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Performance Assessment Modeling of a Generic Salt Disposal System for High-Level Radioactive Waste

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U.S. Nuclear Waste Technical Review Board Meeting

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Participants in Performance Assessment (PA) and Coupled Process Modeling

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- **SNL**
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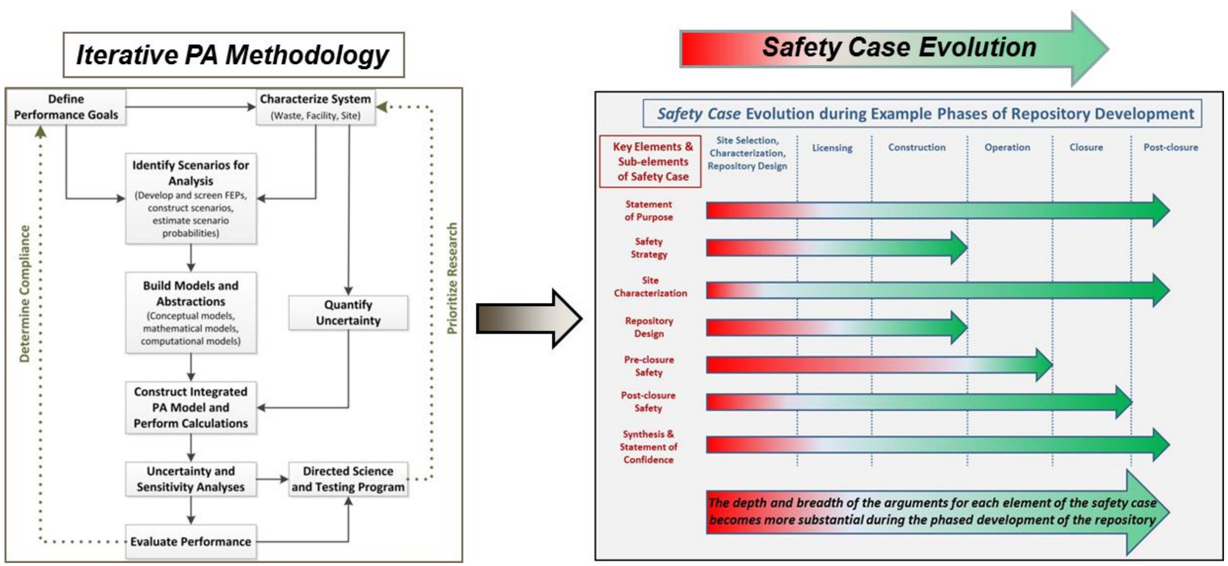
Outline of Presentation

- **Objectives**
- **PA methodology**
  - FEPs analysis, reference case
- **PA model/code development**
  - High-performance computing (HPC) environment
- **Demonstration simulation**
  - Generic salt repository example (for SNF)
- **Source-term process model integration with PA system model**
- **Summary and future work**

Objectives

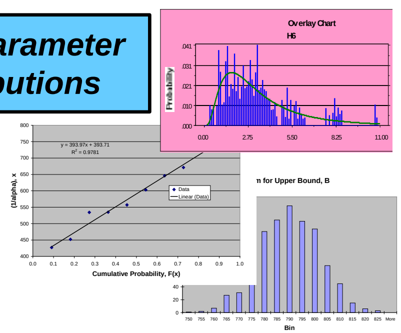
- **Develop a PA capability that readily evolves throughout the program lifecycle (site selection and characterization, construction, licensing, etc.) to**
  1) Evaluate potential SNF/HLW disposal sites in salt host rock (and other generic media)
  2) Help prioritize generic RD&D activities (later, site-specific)
  3) Support safety case development during all phases



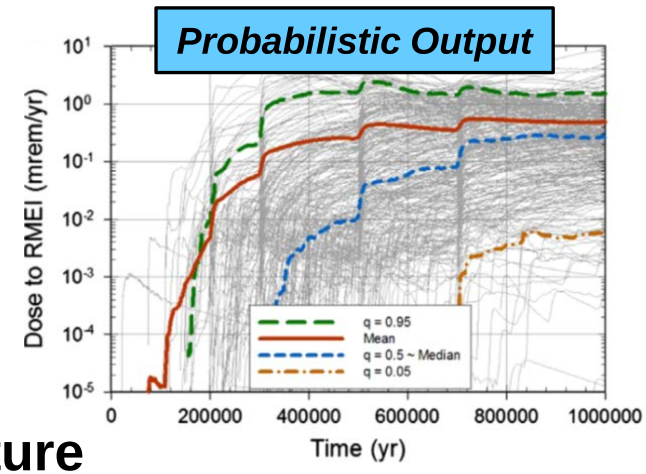
PA Model Development Methodology

- **Direct representation of important coupled multi-physics processes:**
  - Minimize conservative assumptions, simplifications, and process abstractions
    - *Enhances transparency and confidence*
  - Allows a realistic spatial-temporal representation of geometry, features, events, and processes (FEPs), and uncertainty (i.e., 3D probabilistic simulation)
    - *Spatial variability in degradation processes and T-H-C-M behavior*
    - Uncertainty quantification (UQ), both aleatory and epistemic, in parameters/processes

Input Parameter Distributions



Sampling:
- ***Monte Carlo***
- ***LHS stratified***

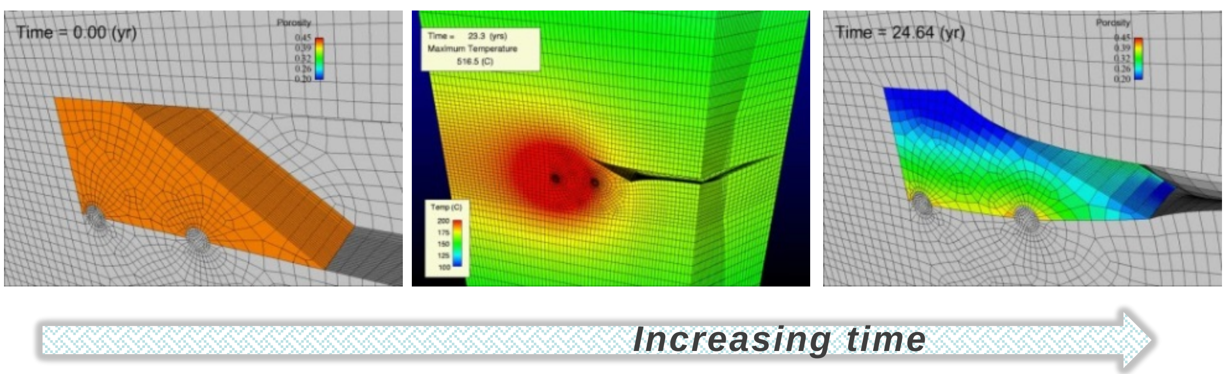


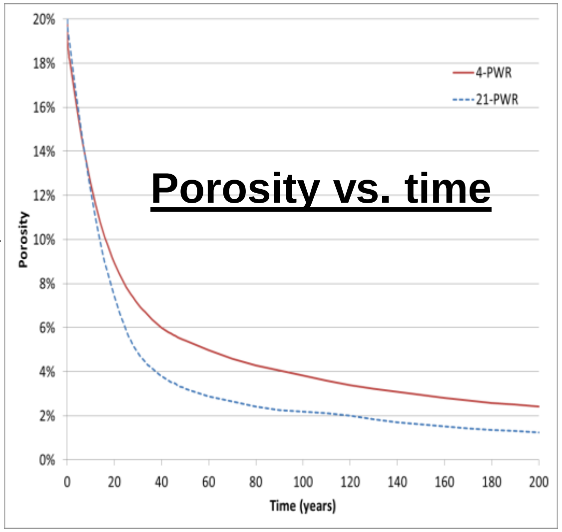
- **High-performance computing (HPC) architecture**
  - Facilitates reasonable probabilistic PA-model runtimes for science-based, 3D multi-physics

* *Fig. 1: J.C. Helton et al. / Reliability Engineering and System Safety 122 (2014) 267–271.*

Multi-Physics Fidelity in PA versus Supporting Process-Level Models

- **We use process-level understanding of salt repository evolution to inform the use of high-fidelity model components in PA code**
- **Process-level detail necessary in a PA is a function of time-scales and importance of underlying processes**
  - e.g., salt creep closure and backfill reconsolidation (THM processes) are short time-scale processes that may need to be represented in PA



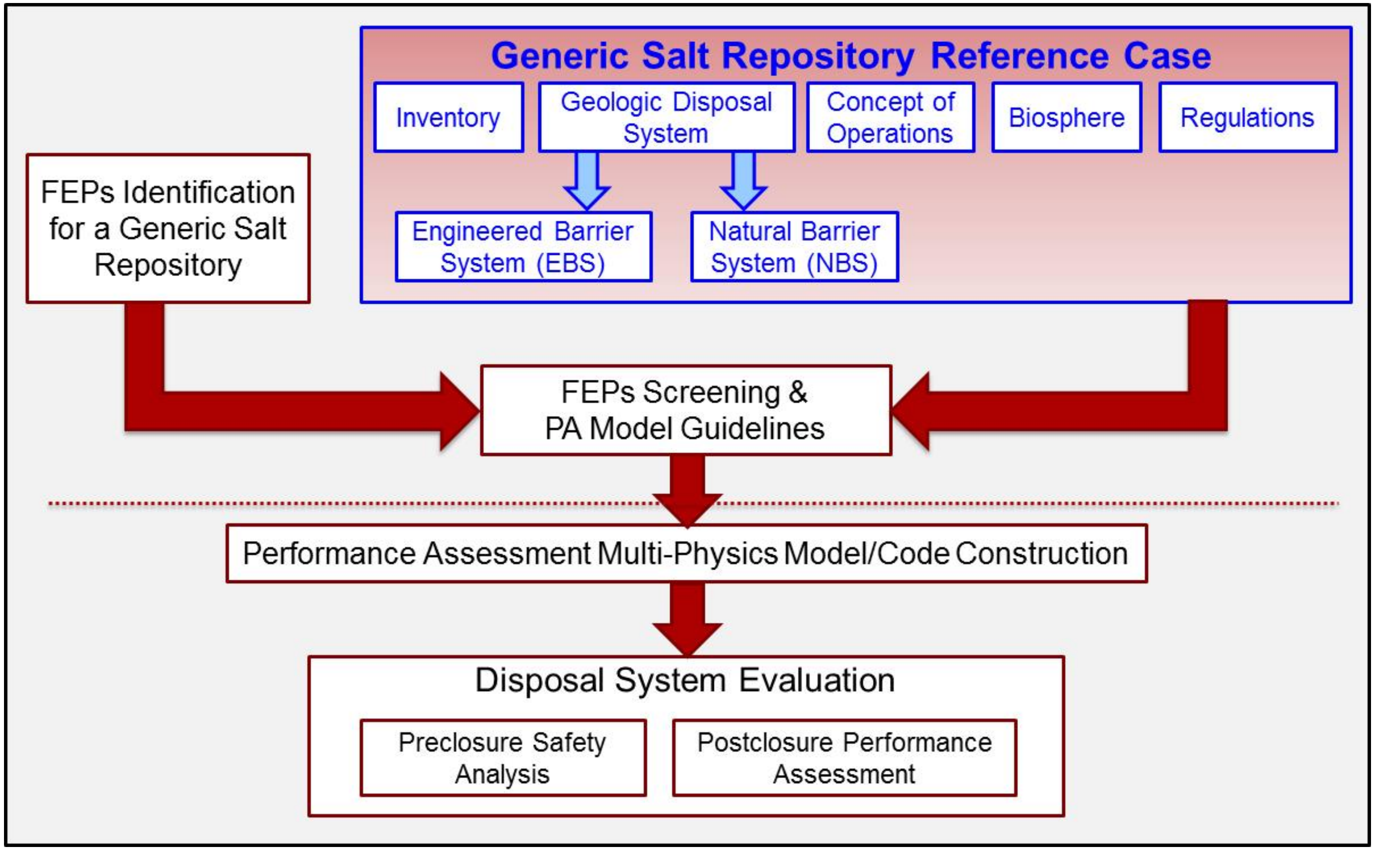


- **Multi-physics-capable PA model will help determine the processes that are important to postclosure repository performance**

