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Enhanced Performance Assessment Models for Generic Deep Geologic Repositories for High-Level Waste and Spent Nuclear Fuel

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Outline of Presentation

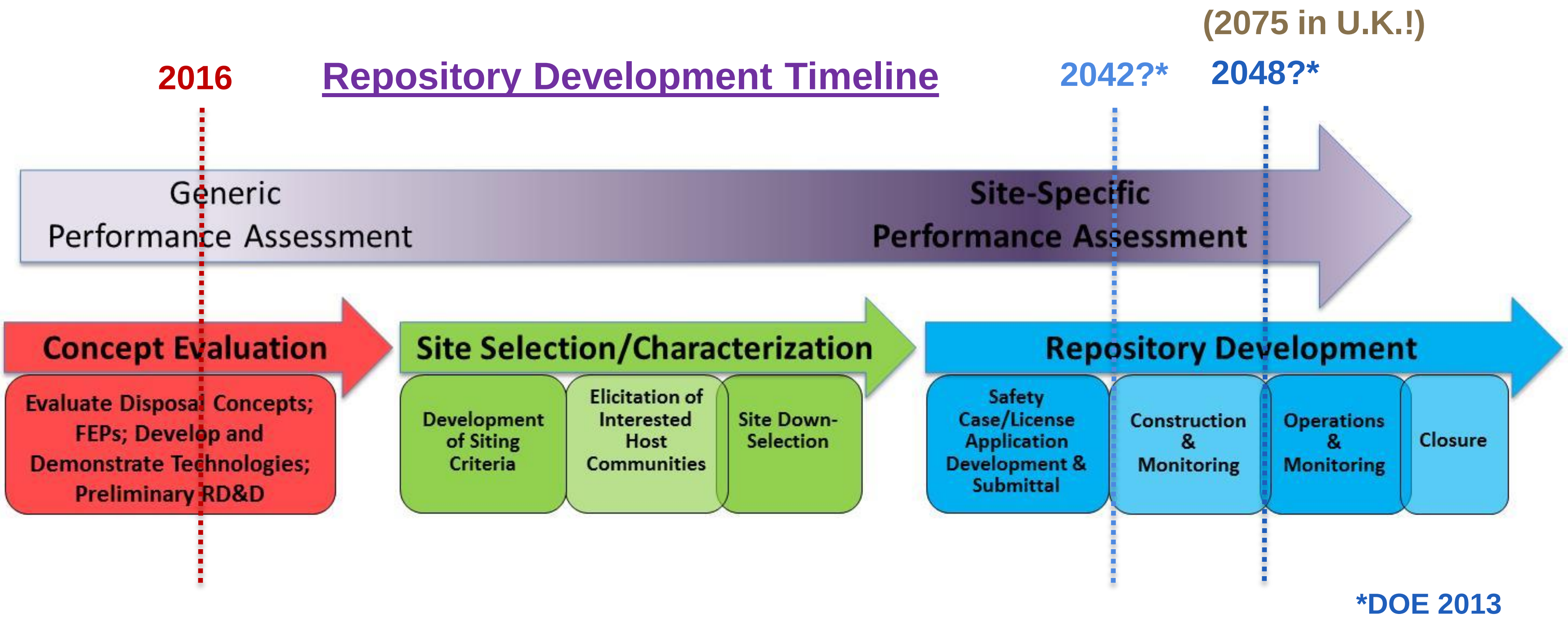
- **Evolution of repository phases, performance assessment (PA) models, computer hardware and software**
- **Performance assessment (PA) model/code development philosophy**
- **Generic Disposal System Analysis (GDSA) framework**
- **Example application of GDSA model**
  - Generic clay/shale repository reference case
  - Demonstration simulations
- **Summary and future work**

