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GDSA Framework: High-Performance Safety Assessment Software to Support the Safety Case

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Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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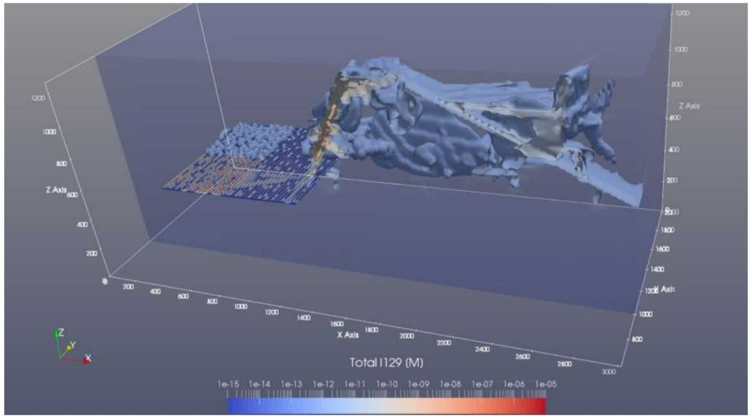
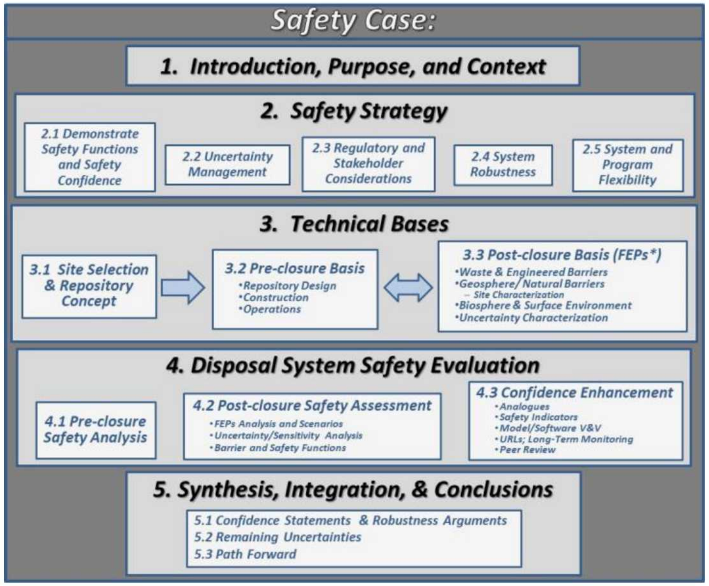
Primary Roles of a Safety Assessment Model

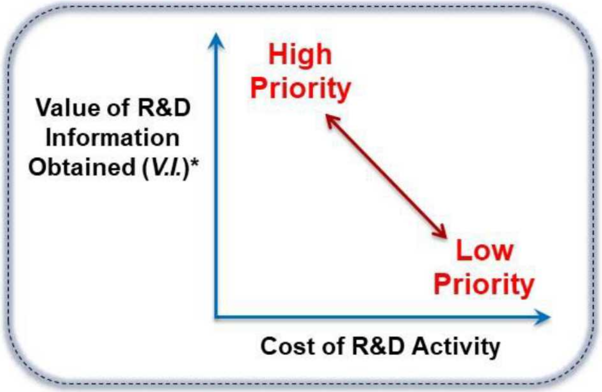
1. Evaluate potential disposal concepts and sites in various host rock media



2. Build confidence in the repository safety case – first *generic*, then *site-specific*



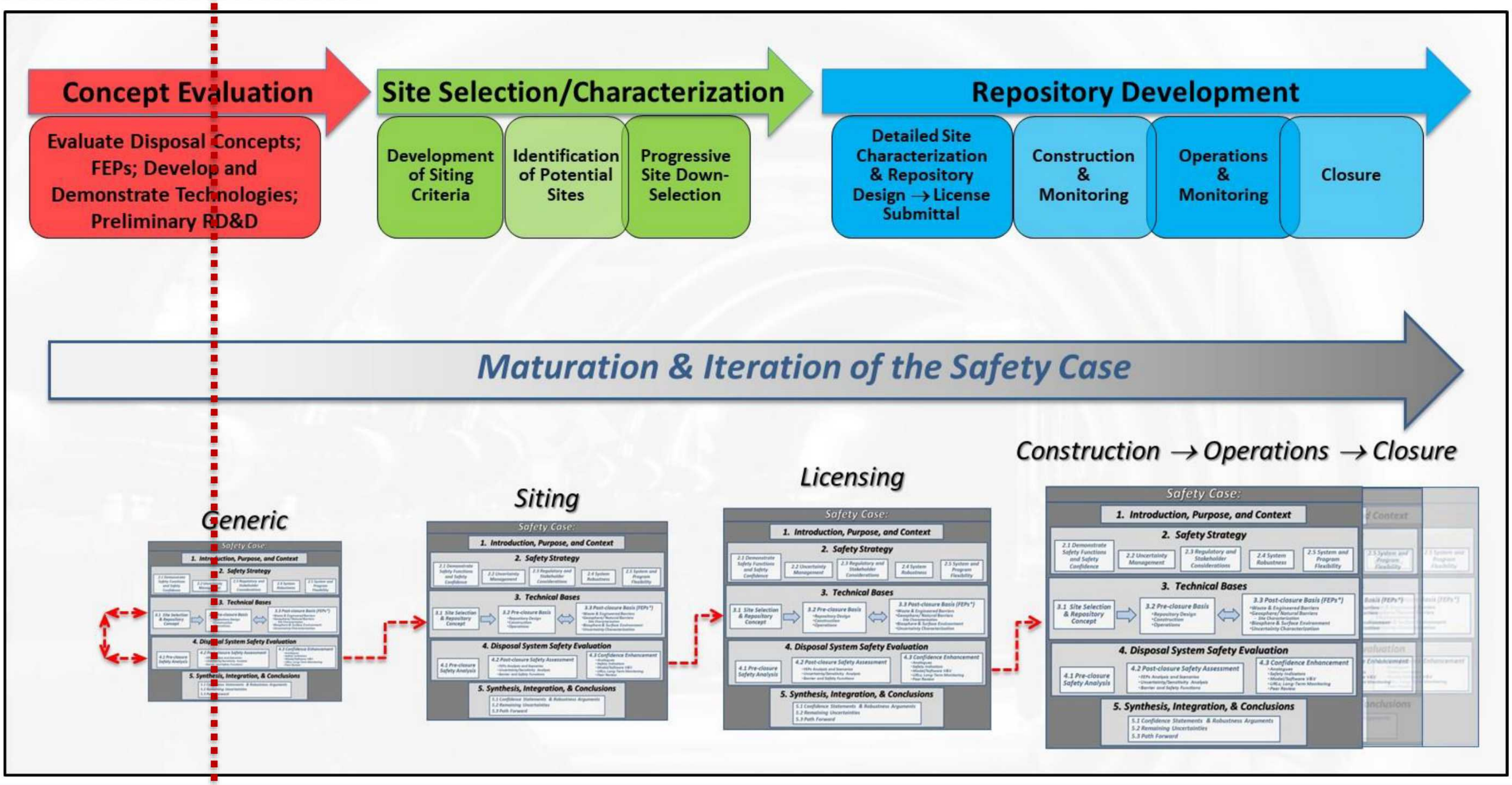
3. Help prioritize R&D activities, through multiple phases of the repository program



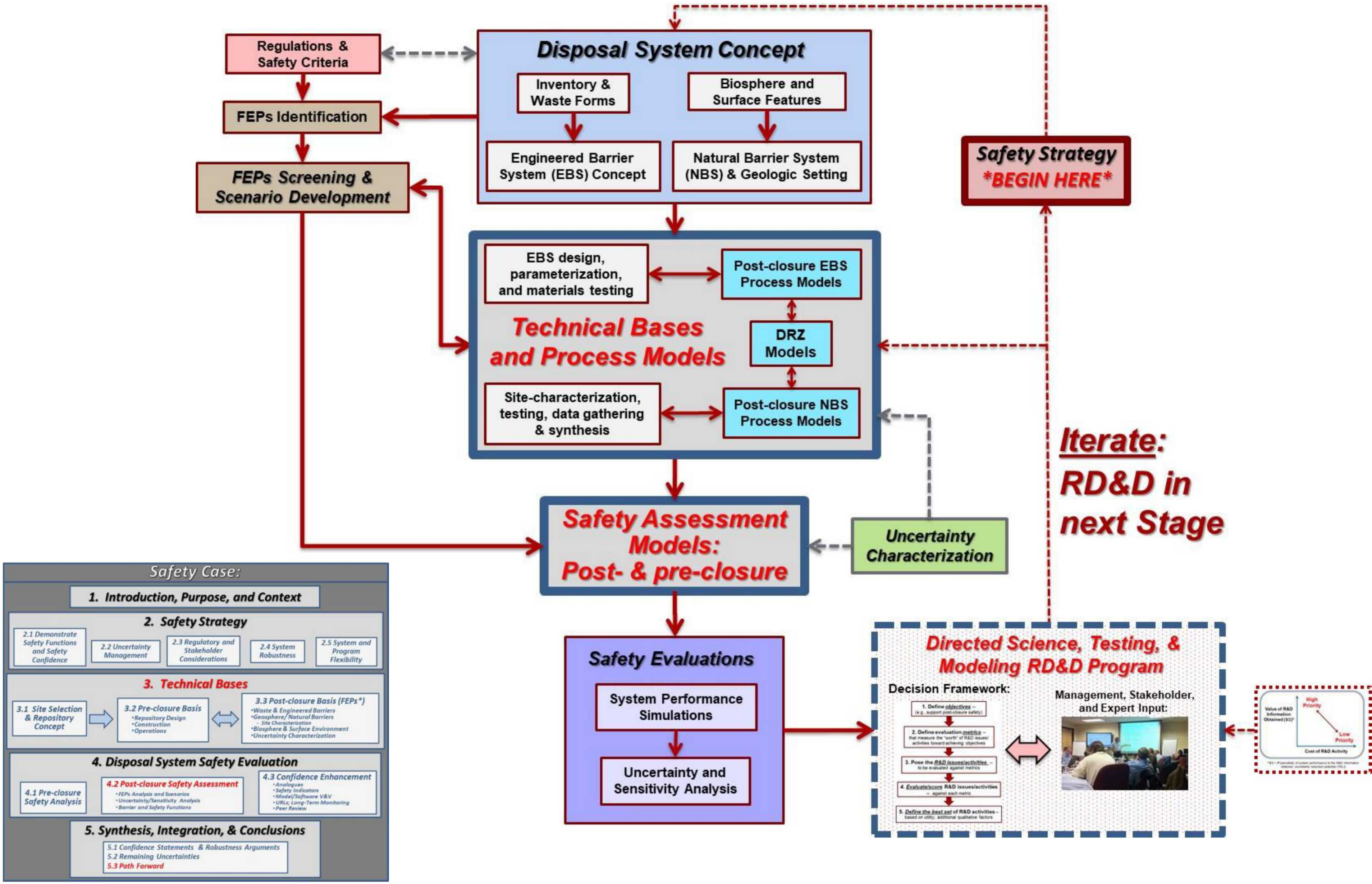
* ***V.I.*** = ***F*** [sensitivity of system performance to the R&D information obtained; uncertainty reduction potential (TRL)]

Phases of a Repository Project
(and maturation of safety case confidence – *Role 2*)

U.S. Program currently:
- Concept Evaluation stage
- “Generic” stage
- Baseline models



