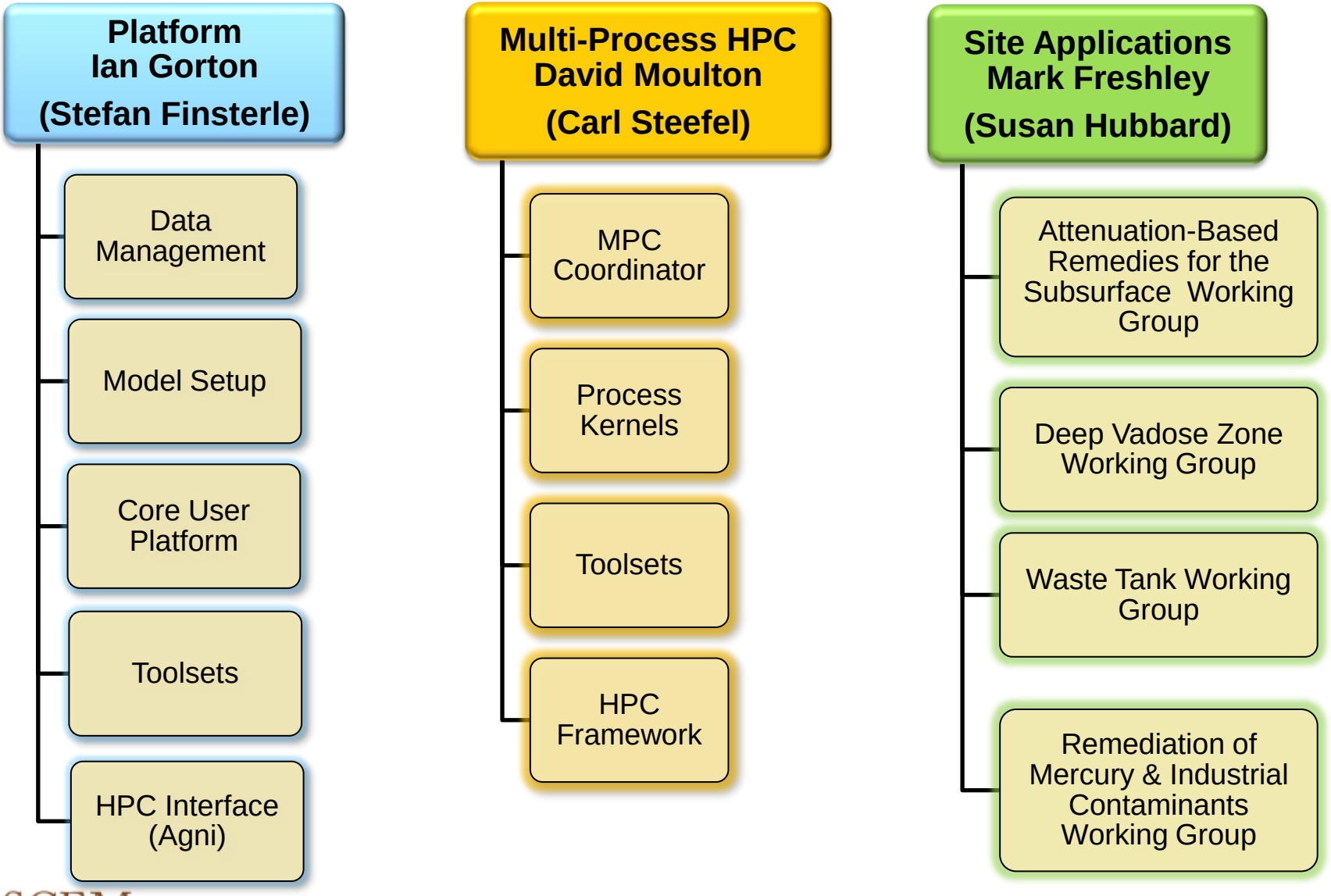
- **Engaged DOE EM end users**
  - Performance Assessment Community of Practice and Low Level Waste Disposal Facility Federal Review Group meetings
  - Interviewed Hanford, Oak Ridge, Paducah, Portsmouth and Savannah River sites
  - Consulted National Laboratories
- **Used recommendations as input to requirements**
  - Use a graded approach to allow the appropriate level of complexity to support a given decision.
  - Take advantage of HPC to reduce need for technical simplifications
  - Recognize data needs as model complexity increases
  - Consider role of modeling as input for regulatory decision making

# ASCEM Approach to Community Code

- We are working toward an **"Open-Source Community Code"** with strong community engagement.