Acknowledgments

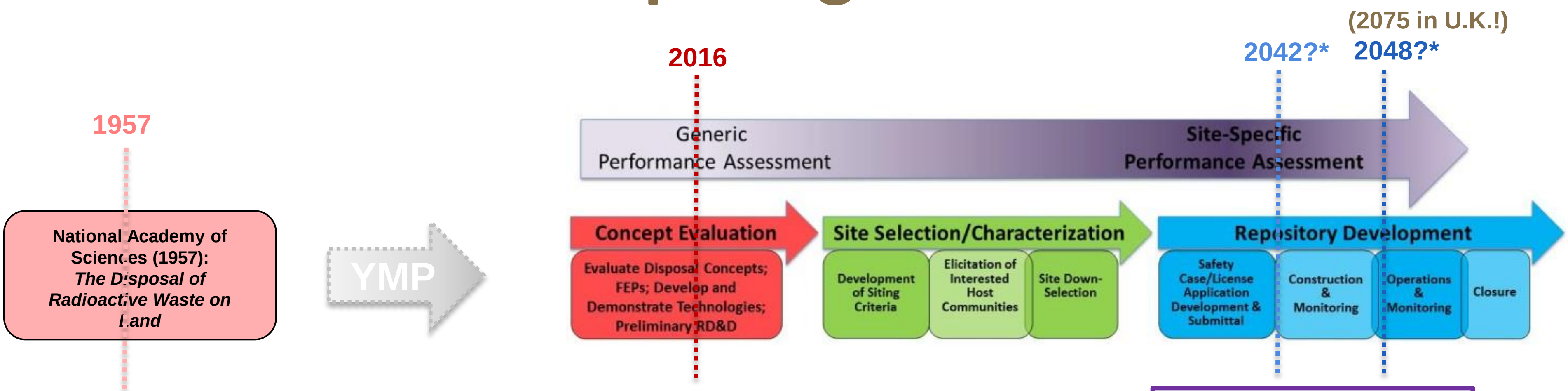
- <u>Code development</u>: Glenn Hammond
- <u>Conceptual model development</u>: Paul Mariner, Emily Stein, Glenn Hammond, Payton Gardner
- <u>Simulations</u>: Emily Stein

Evolution of a Repository Project

- **Key repository phases, and nature of PA:**
  - **Concept Evaluation (the current phase)—generic PA**
  - **Site Selection/Characterization—generic to site-specific PA**
  - **Repository Development—site-specific PA**



Evolution of Computing Power

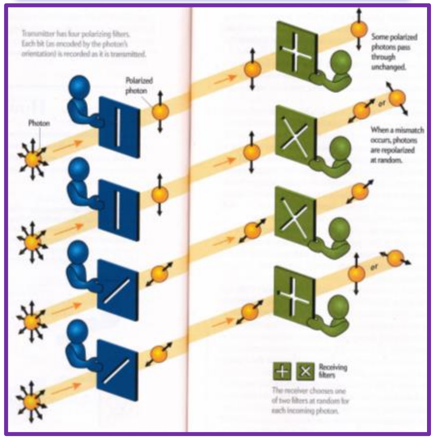


<u>1964</u>:
IBM 360/Model 30
35 x 10^3 IPS
1 CPU, 8 KB Memory

<u>2012</u>:
IBM Blue Gene/Q
10 x 10^{15} FLOPS
786,432 CPUs; 7.86 x 10^{11} KB DRAM

