ASCEM: Advanced Simulation Capability for Environmental Management

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Presentation to the PA Community of Practice
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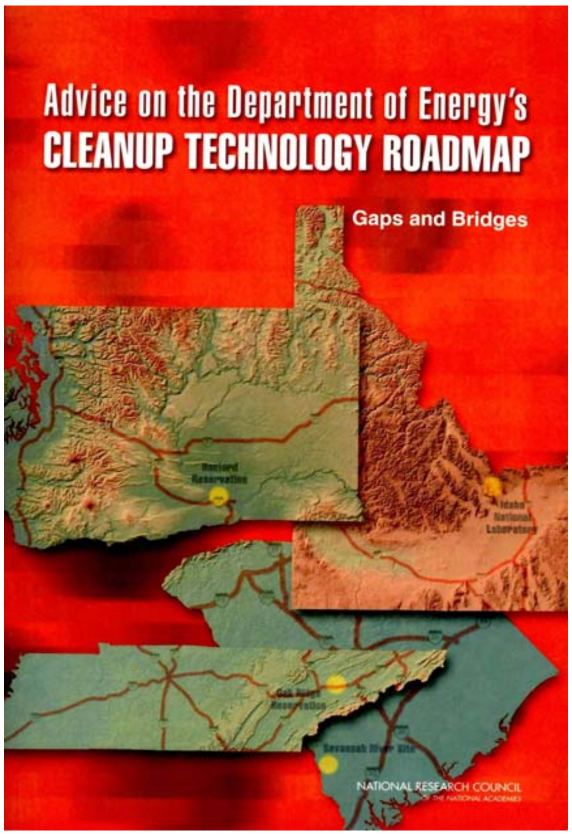
Needs Identified in Workshops & Reviews

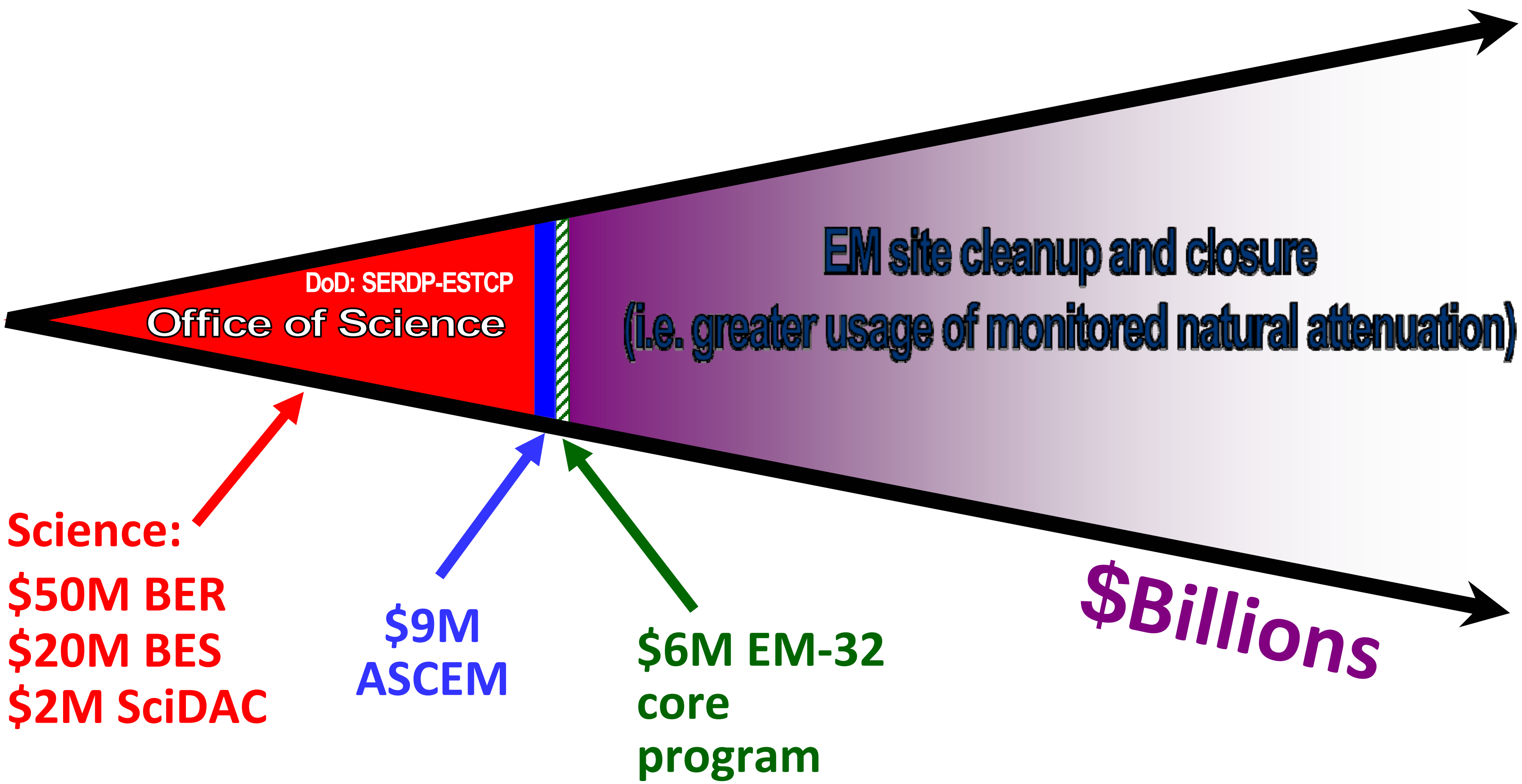


National Academies' Advice on DOE EM Roadmap:

- **GS-1: Subsurface contaminant behavior poorly understood (High Priority)**
- GS-2: Site and contaminant source characteristics may limit the usefulness of EM's baseline subsurface remediation technologies (Medium Priority)
- **GS-3: Long-term trench cap, liner, and reactive barrier performance not currently assessable (Medium Priority)**
- **GS-4: Long-term ability of cementitious materials to isolate wastes not demonstrated (High Priority)**

Scientific Opportunities to Reduce Remediation Risk:

Translating Fundamental Science into Applied Solutions

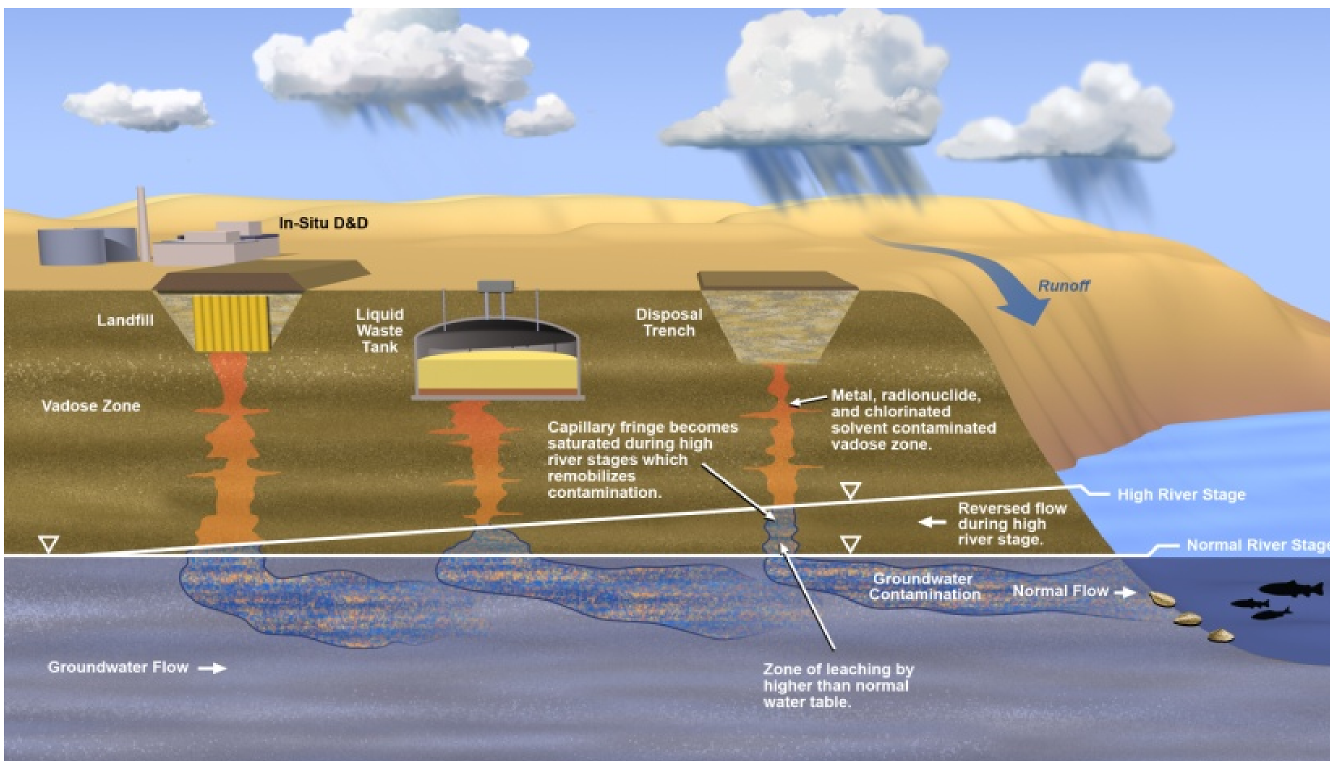


What is ASCEM?

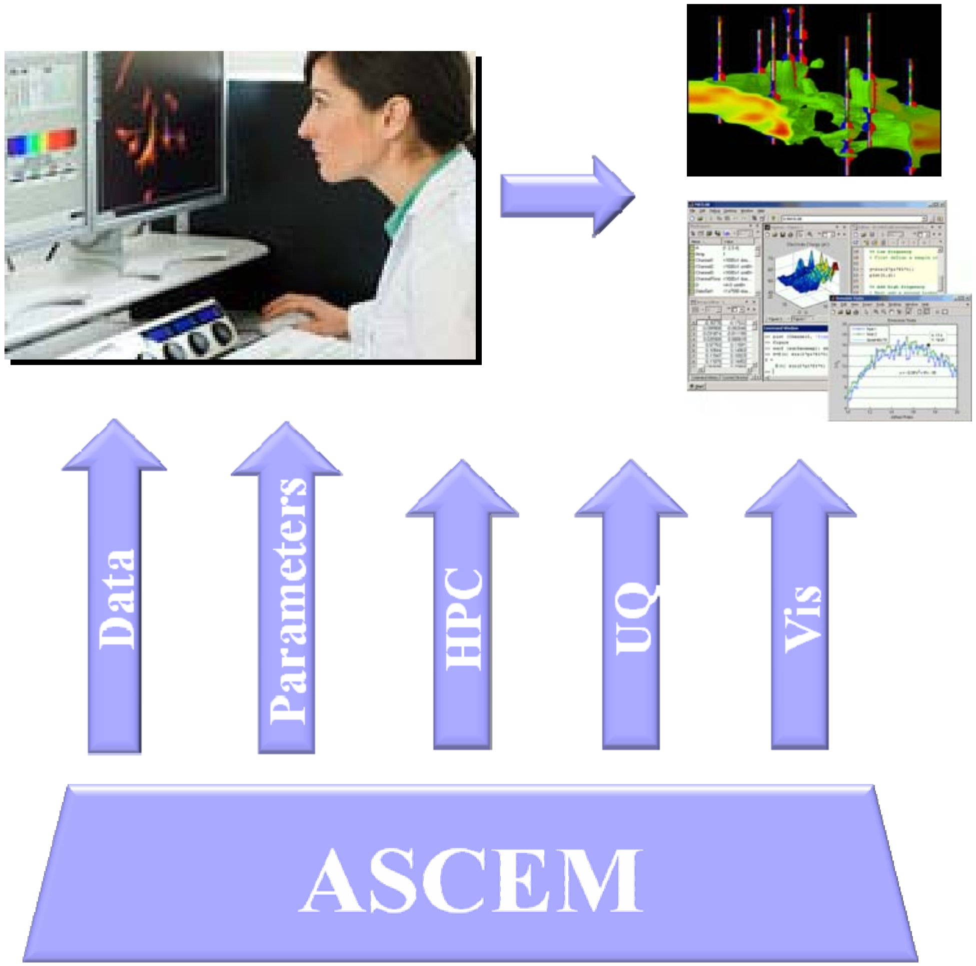
"ASCEM is a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. The modular and open source high performance computing tool will facilitate integrated approaches to modeling and site characterization that enable robust and standardized assessments of performance and risk for EM cleanup and closure activities. "

What Does ASCEM Do?

- Provide the technical underpinnings for DOE EM cleanup decision by implementing the next generation performance and risk assessment tools for DOE EM
- Leverages recent advances in high performance computing technologies
- Collaborates with NNSA (ASCI), ASCR (SciDAC), CBP and OBER (SBR)

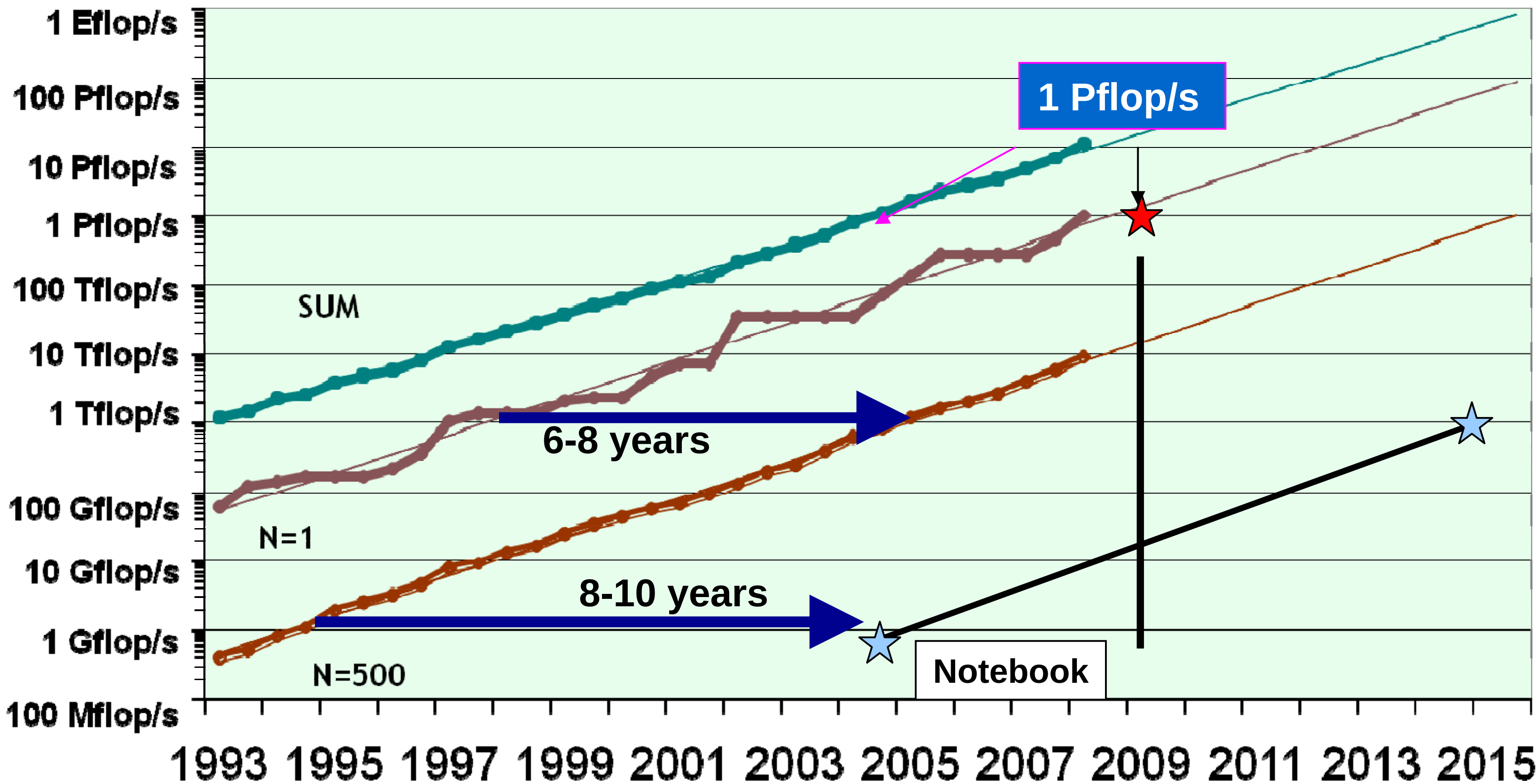


Technical Underpinnings



- Graded, iterative and modular toolsets to accurately represent complex EM sites based on user community input
- Formal uncertainty quantification and decision support analysis in a standardized framework
- Portable from laptops to supercomputers