- ***Flexible:*** easy to apply to a range of problems (range of complexity).
- ***Extensible:*** members of the community can extend the code to meet their specific needs (different levels).
- ***Accessible:***
  - We are adopting a coding standard for easy update/change.
  - Well commented code, documentation.
  - Readily downloaded, updated, and built.
- ***Efficient:*** Does not require but can use advanced/emerging architectures (parallel, multi/many-core).
- Graded and well documented QA approach.
- Leverage existing open-source/community capabilities.

# ASCEM is Organized Around Three Thrust Areas



# Current ASCEM Capabilities

- **Tool development and integration of components :** User Release 1.0 and Phase II Demonstrations in FY12.

## ASCEM User Release 1.0

**"Core Platform"**

**Akuna**

**Data Management**
**Model Setup Toolset**
**Parameter Estimation Toolset**
**Uncertainty Quantification Toolset**
**Visualization**

**AGNI**
**Toolset**
**Driver**

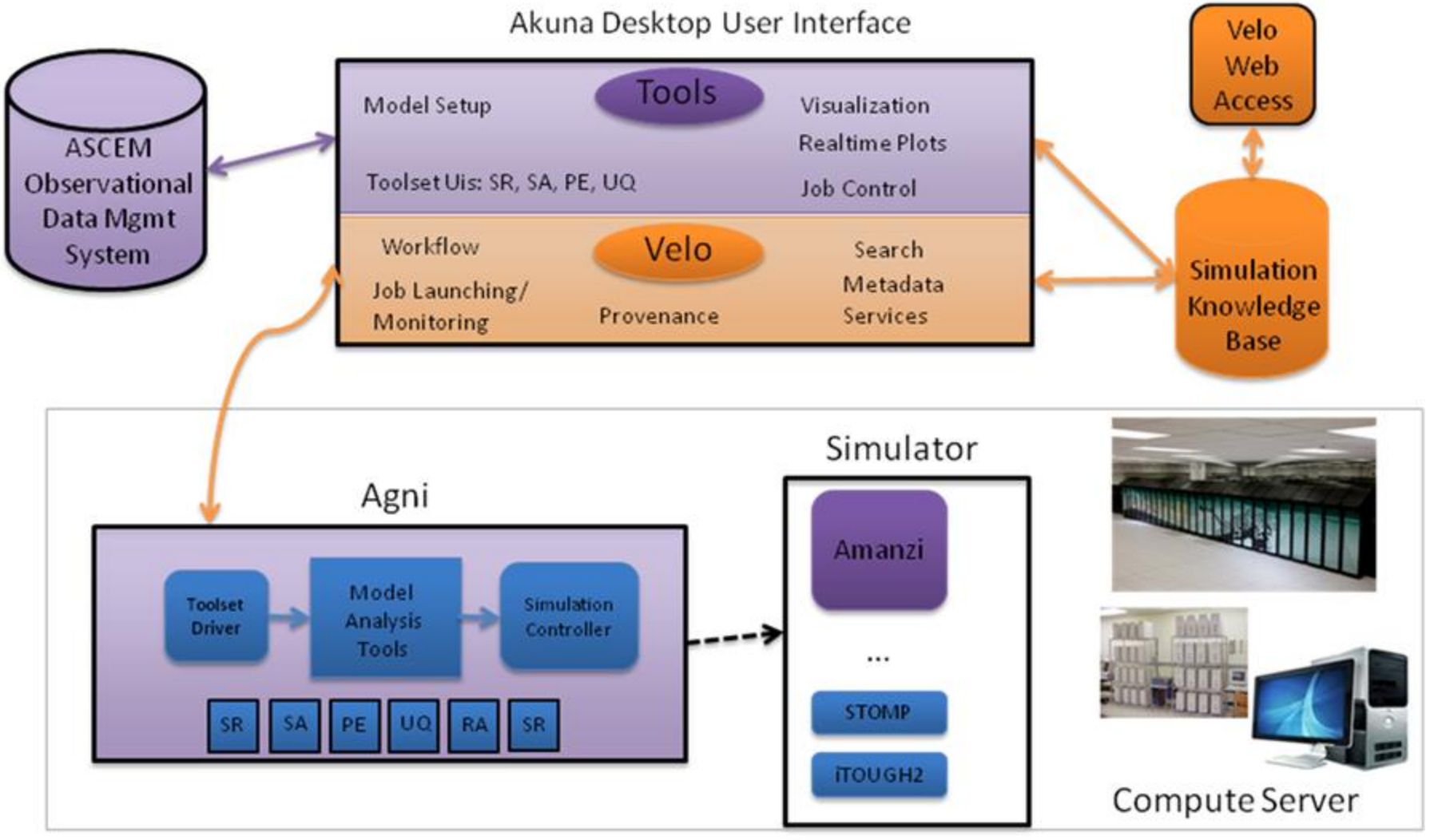
**"HPC Simulator"**

**Amanzi**

**Unstructured polyhedral meshes**
**Structured meshes (AMR)**
**Transient flow and boundary parameters**
**Improved discretization methods**
**Enhanced reactions Toolkit**
**Parallel I/O**

- Working groups for SRS F Area, Hanford Deep Vadose Zone, Waste Tank Performance Assessment and DOE EM small sites (LANL, NNSS)
- Initiate ASCEM user and training facilities (UNLV test case)
- Continue communication and integration with other DOE Simulation efforts…..