three decades

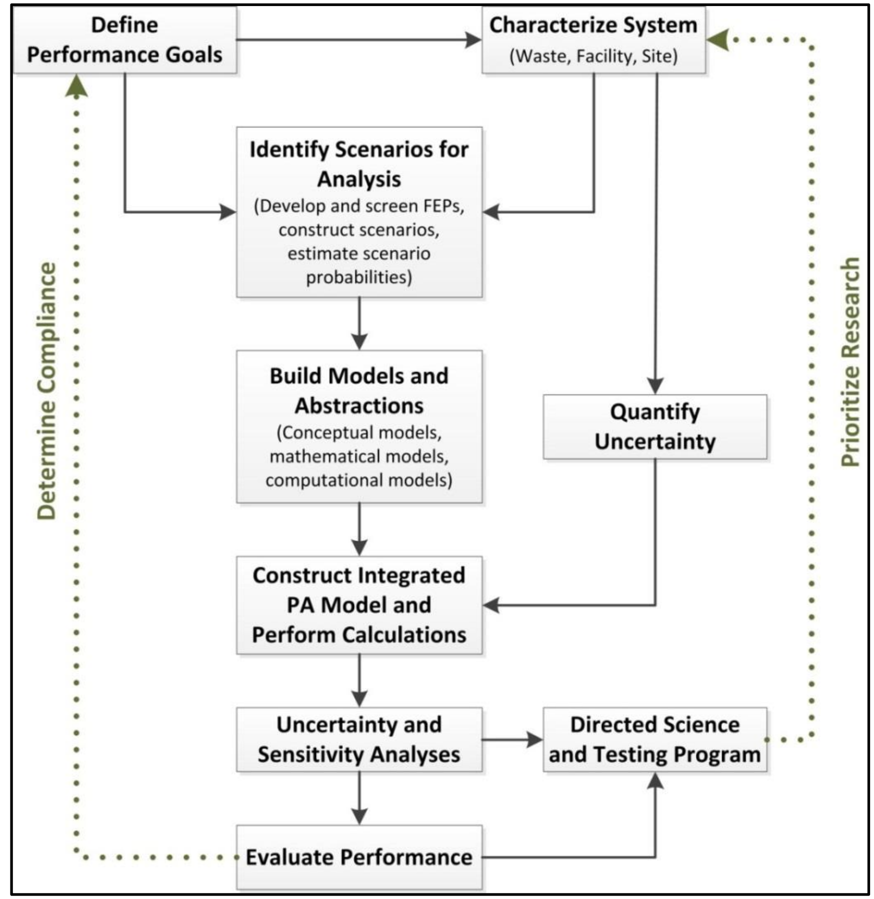
<u>2042-48?</u>
IBM Quantum
$10^{???}$ FLOPS



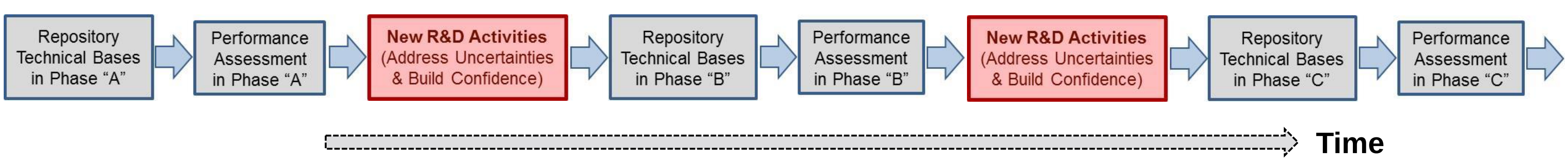
"IBM System360 Model 30" by Dave Ross - Flickr: IBM System/360 Model 30. Licensed under CC BY 2.0 via Wikimedia Commons
"Mira - Blue Gene Q at Argonne National Laboratory - Skin" by Courtesy Argonne National Laboratory. Licensed under CC BY 2.0 via Wikimedia Commons
"The Quantum Hack" by Tim Folger,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

Evolution/Iteration of Performance Assessment

- **Primary ongoing <u>functions</u> of PA framework, throughout repository phases:**
  1. <u>Evaluate</u> potential disposal concepts and sites in various host rock media
  2. Help prioritize <u>RD&D activities</u> (initially *generic*; later *site-specific*)
  3. Support <u>safety case</u> development during all phases of lifecycle