PA Methodology: Reference Case

- **Reference Case is a surrogate for site- and design-specific information**
  - Documents information and assumptions needed for *generic* disposal system models
  - Helps ensure consistency across analyses (e.g., PA, process modeling, UA/SA)

Major steps in PA Methodology



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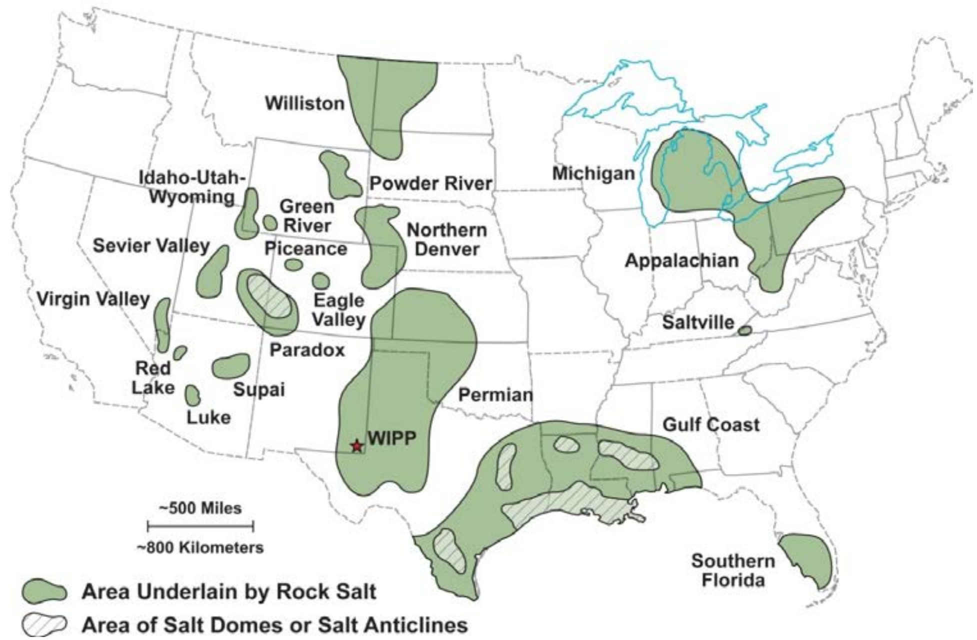
Salt Reference Case Details – Natural Barrier System (NBS)

- **Salt host rock:**
  - Use information and characteristics representative of five major bedded salt basins in the U.S.
    - *Stratigraphy: depth, thickness, lateral extent*
    - *Formation properties: hydraulic gradient, porosity, permeability, diffusivity, sorption*
    - *Fluid (brine) chemistry*

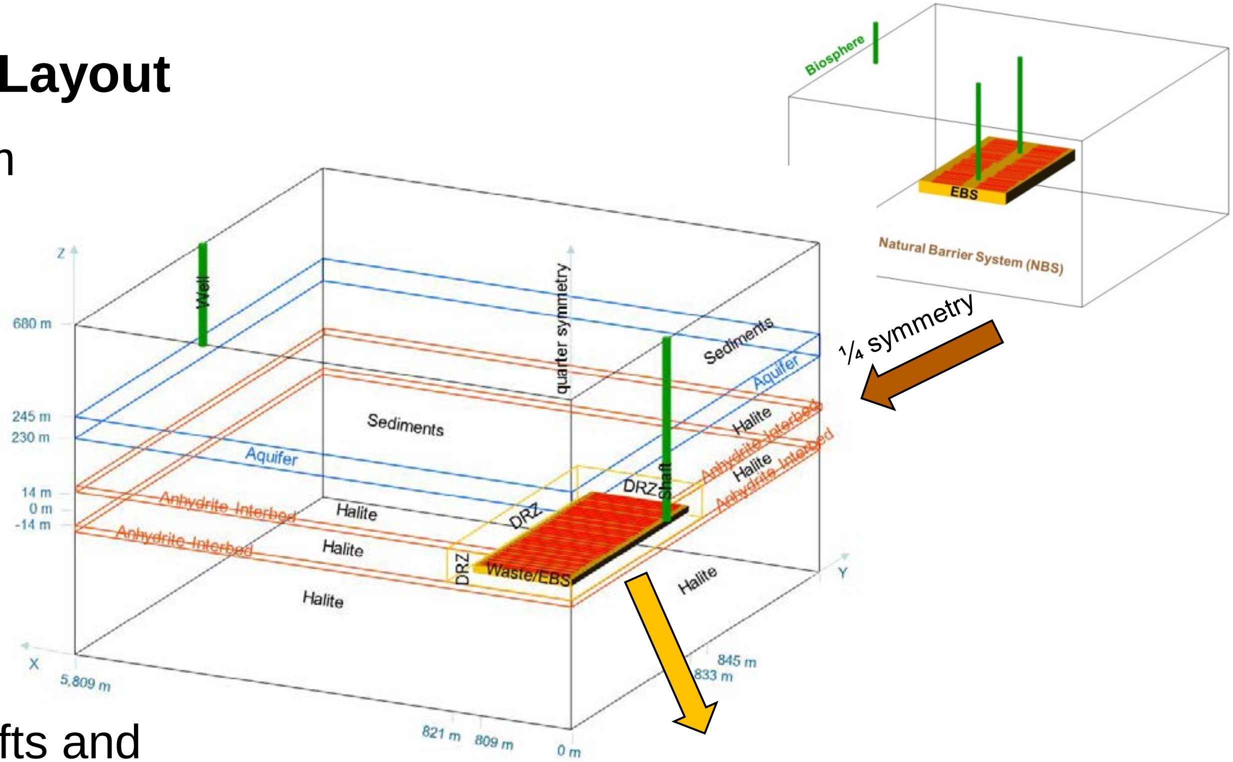


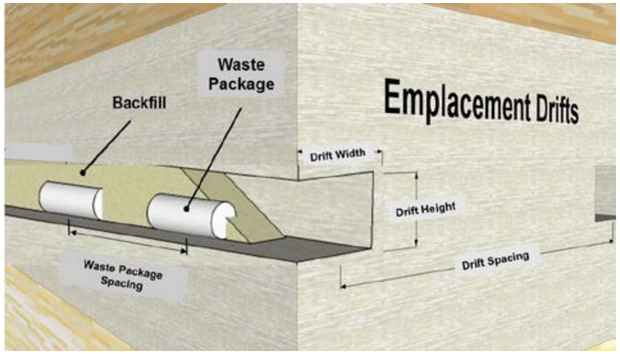
- **Disturbed rock zone (DRZ):**
  - Typical properties from international studies and from WIPP
- **Interbeds:**
  - Types (e.g., dolomite, anhydrite) and frequency
  - Dimensions, locations (near DRZ), and properties
- **Representative aquifer:**
  - A single-porosity, saturated, sedimentary formation
  - Depth above repository, thickness, physical and chemical characteristics

Salt Reference Case Details – EBS and Concept of Operations

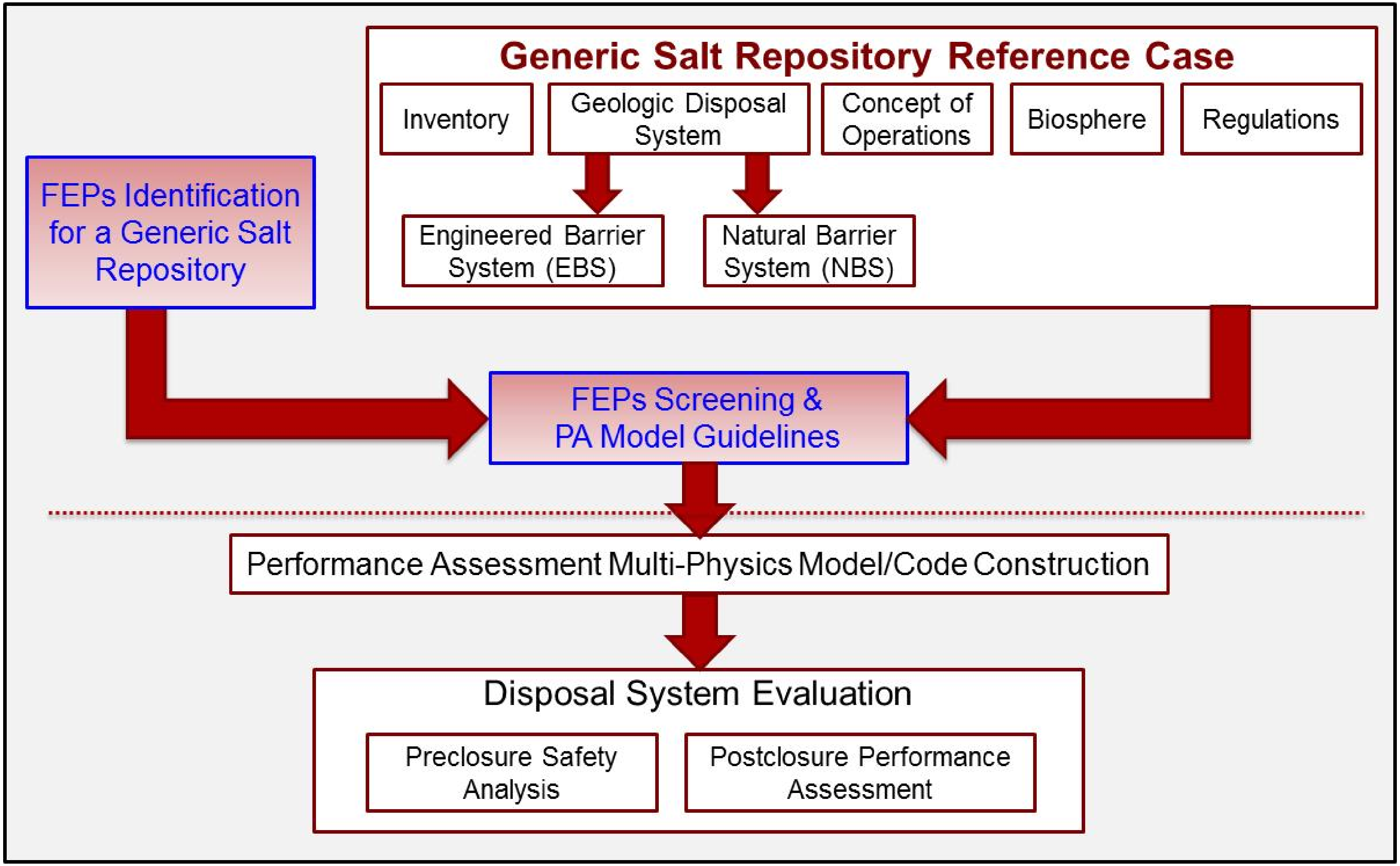
Disposal Concept and Layout

- Repository depth = 680 m
- Waste inventory
  - *~70,000 MTHM UNF*
  - ~13,400 WPs
  - Burn-up = 60 GWd/MT
- Drift spacing and WP loading based on 200°C thermal limit for salt
  - 12 PWR assemblies per WP
  - 7.5 kW/WP
- Geometry — layout of drifts and shafts
  - 84 pairs of 800-m drifts
    - Drift spacing = 20 m
    - 80 5-m-long WPs per drift with 10 m spacing
  - Crushed salt backfill in drifts
  - Sealed shafts (similar to WIPP)



