Advanced Simulation Capability for Environmental Management

Roger Seitz (End User Interface)
Paul Dixon (Multi-Laboratory Project Manager)
Justin Marble (DOE-EM Project Manager)
Tim Scheibe (Platform and Integrated Toolsets Lead)
David Moulton (Multi-Process HPC Simulator HPC Lead)
Mark Freshley (Site Applications Lead)
Stefan Finsterle (Platform and Integrated Toolsets Deputy)
Carl Steefel (Multi-Process HPC Simulator HPC Thrust Deputy)
Susan Hubbard (Site Applications Deputy)

SRS CAB FD&SR Committee Meeting
June 11, 2013
Purpose

- Provide an overview of the DOE-EM sponsored project to develop the Advanced Simulation Capability for Environmental Management (ASCEM) to fulfill a Facilities Disposition & Site Remediation (FD&SR) 2013 Work Plan item
ASCEM Is Delivered Through a National Laboratory Consortium
Why Do We Use Models?

Improve our understanding of system behavior

- Projecting future migration of contamination (10s, 100s or 1,000s of years)
- Managing uncertainties – identifying what is important
- Prioritizing data collection and monitoring activities
- Evaluating potential effectiveness of remediation and closure options
- Optimizing designs
- Regulatory compliance

ASCEM
Modeling Example
Challenges

- Move towards more **standardized and consistent** environmental modeling approaches across the DOE Complex
- Improve model support for **decision-making and demonstrations of regulatory compliance** during and at the conclusion of assessment efforts
- Provide tools that help to **explain complex information in an understandable way**
- Provide capability to **explore problems in greater detail**, where needed to address the most challenging remediation/disposal efforts

![Active DOE-EM Sites](ascemdoe.org)
A State-of-the-art tool for predicting movement of contaminants through natural and engineered systems

Freely available and expandable to incorporate existing modeling tools

Designed to take advantage of modern computing architectures (e.g., multi-core) from laptops to supercomputers
User Interactions Helped Shape ASCEM Development

- The ASCEM team has actively reached out to a variety of potential users around the DOE Complex for suggestions, including regulators, programmatic/management, and modeling practitioners.

- Used recommendations as input to requirements:
  - A **Graded Approach** is needed to allow the use of the appropriate level of complexity to support a given decision.
  - Consider role of modeling as input for regulatory decision making.
  - Take advantage of new tools to reduce reliance on simplifications.
  - Recognize increased data needs as model complexity increases.
**ASCEM Key Components**

- **Akuna** – The graphical user interface and platform with the tools to help manage data, setup and run models, and process results from simulations.

- **Amanzi** – The computational engine that solves all of the equations needed to model movement of water and contaminants in the environment.

- Akuna and Amanzi integrate many tools that have been developed through other activities.
Example Akuna Tools
Example Amanzi Results