Performance Projection



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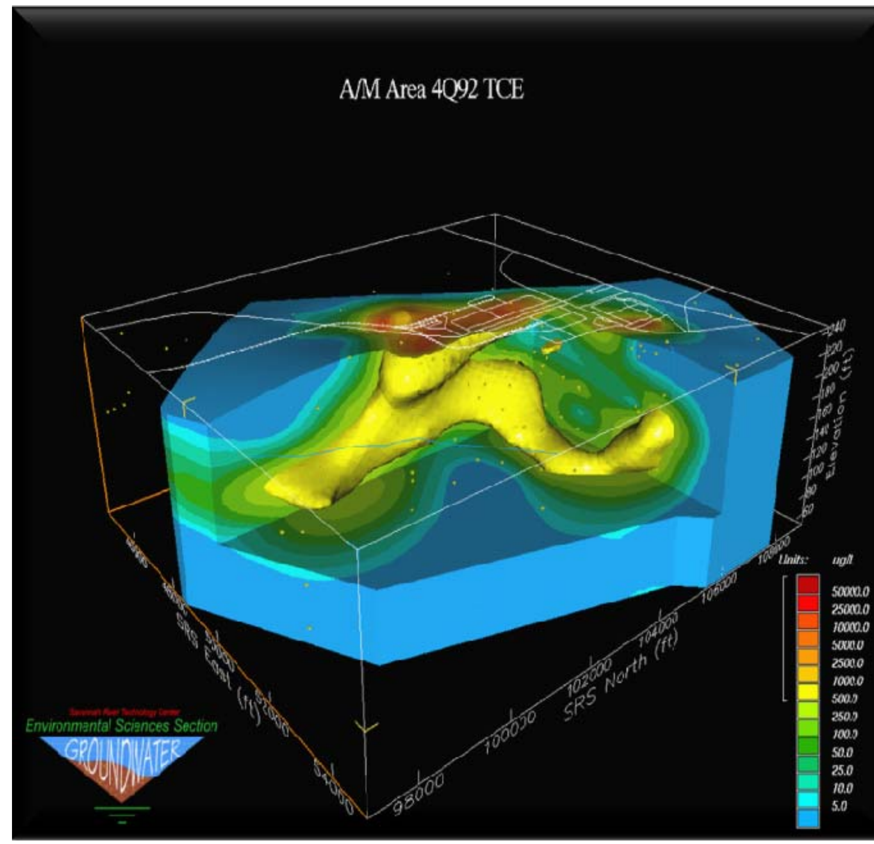
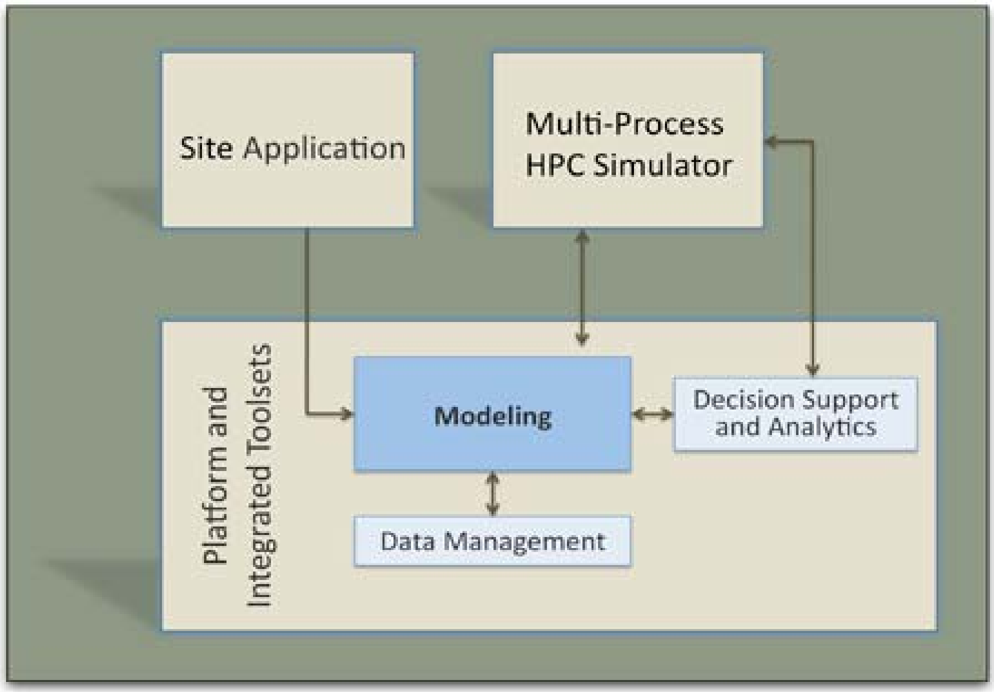
ASCEM Project Goals

- Provide DOE EM with transformational and enduring next-generation Risk and PA models
- Integrate scientific data and understanding with modeling and decision-making to reduce programmatic risk
- Exploit advances in computational methods and computing resources
- Reduce “conservative assumptions” and “abstractions” in current modeling approaches
- Improve consistency of PA methods and applications across the EM complex
- Recognize and support the maintenance of existing simplified Risk/PA models

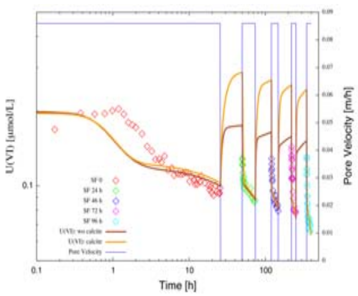


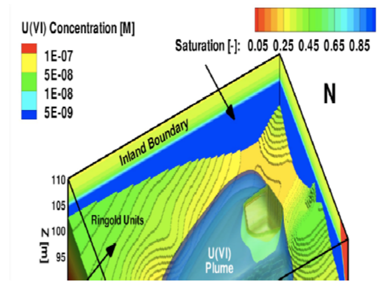
ASCEM Overall Structure



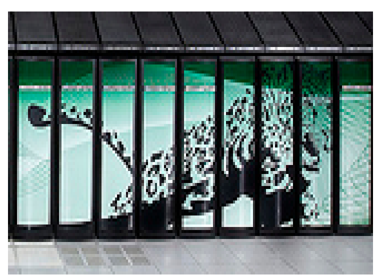
- **Multi-Process High Performance Computing Simulator**
  - Modular simulation capability for barrier and waste form degradation, multiphase flow and reactive transport
- **Platform and Integrated Toolsets**
  - Facilitate model development and execution, parameter estimation, uncertainty quantification, decision support, risk analysis
- **Site Applications**
  - Demonstration sites
  - Actively engage site user community to develop and test ASCEM tools

