Advanced Simulation Capability for Environmental Management

ASCEM

ASCEM Software Capabilities and Performance Assessment Deployments

Greg Flach

ASCEM Site Applications Team

Performance & Risk Assessment Community of Practice
Technical Exchange Meeting

December 11-12, 2014

Las Vegas NM

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ASCEM Points of Contact

- **HPC Thrust**
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- **Platform Thrust**
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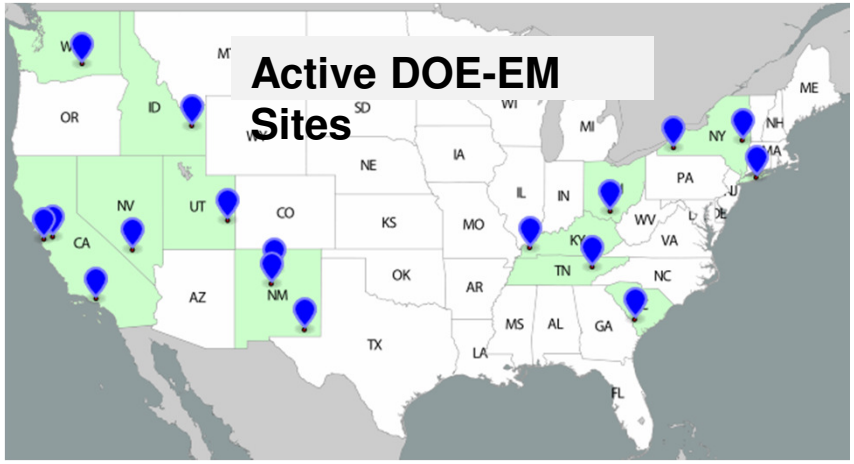
Why ASCEM?

- **<u>Standardized and consistent</u> modeling approaches across DOE Complex**
- **Tools that help <u>explain complex information</u> in an understandable way to all constituents (e.g, public, regulators)**
- **Capability to <u>explore problems in greater detail</u>**
  - Manage uncertainty and reduce reliance on over-conservatism that can lead to costly decisions
  - Scientist determines desired complexity



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Advanced Simulation Capability for Environmental Management (ASCEM)

➢HPC (Amanzi) Thrust

- State-of-the-art subsurface flow and reactive transport simulator
- Designed to take advantage of modern computing architectures (e.g., multiple cores)

➢Platform (Akuna / Agni / Velo) Thrust

- Integrated toolset to address entire modeling workflow:
- Amanzi simulation, visualization, UQ, SA, PE, data management, and more

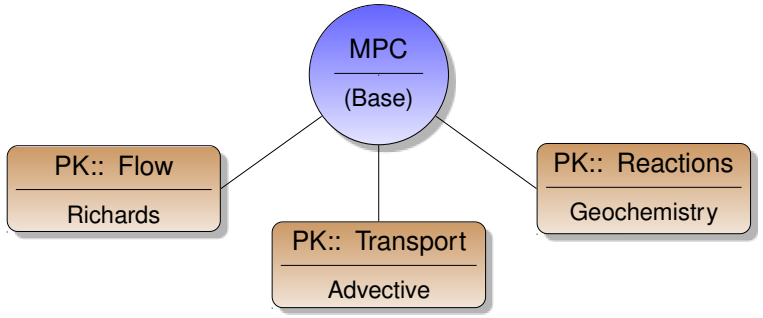
➢Site Applications Thrust

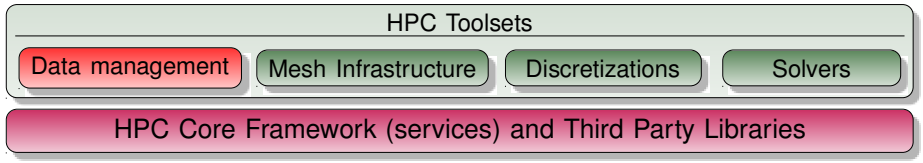
- ASCEM testing, demonstration and deployment

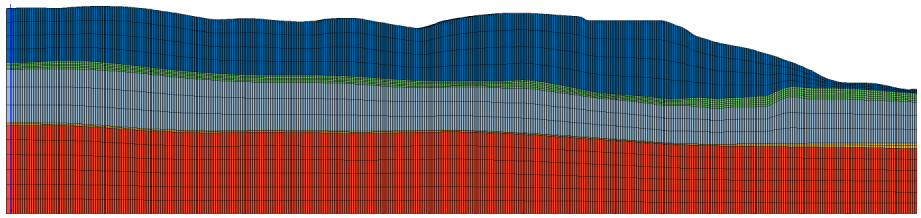
Amanzi Multi-Process Flow and Reactive Transport Simulator

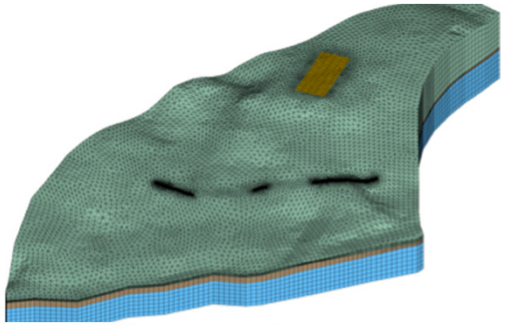
Salient Features

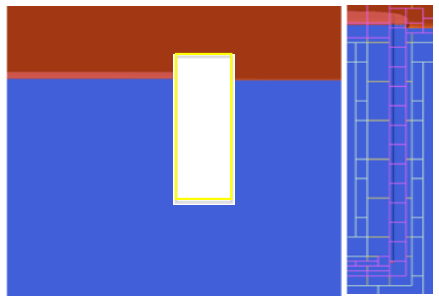
- Selection of governing equation
  - Transient unsaturated flow with Richards equation
  - Transient single-phase flow with specific storage/yield
- Uniform interface to access existing biogeochemistry codes thru Alquimia
  - PFLOTRAN
  - CRUNCHFLOW
- Meshing
  - Internal mesh generation for rectangular domains
  - Unstructured with polyhedral cells
  - Block-structured adaptive mesh refinement
- Tight integration with Platform Software
  - Parallel computing accessible











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ASCEM Platform and Integrated Toolsets

- **Akuna**
  - Mesh generation
  - Input file generation
    - Multiple simulations (e.g., sensitivity analysis [SA], uncertainty quantification [UQ], parameter estimation [PE])
  - Results visualization
    - VisIt integration for spatial viz
- **Velo**
  - Workflow
  - Job launching and monitoring
  - Data and simulation provenance and management
- **Agni**
  - Simulation controller
  - Analysis tool for SA, UQ, PE

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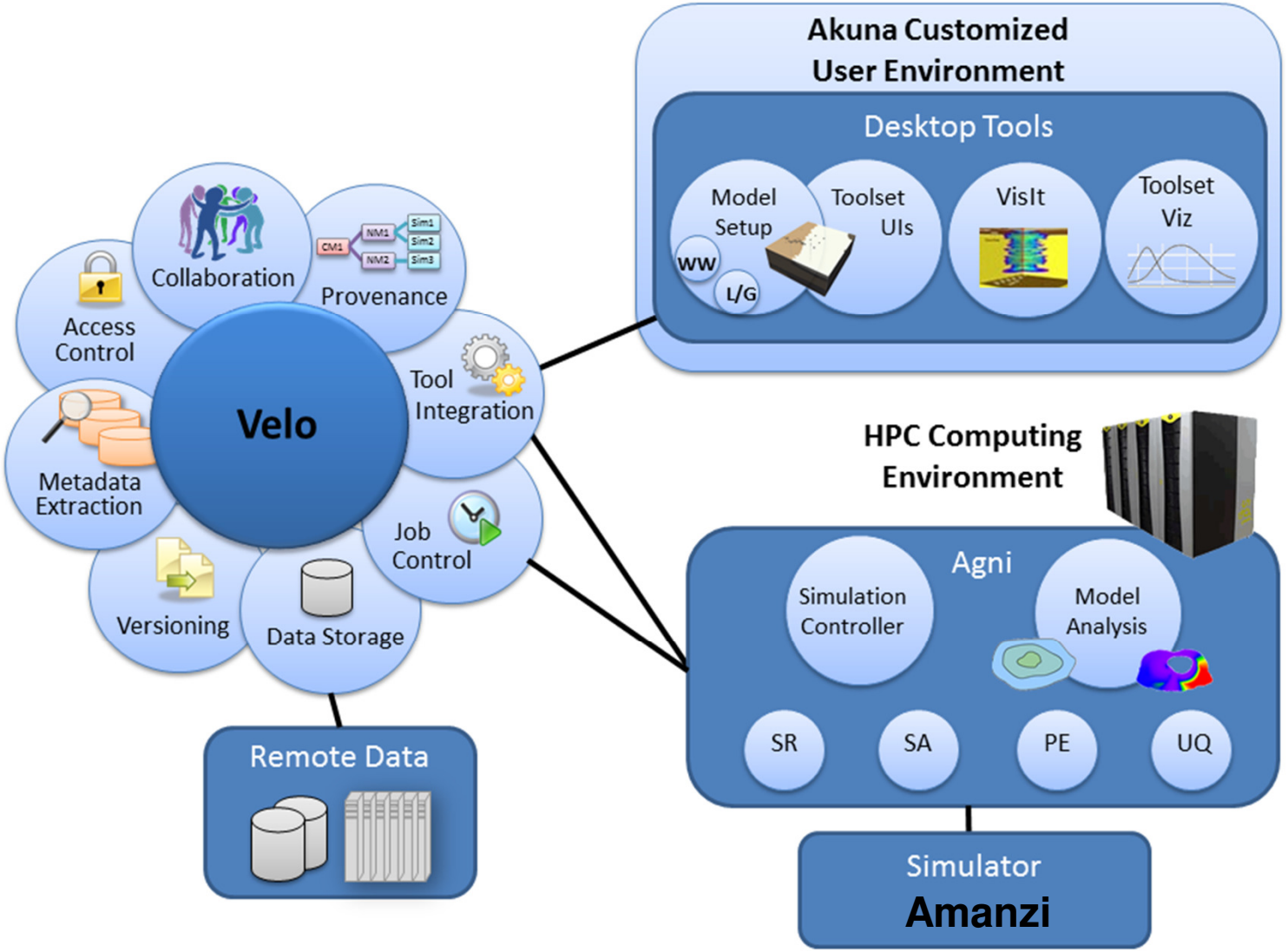
ASCEM Platform and Integrated Toolsets