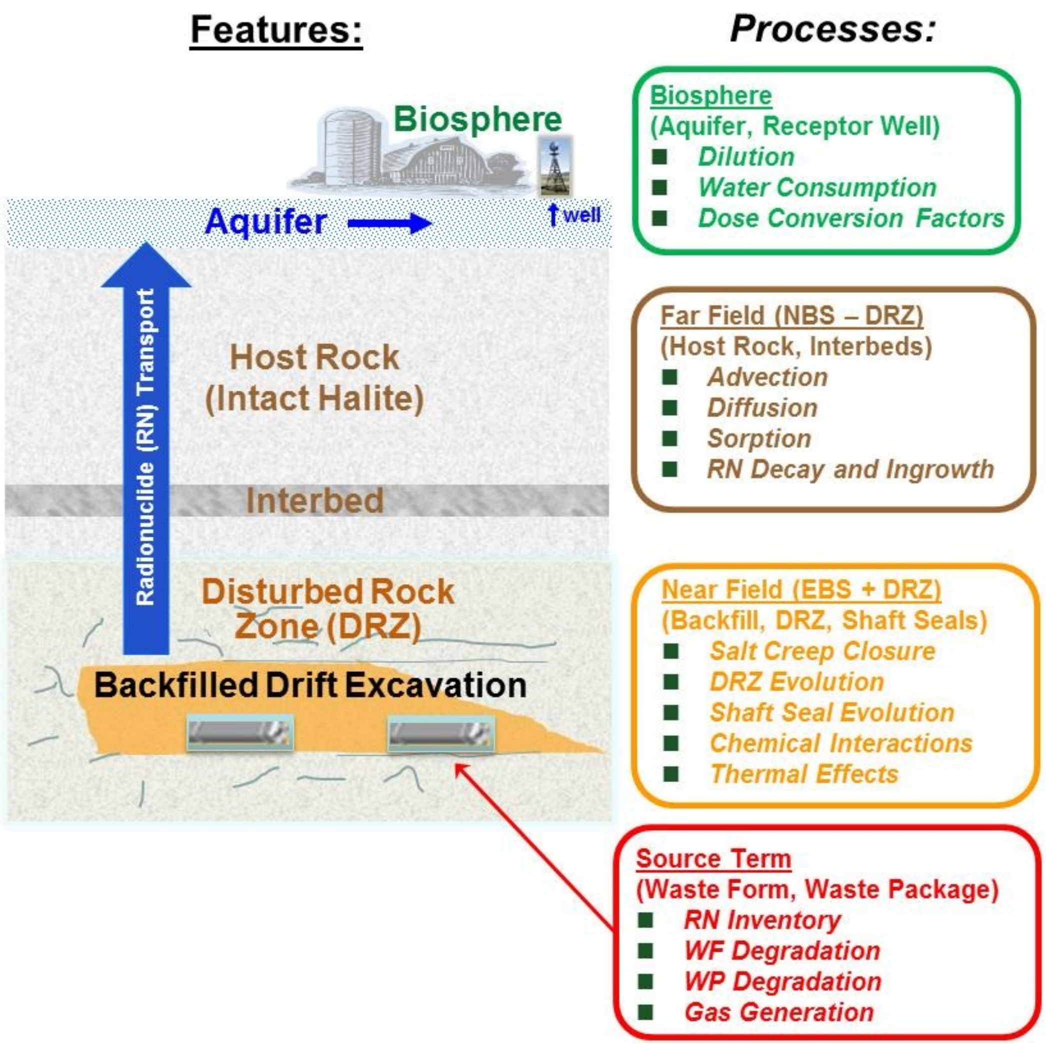


PA Methodology – Features, Events, Processes (FEPs) Analysis



Features, Events, Processes (FEPs) Analysis

- **FEP analysis supports safety assessments and safety cases**
  - Development of system models
  - Prioritization of research
  - Licensing/safety case (completeness)
  - Identification of risks and hazards
- **FEP analysis is used in all advanced repository programs**
  - U.S. DOE-NE Used Fuel Disposition
  - U.S. DOE-EM Waste Isolation Pilot Plant (WIPP)
  - U.S. OCRWM Yucca Mountain Project
  - German VSG (Gorleben)
  - Nuclear Energy Agency (NEA) International FEP Database
    - Sweden, Switzerland, Belgium, U.K., Canada



FEPs Analysis/Screening to Inform PA Model Guidelines

- ***FEPs identification*** **– comprehensive list of FEPs that capture the entire range of phenomena potentially relevant to long-term performance of the repository**
- ***FEPs screening*** **– subset of important FEPs that individually, or in combination with other FEPs, contribute to long-term performance**
  - FEPs may be *excluded* based on low probability, low consequence, or regulation
- ***PA model requirements*** **– Review/analysis of included FEPs will provide guidance on how to include them in the PA component models:**
  - Fidelity & dimensionality of T-H-M-C processes in PA

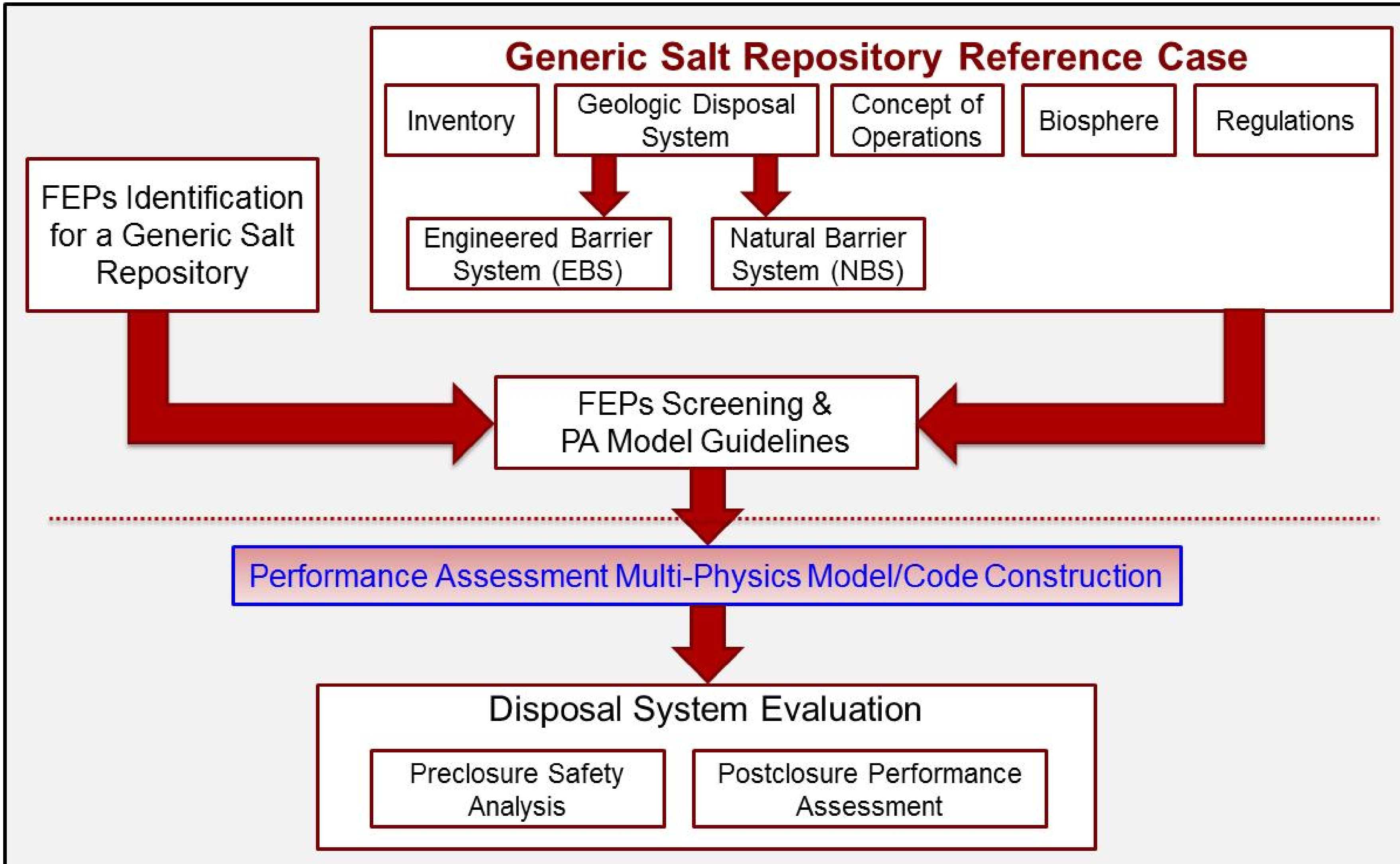
Broad FEP description provided in the "Description" column

Additional detail provided in the "Associated Processes" column

"Screening Decision" may be dependent on design and siting

UFD FEP Number	Name/Description	Associated Processes	Screening Recommendation for a Generic Salt Site
2.1.09.11	Electrochemical Effects in EBS	- Enhanced metal corrosion	**Likely Excluded**, but reevaluate once a more detailed design is available.

PA Methodology – Code Construction (Guidelines)



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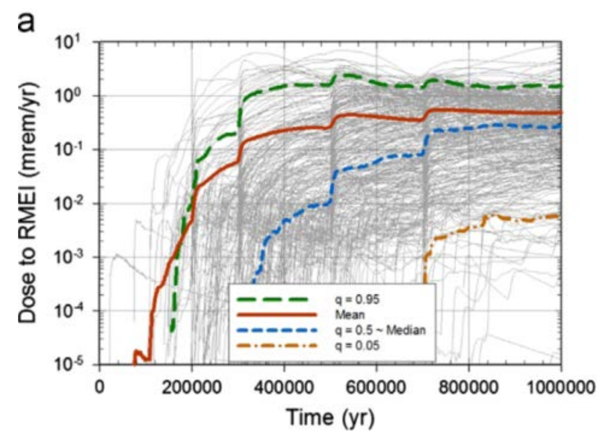
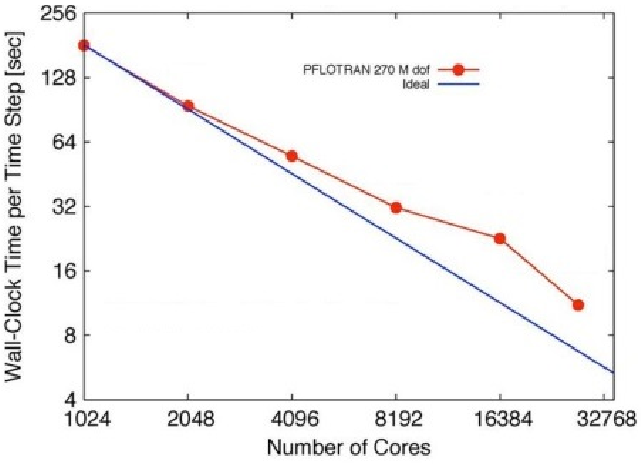
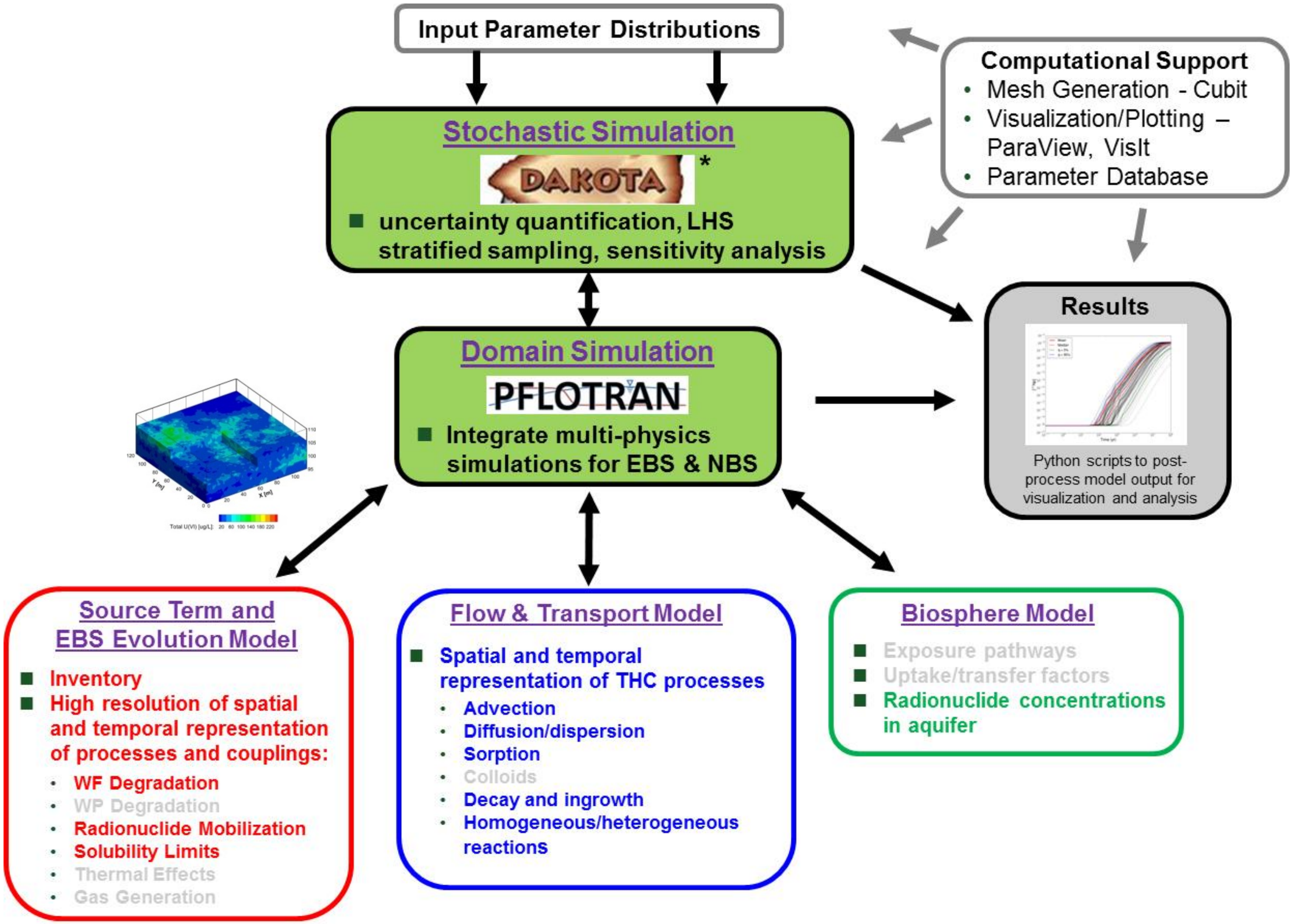
PA Code Construction (Guidelines)