from Meacham et al. 2011



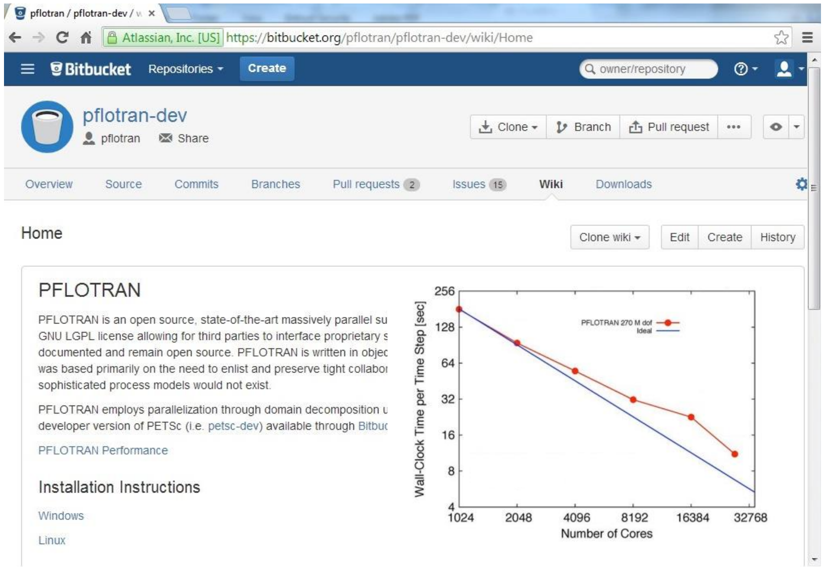
PA Model/Code Development Philosophy

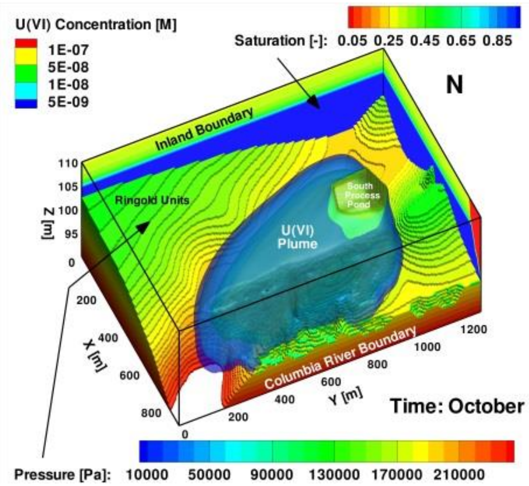
- **Goals**:
  - Elevate confidence and transparency in disposal system safety case through various phases of the repository project
  - Enable better decisions (technical, political, fiscal) through time
- **Methods**:
  - Implement a numerical solution and code architecture that can evolve throughout the repository lifecycle (decades!) and is able from the outset to use the most advanced hardware and numerical solvers available
  - Direct representation in PA 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*
  - Realistic spatial resolution of features and processes
    - *Explicit representation of all waste packages*
  - Quantification and propagation of uncertainties, both aleatory and epistemic, based on model form and data availability at various spatial scales

PFLOTRAN Capabilities

- **Petascale, 3-D, reactive multiphase flow and transport code, with ability to couple with other process models, which can run at identical or dissimilar time scales**
- **High-performance computing (HPC)**
  - *Massively parallel; built on PETSc 3-D solvers*
  - *Structured and unstructured grids*
  - *Scalable from laptop to supercomputer*
- **Domain scientist "friendly", e.g., Fortran 2003/2008**
- **Open source development and distribution**
  - *Transparency*
  - *Shareable among experts and stakeholders*
- **Flexible and extensible**
  - *Modular implementation of simple and/or advanced PA component models and FEPs*
- **Leverage existing computational capabilities**
  - *Meshing, visualization, HPC solvers, etc.*

PFLOTRAN





Hammond and Lichtner, WRR, 2010

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DAKOTA

- Interface Control
- Uncertainty Sampling and Quantification
- Sensitivity Analysis

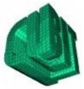
Input Parameters

Parameter database

Computational Support

Processing (Python, etc.)

Mesh generation

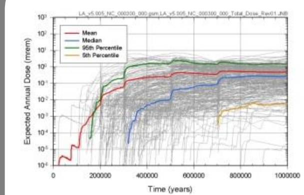


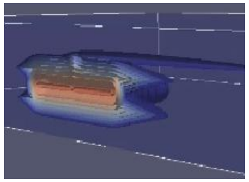
Visualization

ParaView — Parallel Visualization Application

VisIt

Results





PFLOTRAN

Multi-Physics Simulation and Integration

Source Term and EBS Evolution Model

- Inventory
- WF degradation
- WP degradation
- Radionuclide mobilization
- Thermal effects
- Gas generation