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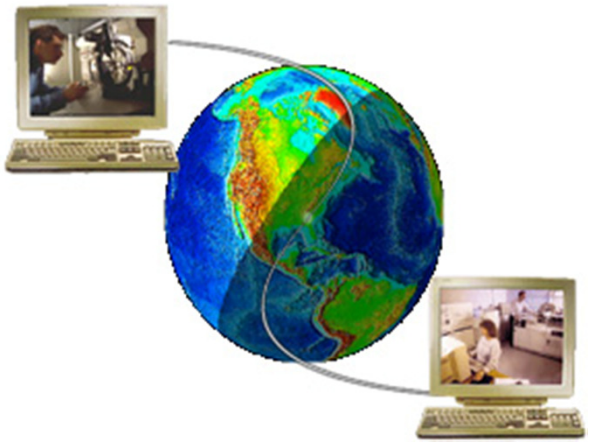
ASCEM Strengths

- **High Performance Computing (HPC)**
  - Computational algorithms that take advantage of modern computing hardware (multiple cores)
- **Toolset integration**
  - More efficient workflows
  - Automated execution of multiple simulations
    - SA, PE, UQ
  - Data and simulation provenance
- **Cloud computing**
  - Enhanced collaboration
  - Ready access to high-performance computing resources

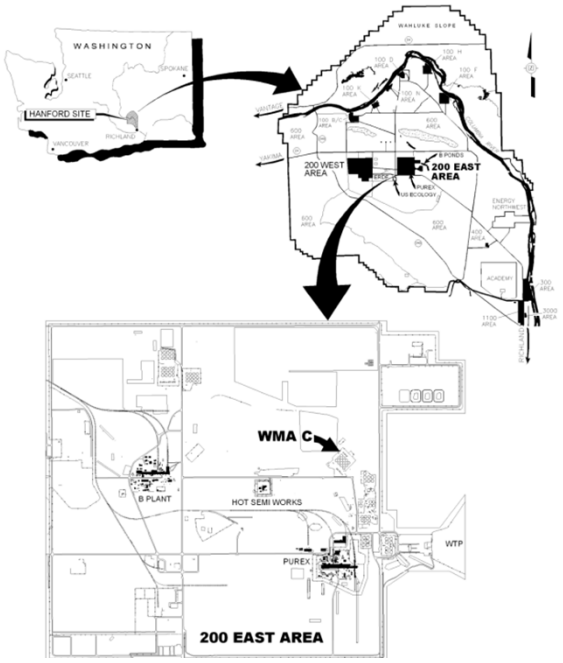


Site Applications Thrust

- Guide software development
- Assist with testing and QA
- Provide site data for model testing and validation
- Conduct demonstrations of Platform and HPC capabilities
- **Facilitate ASCEM deployments, for example,**
  - Hanford Waste Management Area (WMA) C
  - Savannah River H-Area Tank Farm (HTF)
  - Collaboration with Cementitious Barriers Partnership (CBP)
  - Savannah River F-Area Seepage Basins Plume

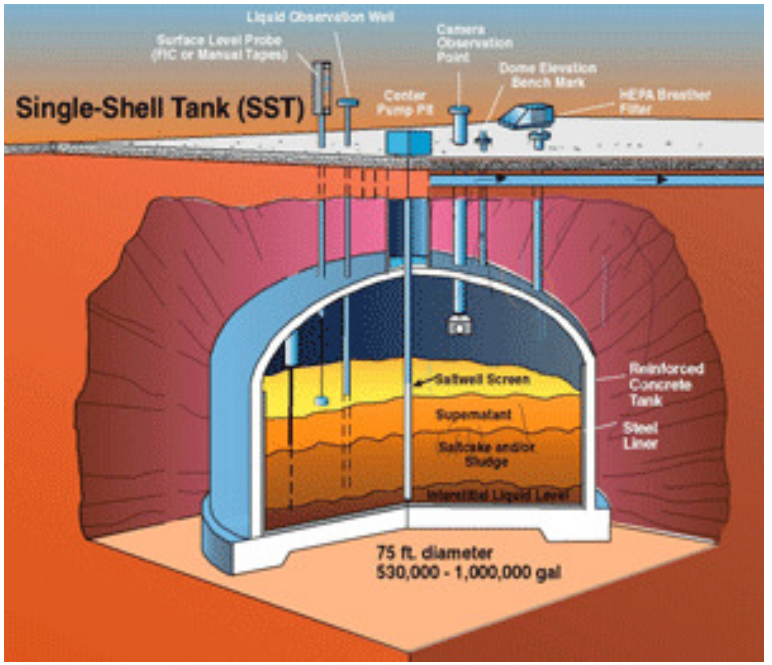
Waste Management Area C (WMA C)

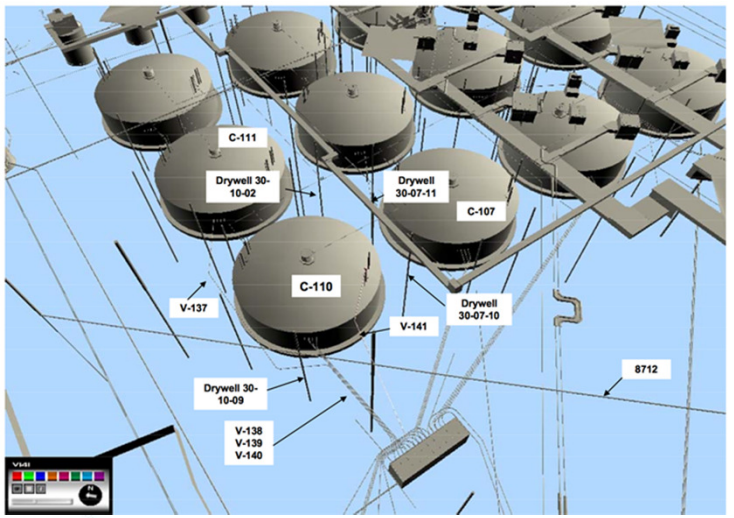
- WMA C is located in the 200 East Area of the Hanford Central Plateau
- Tank farm consists of
  - 16 tanks
  - Waste transfer pipelines
  - Tank ancillary equipment (e.g. diversion boxes, valve boxes)
- Tanks in WMA C have stored high-level waste from defense-related nuclear research, development, and weapons production since the late 1940s
- Multiple unplanned releases have occurred



Modeling WMA C Closure

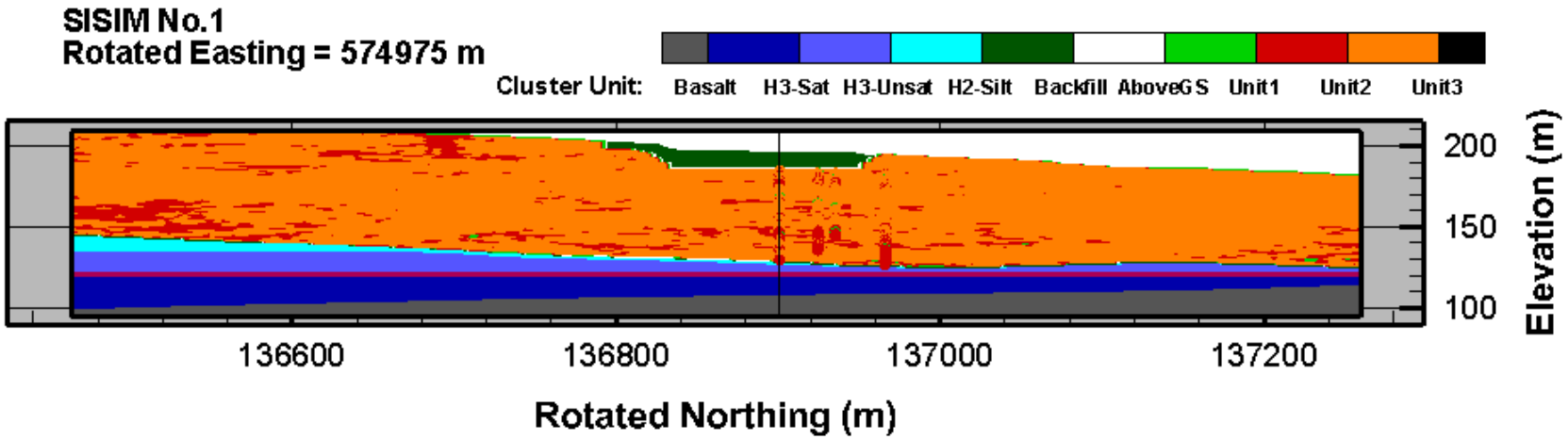
- Preparations for final closure of WMA C is underway
  - Closure follows retrieval of as much tank waste that is technically and economically practical
  - Tanks will be backfilled with grout
  - Will be closed on site as a landfill
- The WMA C Performance Assessment will be used to evaluate risks from landfill closure (i.e., waste left in place at WMA-C)
  - To obtain a ROD, risks from wastes left in place need to be assessed