# ASCEM Integrated Modeling Workflow



# Data Management: Data Analysis and Browsing

Wiki

Database

File Store/ Archive

Code repository

Data storage – Reports, simulation inputs/outputs, measurement data, etc

Data Post-processing

Indexes

Maps

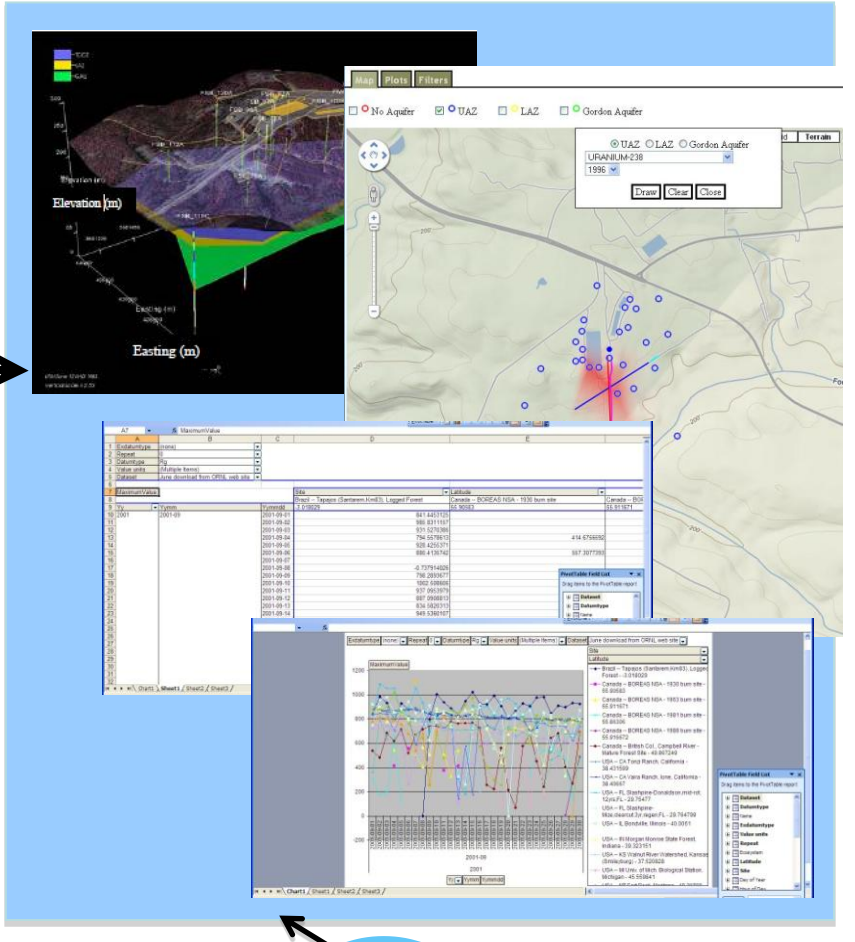
VisIt

Data Mining Tools

Browsing, Searching, Subsetting

Data analysis, browsing, and support infrastructure