Flow and Transport Model

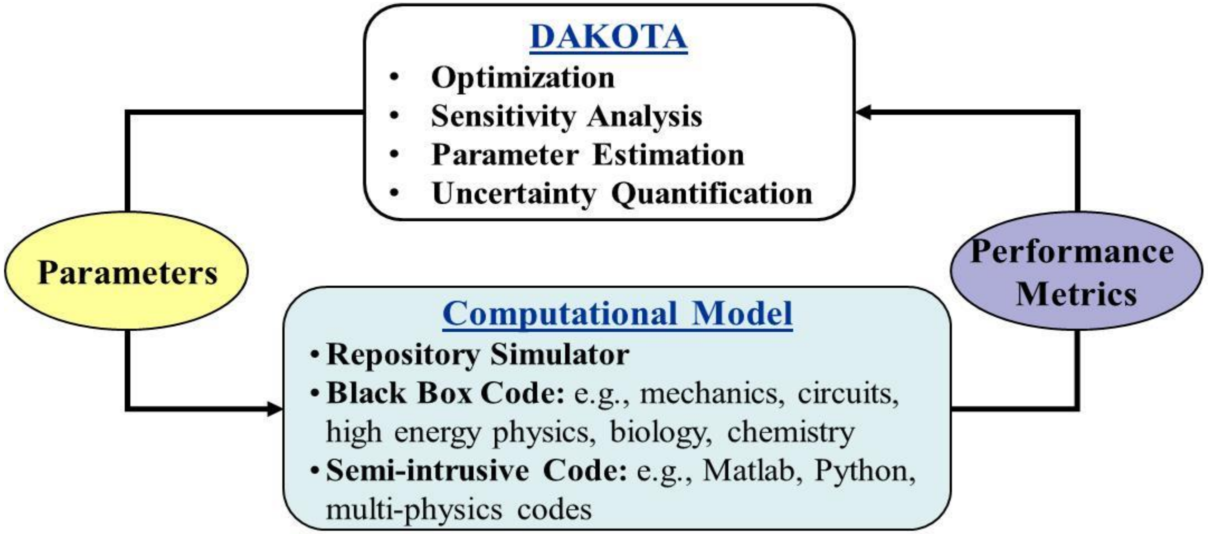
- THC processes
  - Advection, diffusion, dispersion
  - Sorption
  - Precipitation, dissolution
  - Decay, ingrowth
  - Colloids
  - Chemical reactions

Biosphere Model

- Exposure pathways
- Uptake/ transfer
- Dose calculations

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
  - Generic interface to simulations



http://dakota.sandia.gov/

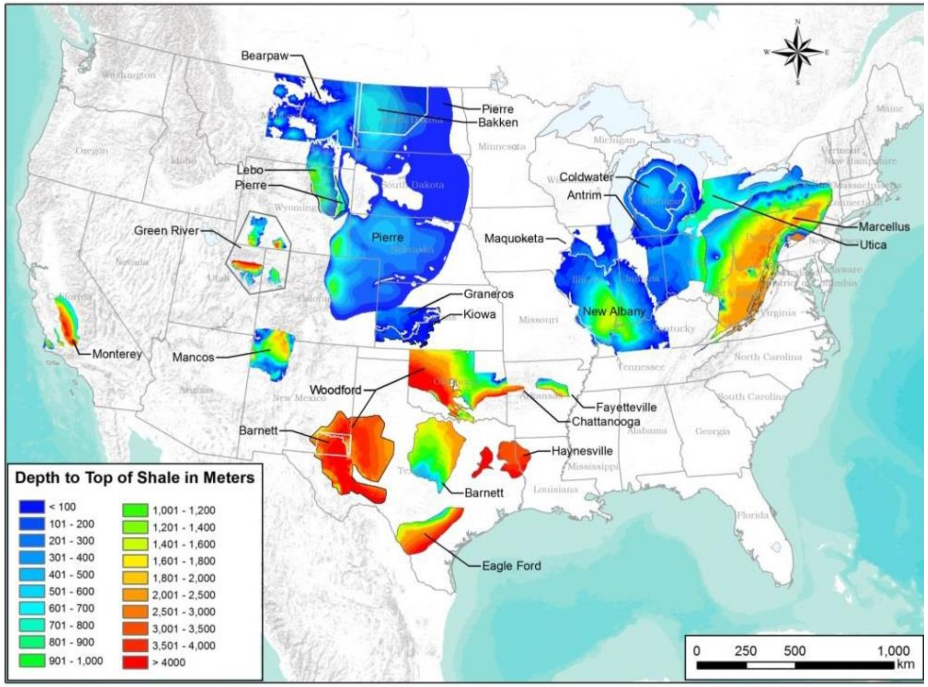
Generic Clay/Shale Reference Case

Clay Reference Case – General Considerations

- ***Reference Case* is a surrogate for site- and design-specific information not yet available during the current Concept Evaluation Phase**
  - Documents information and assumptions needed 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)