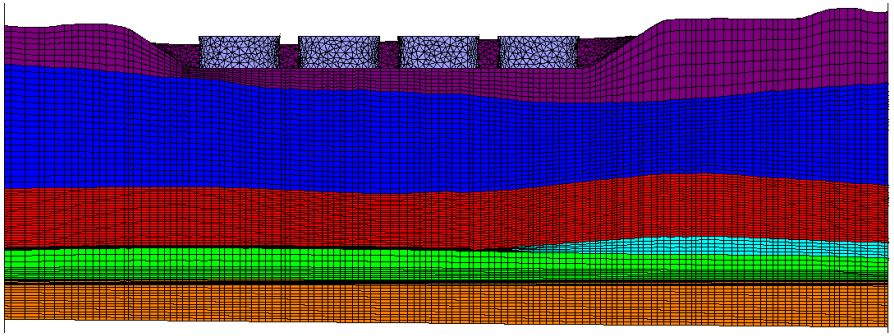
WMA C Applications

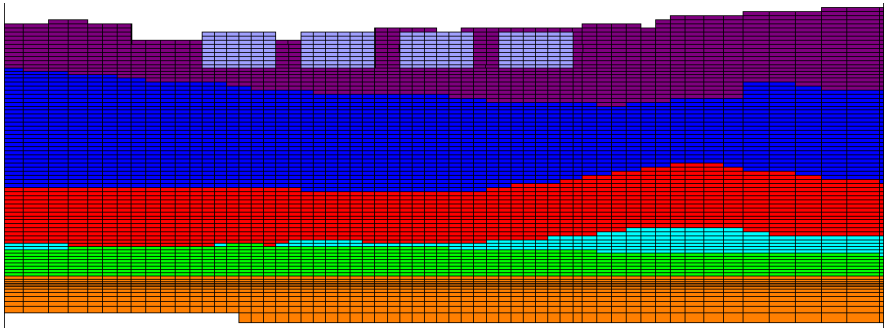
- **ASCEM investigating impacts of**
  - Small-scale heterogeneities on flow and transport under closure and past leak conditions
  - Generate multiple realizations of lithofacies distribution using indicator simulation methods
    - Each realization honors borehole data, then reproduces spatial model of lithofacies continuity between boreholes
    - Incorporates heterogeneity of lithofacies, rather than treating stratigraphic units as homogeneous layers



WMA C Applications

- **ASCEM investigating impacts of**
  - Use of orthogonal grids in representing the geologic conceptual model





SRS Submerged Waste Tank Concern

- **Several SRS waste tanks are fully or partially submerged below water table aquifer**
- **Closure requires isolation from subsurface flow**. A low-permeability cover will not isolate these tanks from subsurface flow, unlike tanks above the water table
- **The NRC has expressed the following concern:**
  The HTF Performance Assessment does not adequately assess waste release from the submerged and partially submerged tanks via a preferential pathway
  (NRC Staff Request for Additional Information 31 July 2013)

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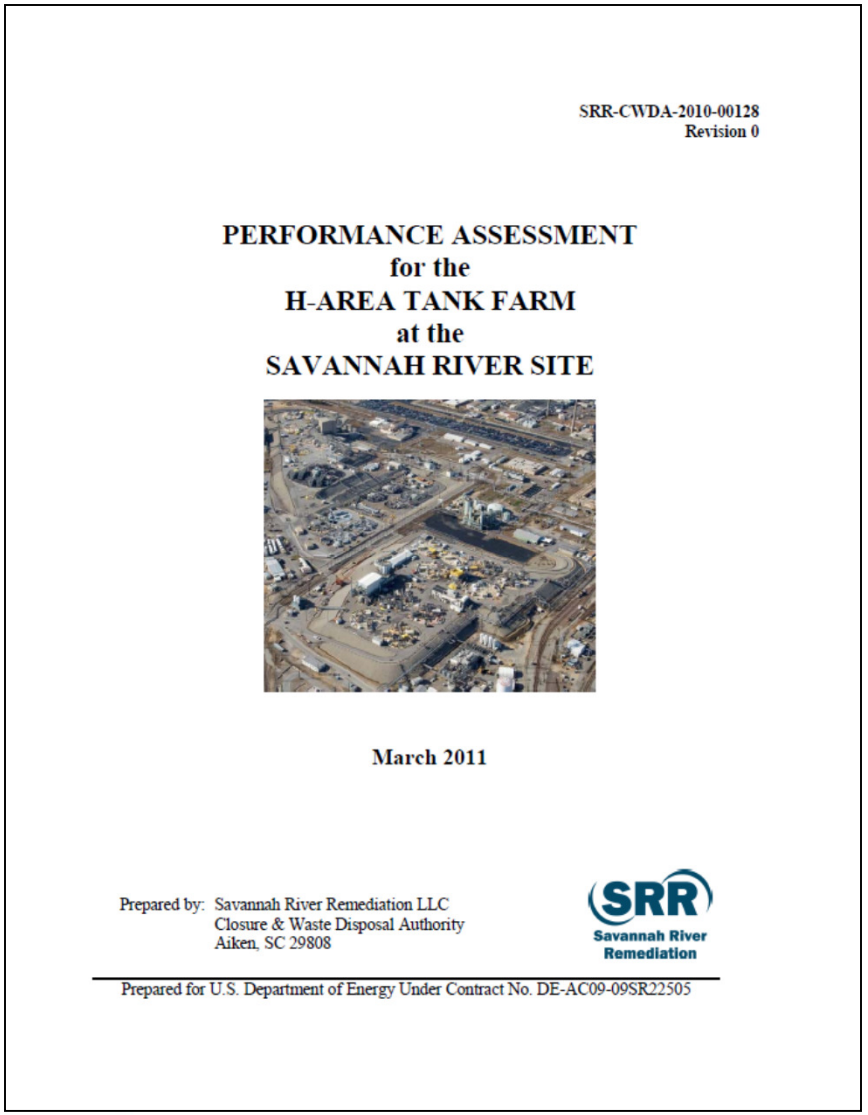
ASCEM Support for SRS H-Tank Farm Performance Assessment (PA)

- **Current base case modeling approach**
  - Two-dimensional axi-symmetric simulation models
  - Approach suited to tanks in the unsaturated zone
  - Grid sizes are limited to 10,000s nodes to achieve reasonable computational times
- **Challenge for Submerged Tanks**
  - Three-dimensional geometry required because of lateral flow
  - Thin features (e.g. preferential pathway) require fine-scale mesh resolution
  - Millions of nodes required
  - Not feasible with current approach
- **ASCEM deployed to addresses challenges**



SRR-CWDA-2010-00128
Revision 0

PERFORMANCE ASSESSMENT
for the
H-AREA TANK FARM
at the
SAVANNAH RIVER SITE

March 2011

Prepared by: Savannah River Remediation LLC
Closure & Waste Disposal Authority
Aiken, SC 29808

SRR Savannah River Remediation

Prepared for U.S. Department of Energy Under Contract No. DE-AC09-09SR22505

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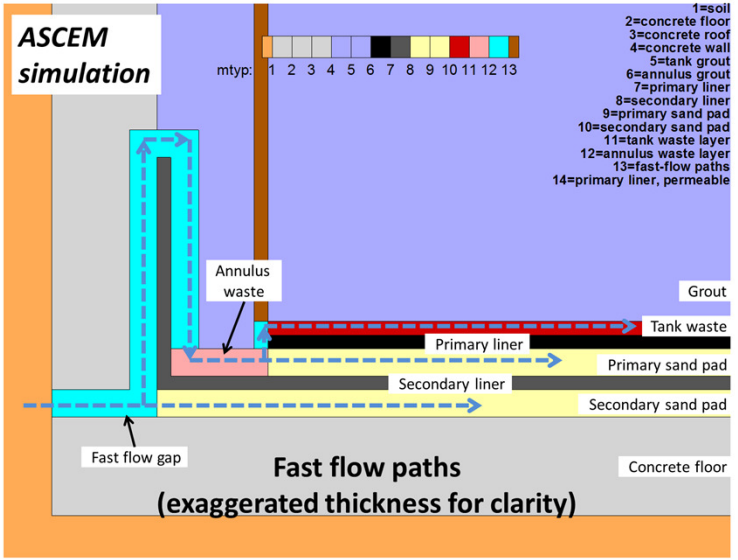
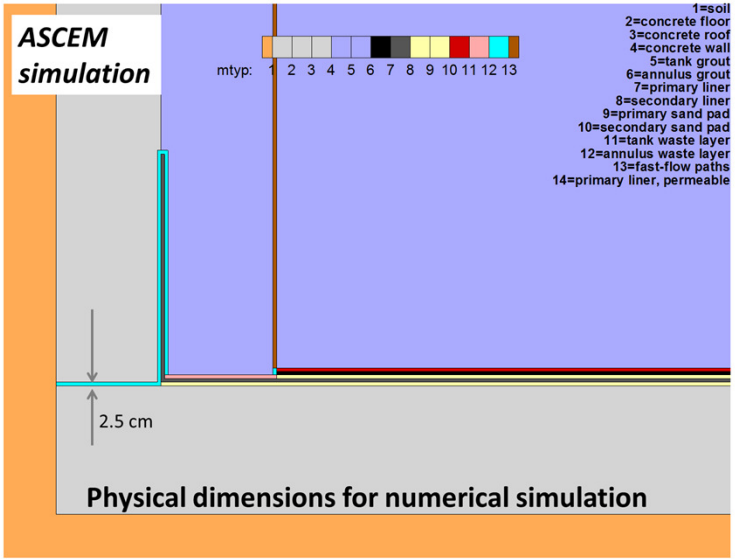
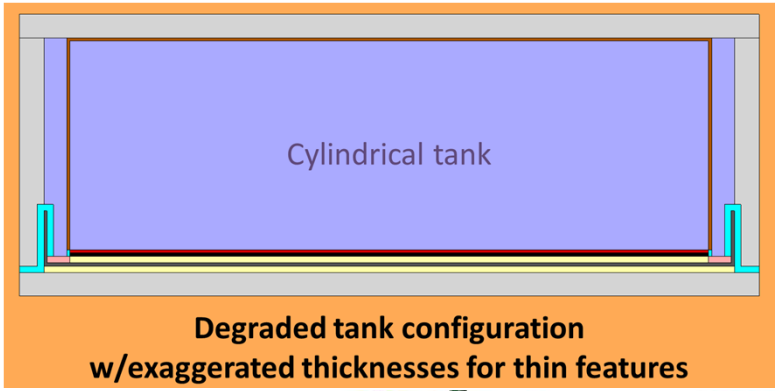
ASCEM Deployment