Interactive maps, search, graph displays, and APIs

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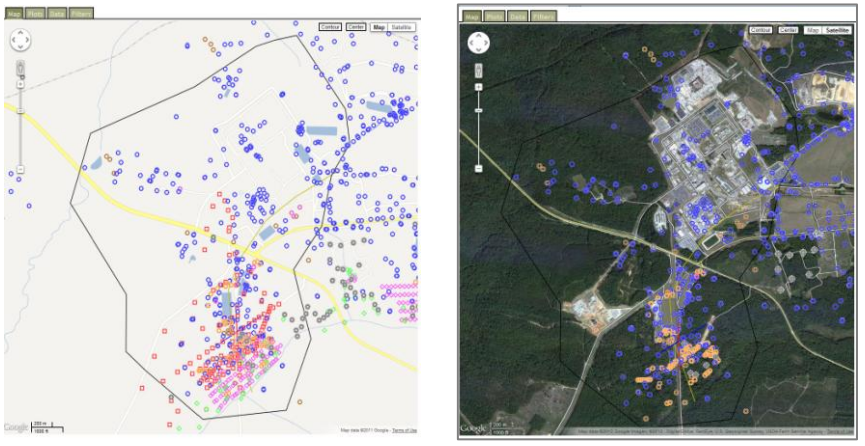
# Site Applications Scope

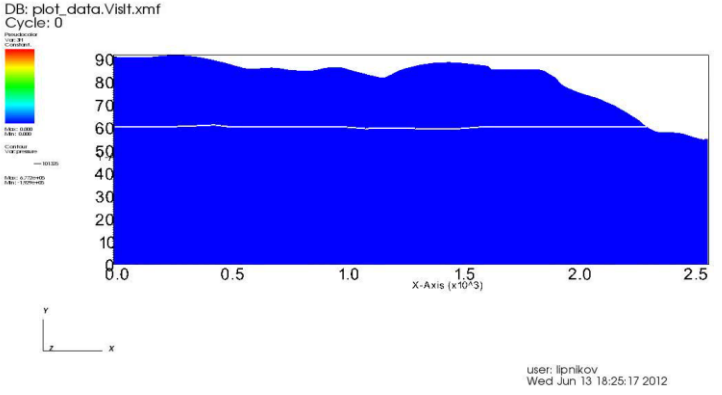
## Goals:

- Solicit input to requirements specification and development activities
- Conduct testing, and model confidence building using EM site data
- Lead demonstrations of the Platform and HPC simulator
- Interface with end users