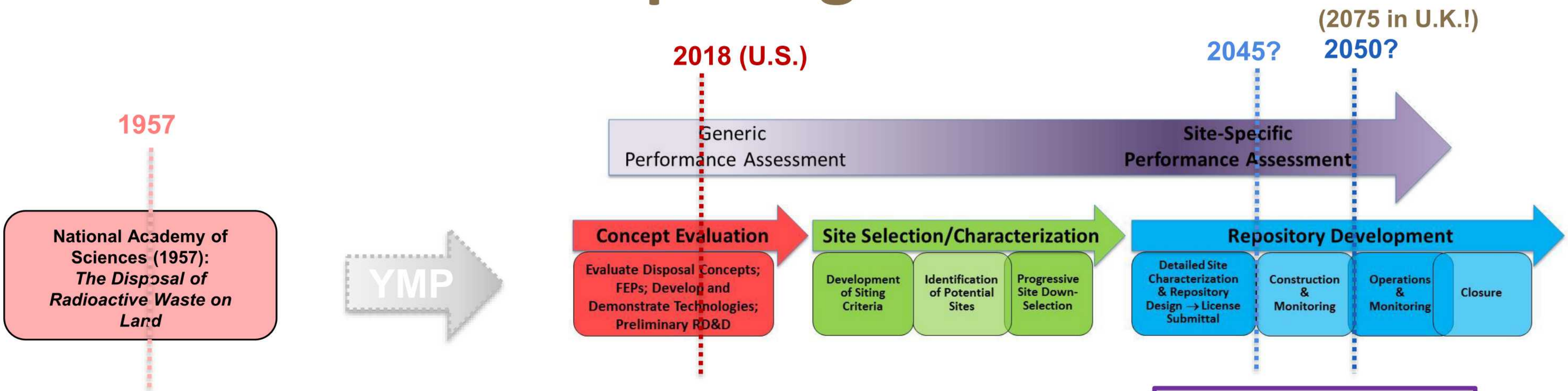
Role 3 – R&D Prioritization Within one Project Phase



Role 1 (and Role 2) – Safety Assessment Model/Software Philosophy

1. **Direct representation in Safety Assessment model of significant coupled multi-physics processes in three dimensions (3-D), over a large heterogeneous domain**
   - *Lessening reliance on assumptions, simplifications, and process abstractions*
2. **Realistic spatial resolution of features and processes**
   - *Explicit representation of all waste packages*
3. **Appropriate quantification and propagation of uncertainties, based on model form and data availability at various spatial scales**
4. **Implementation of a numerical solution and code architecture that uses evolving (a) computer architecture (parallel HPC), (b) software languages, and (c) numerical solution algorithms**

Evolution of Computing Power

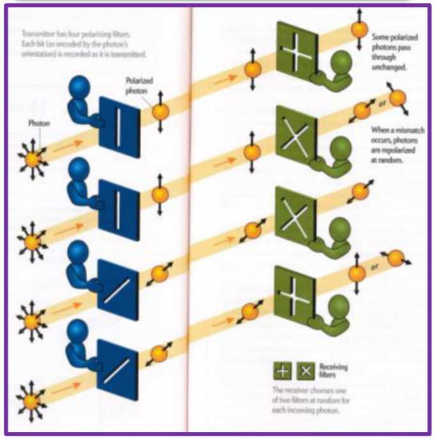


1964:
IBM 360/Model 30
35 x 10^3 IPS
1 CPU, 8 KB Memory

2012:
IBM Blue Gene/Q
10 x 10^{15} FLOPS (petaflops)
786,432 CPUs; 7.86 x 10^{11} KB DRAM

three decades

2045-50?
IBM Quantum
$10^{???}$ FLOPS



"IBM System360 Model 30" by Dave Ross - Flickr: IBM System/360 Model 30. Licensed under CC BY 2.0 via Wikimedia Commons
"Mira - Blue Gene Q at Argonne National Laboratory - Skin" by Courtesy Argonne National Laboratory. Licensed under CC BY 2.0 via Wikimedia Commons
"The Quantum Hack" by Tim Folger, Scientific American, February 2016

(Geologic Disposal Safety Assessment)
GDSA Framework

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Input Parameters
- Parameter database

Computational Support
- Uncertainty Sampling and Sensitivity Analysis — DAKOTA (Explore and predict with confidence.)
- Pre-/Post-Processing — python, dfnWorks
- Visualization — ParaView (Parallel Visualization Application), VisIt

Multi-Physics Simulation and Integration

PFLOTRAN

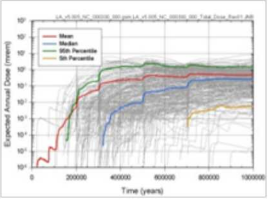
Source Term and EBS Evolution Model
- Inventory
- Decay, ingrowth
- WF degradation
- WP degradation
- Radionuclide release
- Thermal, mechanical
- Gas generation

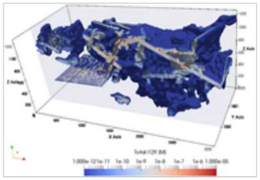
FMDM

Flow and Transport Model
- Advection, diffusion, dispersion
- Discrete fracture networks
- Sorption, solubility, colloids
- Isotope partitioning
- Decay, ingrowth
- Thermal effects
- Chemical reactions

Biosphere Model
- Exposure pathways
- Uptake/ transfer
- Dose calculations

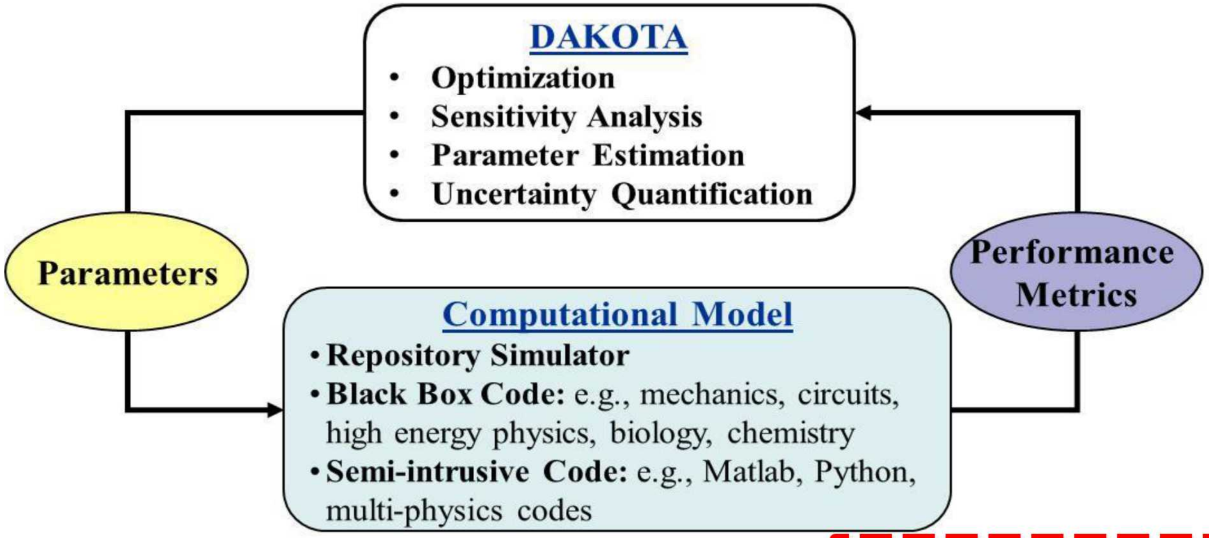
Results





DAKOTA Modeling Capabilities

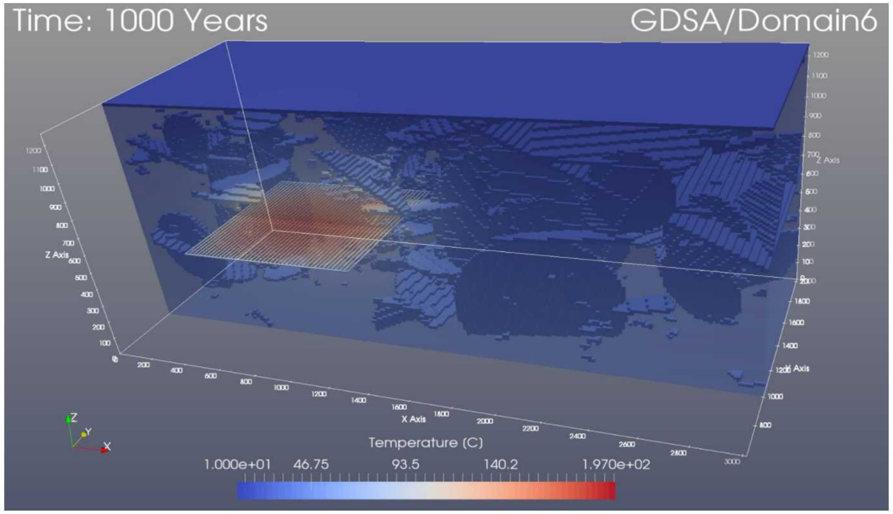
- **Interface between input parameters and domain simulation (PFLOTRAN)**
- **Manages uncertainty quantification (UQ), sensitivity analyses (SA), optimization, and calibration**
  - Object-oriented code; open source
  - Supports scalable parallel computations on clusters
  - Mixed deterministic / probabilistic analysis; aleatory and epistemic uncertainty



http://dakota.sandia.gov/

What is PFLOTRAN?

- **A porous-medium continuum code for modeling:**
  - Multicomponent, multiphase flow & transport
  - Heat conduction & convection
  - Biogeochemical reaction
  - Geomechanics
  - Isotope decay & ingrowth

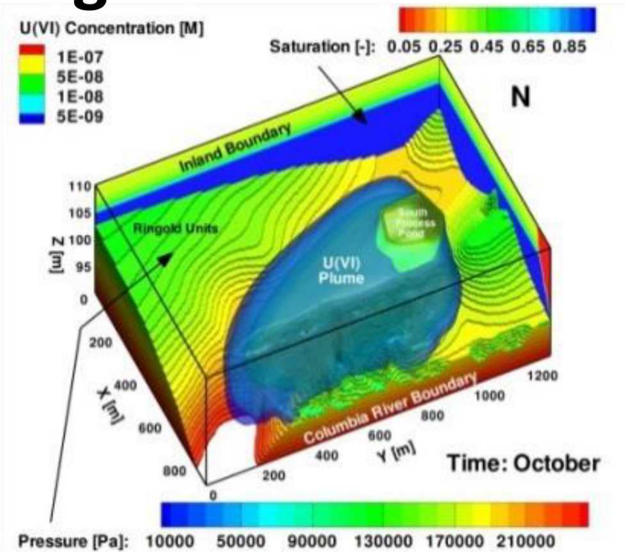


GDSA Framework **Website**

- At http://pa.sandia.gov
- Past reports, latest developments, contact information

Typical Applications of PFLOTRAN

- **Nuclear waste disposal**
  - US DOE – new geologic repository concepts for spent fuel
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - SKB Forsmark spent fuel repository (Sweden, Amphos[21])
- **Climate: coupled overland/groundwater flow**
- **3-D contaminant transport modeling**
- **CO_2 sequestration**
- **Enhanced geothermal energy**
- **Radioisotope tracers**
- **Colloid-facilitated transport**



Hammond and Lichtner, WRR, 2010

Applications of PFLOTRAN

Information from a survey of PFLOTRAN users:

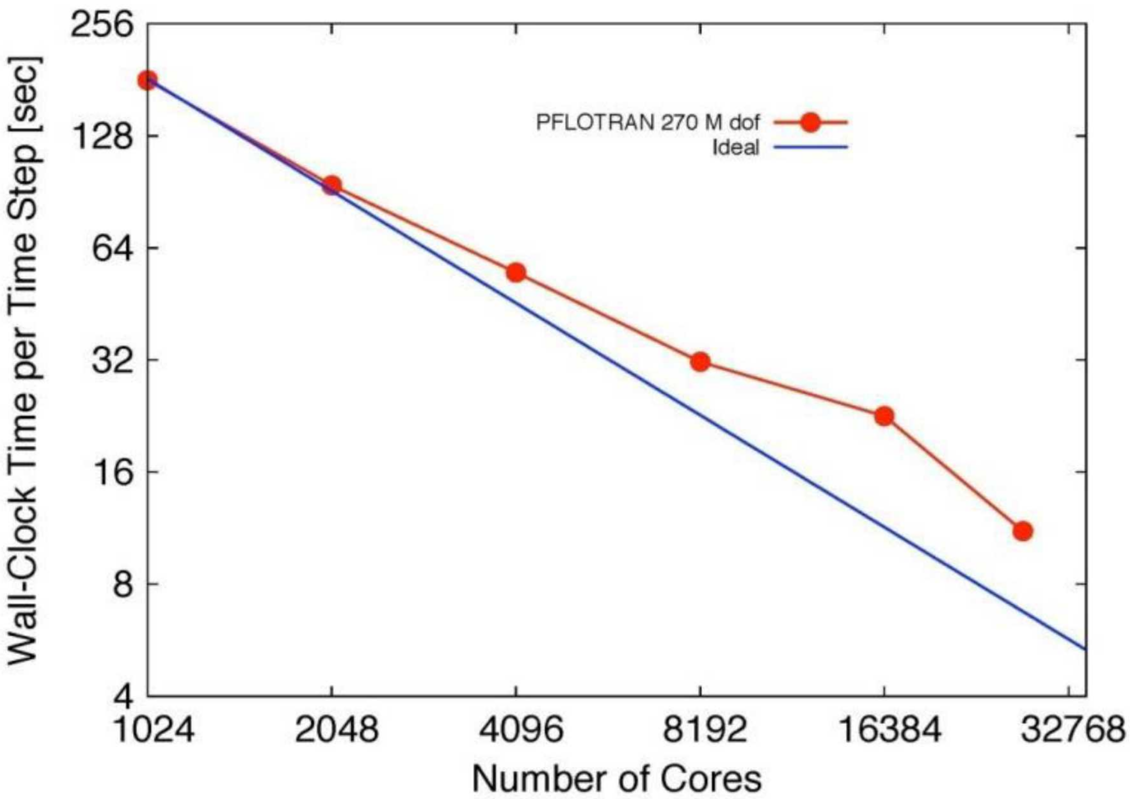
- 3D near-field models of nuclear waste repositories
- Agriculture
- Apatite reactive barrier
- Behind-casing pressure development in well annulus due to N2 injection
- Biogeochemical hot spots/hot moments
- Biogeochemistry within groundwater-river water exchange zones
- CO2 sequestration
- CO2 storage
- Coupled surface/subsurface land mode
- Geothermal Systems
- Groundwater age
- Groundwater management
- Hydrogeochemical evolution
- Interpretation of in-situ through-diffusion experiments
- Modelling of enhanced oil recovery (using CO2 as solvent)
- Modelling of oil and gas reservoirs
- Mountain block recharge beneath soil mantled hill slopes
- Multicomponent transport of trace gases
- Nuclear waste repository performance assessment
- Permafrost modeling
- pH sweep and water quality data analysis
- Radioactive waste management
- Radionuclide transport
- Redox gradients within hyporheic zones
- Remediation design
- Species specific diffusion and Donnan equilibrium in clays
- Subsurface hydrology and geochemistry
- Surface/hill slope hydrology

Why use PFLOTRAN?

- **Open source licensing: LGPL**
  - Freely available
- **Modularly programmed in modern object-oriented Fortran**
- **Founded upon established and supported open source libraries**
  - MPI, PETSc, HDF5, METIS/ParMETIS/CMAKE
- **Demonstrated performance on supercomputers**
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom
  - Scales well to over 10,000 processes

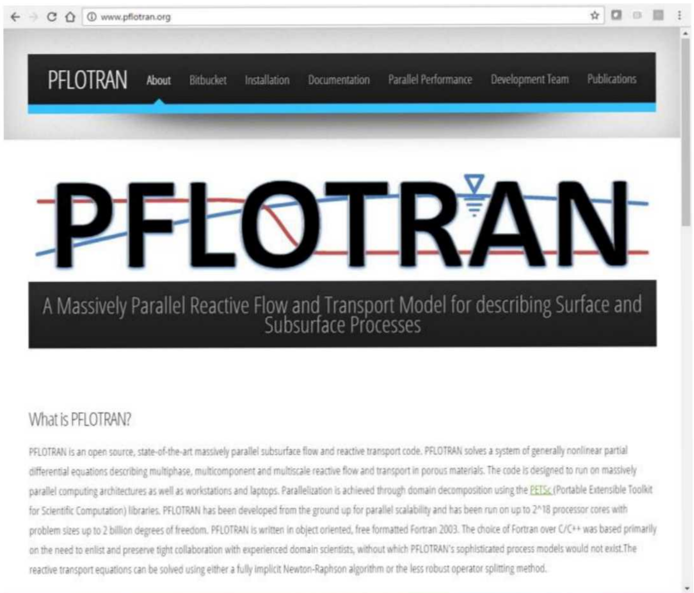
How well does PFLOTRAN scale?

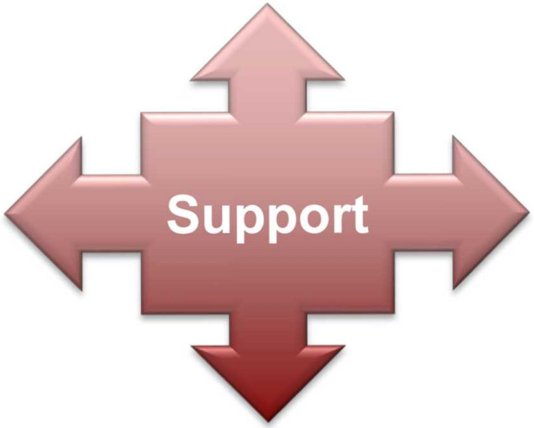
- **Doubling the number of cores nearly cuts run time in half (up to and beyond 10,000 cores)**



Support for PFLOTRAN

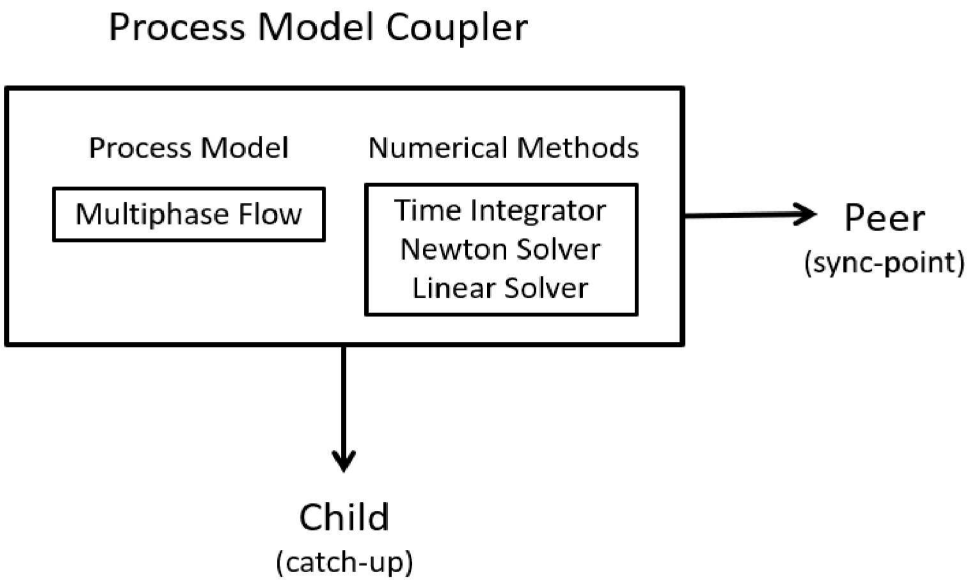
- **Active support infrastructure: www.pflotran.org**
  - Online documentation: documentation.pflotran.org
  - Online access to source code:
    - Git clone bitbucket.org/pflotran/pflotran
  - Automated testing: travis-ci.org/pflotran/pflotran
  - User mailing list: pflotran-users@googlegroups.com





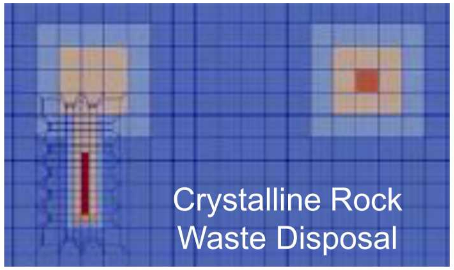
Flexible Process Model Coupling

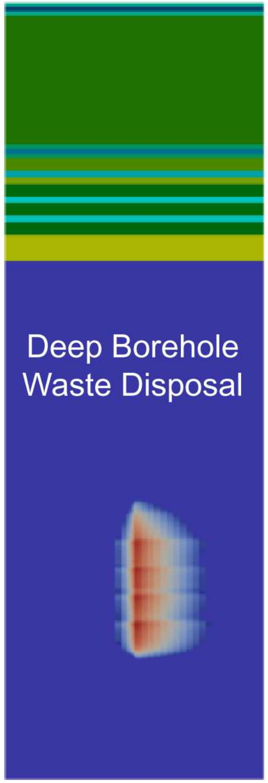
- **Customizable linkage between process models**
  - Flow
  - Transport
  - Reaction
  - Updates to material properties at select times
- **Flexible time stepping**
  - Individual processes may run at their own time scale
- **Modularity for incorporating new process models**
  - Time stepping loops for existing process models are not impacted



Discretization and Numerical Methods

- **Spatial discretization**
  - Finite volume (2-point flux default)
  - Structured and unstructured grids
- **Time discretization: fully-implicit backward Euler**
- **Nonlinear solver**
  - Newton-Raphson
  - Line search/damping with custom convergence criteria
- **Linear solver: direct (LU) or iterative (BiCGStab)**
- **Multi-physics coupling**
  - Flow and transport/reaction: sequential
  - Transport and reaction: global implicit
  - Geomechanics and flow/transport: sequential
  - Geophysics and flow/transport: sequential





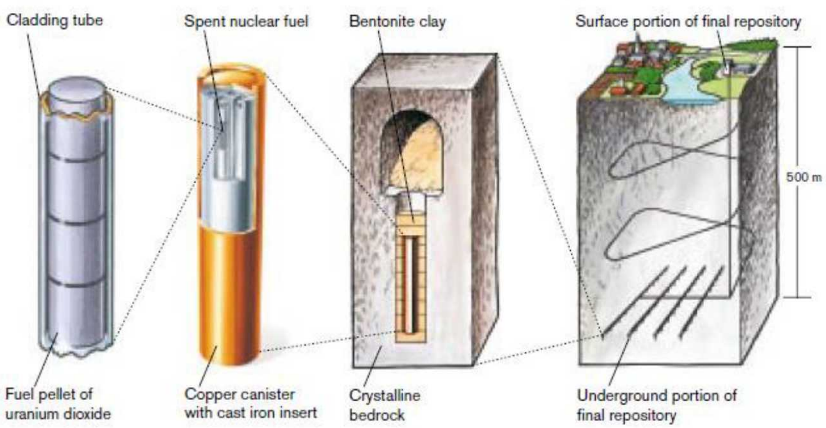
Stein 2015

Generic Repository Reference Case

- ***Reference Case* is a surrogate for site- and design-specific information not yet available during the current Concept Evaluation Phase**
  - Documents information and assumptions for *generic* disposal system models
  - Helps ensure consistency across analyses (e.g., PA, process modeling, UA/SA)
  - Initial focus on the undisturbed scenario (e.g., performance in the absence of external natural or human-induced events)