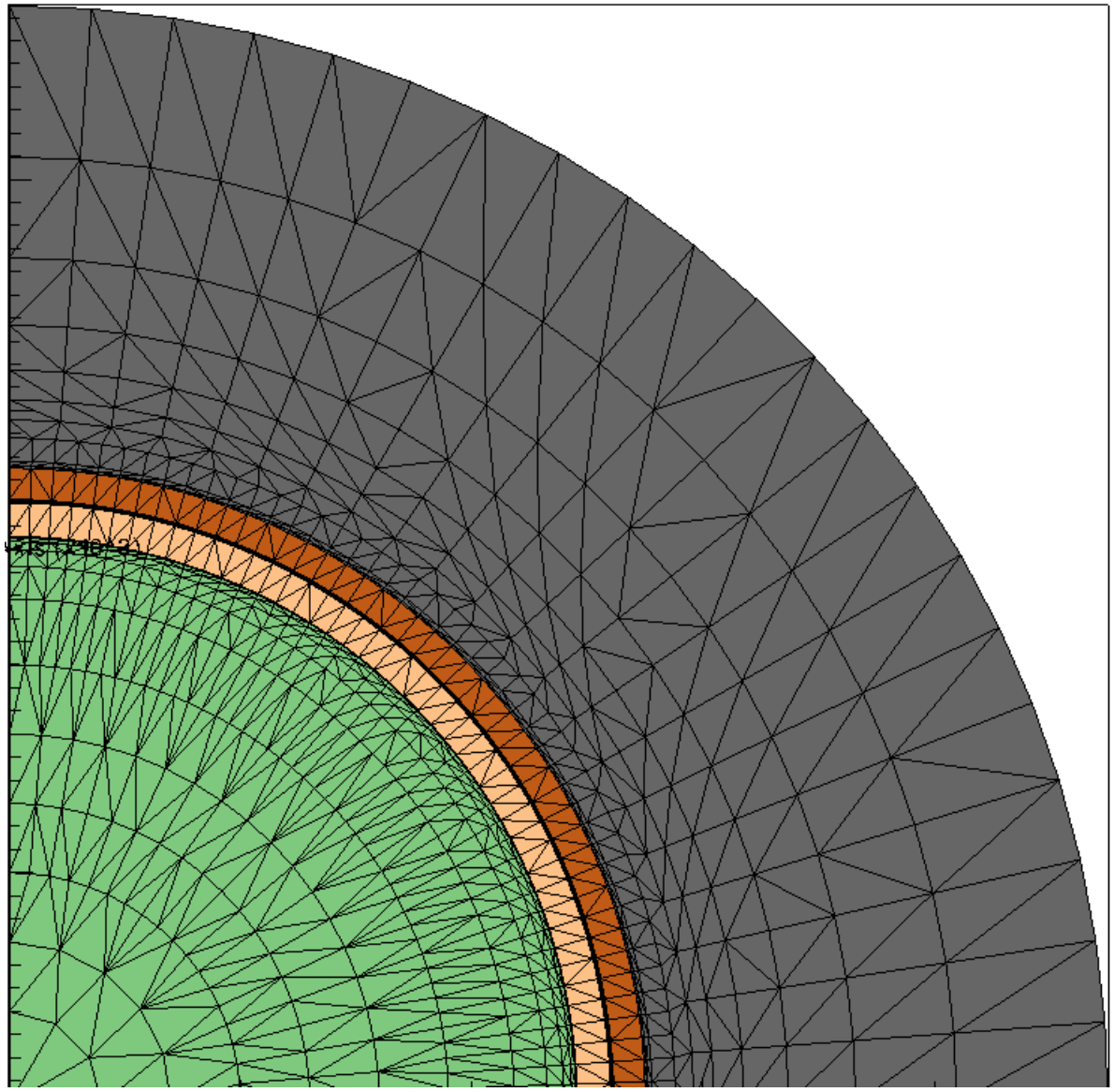
- **ASCEM Deployment**
  - Use HPC software and hardware to achieve feasible computational runtimes
- **FY14 ASCEM Deployment**
  - Collaboration with PA Contractor to define scenario of interest to address NRC concern
  - 3D mesh with local resolution of steel liners and fast-flow pathways
  - Scale up of problem to millions of nodes with Adaptive Mesh Refinement