- **High-performance computing (HPC) environment facilitates:**
  - Three-dimensional (3D) multi-physics in PA
  - Multiple realizations over uncertain inputs
  - Future advances in computational methods and hardware
- **Code capabilities:**
  - Open source development and distribution
    - *Transparency*
    - *Shareable among multi-lab subject matter experts and stakeholders*
  - Flexible and extensible; scalable
    - *Modular implementation of simple and/or advanced PA component models and FEPs*
  - Leverage existing computational capabilities
    - *Meshing, visualization, HPC solvers, etc.*
  - Appropriate Configuration Management (CM) and Quality Assurance (QA)





Current Integrated PA Code Capabilities

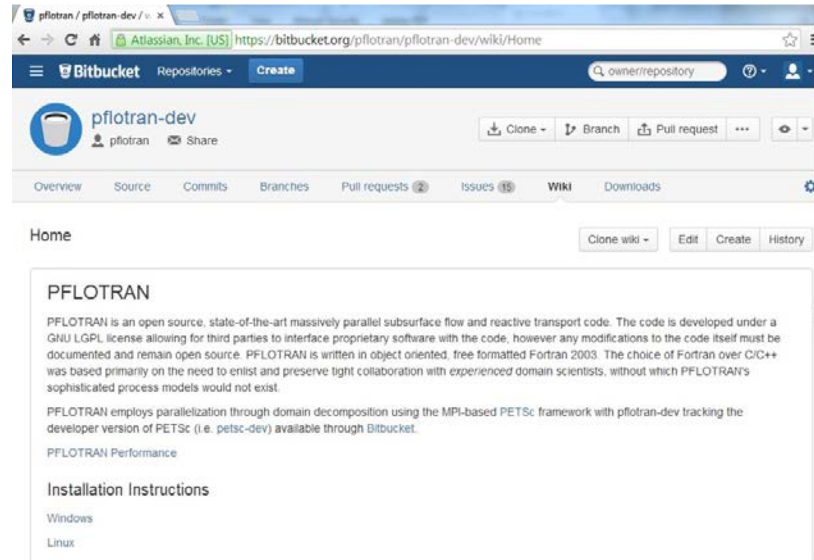


*Design Analysis Kit for Optimization and Terascale Applications

PFLOTRAN Capabilities

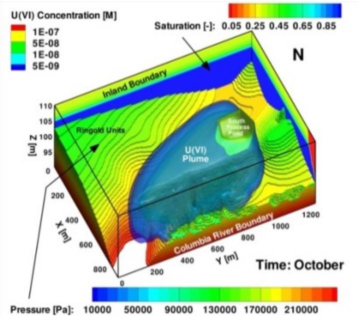
- **Multi-physics**
  - Multi-phase flow and heat
  - Multi-component reactive transport
  - Biogeochemistry processes
- **High-Performance Computing**
  - Mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- **Open Source Collaboration**
  - Leverages diverse scientific community
- **Modern Fortran (2003/2008)**
  - Domain scientist friendly
  - Modular framework for adding new capability

PFLOTRAN

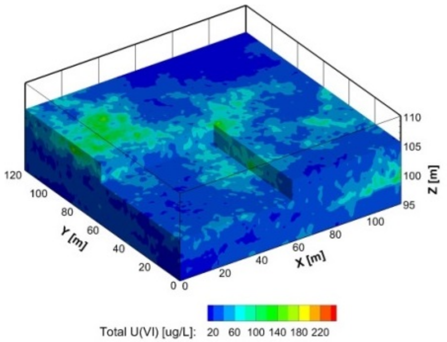


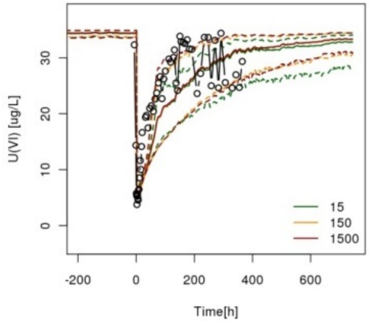
PFLOTRAN Process Modeling

- **Flow**
  - Multiphase gas-liquid
  - Constitutive models and equations of state
- **Reactive Transport**
  - Advection, dispersion, diffusion
  - Multiple interacting continua
- **Energy**
  - Thermal Conduction and Convection
- **Geochemical Reaction**
  - Aqueous speciation (with activity models)
  - Mineral precipitation-dissolution
  - Surface complexation, ion exchange, isotherm-based sorption
  - Radioactive decay with daughter products