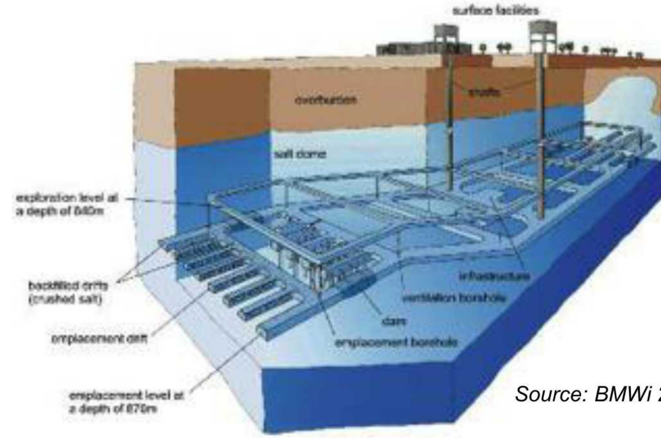
Disposal Concepts Being Examined (with corresponding generic reference cases)

Mined repository in granite or other hard rock



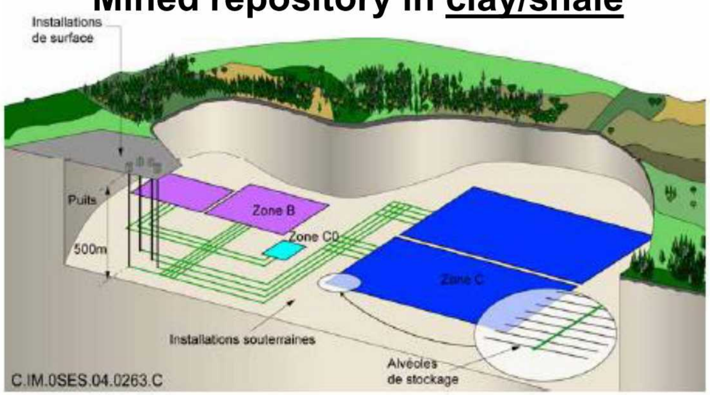
Source: SKB 2011, Figure S-1.

Mined repository in bedded salt



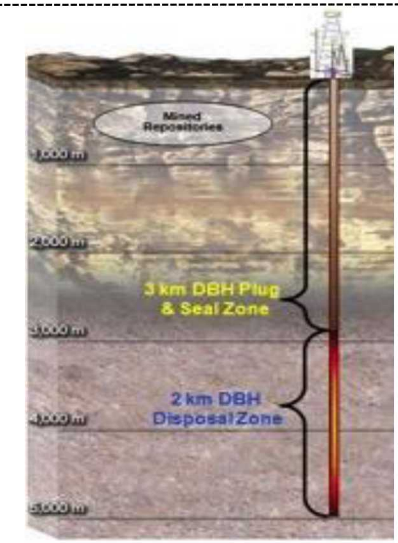
Source: BMWi 2008, Figure 15.

Mined repository in clay/shale

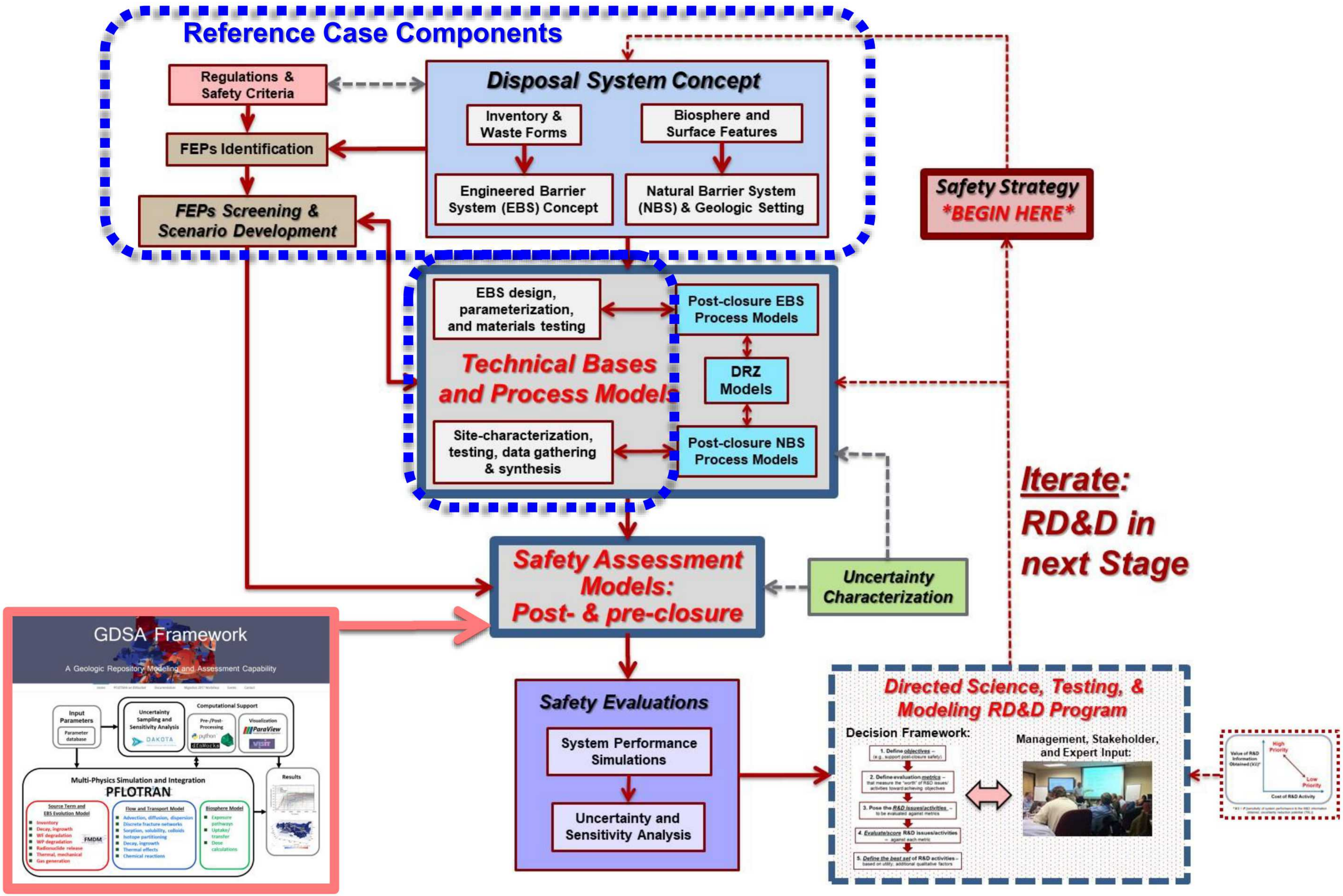


Source: ANDRA 2005b.

Deep borehole in crystalline basement rock

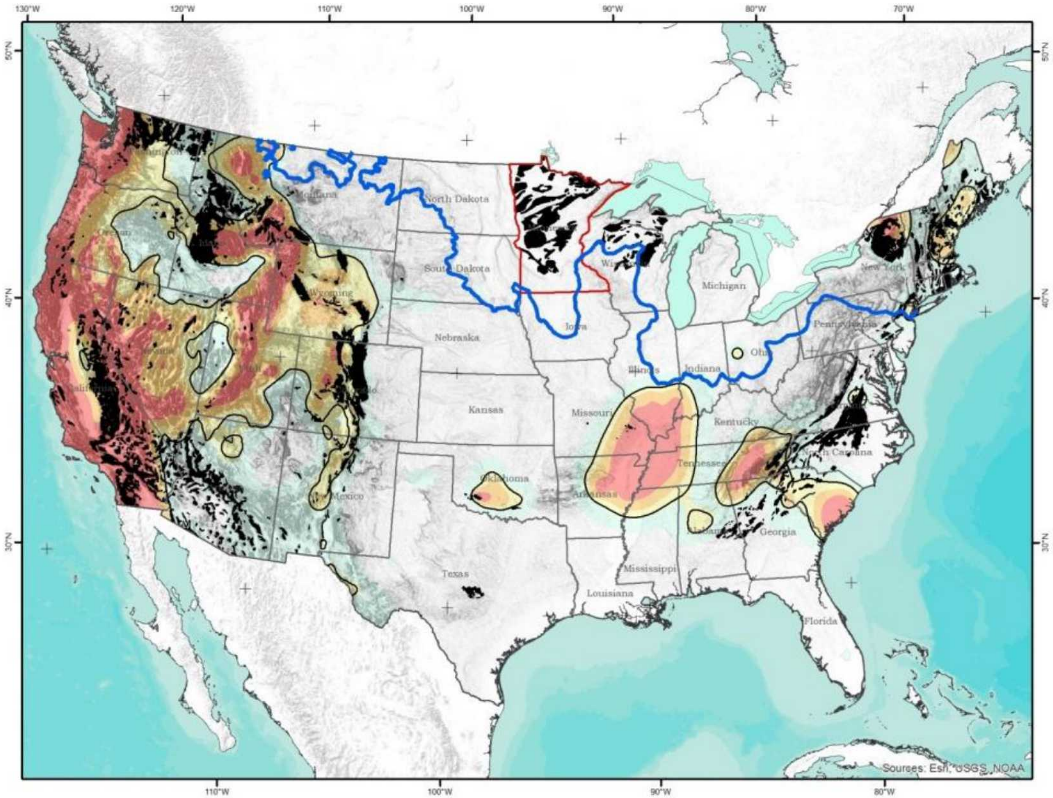


Reference Case Components of Safety Assessment



Crystalline Reference Case

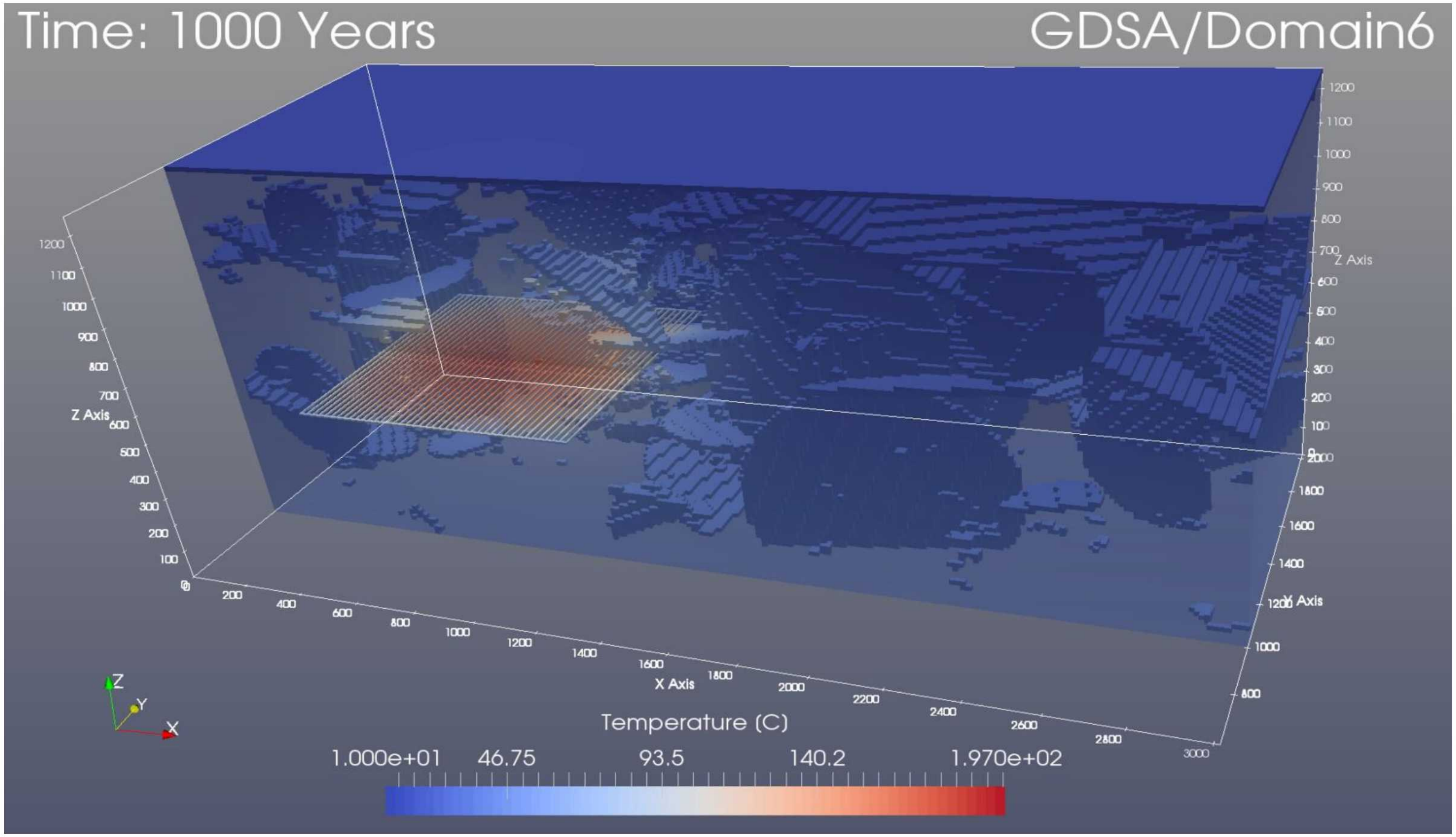
- **Characteristics of *crystalline rock* as a geologic disposal medium:**
  - High structural strength, which stabilizes engineered barriers (unique)
  - Low permeability (~ 10^{-20} m^2)
  - Typically reducing pore waters (which limit radionuclide solubility)
  - High sorption capacity
  - Potentially connected fracture network – adversely affecting isolation if present