Unstructured Grid Capability



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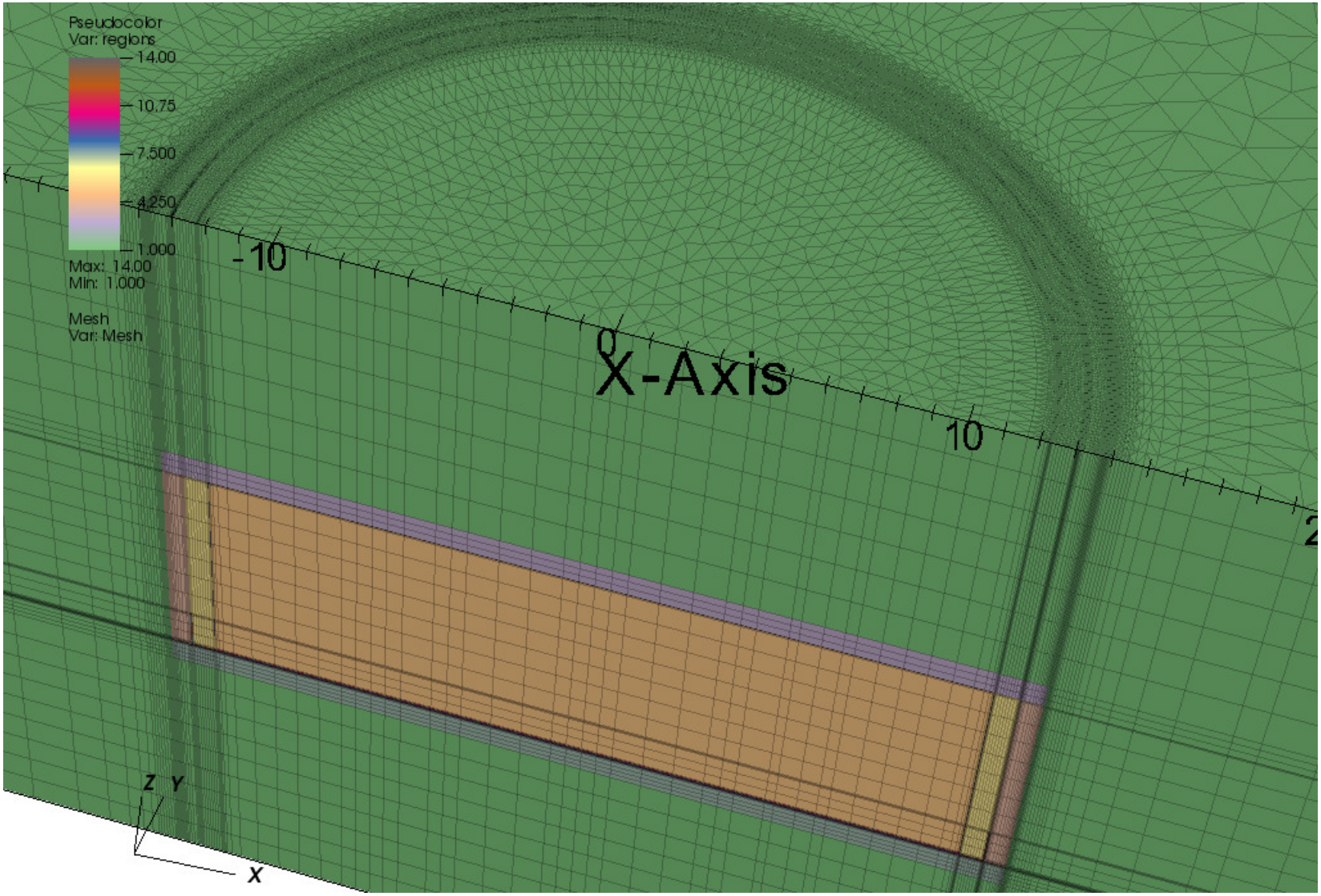
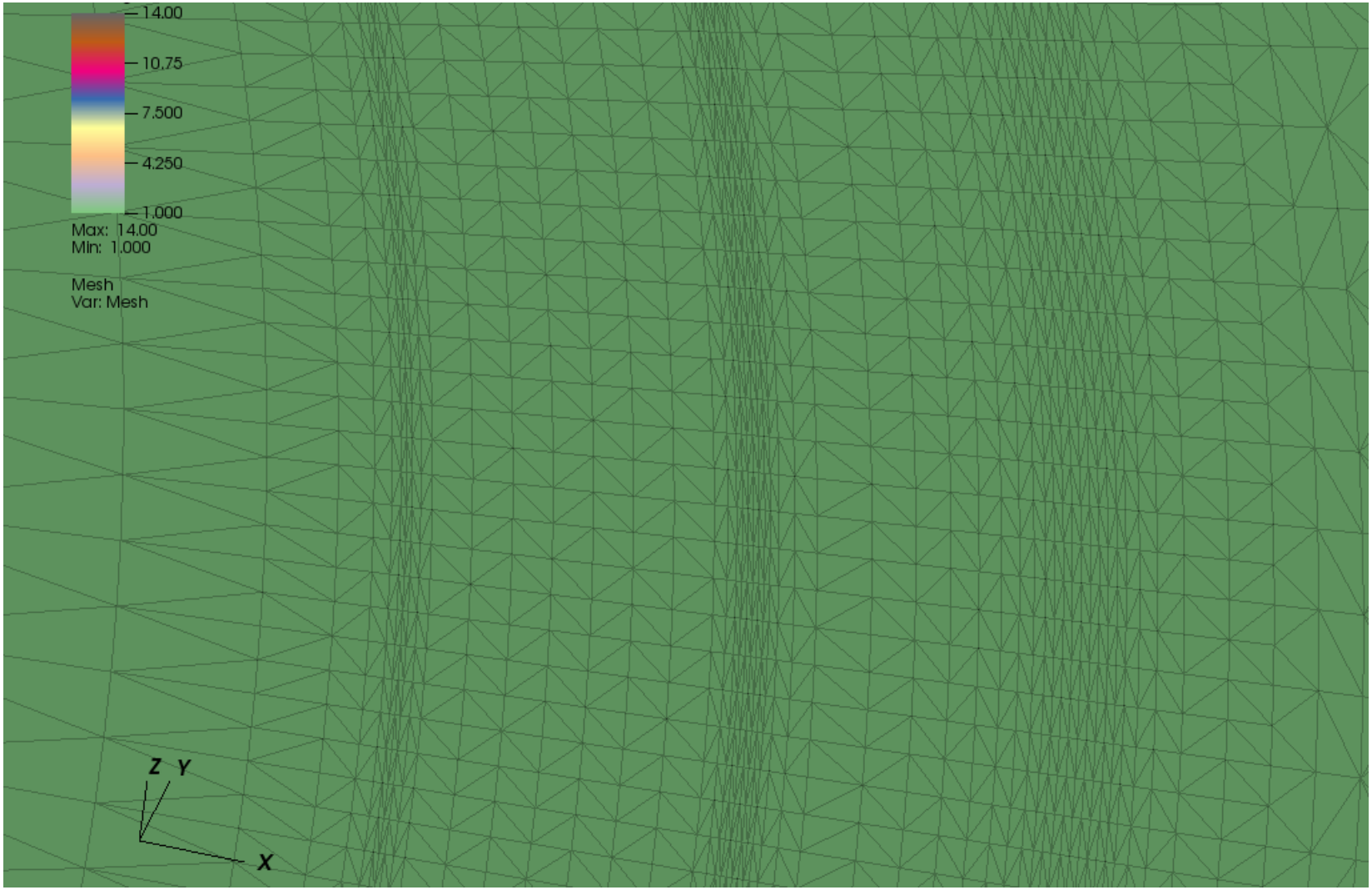
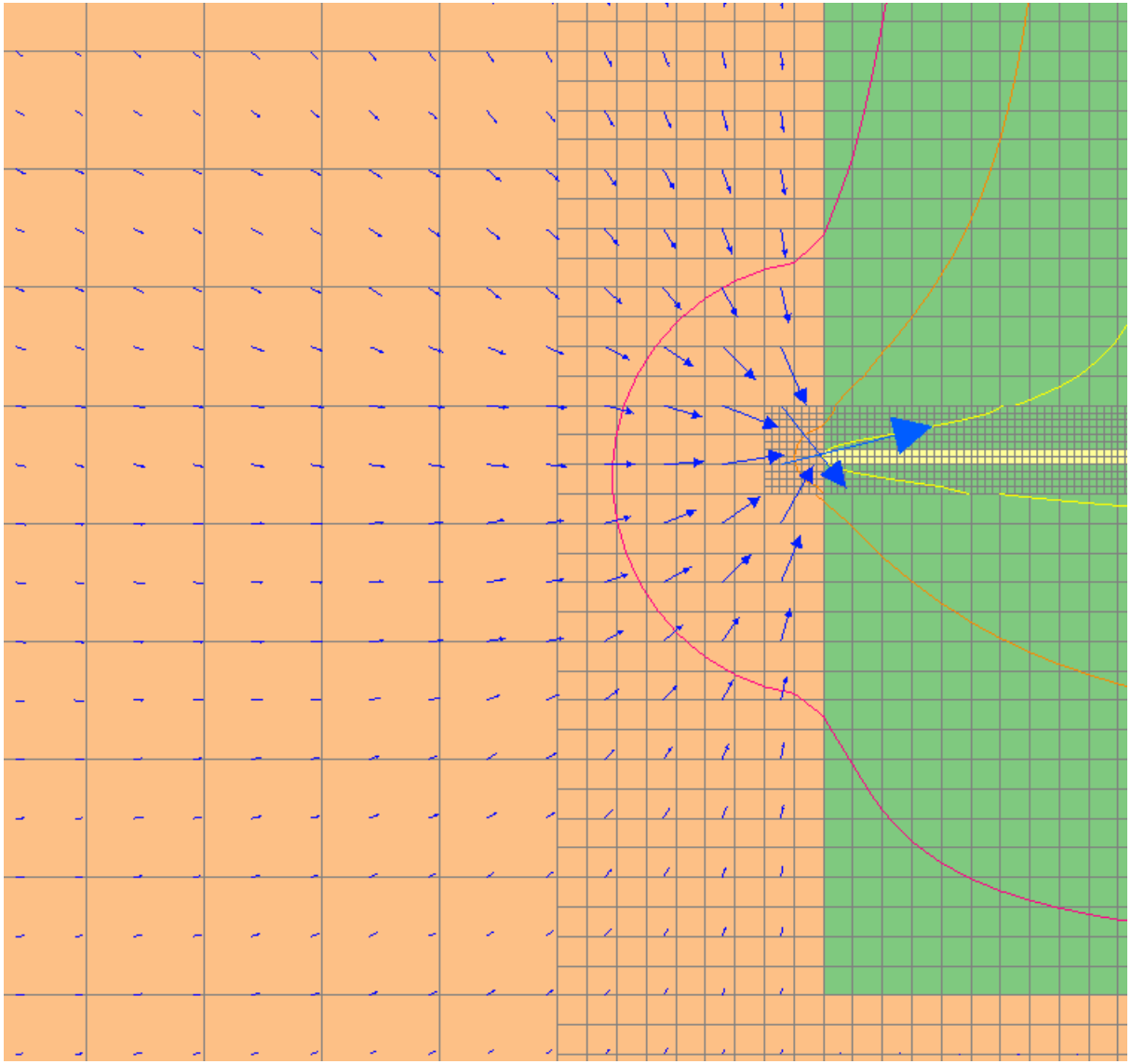