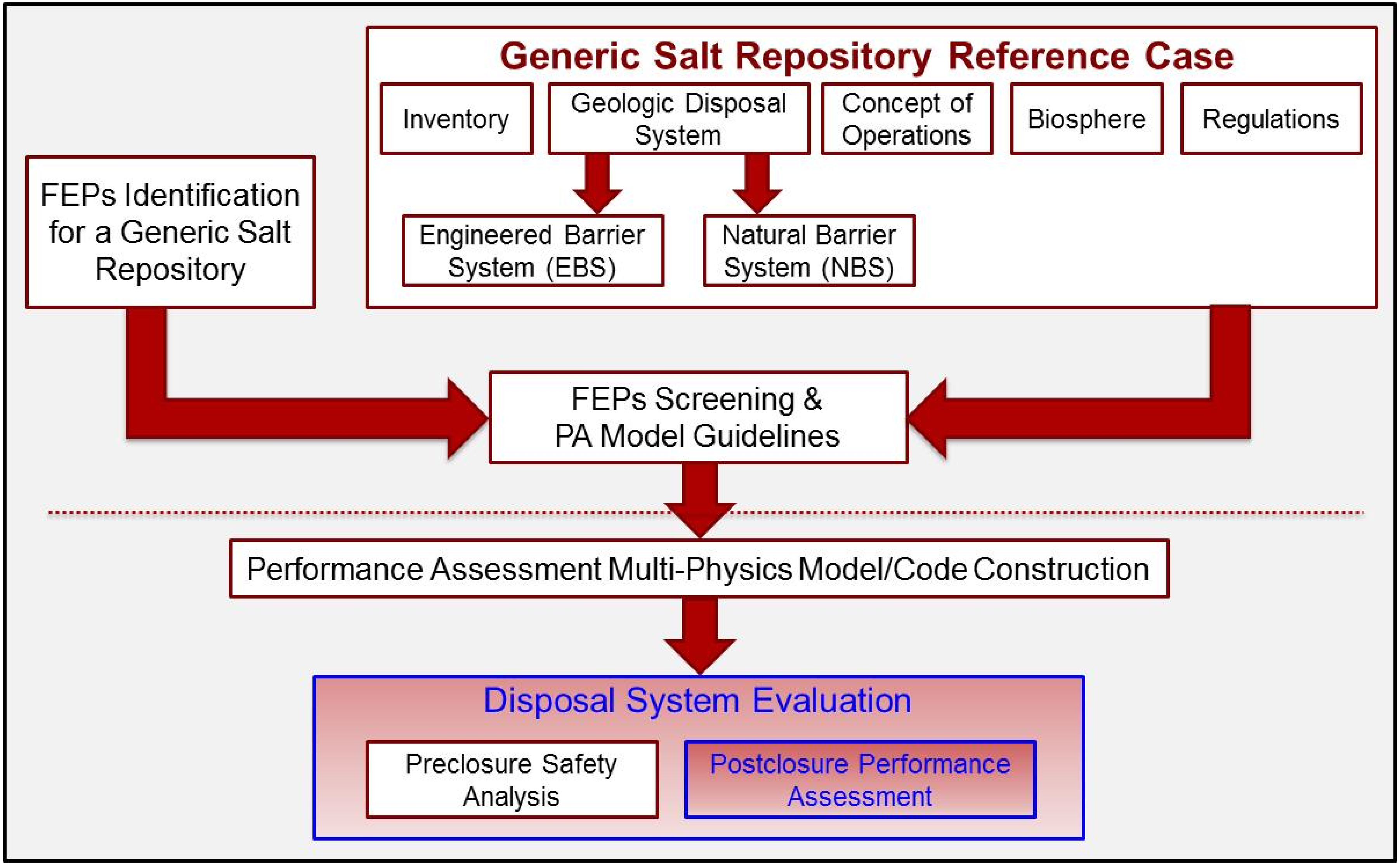


Hammond and Lichtner, WRR, 2010





PA Methodology – Disposal System Evaluation



Generic Salt Repository PA Demonstration Case

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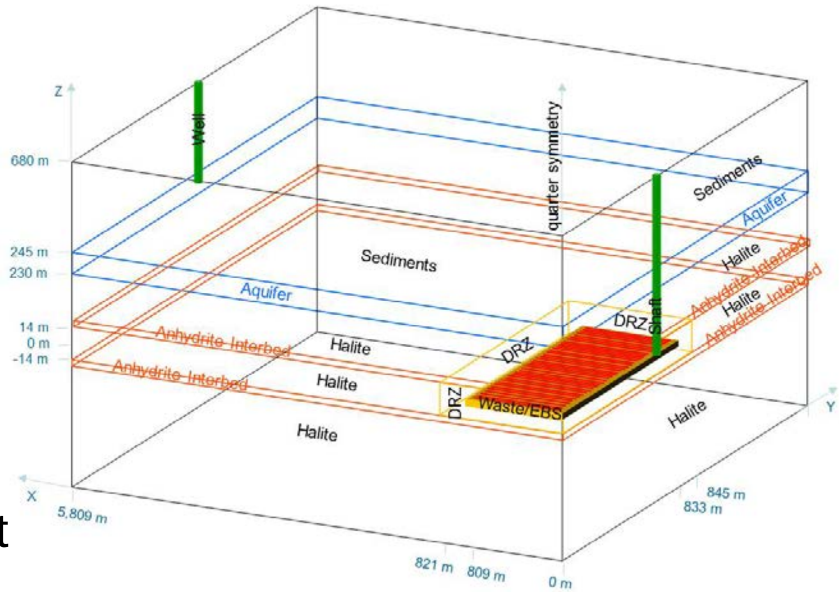
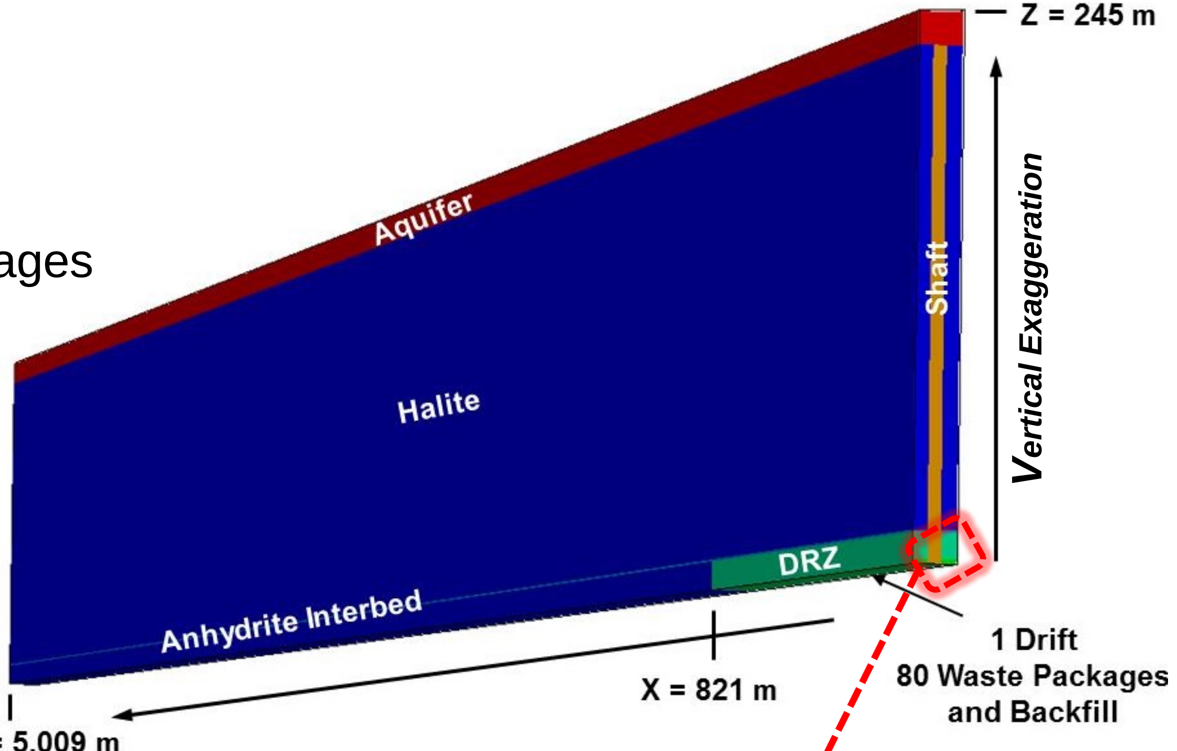
- **Undisturbed scenario**
- **Uncertainty quantification (DAKOTA)**
  - Latin Hypercube sampling of input parameter distributions
  - Sensitivity analysis
- **Coupled domain processes (PFLOTRAN)**
  - **NBS:** 3D flow and radionuclide transport
    - *Diffusion through DRZ and bedded salt*
    - *Advection through aquifer*
  - **EBS:** realistic source term
    - *5 radionuclides:*
      - ^{129}I, ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th
    - *Waste form (SNF) degradation rate controlled by kinetic rate of reaction*
    - *Solubility limits*
      - Dissolved radionuclides that reach solubility will precipitate

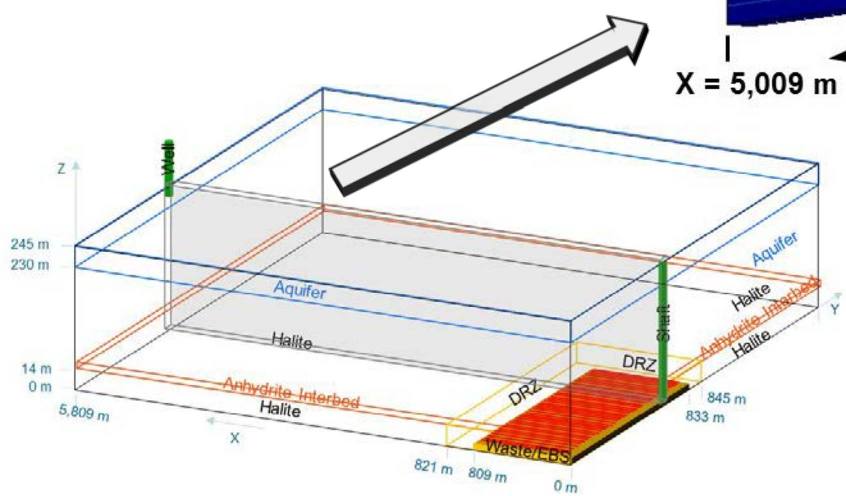


Generic Salt Repository PA Demonstration – 3D Model Domain

- **Simulation domain**
  - 3D vertical slice
  - 20-m wide pillar to pillar
  - 1 drift with 80 waste packages and backfill

X	*= 5009 m*	*NX*	*= 242*
Y	*= 20 m*	*NY*	*= 5*
Z	*= 245 m*	*NZ*	*= 38*
		Cells	*= 45,980*

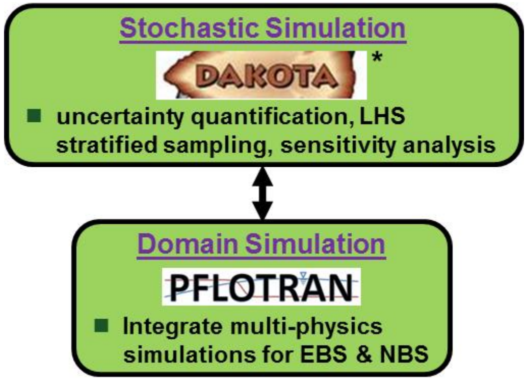




Drift detail
8 of 80 waste packages shown

Generic Salt Repository PA Demonstration – Simulations

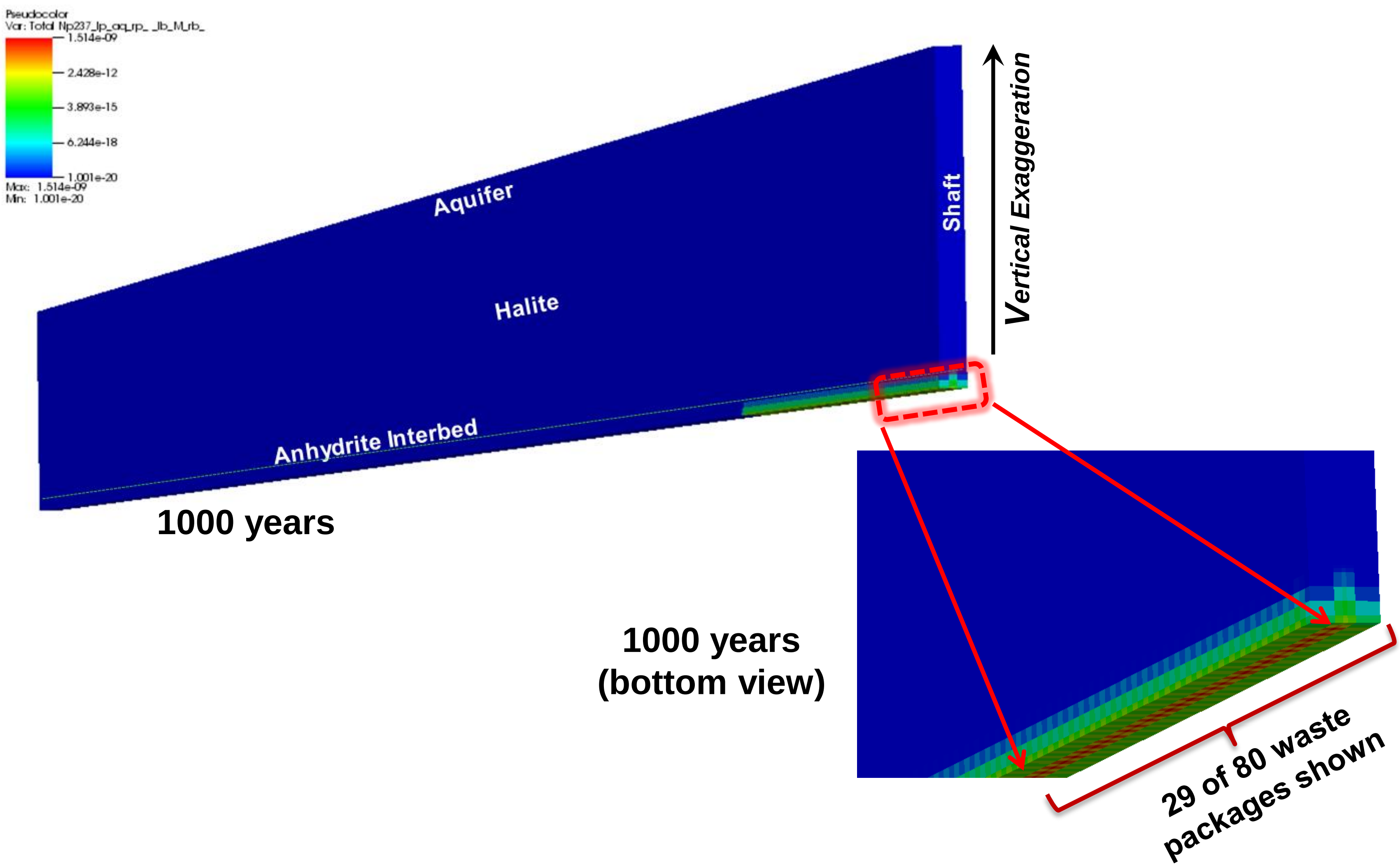
- **DAKOTA / PFLOTRAN simulations:**
  - Deterministic simulation with mean values
  - 100-realization probabilistic simulation with 9 sampled parameters
  - Run on SNL Red Sky HPC cluster
    - *Nested parallelism*
    - *Many concurrent realizations*
    - *Each realization distributed across many processors*



- Total nodes: 2,816 nodes / 22,528 cores
- 505 TeraFlops peak

Generic Salt Repository PA Demonstration – Deterministic Simulation Results

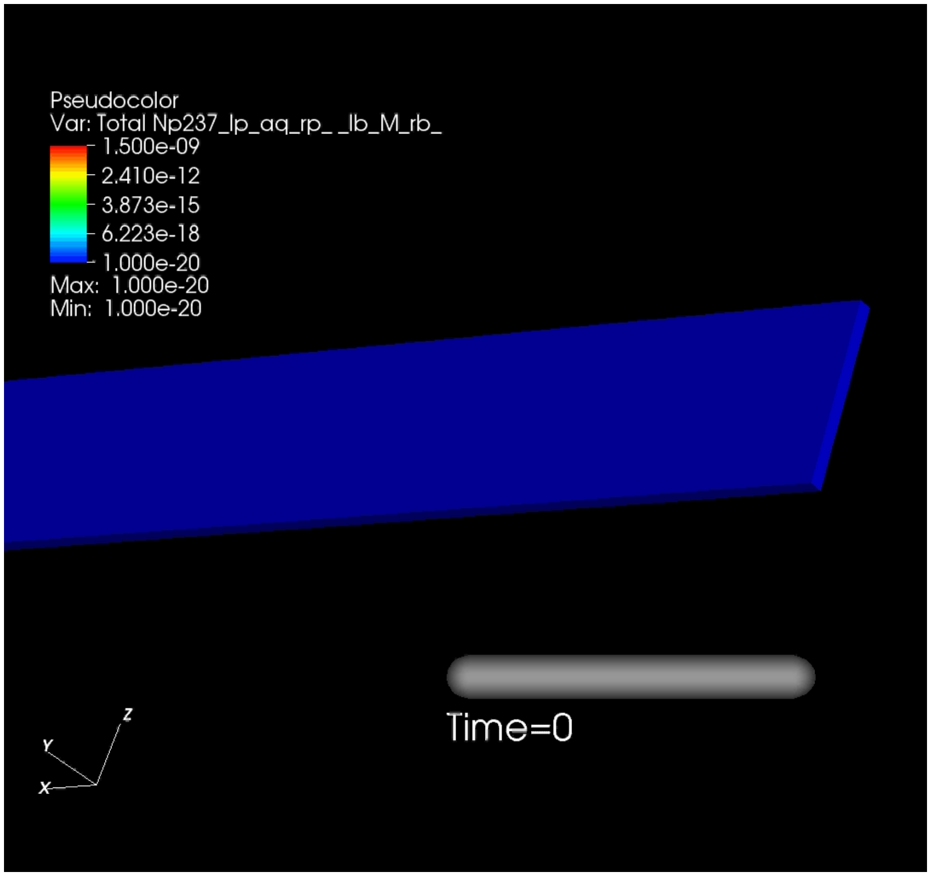
- ^{237}Np dissolved concentration at 1000 years, showing drift detail