Locations of crystalline rock outcrop and near-surface subcrop in the US (black). **Regions of high seismic hazard shown in warm color shading.** **Blue line is the maximum extent of the last glacial maximum (Perry et al. 2016)**

Crystalline Reference Case

- **Crystalline Host-Rock Repository**
  - In drift 12-PWR disposal, 3360 WPs (1/4 size), 168 drifts, 20 m apart
  - Fractures generated by dfnWorks, mapped to porous media mesh



Crystalline Reference Case

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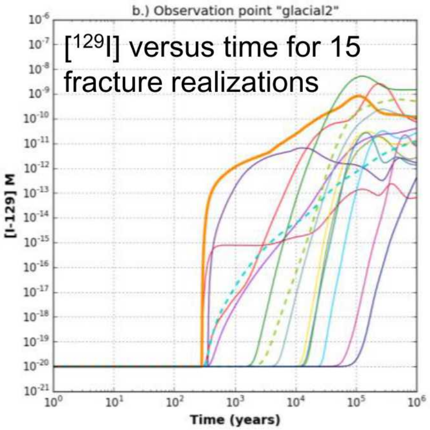
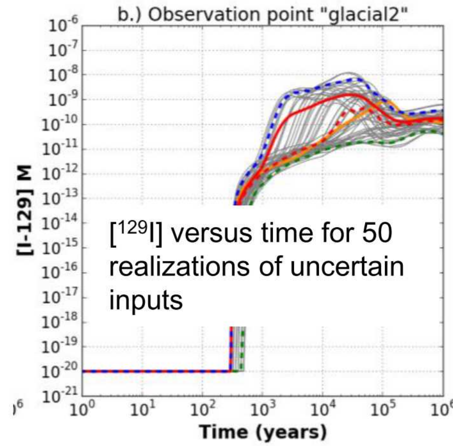
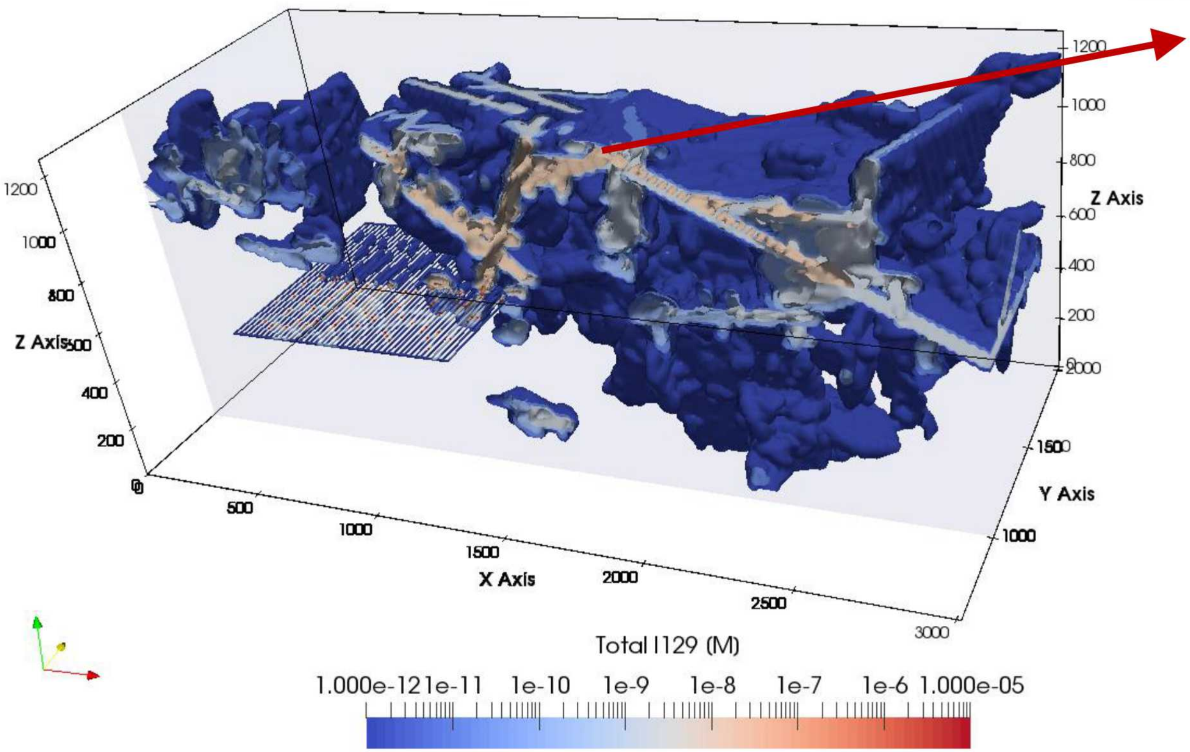
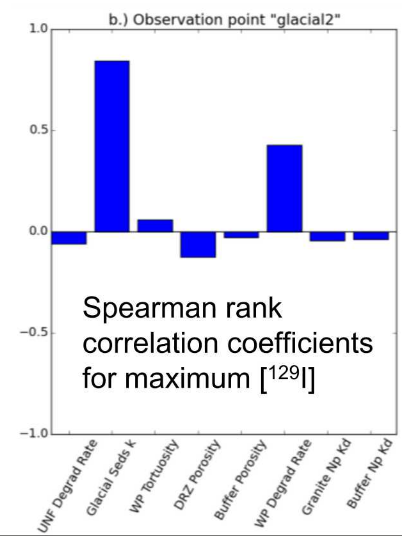
- **Crystalline Repository Simulations**
  - Breakthrough of ^{129}I (at surface) highly sensitive to fracture distribution
    - Also sensitive to sediments permeability and waste package degradation rate









Parameter	Range	Units	Distribution
UNF Dissolution Rate	10^{-8} – 10^{-6}	yr^{-1}	log uniform
Mean Waste Package Degradation Rate	$10^{-5.5}$ – $10^{-4.5}$	yr^{-1}	log uniform
Waste Package τ	0.01 - 1.0		log uniform
Bentonite ϕ	0.3 - 0.5		uniform
DRZ ϕ	0.005 - 0.05		uniform
Np K_d bentonite	0.1 – 702	m^3kg^{-1}	log uniform
Np K_d natural barrier	1.26 x 10^5 – 5.37 x 10^7	m^3kg^{-1}	log uniform

Other Recent Repository Applications

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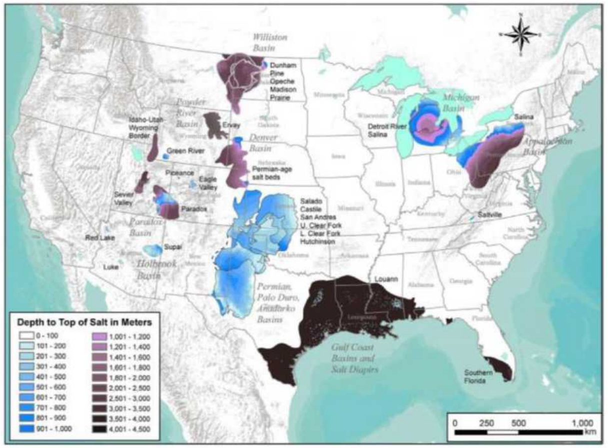
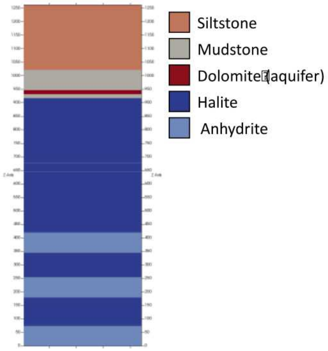
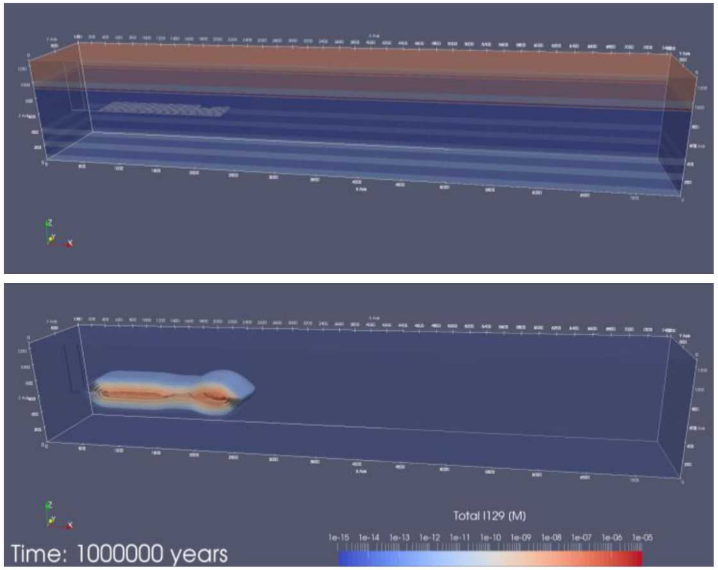
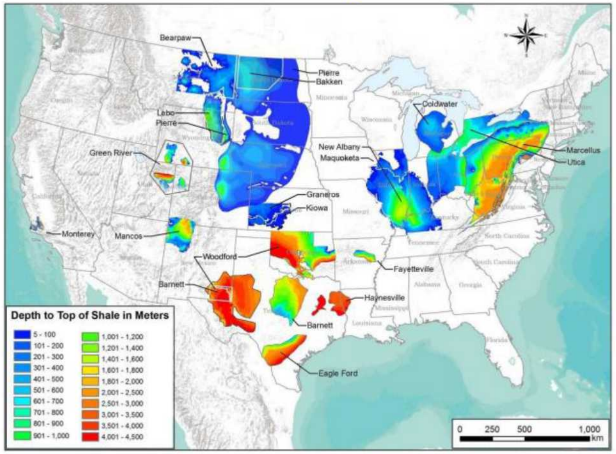
Generic Bedded Salt

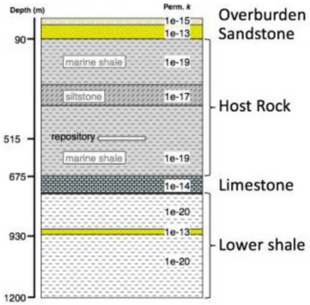


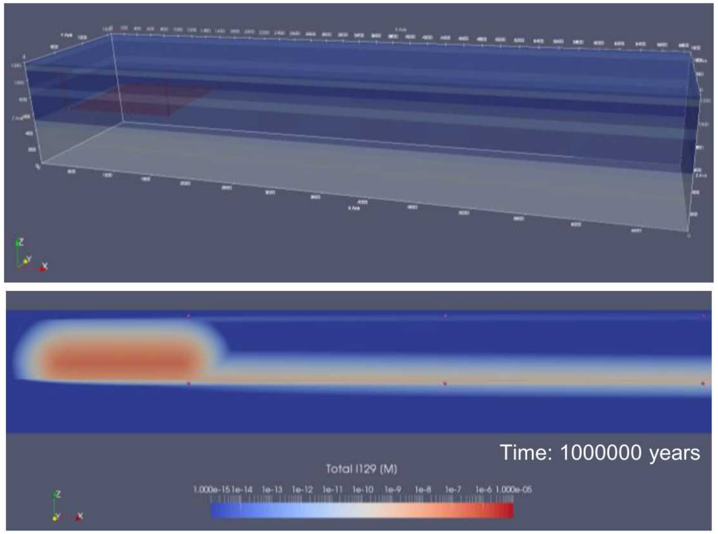




Generic Clay/Shale







Questions?