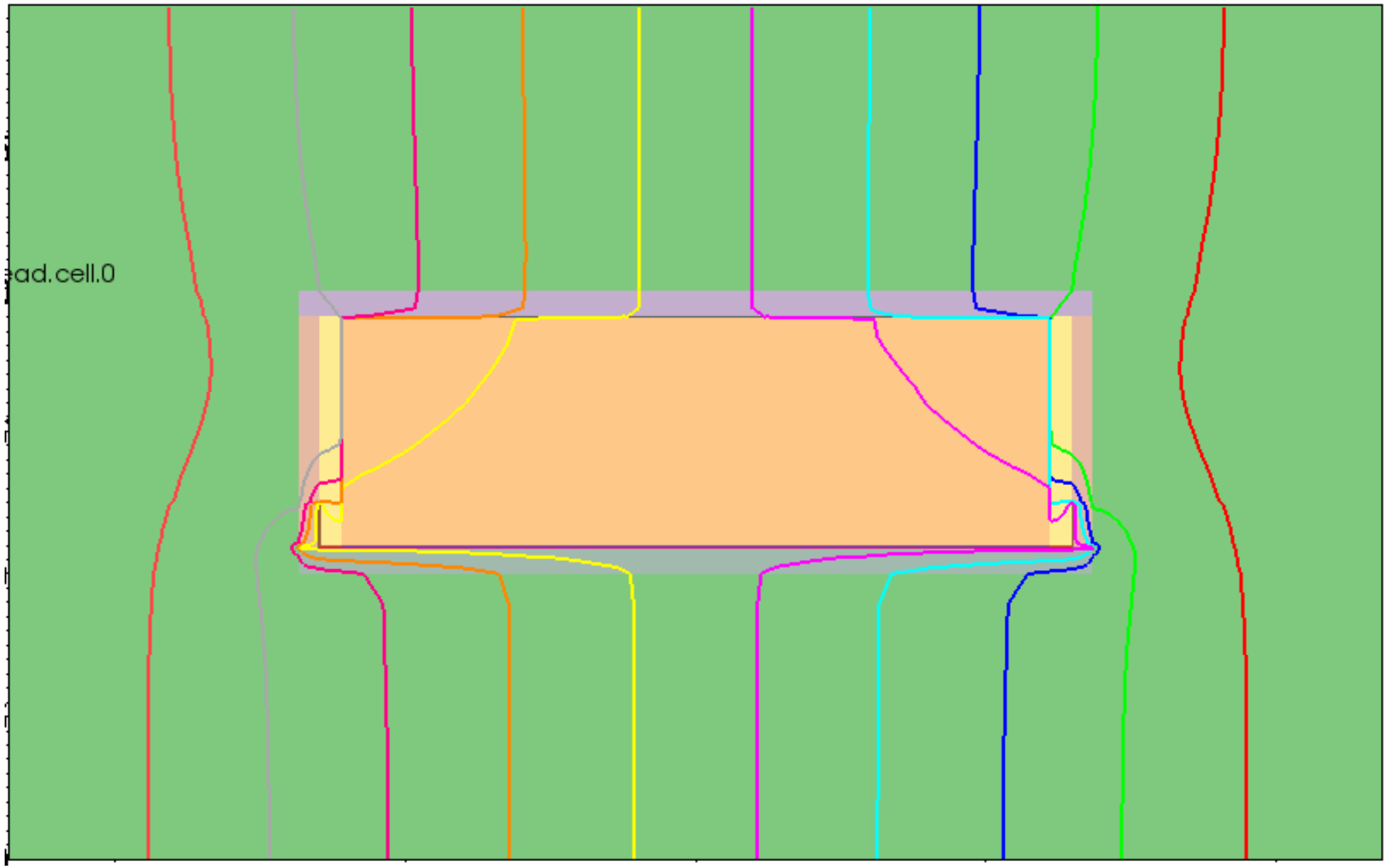
Unstructured Grid Capability



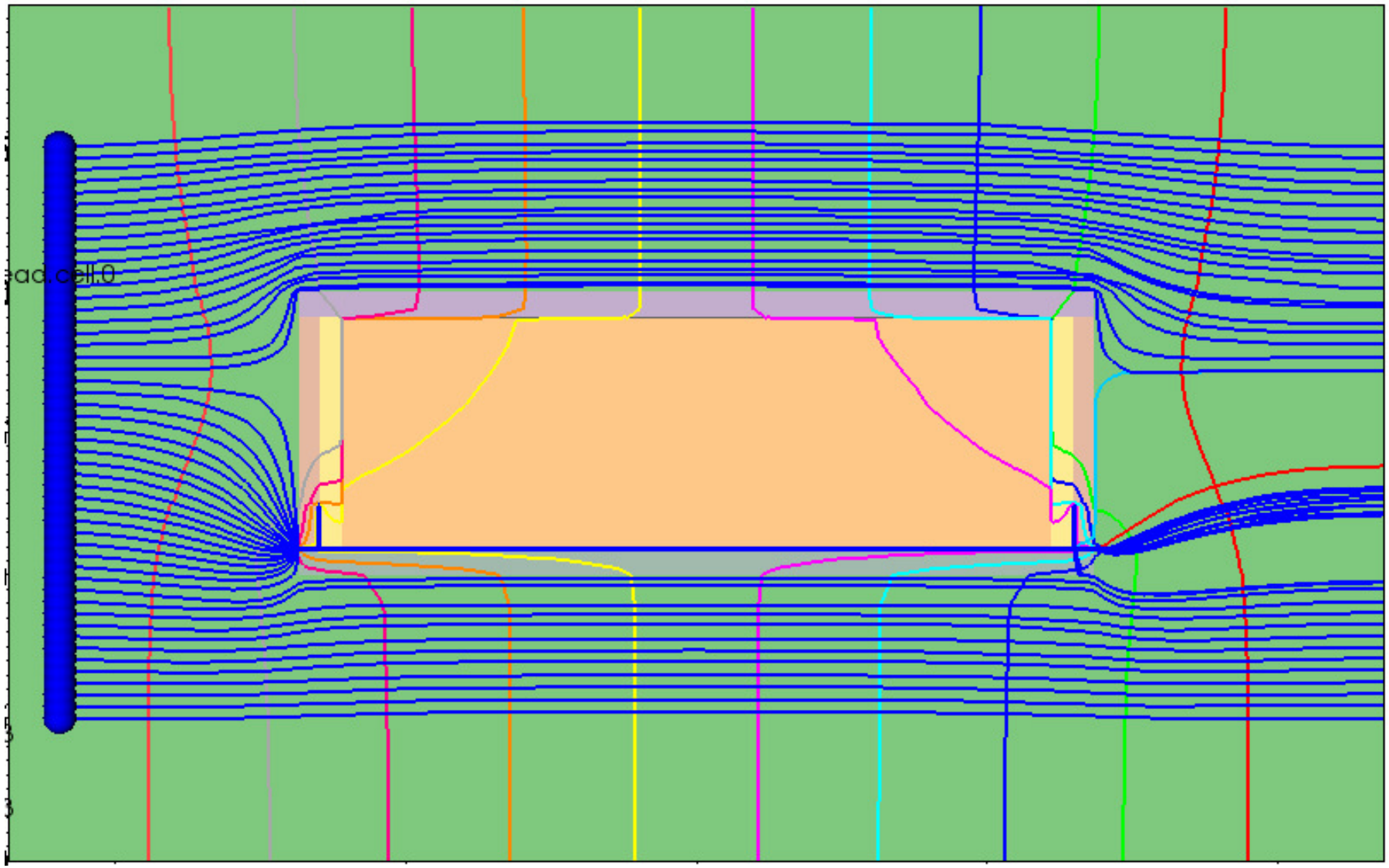
Structured Grid AMR Capability



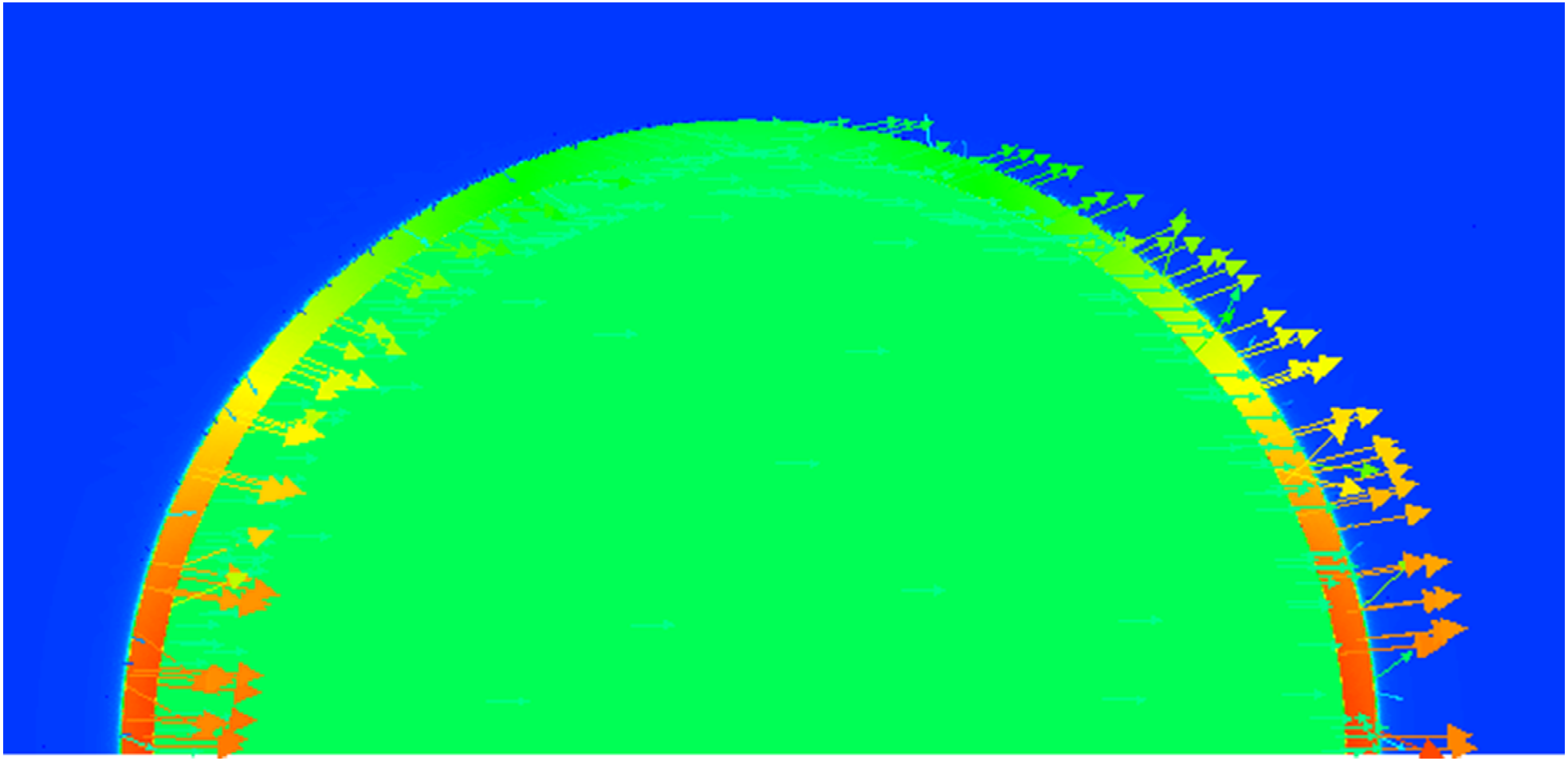
Hydraulic Head Simulation



Streamtraces



Velocity Field



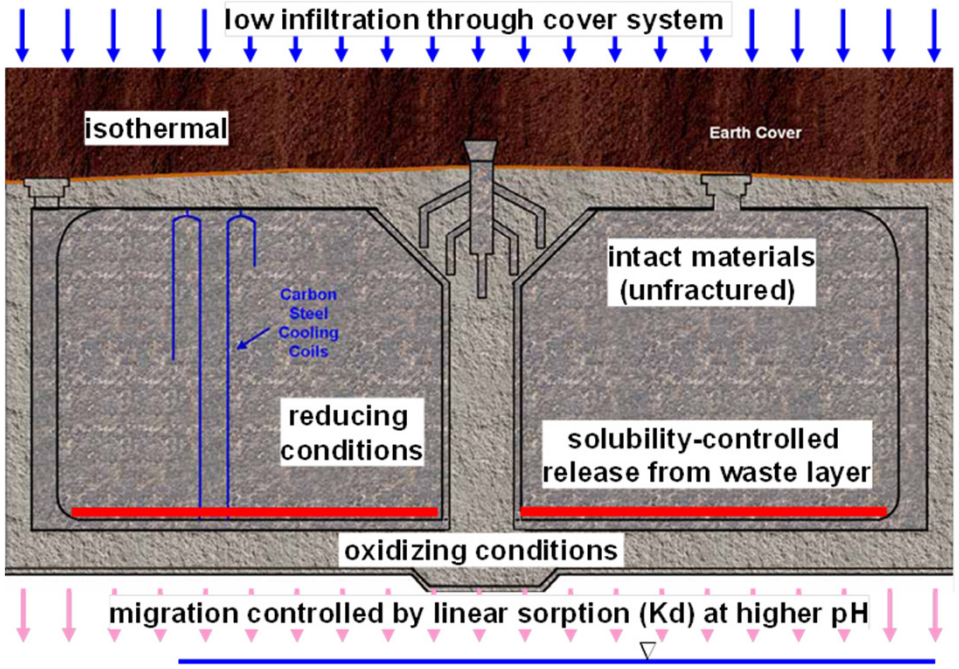
Anticipated Next Steps

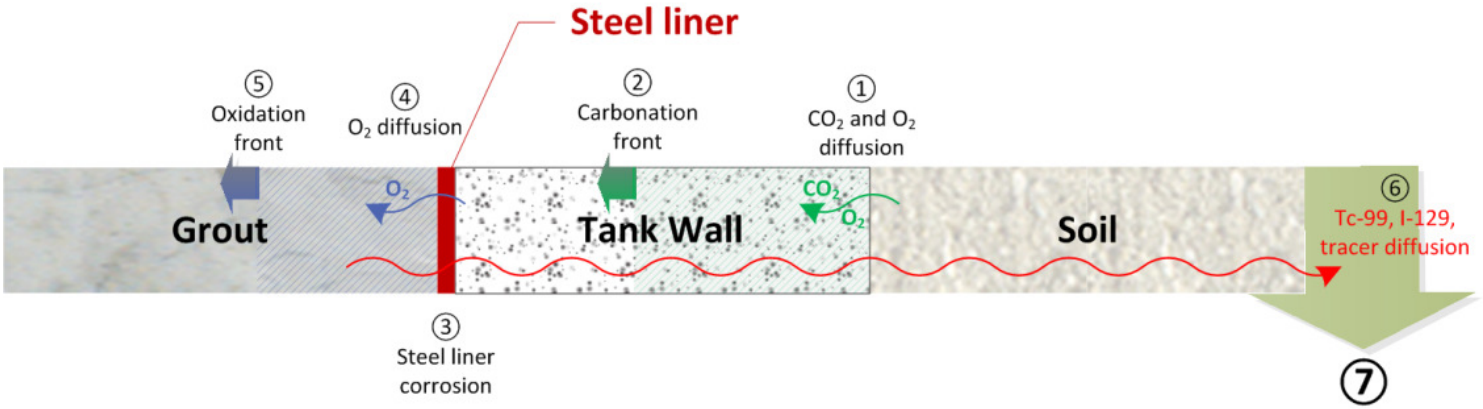
- **Transport simulations for Sr-90 and Cs-137**

- **Scenario refinements**
  - More realistic fast-flow path configurations
  - Patch corrosion of steel liners
  - Time-dependent material degradation