Generic Salt Repository PA Demonstration – Deterministic Simulation Results

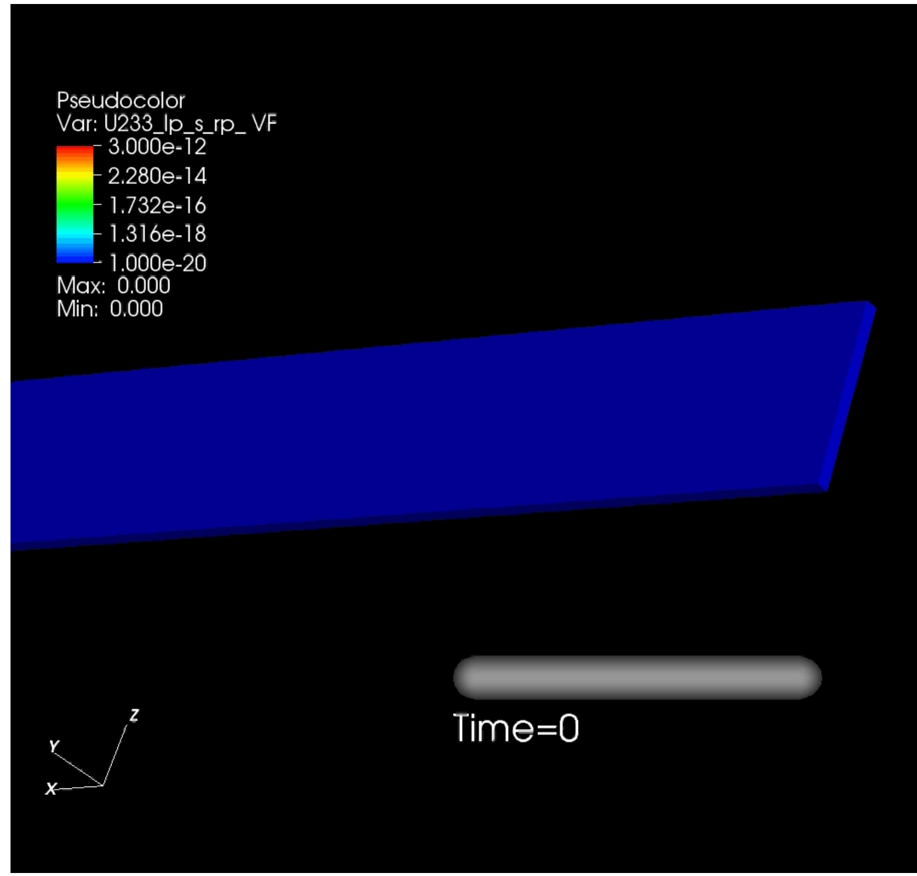
- ^{237}Np dissolved concentration

Repository domain ~ 1000 m



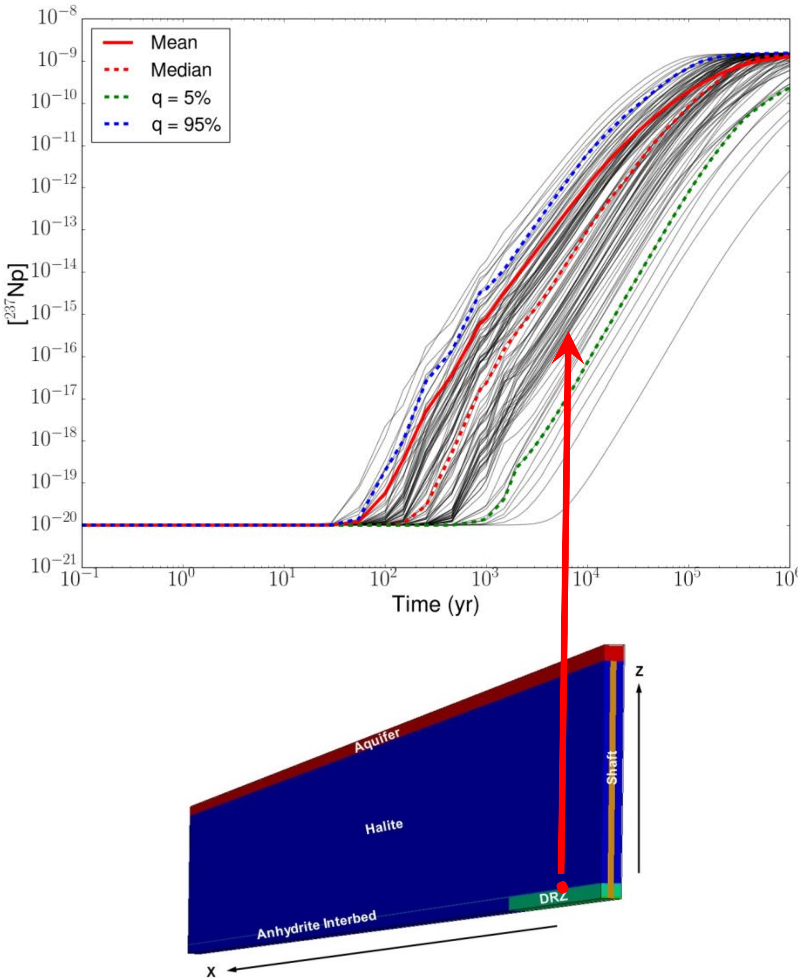
- ^{233}U precipitated concentration

Repository domain ~ 1000 m

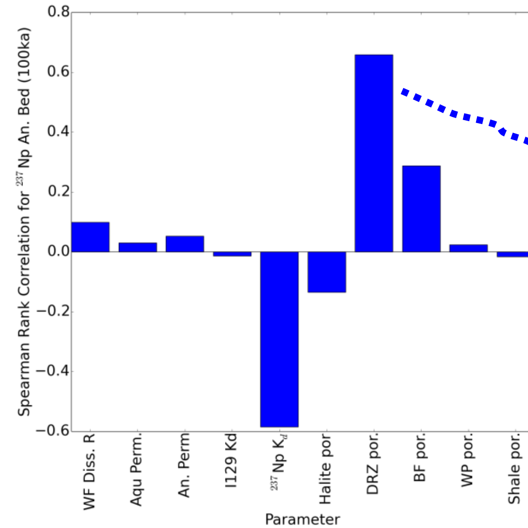


Multi-Realization Analysis

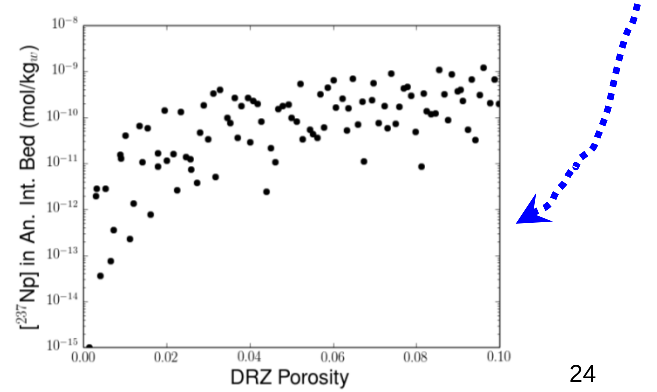
- **^{237}Np dissolved concentration vs. time in anhydrite interbed at x = 400 m (DAKOTA probabilistic output of 100 realizations)**



- **DAKOTA rank correlation analysis: ^{237}Np output concentration at 100K years versus input parameter uncertainty**



- **Scatterplot: ^{237}Np output concentration at 100K years versus DRZ porosity**

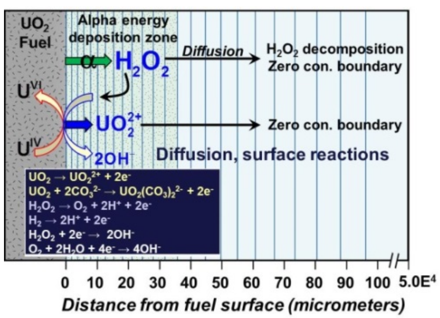


Example of Flexible PA Model Architecture

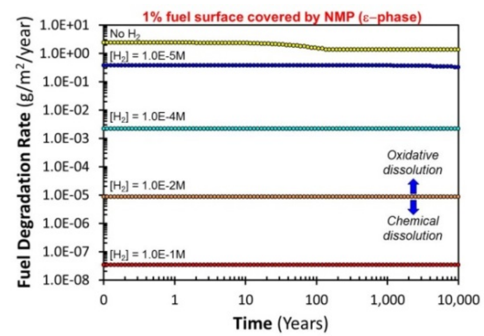
- **Coupling with Process-Level Mixed Potential Model (MPM) for SNF Degradation:**

System Level Model (Performance Assessment)

Solution Chemistry



Fuel matrix degradation rate + IRF



SNF Waste Form Degradation Model

Radiolysis Module ⇄ ***Mixed Potential Module*** + ***Instant Release Fraction Module***

Summary and Future Work

- **A PA modeling/analysis capability has been developed to:**
  - Evaluate generic and/or specific disposal sites with a high-fidelity representation of coupled processes in 3D:
    - *Based on HPC architecture and software, and adaptable to future advances*
    - *Use extensive current knowledge base in salt to inform model development*
    - *Includes appropriate representation of uncertainty and heterogeneity*
  - Support prioritization of UFD RD&D activities
  - Enhance confidence and transparency in the eventual safety case
- **Demonstration of new capability by application to a generic salt repository reference case**
- **FY14 ongoing work includes**
  - Further code refinement, as necessary
  - Further reference case development, simulations, and testing for salt, as well as granite and argillite
  - Integration with SNF degradation process-level models

Thank you for your attention!

Questions?