Backup Slides

Components of Generic Safety Case

Safety Case:

1. Introduction, Purpose, and Context

2. Safety Strategy

2.1 Management Strategy
- a. Organizational/mgmt. structure
- b. Safety culture & QA
- c. Planning and Work Control
- d. Knowledge management
- e. Oversight groups

2.2 Siting & Design Strategy
- a. National laws
- b. Site selection basis & robustness
- c. Design requirements
- d. Disposal concepts
- e. Intergenerational equity

2.3 Assessment Strategy
- a. Regulations and rules
- b. Performance goals/safety criteria
- c. Safety functions/multiple barriers
- d. Uncertainty characterization
- e. RD&D prioritization guidance

3. Technical Bases

3.1 Site Selection
- a. Consent-based siting methodology
- b. Repository concept selection
- c. FEPs Identification
- d. Technology development
- e. Transportation considerations
- f. Integration with storage facilities

3.2 Pre-closure Basis
- a. Repository design & layout
- b. Waste package design
- c. Construction requirements & schedule
- d. Operations & surface facility
- e. Waste acceptance criteria
- f. Impact of pre-closure activities on post-closure

3.3 Post-closure Bases (FEPs)

3.3.1 Waste & Engineered Barriers Technical Basis
- a. Inventory characterization
- b. WF/WP technical basis
- c. Buffer/backfill technical basis
- d. Shafts/seals technical basis
- e. UQ (aleatory, epistemic)

3.3.2 Geosphere/ Natural Barriers Technical Basis
- a. Site characterization
- b. Host rock/DRZ technical basis
- c. Aquifer/other geologic units technical basis
- d. UQ (aleatory, epistemic)

3.3.3 Biosphere Technical Basis
- a. Biosphere & surface environment:
  - Surface environment
  - Flora & fauna
  - Human behavior

Most generic R&D issues/activities are for these two major safety case elements

4. Disposal System Safety Evaluation

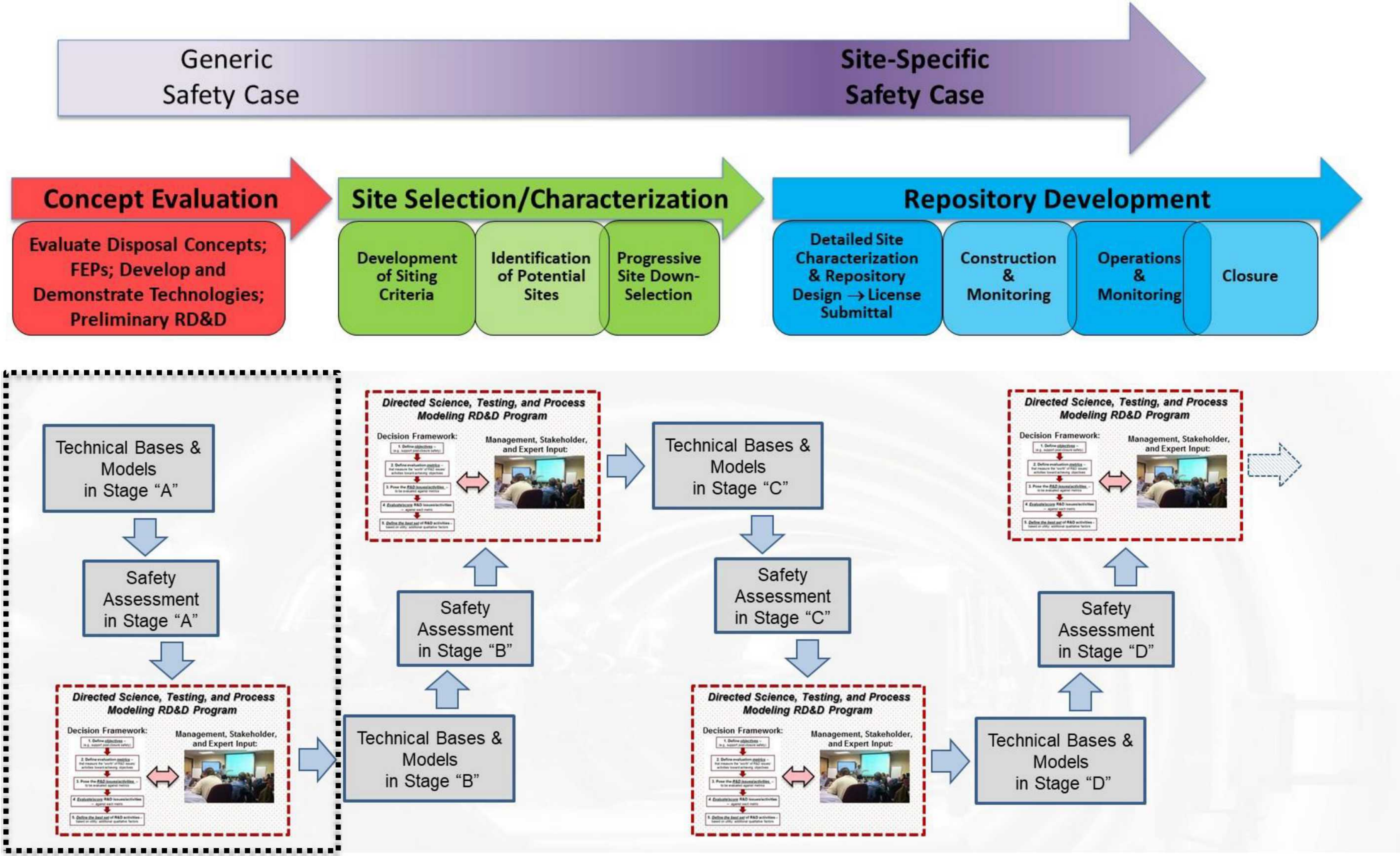
4.1 Pre-closure Safety Analysis
- a. Surface facilities and packaging
- b. Mining and drilling
- c. Underground transfer and handling
- d. Emplacement operations
- e. Design basis events & probabilities
- f. Pre-closure model/software validation
- g. Criticality analyses
- h. Dose/consequence analyses

4.2 Post-closure Safety Assessment
- a. FEPs analysis/screening
- b. Scenario construction/screening
- c. PA model/software validation
- d. Barrier/safety function analyses and subsystem analyses
- e. PA Model Analyses/Results
- f. Uncertainty characterization and analysis
- g. Sensitivity analyses

4.3 Confidence Enhancement
- a. R&D prioritization
- b. Natural/anthropogenic analogues
- c. URL & large-scale demonstrations
- d. Monitoring and performance confirmation
- e. International collaboration & peer review
- f. Verification, validation, transparency
- g. Qualitative and robustness arguments

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

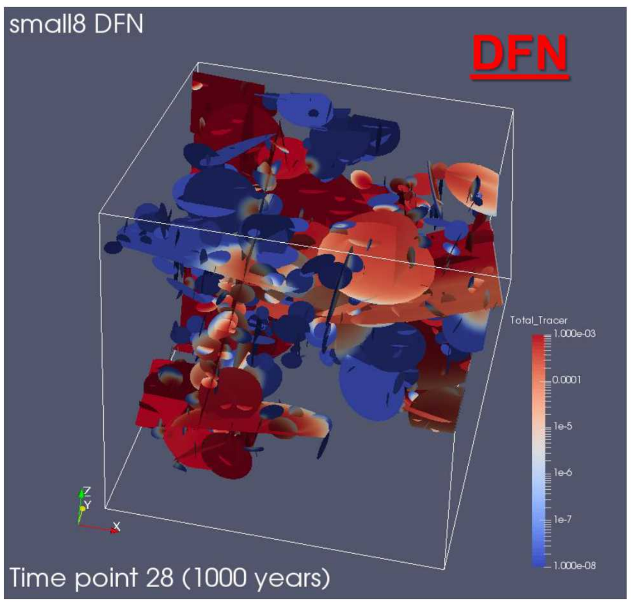
Evolution/Iteration of Technical Bases & Safety Assessment through R&D – *Role 3*

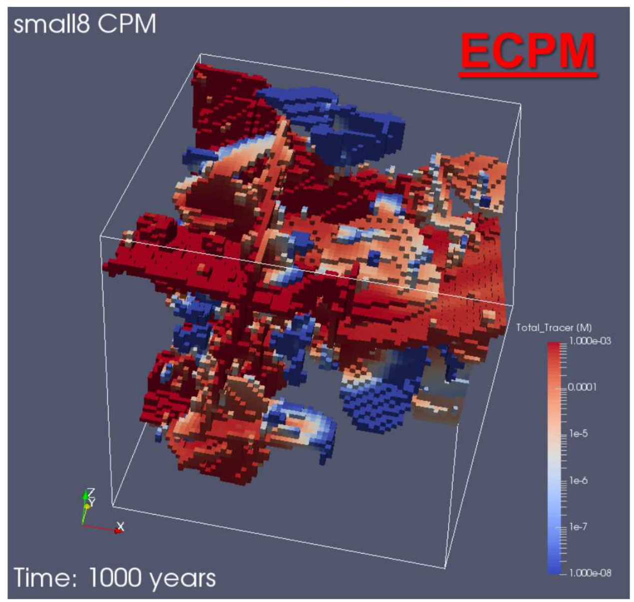


Representation of Flow in Fractures

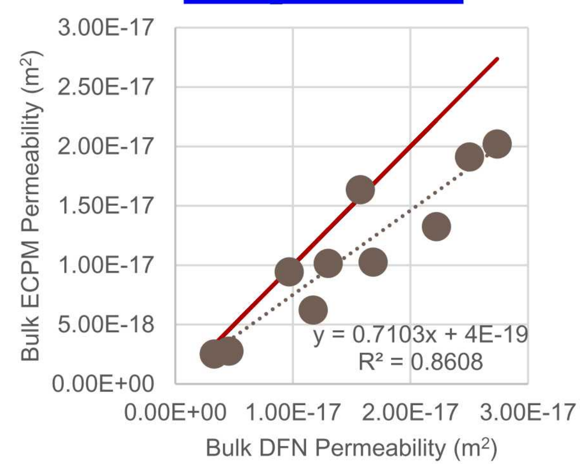
- **Discrete fracture networks (DFNs) are commonly used to model isothermal fluid flow and radionuclide transport in fractured rock:**
  - Stochastically generated network of 2-D fracture planes distributed in 3-D domain
  - Does not include the effects of heat on fluid flow
- ***GDSA Framework* has mapped a DFN (generated with dfnWorks) to an equivalent continuous porous medium (ECPM) in PFLOTRAN**
  - Determines which ECPM 3-D grid cells are intersected by DFN fracture planes
  - Adjusts anisotropic permeability and porosity of ECPM “fracture cells” to represent those same properties of the DFN