Waste Tank Performance Assessment Working Group
Joint ASCEM-CBP Demonstration

- Collaborate with DOE-EM Cementitious Barriers Partnership (CBP) for interface of processes within a cement barrier
- Use ASCEM HPC processes outside the cement barrier





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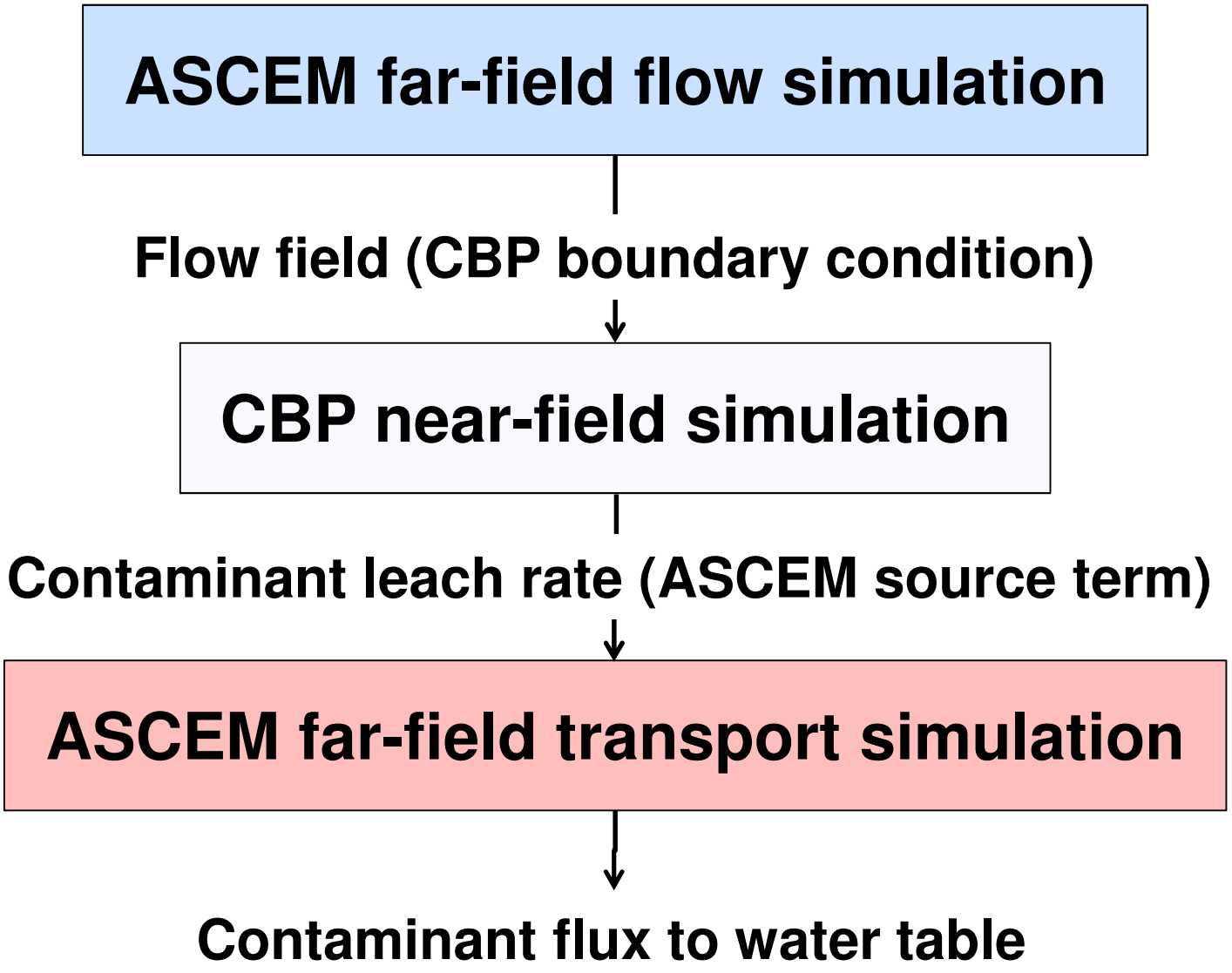
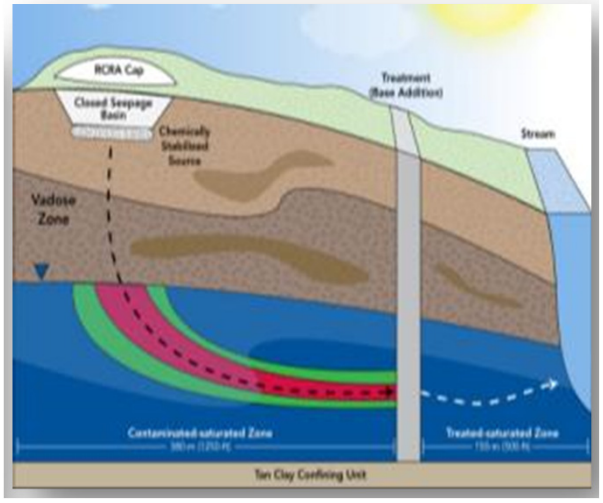
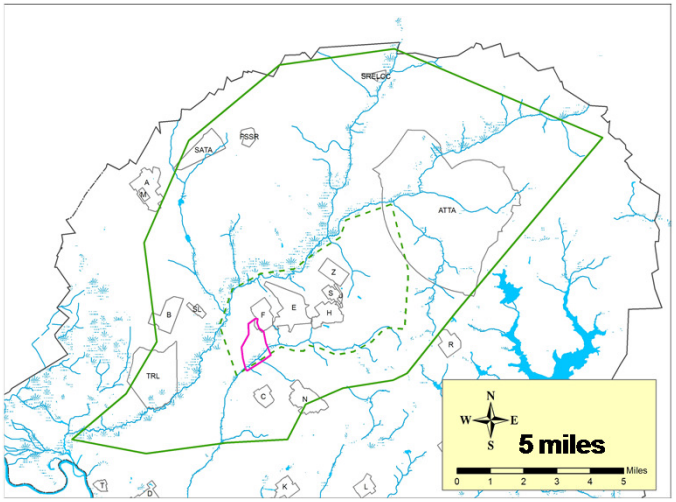
Interfaces (Information handoffs)



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.