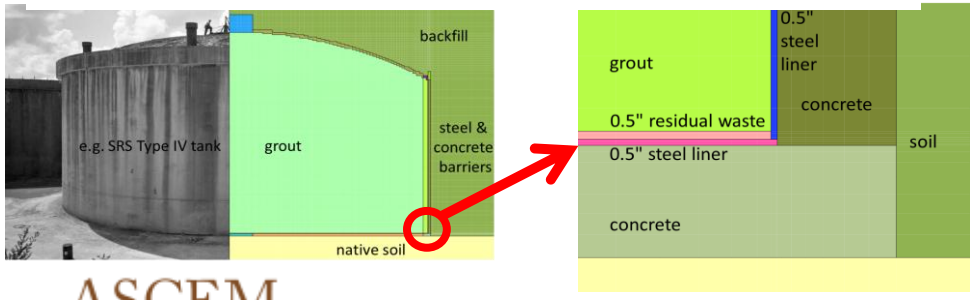
### F-Area Data Management



### F-Area Simulation with Amanzi




### Waste Tank Performance Assessment

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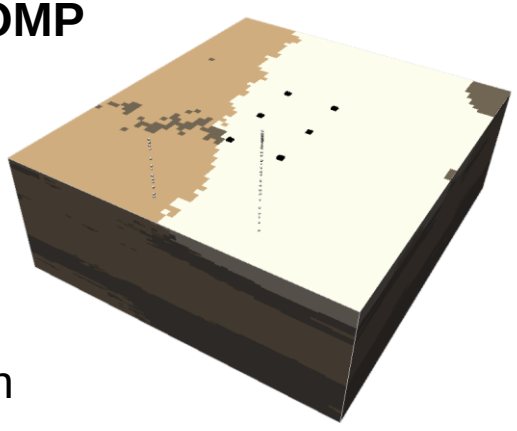
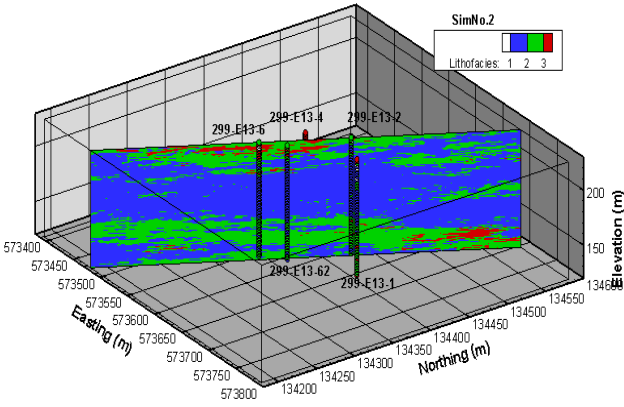
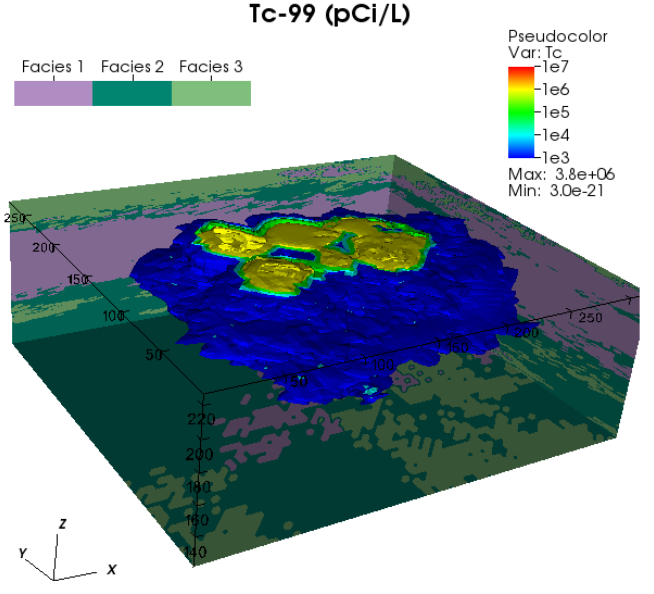
# High Performance Computing and Uncertainty Analysis

- **Akuna Model Setup Tool used to translate conceptual model to grid and generate input for simulator (eSTOMP and Amanzi)**
  - Hanford BC Cribs
  - Site characterized by sparse data
  - Water and contaminant releases occurred 1956 to 1958
  - $^{99}$Tc released to cribs with partition coefficient of zero