Multi-Process HPC Simulator





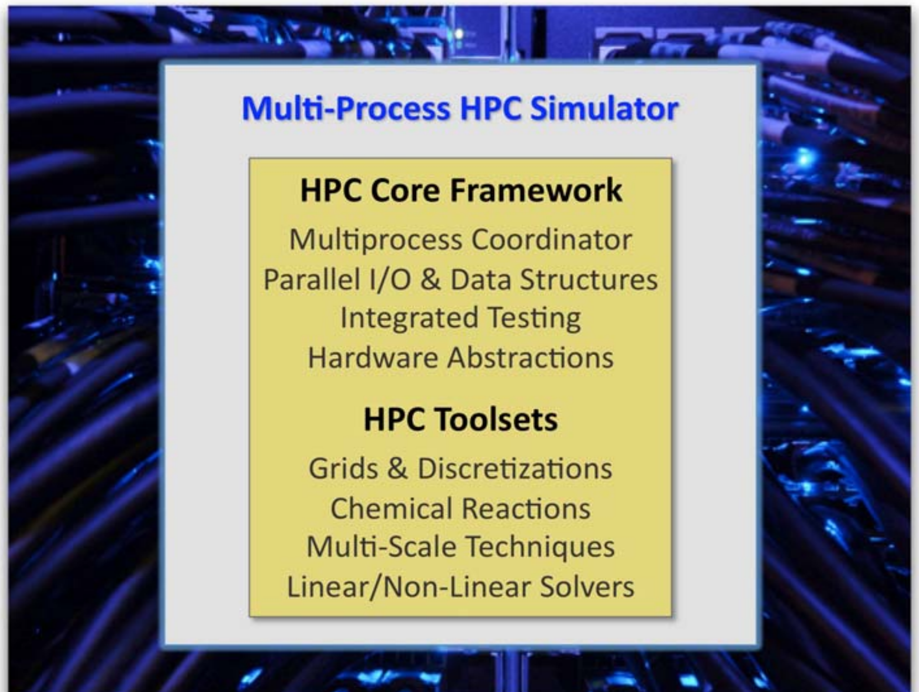
Wide Range of Complexity



Wide Range of Platforms

- Modular HPC simulation capability for waste form and engineered barrier degradation ,multiphase flow and reactive transport
- Efficient, robust simulation from supercomputers to laptops
- Design and build for emerging multi-core and accelerator-based systems
- Open-source project with strong community engagement

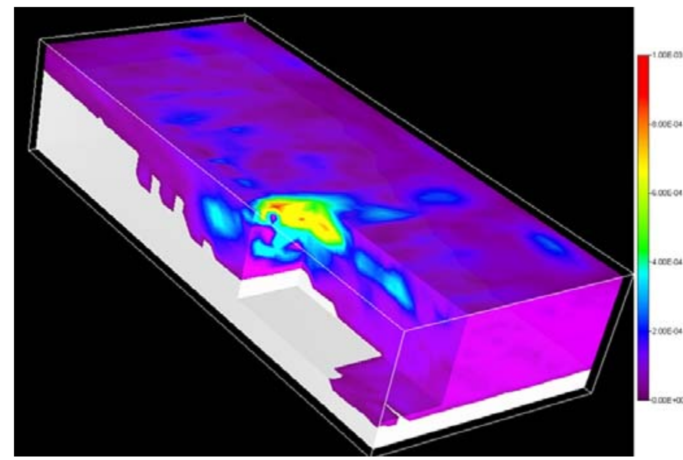
Multi-Process HPC Simulator



- ***Process models:*** Provide the mathematical description of the processes that play a role in the release and transport of contaminants in the environment.
- ***HPC Core Framework:*** Provide key infrastructure to facilitate modular design of the HPC Simulator, portability and a graded Quality Assurance approach..
- ***HPC Toolsets:*** Provide the building blocks that transform the mathematical description of the process models into a discrete form suitable for computer simulation.

Process Models (The Core of ASCEM)

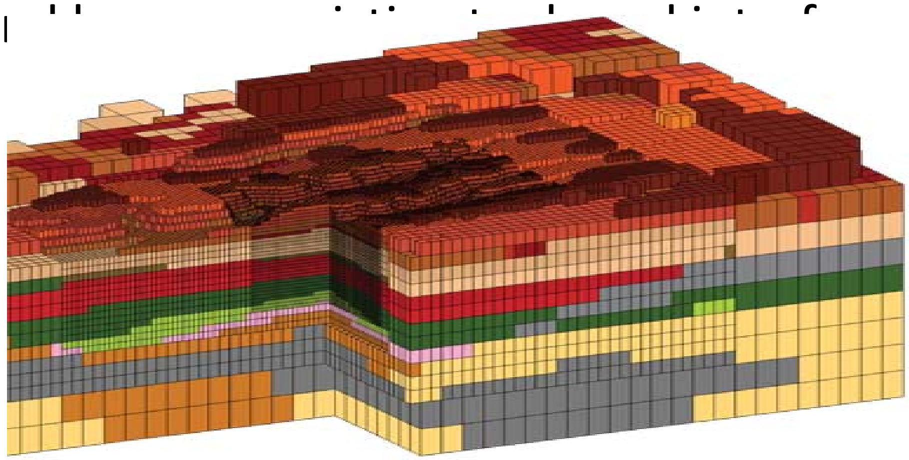
Provide the mathematical description of the processes that play a role in the release and transport of contaminants in the environment.



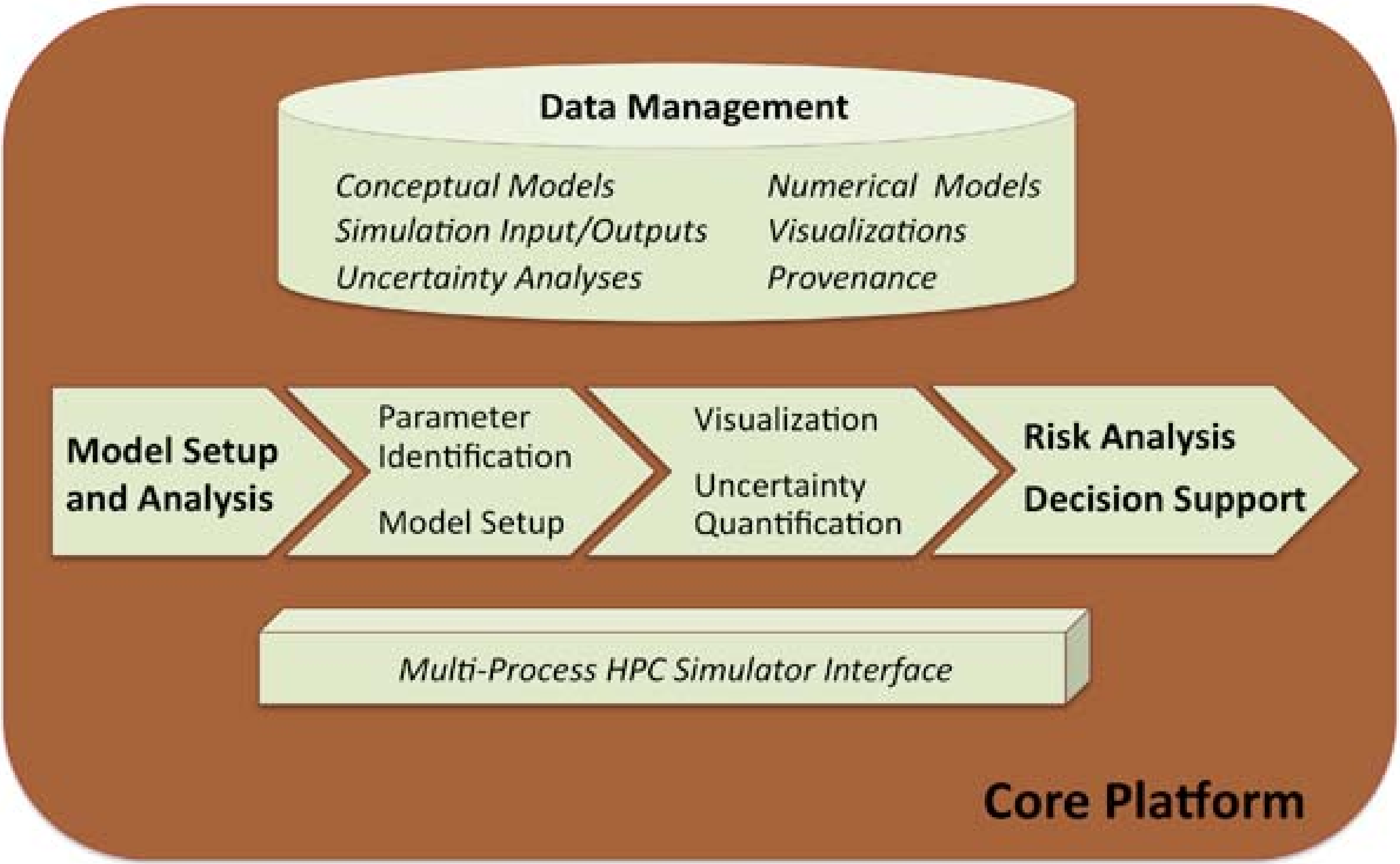
- Define process models for:
  - Single/multiphase flow and infiltration processes
  - Multicomponent transport processes
  - Chemical/geochemical and biological processes
  - Complex source terms (e.g., cementitious barriers)
  - Degradation processes (both mechanical and chemical)
- Analyze properties of the models that impact the HPC Simulator.
- Prioritize the process models and their coupling - **end user input.**
- Develop objects and interface designs for flexible, high level representation models accessible to end user scientists and regulators