Tracer distribution comparison at 1000 years:



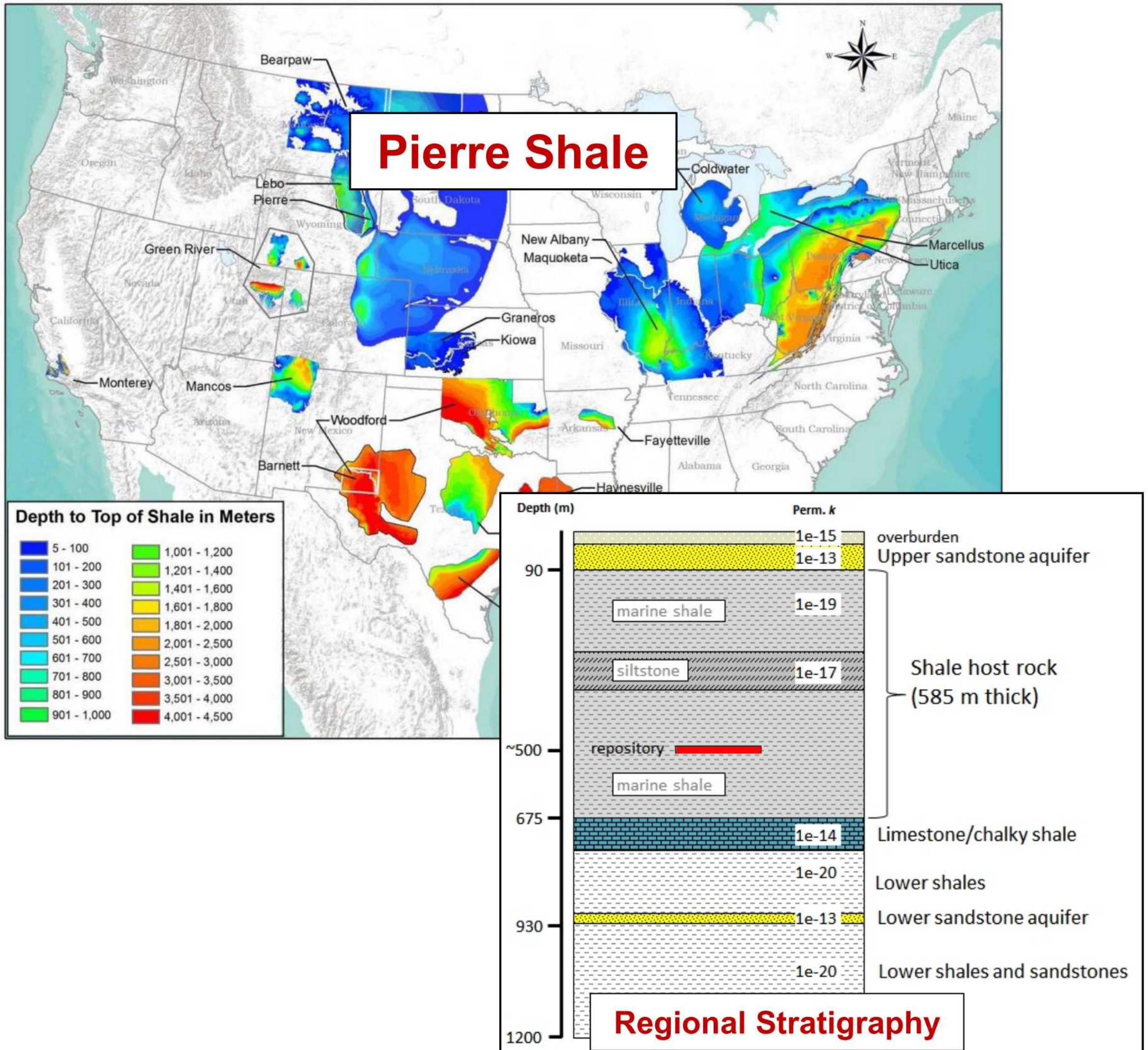


Bulk permeability comparison:*



* Stein et al. 2017 (at IHLRWM 2017 in Charlotte)

Argillite Reference Case

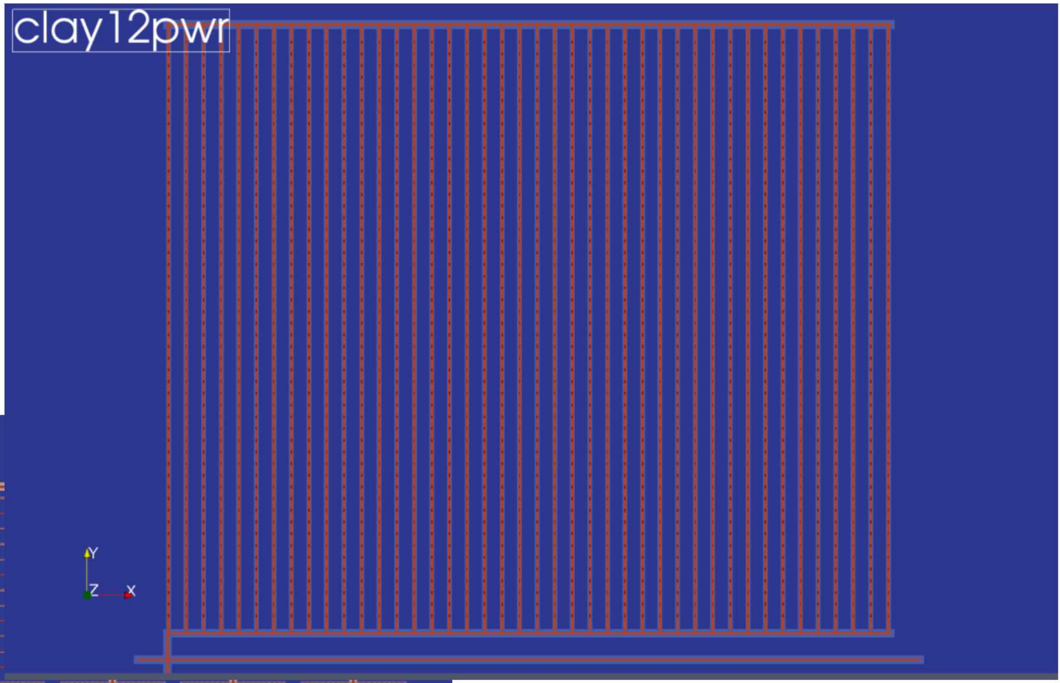


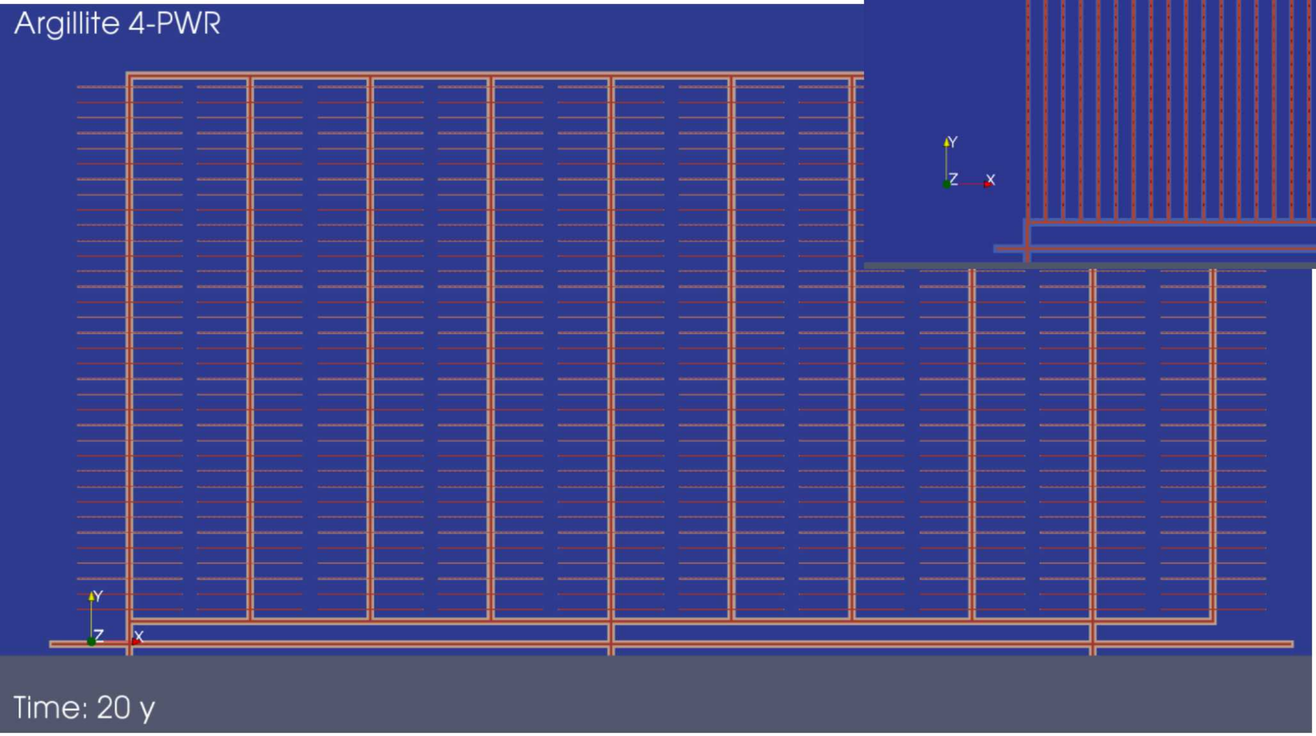
Data feeds and conceptual model to support GDSA reference case

- Hydrologic properties of the Pierre Shale host rock and adjacent formations
- Implications of fluid pressure anomalies in shale
- Groundwater chemistry
- Other processes or events relevant to the safety case (seismicity, human intrusion)

Argillite Reference Case

- **Two shale repository models**
  - In drift 12-PWR disposal
  - Horizontal borehole 4-PWR disposal