- **Generated three-dimensional realizations of subsurface geology and recharge to evaluate uncertainty of baseline conditions**
  - Capture fine-scale heterogeneities
  - Parameter estimation 1956 to 2008
  - Uncertainty quantification 2008 to 3000




**Simulated technetium distribution under the BC-cribs area at Hanford**

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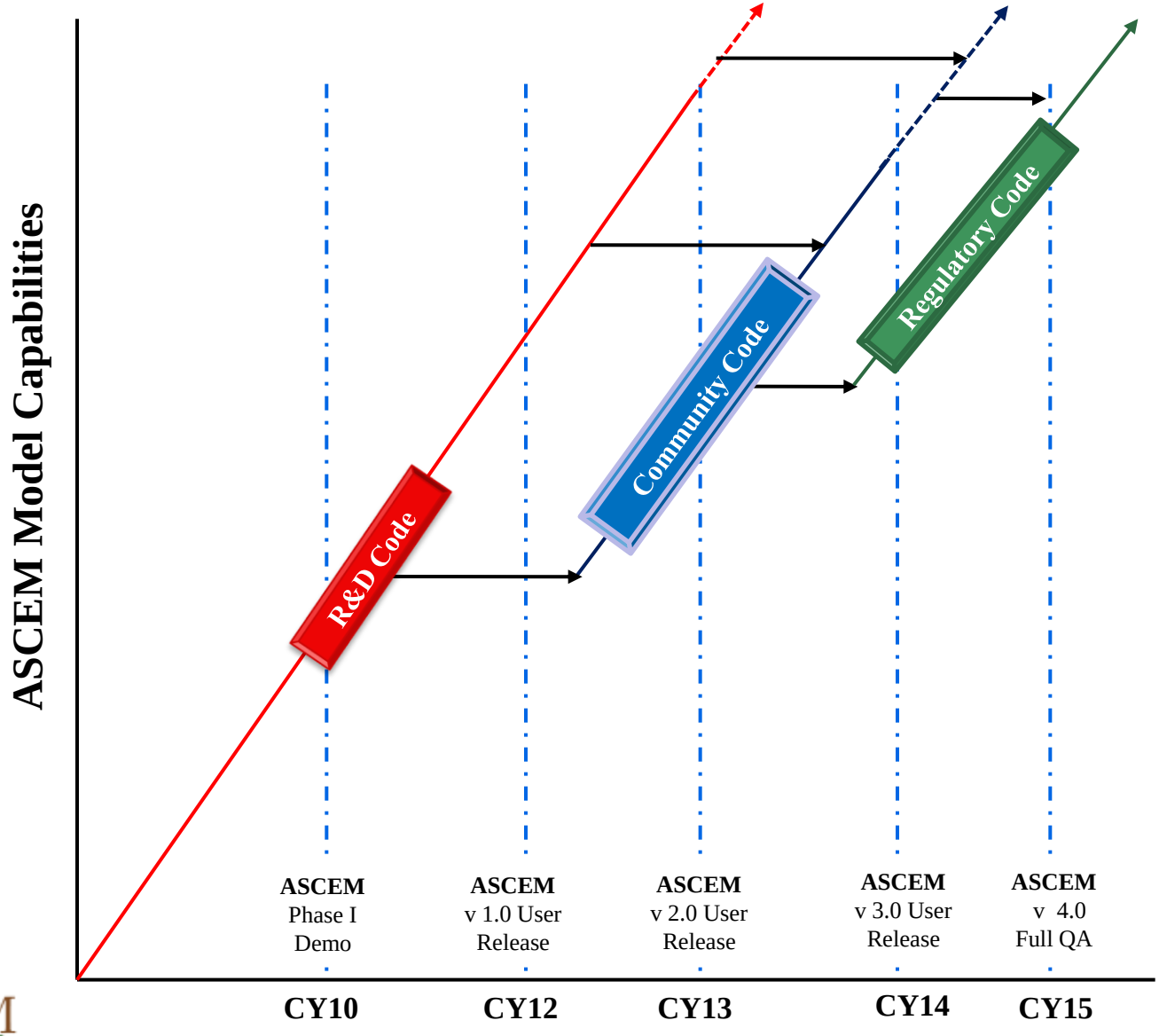
# Future ASCEM Capability Development Efforts