HPC Toolsets Example: Meshing

- The ***Meshing Toolset*** provides distributed parallel mesh data structures that serve to bridge the conceptual model and numerical methods.
  - Support a variety of mesh types ranging from logically structured (stratigraphy fit) to fully unstructured (general polyhedral elements)
  - Design for potential use of adaptive mesh refinement (or adaptive coarsening) in the future
  - Explore a



Platform and Integrated Toolset Tasks



Platform & Integrated Toolset: Goals and Approach

Goals

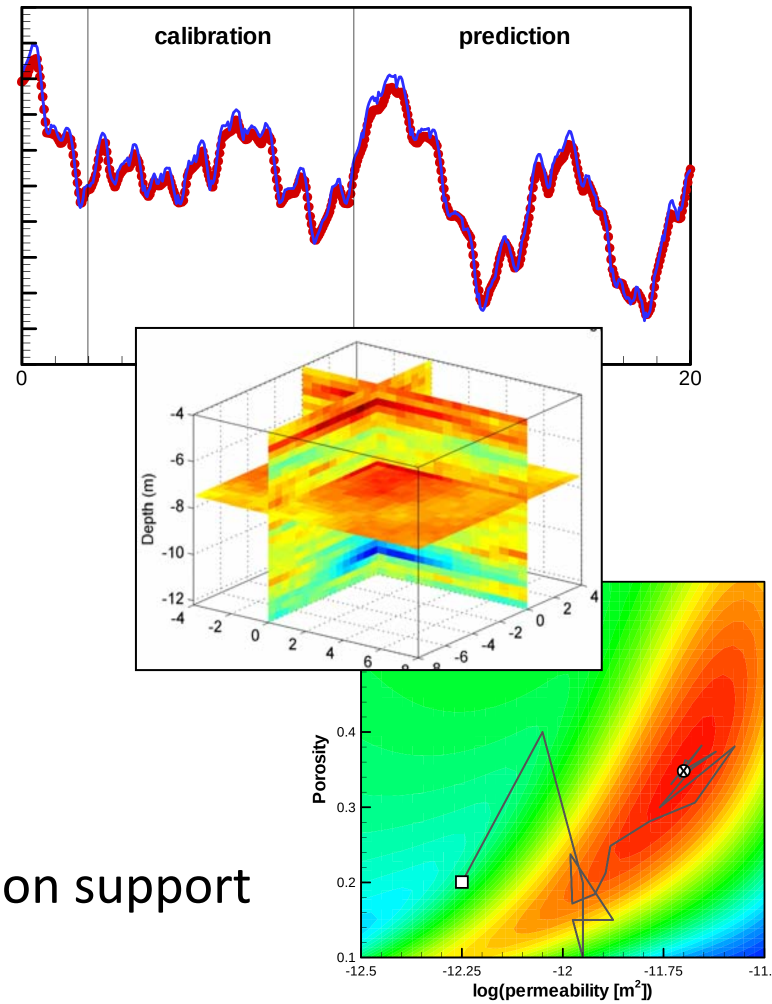
- Facilitate application of HPC simulation to environmental management tasks
- Provide support for conceptual to numerical model development as well as analysis tasks including uncertainty quantification
- Manage a wide range of heterogeneous modeling and simulation data

Approach

- Create a collaborative user environment to support site application user teams
- Integrate with the HPC core to support parameter estimation, uncertainty quantification, risk analysis, and decision support
- Provide advanced visualization, analysis and data access/ management tools

Parameter Estimation Toolset Example

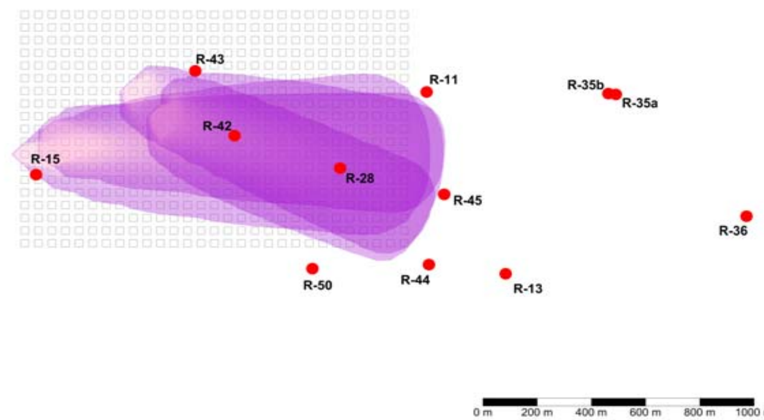
- Estimates model-related parameters based on available site or testing data
- Automatically calibrates model
- Evaluates parameter sensitivities
- Evaluates information content of measured data
- Evaluates estimation uncertainty
- Evaluates goodness-of-fit and other model identification criteria
- Provides optimization algorithms for decision support toolset

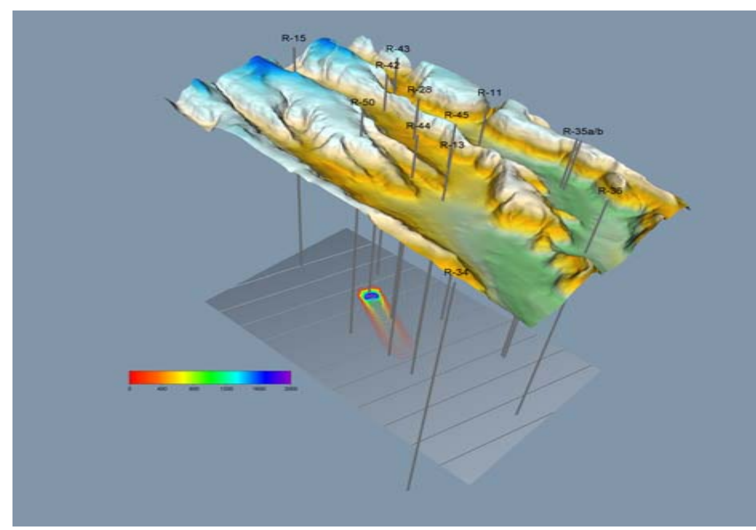


ASCEM

Example Decision Support Demonstration

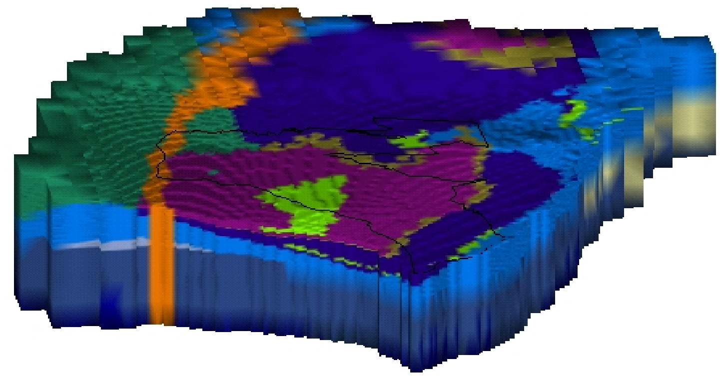
- Decision-support analyses of model predictions provide critical information related to:
  - Processes and assumptions effecting contaminant transport,
  - spatial distribution of contaminant mass,
  - plausible source locations and contaminant flux at the regional aquifer,
  - design of the next phase of site-characterization activities,
  - optimization of monitoring-network design, and
  - environmental risk.