Backup Slides

Detailed Elements of the Safety Case

1. Introduction, Purpose, and Context

2. Safety Strategy

2.1 Management strategy
- Organizational/mgmt. structure
- Safety culture & QA
- Planning and Work Control
- Knowledge mgmt
- Oversight groups

2.2 Siting & Design strategy
- NWPA
- Site selection basis
- Design requirements
- Disposal concepts

2.3 Assessment strategy
- Regulations (10 CFR 60)
- Performance goals/safety criteria
- Safety functions/multiple barriers
- Uncertainty characterization
- RD&D prioritization guidance

3. Assessment Basis

3.1 Design, Construction, & Operations
- Repository design & layout
- Waste package (WP) design
- Construction requirements & schedule
- Operations & surface facility
- Waste acceptance criteria

3.2 Waste & Engineered Barriers Technical Basis
- Inventory characterization
- WP technical basis
- Buffer/backfill technical basis
- Shafts/seals technical basis
- International collaboration & peer review

3.3 Geosphere/ Natural Barriers Technical Basis
- Site characterization
- Host rock/DRZ technical basis
- Aquifer/other geologic units technical basis
- International collaboration & peer review

3.4 Biosphere & Surface Environment Technical Basis
- Biosphere & surface environment:
  - Surface environment
  - Flora & fauna
  - Human behavior
- International collaboration & peer review

4. Disposal System Safety Evaluation

4.1 Preclosure Safety Analysis
- Surface facilities, handling & acceptance
- Underground transfer
- Emplacement operations
- Design basis event construction
- Preclosure model/software development

4.2 Postclosure Safety Assessment
- FEPs analysis/screening
- Scenario construction/screening
- TSPA model/software development
- Performance assessment analyses
- Barrier/safety function analyses and subsystem analyses
- Uncertainty/sensitivity analyses

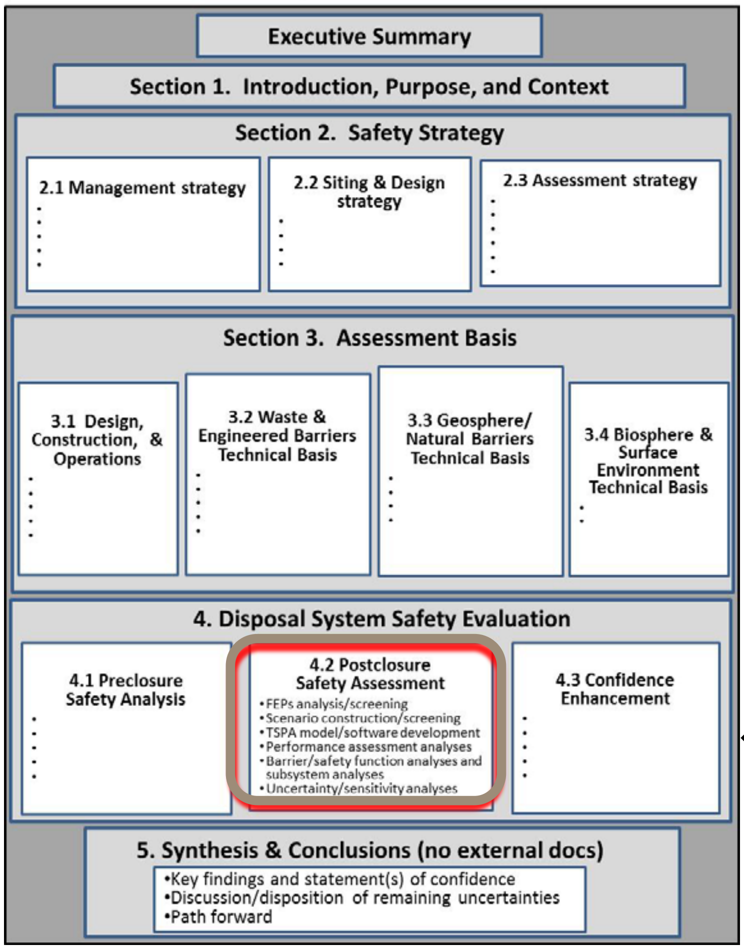
4.3 Confidence Enhancement
- RD&D prioritization
- Natural/anthropogenic analogues
- URL & large-scale validation
- Monitoring and performance confirmation
- International collaboration & peer review

5. Synthesis & Conclusions
- Key findings and statement(s) of confidence
- Discussion/disposition of remaining uncertainties
- Path forward

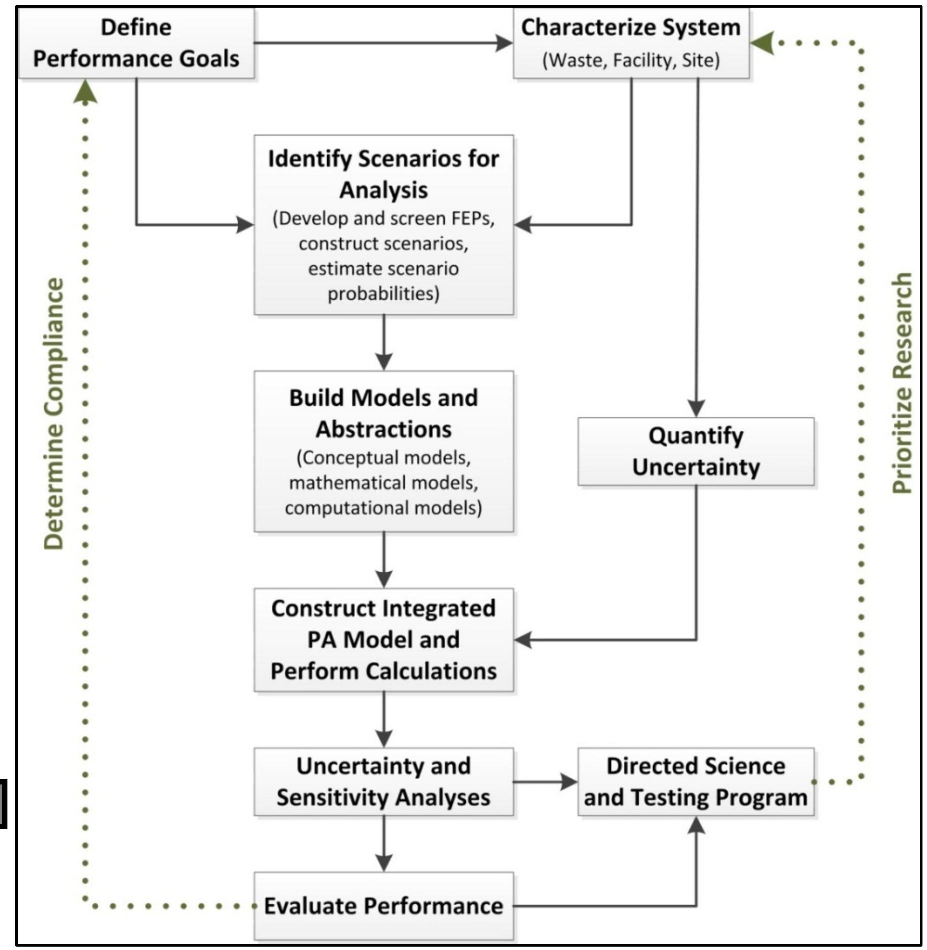
Role of PA in the Safety Case

- ***"Performance assessment is arguably the most important part of the safety case..."*** **(NWTRB 2011)**

Safety Case Structure



Iterative PA Methodology



Role of RD&D in Evolution of the Safety Case

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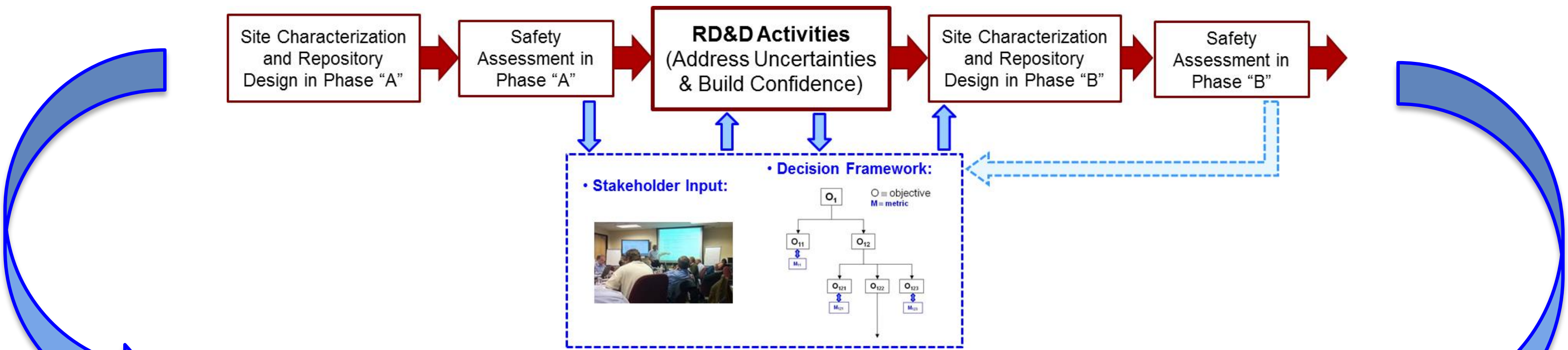
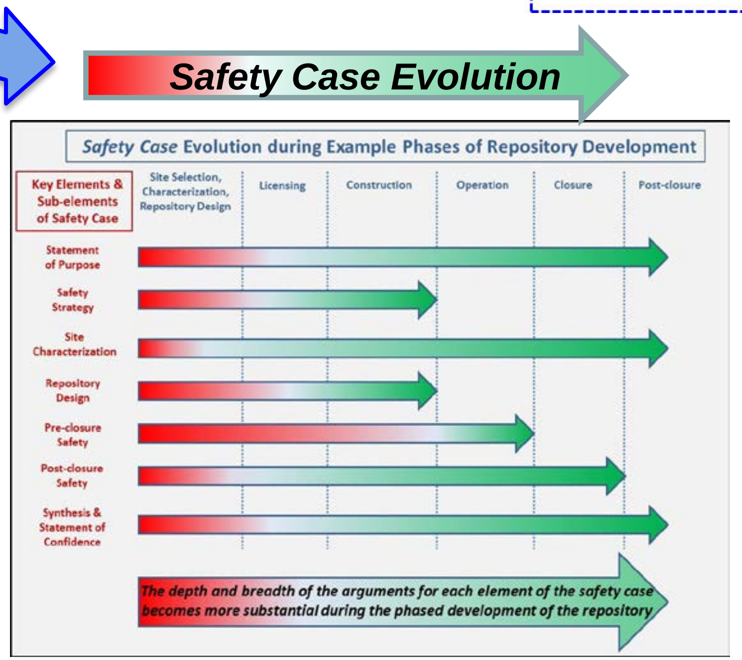
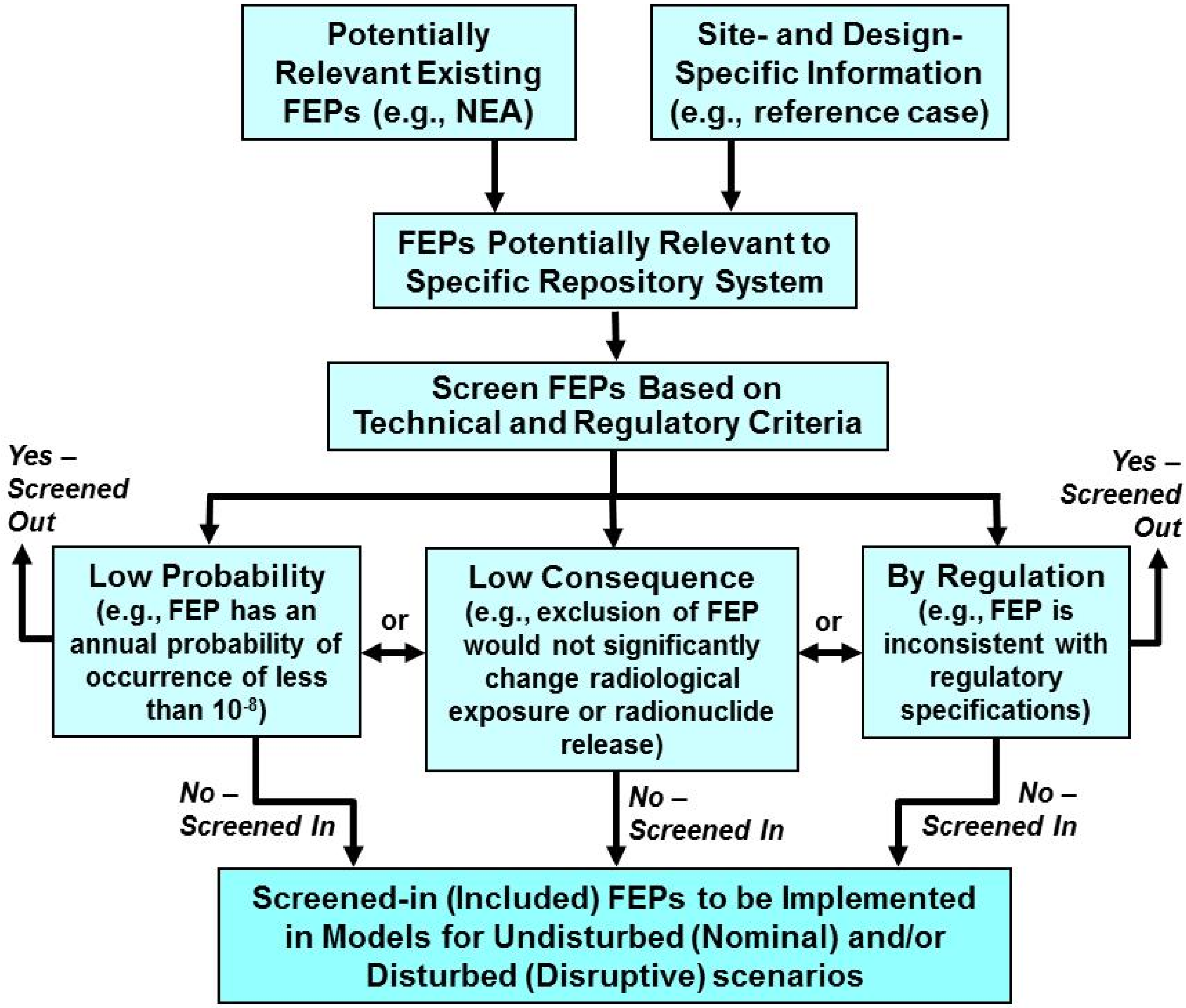
- **Iteration of Safety Assessment and Site Characterization/Design:**