- **AKUNA:**
  1. Enhanced numerical modeling tools (FY13)
  2. Initial Decision Support Toolset (FY13)
  3. Enhanced UQ, PE, SA capabilities (FY13)
  4. Powerful integrated visualization and analysis (FY13)
  5. Usability enhancements based on user feedback (FY13)
  6. Incorporation of Risk Evaluation toolset (FY14)
- **AMANZI**
  1. More flexible input specification to streamline model representations (FY13)
  2. Enhanced performance on emerging architectures (FY13)
  3. Accurate modeling of truly three-dimensional structural features (FY13)
  4. Flexible and extensible interface for alternative geochemistry process kernels (FY13)
  5. Initial prototyping of surface water processes (FY13/FY14)
  6. Multi-phase flow with thermal processes for modeling desiccation (FY14).
- **Solicit University Collaborations with ASCEM user and training facilities**
- **Support major international benchmarking workshop with ASCEM**
- **NQA-1 qualification of ASCEM codes for regulatory release (Begin FY14 and complete FY15)**

# Graded Approach to ASCEM Code and QA Development

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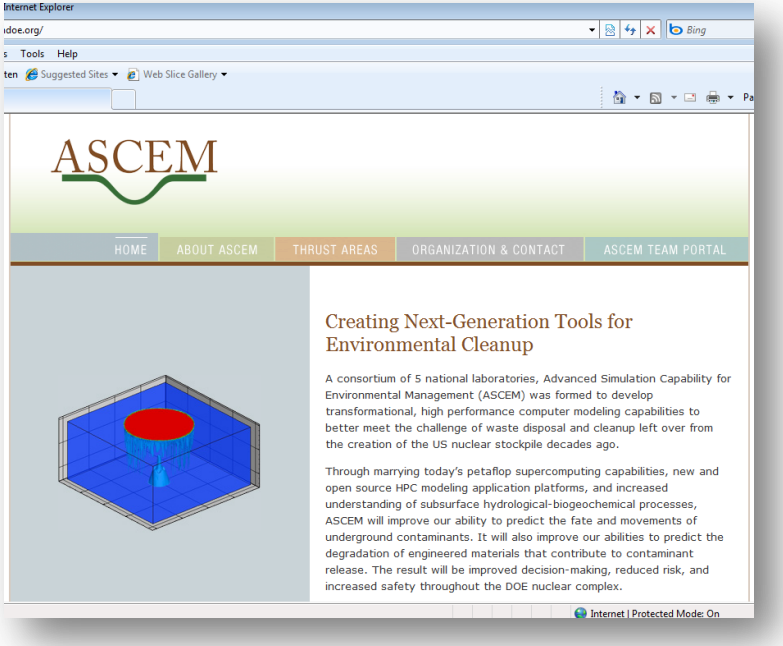
# More Information about ASCEM

- **Mathematical Formulation Requirements and Specifications for the Process Models;** ASCEM-HPC-2011-01, 2011
- **High-Level Design of Amanzi: The Multi-Process High Performance Computing Simulator;** ASCEM-HPC-2011-03, 2011
- **2011 ASCEM Platform Thrust Design Document;** ASCEM-PIT-2011-01, 2011
- **ASCEM Phase II Demonstration Plan;** ASCEM-SITE-2011-01, 2011
- **ASCEM User Needs Report – FY 2011;** ASCEM-SITE-2011-02, 2011
- **ASCEM Phase 1 Demonstration;** ASCEM-SITE-102010-01, 2010
- **Advanced Simulation Capability for Environmental Management (ASCEM): An Overview of initial Result;** *Technology and Innovation, Vol. 13, pp. 175–199, 2011.*




**http://ascemdoe.org/**

**Currently under redesign and new version publically available May 2011**

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Questions