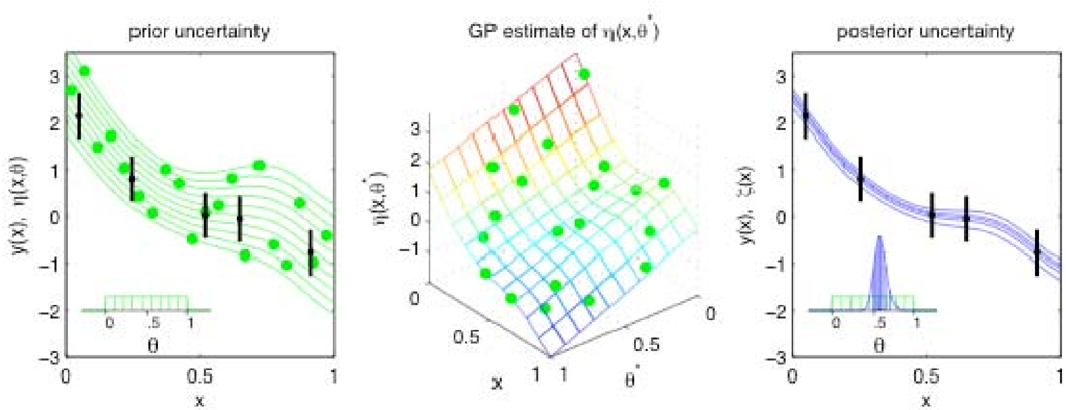
Uncertainty Quantification Example

Computational models encode physical structure and information to leverage relatively small amounts of physical data for useful predictions and inference



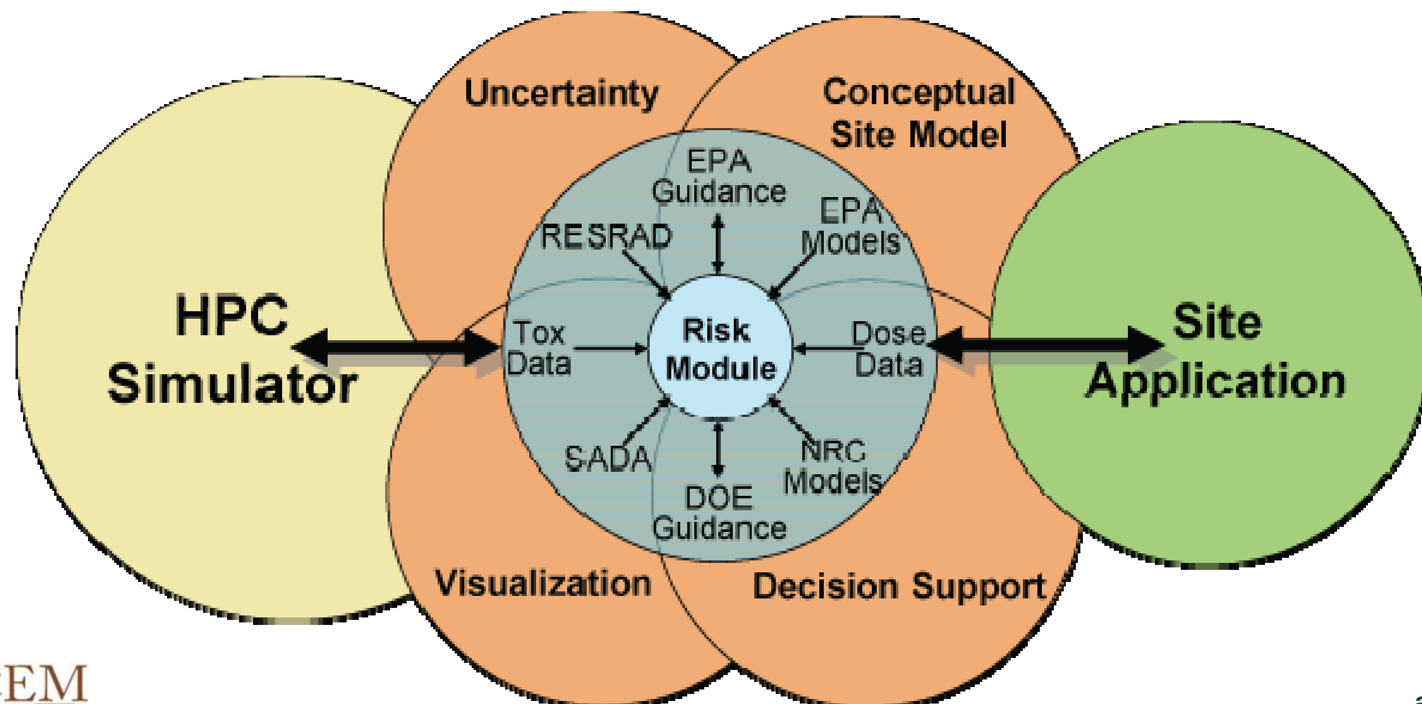
- Null-space Monte Carlo
- Bayesian inference and computation: e.g. Markov chain Monte Carlo
- Optimization
- Reduced models, response surfaces, tangent models
- Constraining uncertainties with physical observations via Bayesian and likelihood-based approaches
- Propagation of error for prediction uncertainty

$$P(x \rightarrow x') = \min\left(1, \frac{\pi(x')}{\pi(x)}\right)$$



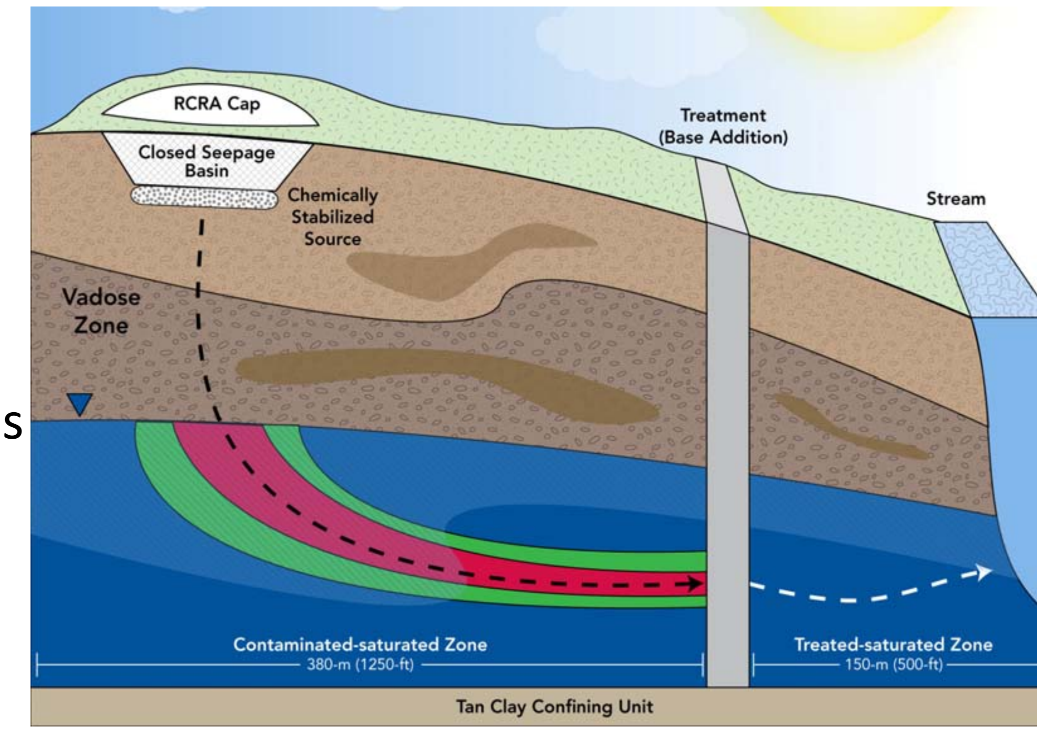
Example Risk Analysis Toolset Demonstration