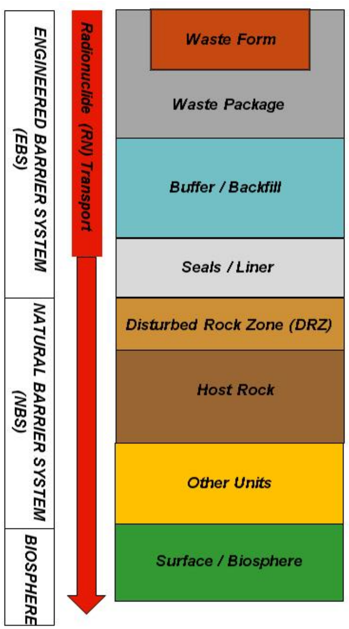
- **Safety case provides a structured framework to assist in prioritizing the technical work in the next phase, to reduce uncertainties and enhance confidence**
- **Safety understanding and the associated technical bases evolve with phases of repository development, via RD&D**

Features, Events, Processes (FEPs) Screening Methodology



FEPs Matrix

Coupled THCMBR Processes and Events

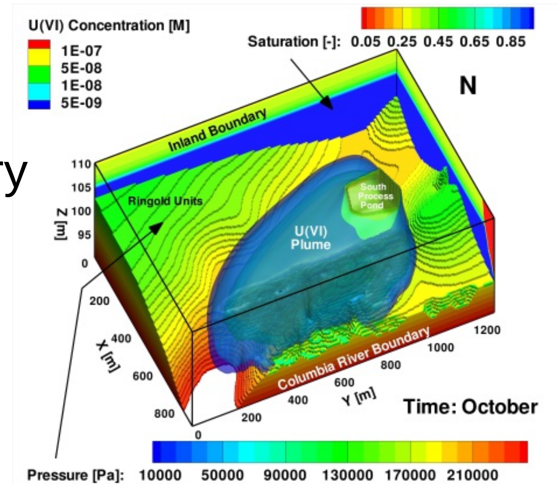


Characteristics, Processes, and Events / Features		Processes											Events					
	Characteristics	Mechanical and Thermal-Mechanical	Hydrological and Thermal-Hydrologic	Chemical and Thermal-Chemical	Biological and Thermal-Biological	Transport and Thermal-Transport	Thermal	Radiological	Long-Term Geologic	Climatic	Human Activities (Long Timescale)	Other	Nuclear Criticality	Early Failure	Seismic	Igneous	Human Activities (Short Timescale)	Other
Waste and Engineered Features																		
Waste Form and Cladding																		
Waste Package and Internals																		
Buffer/Backfill																		
Emplacement Tunnels/Drifts and Mine Workings																		
Seals/Plugs																		
Geosphere Features																		
Host Rock (Repository Horizon)																		
Other Geologic Units (non-Repository Horizon)																		
Surface Features																		
Biosphere																		
System Features																		
Repository System																		

Nuclear Energy

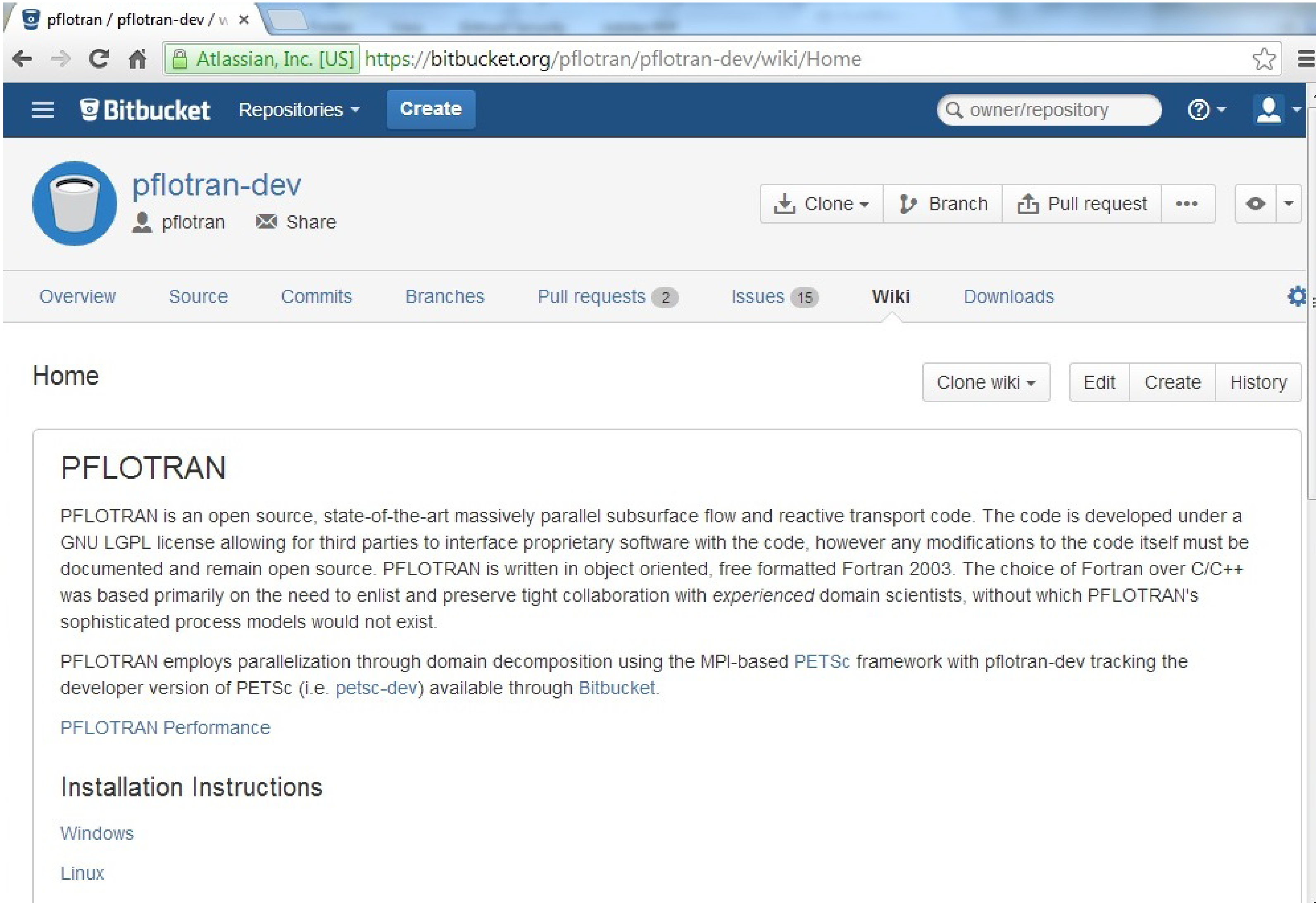
Major Projects Leveraging PFLOTRAN

- **Nuclear Waste Disposal**
  - Waste Isolation Pilot Plant (WIPP)
  - SKB Forsmark Spent Fuel Nuclear Waste Repository
- **Climate (CLM-PFLOTRAN)**
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- **Fate and Transport of Contaminants**
  - PNNL SBR Science Focus Area (Hanford 300 Area)
  - ASCEM (i.e. PFLOTRAN geochemistry)
- **CO2 Sequestration**
  - DOE Fossil Energy: Optimal Model Complexity in Geological Carbon Sequestration (U. Wyoming)
  - DOE Geothermal Technologies: Interactions between Supercritical CO2, Fluid and Rock in EGS Reservoirs



Hammond and Lichtner, WRR, 2010

PFLOTRAN Bitbucket Wiki



PFLOTRAN

PFLOTRAN is an open source, state-of-the-art massively parallel subsurface flow and reactive transport code. The code is developed under a GNU LGPL license allowing for third parties to interface proprietary software with the code, however any modifications to the code itself must be documented and remain open source. PFLOTRAN is written in object oriented, free formatted Fortran 2003. The choice of Fortran over C/C++ was based primarily on the need to enlist and preserve tight collaboration with *experienced* domain scientists, without which PFLOTRAN's sophisticated process models would not exist.

PFLOTRAN employs parallelization through domain decomposition using the MPI-based PETSc framework with pflotran-dev tracking the developer version of PETSc (i.e. petsc-dev) available through Bitbucket.

PFLOTRAN Performance

Installation Instructions

Windows

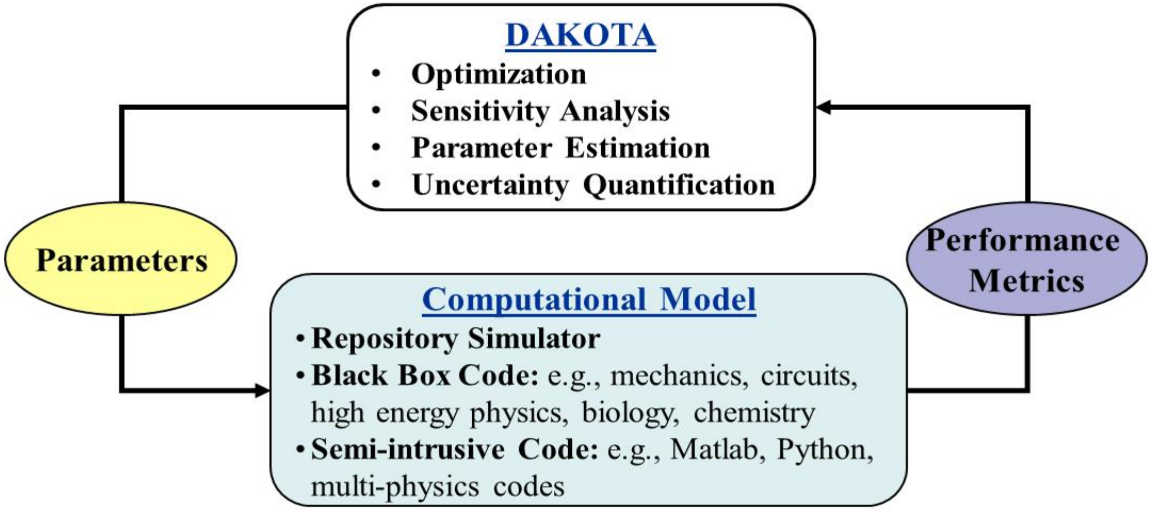
Linux

PFLOTRAN Support Infrastructure

- Mercurial: distributed source control management tool
- Bitbucket: online PFLOTRAN repository
  - `hg clone https://bitbucket.org/pflotran/pflotran-dev`
  - Source tree
  - Commit logs
  - Wiki
    - Installation Instuctions
    - Quick Guide
    - FAQ (entries motivated by questions on mailing list)
  - Change Requests
  - Issue Tracker
- Google Groups: pflotran-users and pflotran-dev mailing lists
- Buildbot: automated building and testing
- Google Analytics: tracks behavior on Bitbucket

DAKOTA Modeling Capabilities

- **Manages uncertainty quantification (UQ), sensitivity analyses (SA), optimization, and calibration**
  - Generic interface to simulations
  - Extensive library of time-tested and advanced algorithms
  - Mixed deterministic / probabilistic analysis
  - Supports scalable parallel computations on clusters
  - Object-oriented code; modern software quality practices



http://dakota.sandia.gov/

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