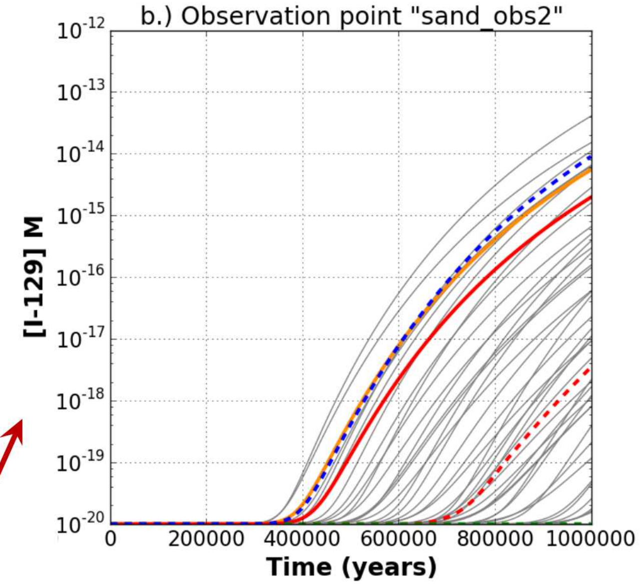


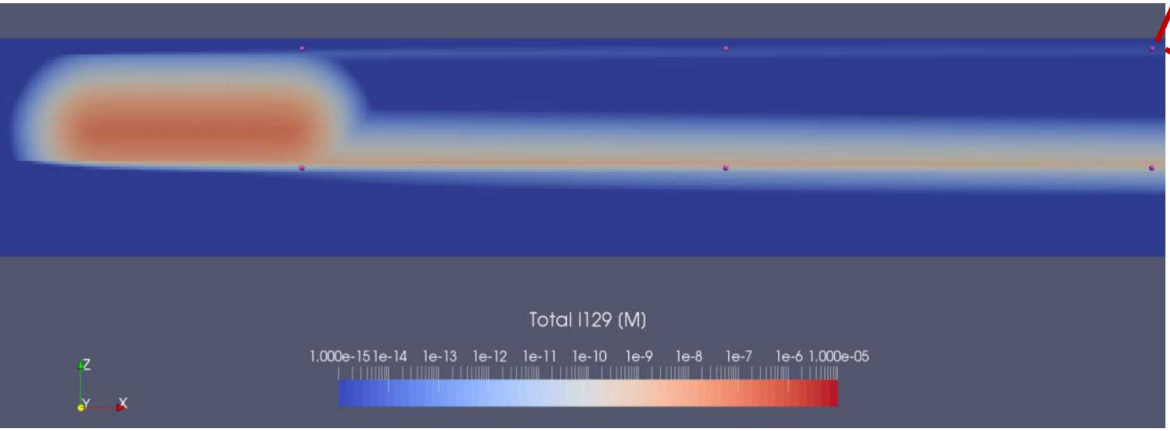


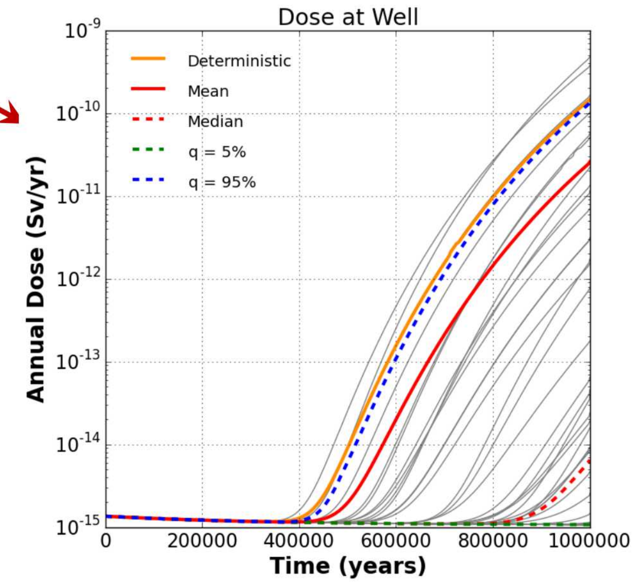
  - Both are mirrored in the negative Y direction

Argillite Reference Case

- **Shale repository simulation**
  - 4-PWR and 12-PWR repository layouts provide similar performance
  - Diffusive transport through shale
  - ^{129}I concentration remains below 10^{-12} M in upper sandy aquifer up to 10^{6} y
    - Dose remains far below IAEA rec. limit of 10^{-3} Sv/yr
  - ^{129}I concentration remains below 10^{-8} M in lower limestone aquifer up to 10^{6} y



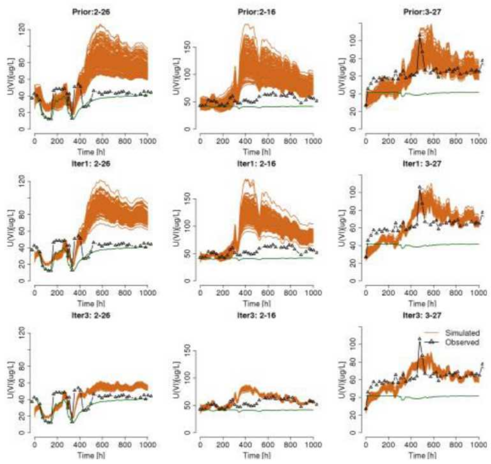




PFLOTRAN Computing Capability

- **High-Performance Computing (HPC)**
  - Increasingly mechanistic process models
  - Highly-refined 3D discretizations
  - Massive probabilistic runs
- **Open Source Collaboration**
  - Leverages a diverse scientific community
  - Sharing among subject matter experts and stakeholders from labs/universities
- **Modern Fortran (2003/2008)**
  - Domain scientists remain engaged
  - Modular framework for customization
- **Leverages Existing Capabilities**
  - Meshing, visualization, HPC solvers, etc.
  - Configuration management, testing, and QA

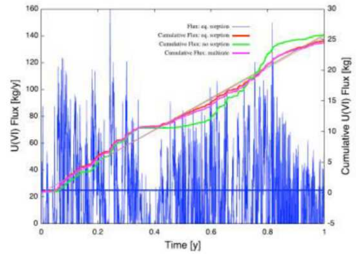
Data Assimilation



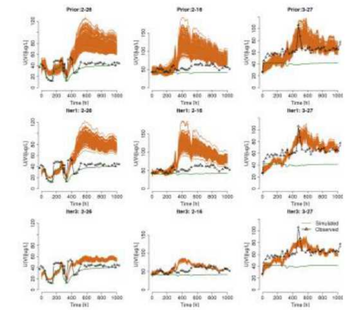
Xingyuan Chen, PNNL, 2011

PFLOTRAN Output Formats

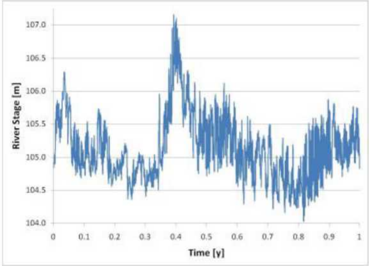
- Excel: *.tec [POINT]
- gnuplot: *.tec [POINT]
- MATLAB: *.tec [POINT], *.h5
- Matplotlib: *.tec [POINT]
- Tecplot : *.tec [POINT, BLOCK, FEBRICK]
- ParaView: *.h5, *.xmf, *.vtk
- R *.tec [POINT], *.h5
- VisIt *.h5, *.xmf, *.vtk



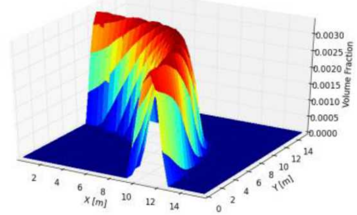
gnuplot



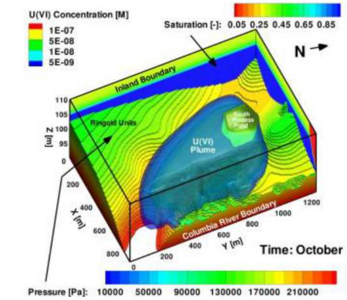
R



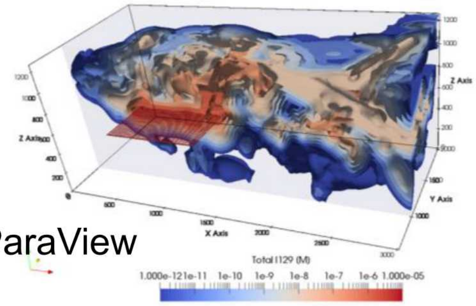
Excel



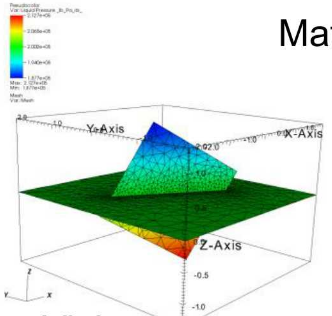
Matplotlib



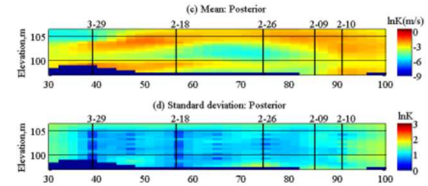
Tecplot



ParaView



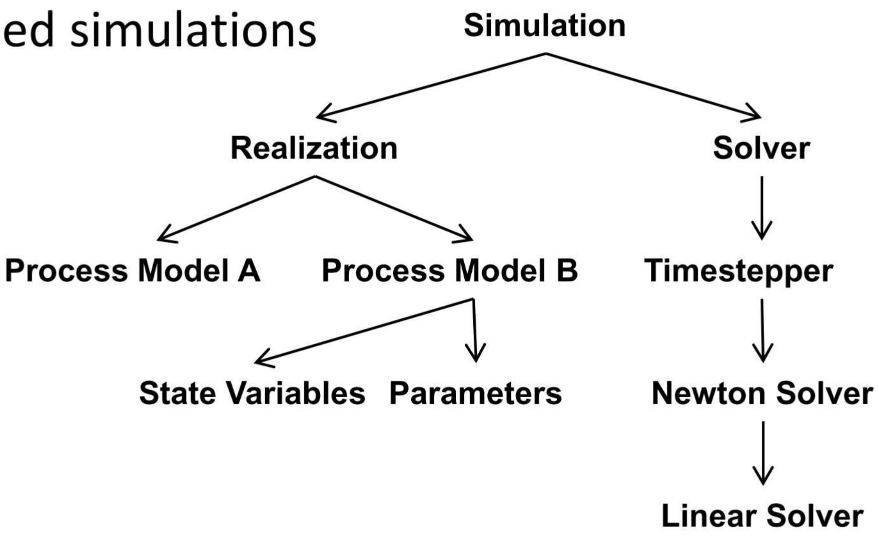
VisIt



MATLAB

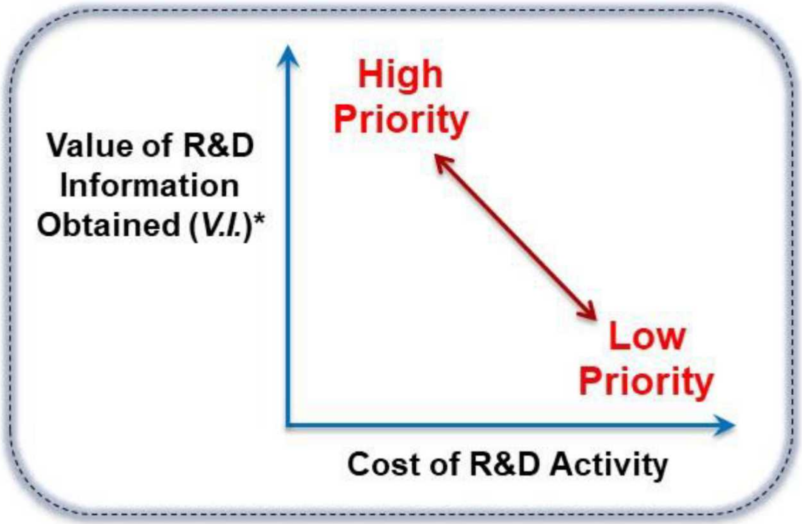
Why Object-Oriented Fortran 2003/2008?

- **Why Fortran?**
  - Experienced domain scientists remain engaged
  - Commonality among all domain scientists
- **Why object-oriented?**
  - Modular data structures
    - Eases code development and debugging – data locality
    - Nesting of processes and data
  - Tree structure enables self-contained simulations
- **Why Fortran 2003/2008?**
  - Classes (extendable derived types)
    - Member functions
    - Inheritance
  - Pointers to procedures
    - E.g. swapping equations of state



Prioritizing R&D Activities

- **R&D Prioritization process can be formalized**
  1. Identify a set of objectives and associated metrics, including
     - Importance to components of the safety case: safety assessment, technical bases, confidence-building
     - Potential to reduce key uncertainties, i.e., increase the TRL (or KRL, or SAL)
     - Other factors, e.g., cost, redundancies, synergies
  2. Evaluate each R&D activity using the metrics
  3. Define a "utility function" to combine the metric scores, to give an overall numerical score
  4. Compare utilities ("rankings") of the activities



* ***V.I.*** = ***F*** [sensitivity of system performance to the R&D information obtained; uncertainty reduction potential (TRL)]