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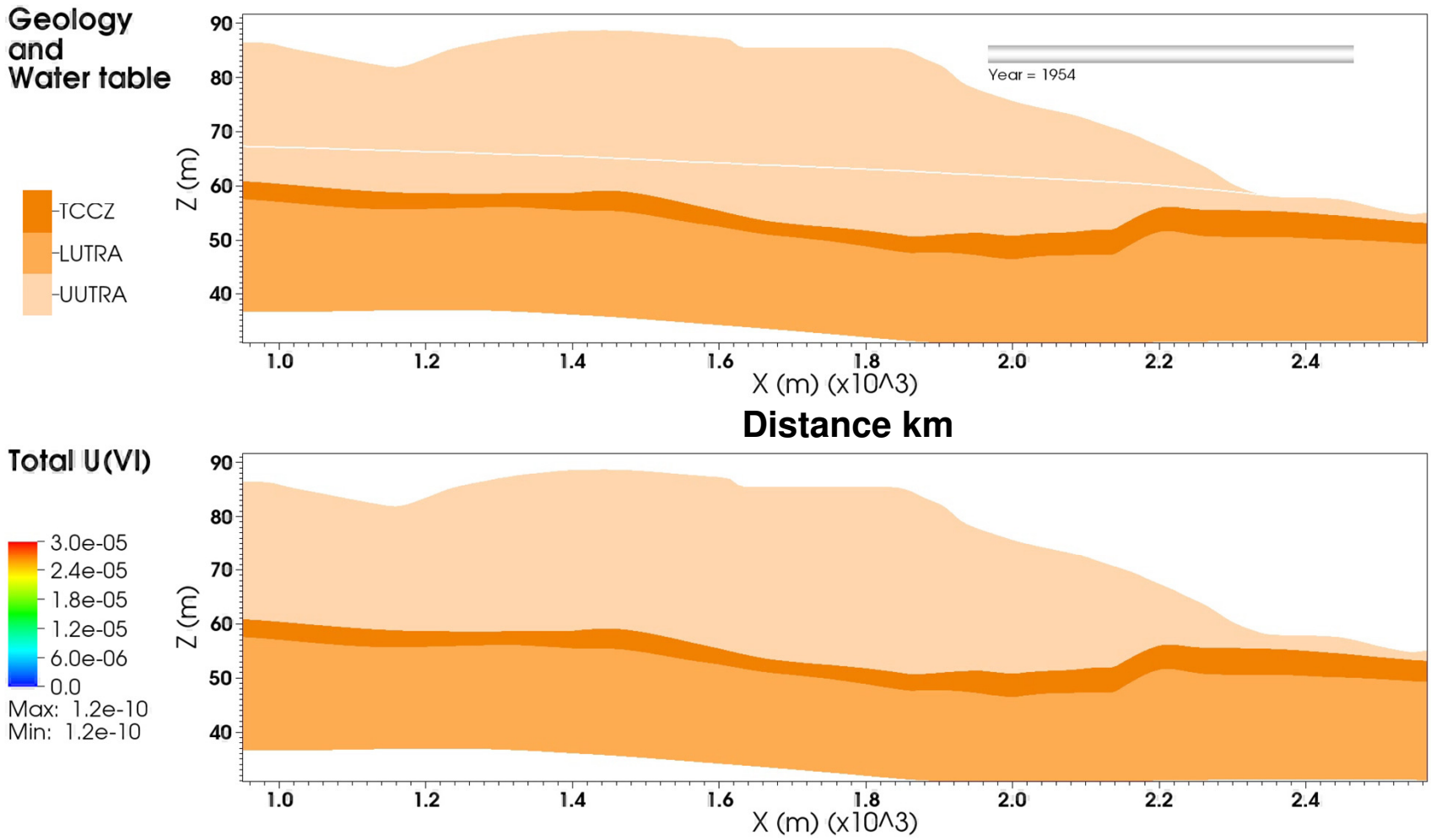
Visualization Communicates the Results of F-Area Uranium Reactive Transport



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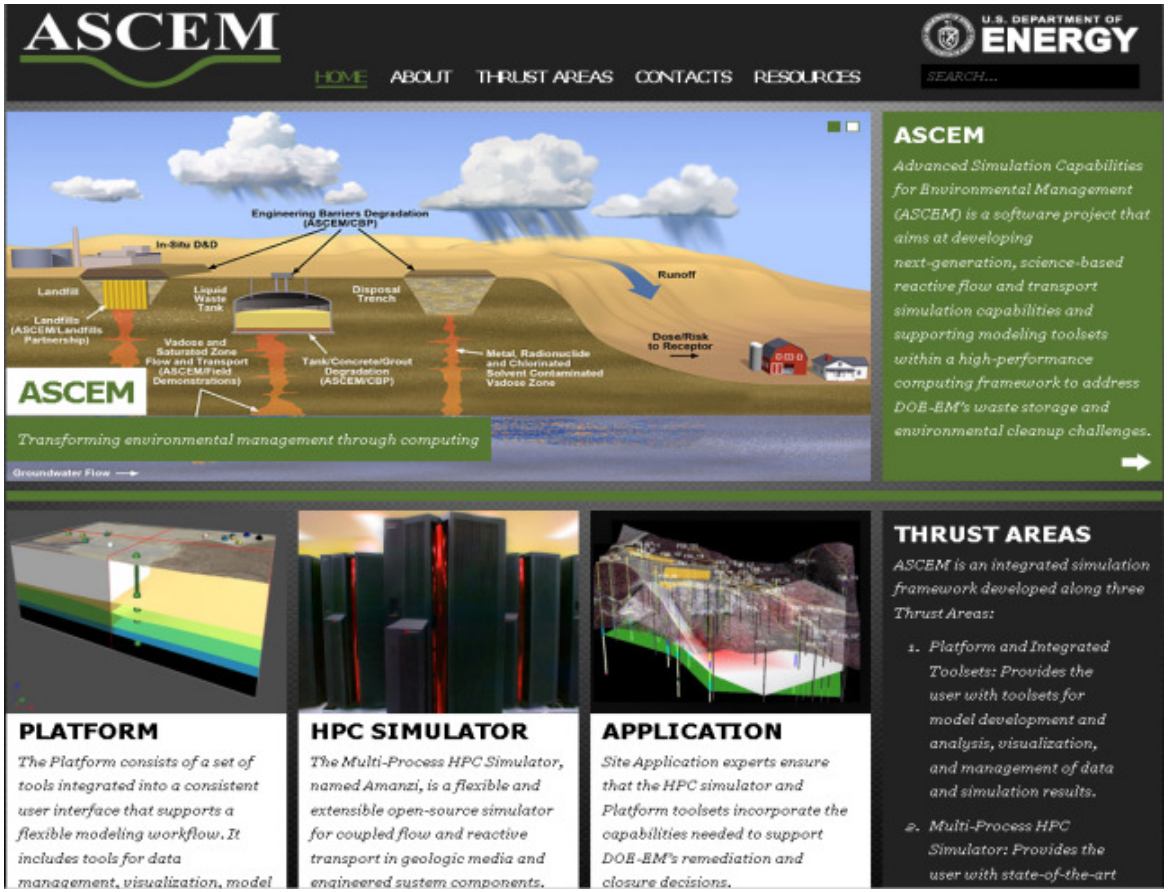
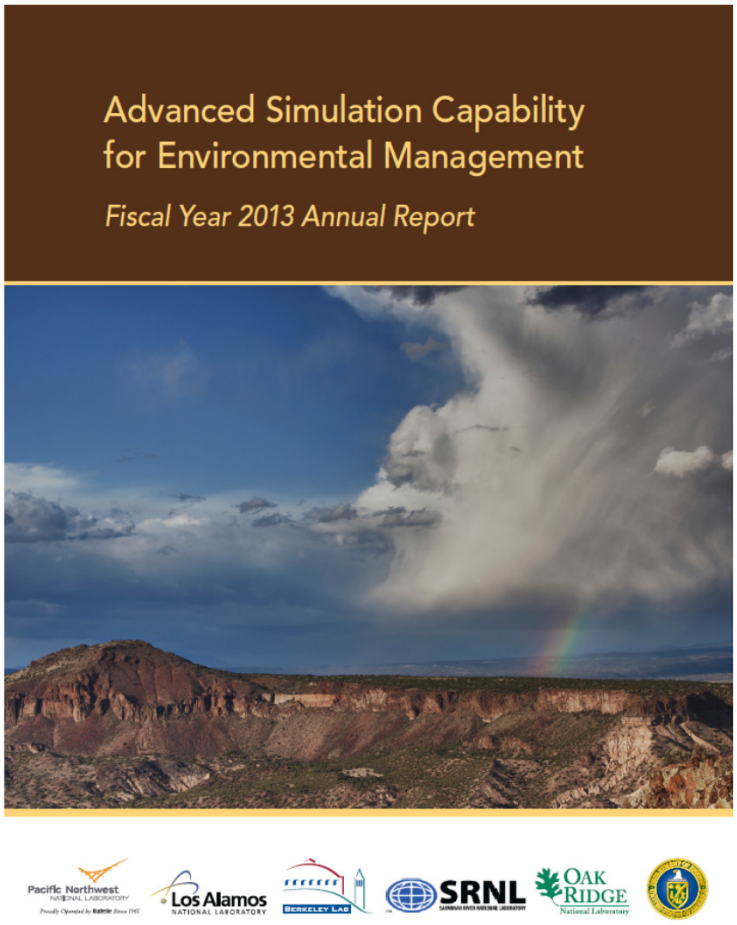
Summary

- ASCEM represents the next-generation **agile, open source, and modular computing framework** 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
  - Multiple simulation launching capability for UQ, SA, PE
- **ASCEM capabilities are being deployed** to support DOE-EM Performance Assessments
- ASCEM v2.0 **Community Code release anticipated in 2015**

Questions?





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