- **Demonstration focus:**
  - Meeting user requirements
  - Integration needed to provide a sound foundation for activities in subsequent years
- **Overarching Objective: Improved application of risk information to the decision process at EM sites.**

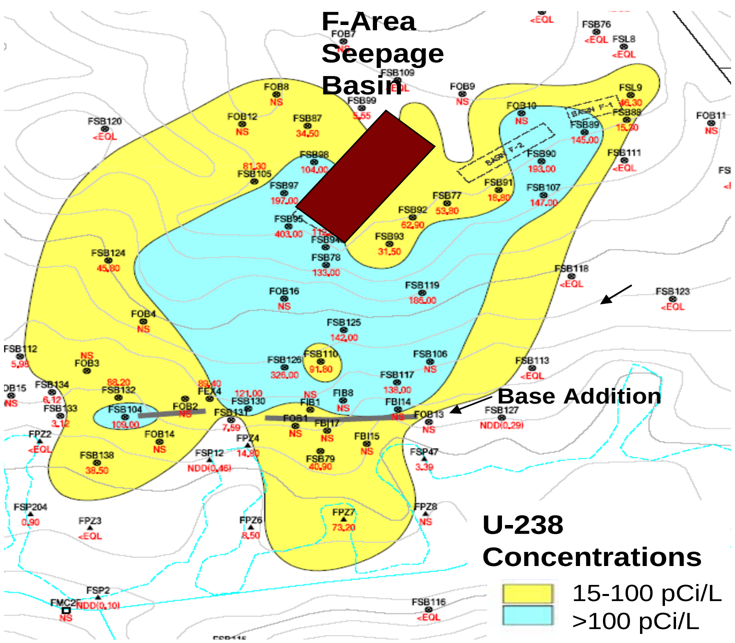


Site Applications Scope

- Provide site data for model development, testing and validation
- Provide sites for demonstrating the platform and HPC simulator
- Establish and maintain interfaces with end users
- Solicit input to requirements specification and development activities



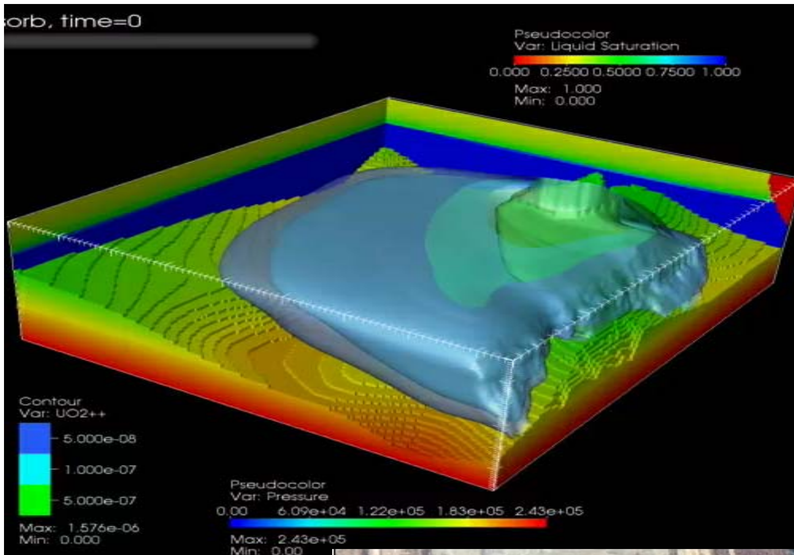
Site Application Example



Savannah River Site F-Area Acidic Plumes (Uranium, Tritium, Iodine, Strontium, Tc)

- Natural attenuation desired closure strategy
- Long term plume mobility governed by natural increases in groundwater pH and by spatial variability of sorption mechanisms that are related to stratigraphy
- 30 Years of groundwater monitoring data available

Site Application Example

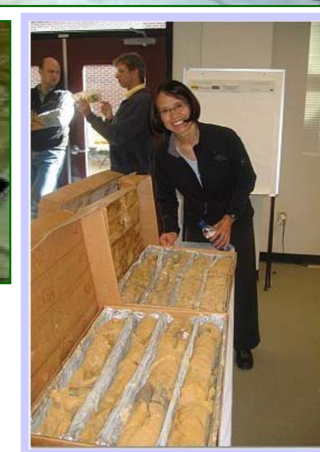


Hanford Site 300 Area

- Regulatory process to identify remediation strategy
- Uranium reactive transport; persistent groundwater plume; capillary fringe source
- Highly variable river stage
- IFRC Site

ASCEM User Interface Goals

- Provide a vehicle for the EM User Community to have input to the ASCEM project requirements design and development
- Facilitate broad user community participation in the development of Site Applications problems, test beds and testing tools
- Draft Charter developed for the User Steering Committee with membership from Senior level contractors, DOE (LFRG), and regulators familiar with PA and PA-like applications
- Review plans and interim products to provide feedback from user and oversight perspective
- Chair of the User Steering Committee is **Roger Seitz (SRNL)**



ASCEM Program - Deliverables

Multi-Process High Performance Computing (HPC) Simulator

- Define the requirements and implement the mathematical models for the core set of processes needed by user sites
- Begin implementation of interface designs for flexible, high-level representation models accessible by domain scientists
- Assemble the HPC modules and interface with the multi-process coordinator to simulate coupled processes

Platform and Integrated Toolsets

- Design and prototype the visualization, analysis and data access and management tools required for the site usage of ASCEM
- Develop, integrate and prototype the tools necessary for parameter estimation, uncertainty quantification, decision support, and risk assessment
- Demonstrate prototype modules of ASCEM and engage site users

Site Application

- Continue to gather input from sites and the end user community to guide requirements for platform and HPC development
- Provide additional data sets from selected sites for platform and HPC core testing and demonstration
- Implement a user environment and interface to support site application teams

Conclusions and Thank You

- ASCEM needed to provide technical underpinnings for DOE EM cleanup decisions through implementation of the next generation performance and risk assessments
- The ASCEM capability will leverage recent advancements in high performance computing technologies
- ASCEM will be used in combination with advanced remedial strategies to reduce risk, cost, and time-line for site closure
- Integration of ASCEM with site programs will provide a transformational, systems-based technical solution
- Success will be found through active coordination with site end users, direct site involvement and leveraging efforts in other DOE offices

Backup Slides

HPC Core Framework

Provide key infrastructure to facilitate modular design of the HPC Simulator, portability and a graded Quality Assurance approach.

- Provide low-level services, such as:
  - Parallel input/output and parallel (distributed) data structures
  - Guide API design and provide HPC related visualization support
  - Leverage elements of existing frameworks such as Trilinos and PETSc
- Develop a unified hierarchical approach to testing, verification and validation, and benchmarking (integrated tests).
- Use automated cross-platform builds to ensure robust and efficient performance on a range of platforms from laptops to supercomputers
- Provide Multiprocess Coordinator (MPC) services that coordinate the assembly of coupled-process simulations from the HPC Toolsets.

HPC Toolsets

Provide the building blocks that transform the mathematical description of the process models into a discrete form suitable for computer simulation.

- The *Meshing Toolset* provides distributed parallel mesh data structures that serve to bridge the conceptual model and the numerical methods.
- The *Discretization Toolset* provides several modules that provide the fundamental building blocks to create the process models.
- The *Solvers Toolset* provides algorithms to solve the discrete nonlinear systems of equations that arise in the simulation for EM applications.

HPC Toolsets: Solvers

- The *Solvers Toolset* provides algorithms to solve the discrete nonlinear systems of equations that arise in the simulation for EM applications.
  - Provide robust and efficient solvers for time evolution, geochemical reaction networks, as well as optimization, and assimilation.
  - Newton-based methods (e.g., Newton-Krylov) provide the basis for the most popular algorithms. Efficiency hinges on preconditioners for the (linear) Krylov iteration.
  - Design preconditioners based on well-established principles and the unique capabilities of the MPC.
  - Leverage existing nonlinear and linear solver packages, particularly robust multilevel/multigrid solvers critical to performance in high-resolution simulations.

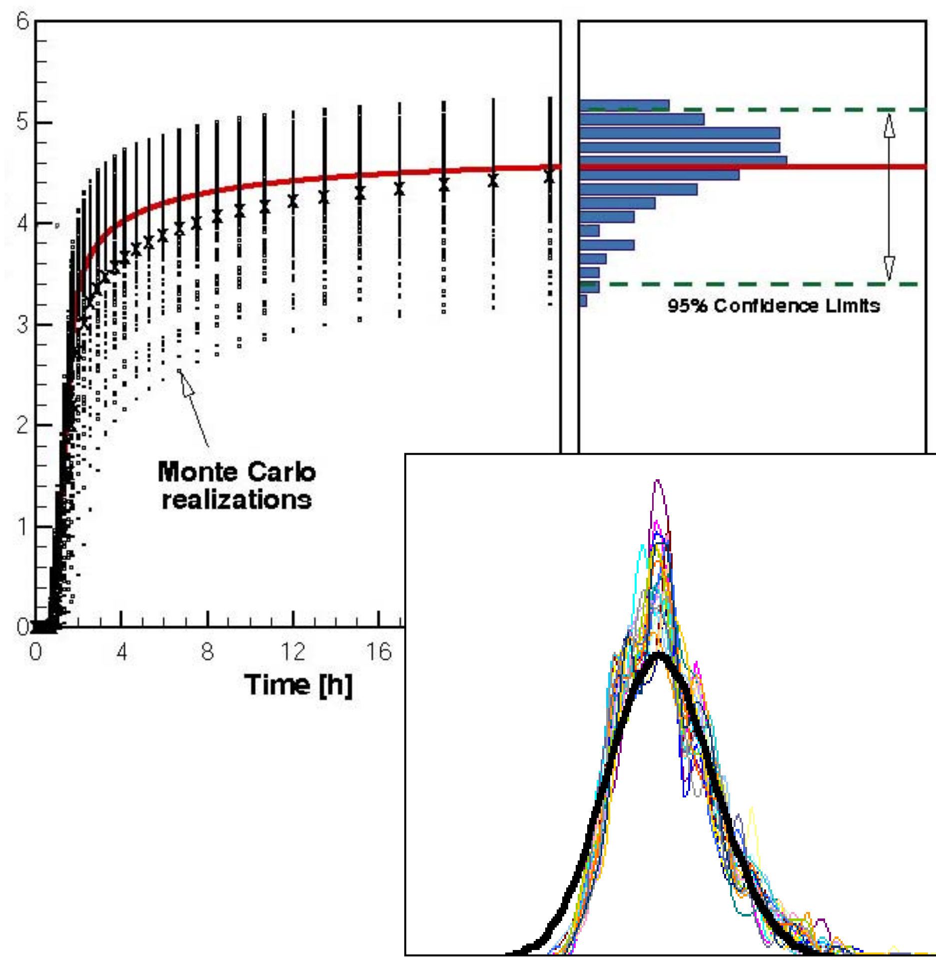
HPC Toolsets: Discretizations

- The *Discretization Toolset* provides several modules that provide the fundamental building blocks to create the process models.
  - Spatial/Temporal discretization modules provide robust and accurate representations of the fundamental mathematical operators on the required meshes with possibly anisotropic parameters.
  - The Geochemistry module supports the required reaction networks.
  - Multiscale and Upscaling methods facilitate the use of multiresolution/multiscale data and methods.
  - Explore and leverage existing algorithms and methods from key communities, including geosciences, applied mathematics and computational science.

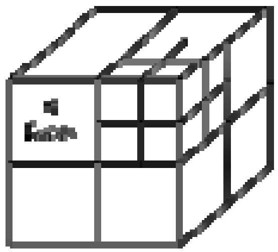
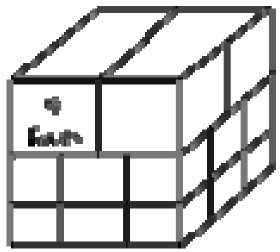
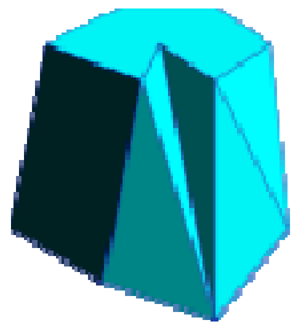
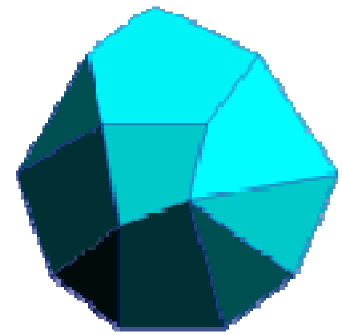
Uncertainty Quantification Toolset

Computational models encode physical structure and information to leverage relatively small amounts of physical data for useful predictions and inference

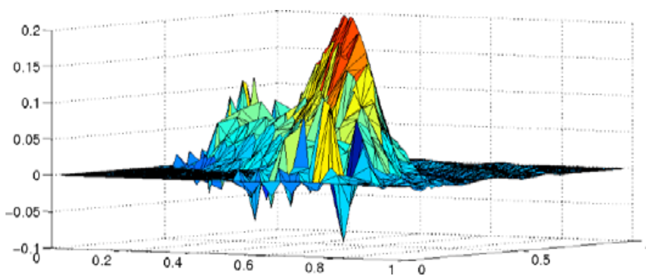
- Propagate input uncertainties through multi-process simulator to model output
- Evaluate parametric and conceptual model uncertainties
- Calculate sensitivities and importance
- Account for statistical correlations among uncertain parameters
- Use advanced sampling methods
- Facilitate analysis of model output, including causes of extreme results
- Provide input to Risk Assessment and Decision Support Toolsets

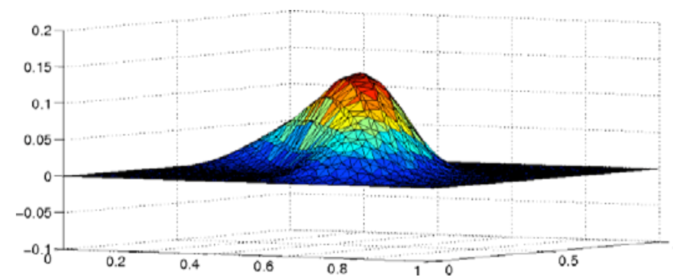


Challenges for Advanced Discretizations

Degenerate polygons/polyhedra can arise in AMR, non-convex elements can arise through mesh motion. Poloygonal/polyhedral elements offer great flexibility for meshing complex geometries. Mimetic methods rigorously treat these problems.





Anisotropic coefficients may destroy important properties of a discretization, such as monotone or positivity of the solution. Negative values appear in the original MPFA solution, while positivity is guarenteed in the new nonlinear Finite Volume scheme.

Example Risk Analysis Toolset Demonstration

- Demonstration focus:
  - Meeting user requirements
  - Integration needed to provide a sound foundation for activities in subsequent years
- Overarching Objective: Improved application of risk information to the decision process at EM sites.