- **Benefits of *clay/shale* as a geologic disposal medium:**
  - Low permeability (~ 10^{-20} m^2)
  - High sorption capacity
  - Typically reducing pore waters (which limit radionuclide solubility)
  - Ability to deform plastically (if not indurated), which promotes self-healing of fractures

Distribution of clay-rich formations in the US (Jove-Colon et al. 2014)



Generic Clay/Shale *Natural Barrier System (NBS)* and Overall Repository Concept

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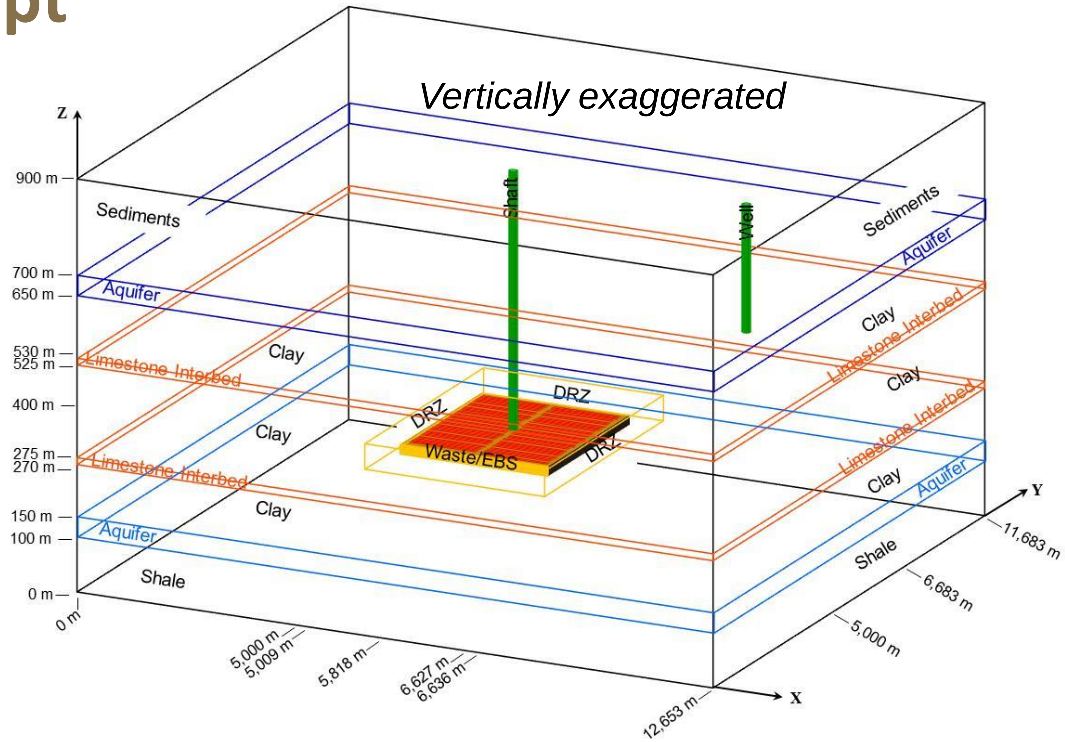
- **General considerations:**
  - Thick (>1000 m) marine depositional sequence, consisting of:
    - Thick layers of low permeability shales and marls, alternating with
    - Thin layers of higher permeability sandstones and limestones
  - Properties and stratigraphy consistent with depositional sequences in the U.S.

- **Specific assumptions:**
  - 500-meter thick shale formation containing a homogeneous repository horizon
  - 9-m disturbed rock zone (DRZ) surrounding the excavated drifts
  - two thin (5 meter) high-permeability interbeds (such as limestone) 125 meters above and below the repository horizon
  - two 50-meter thick sandstone aquifers above and below the 500-meter shale formation
  - 200 meters of generic (non-lithified) sediments above the upper aquifer
  - 100-meter thick low-permeability confining layer below the lower aquifer

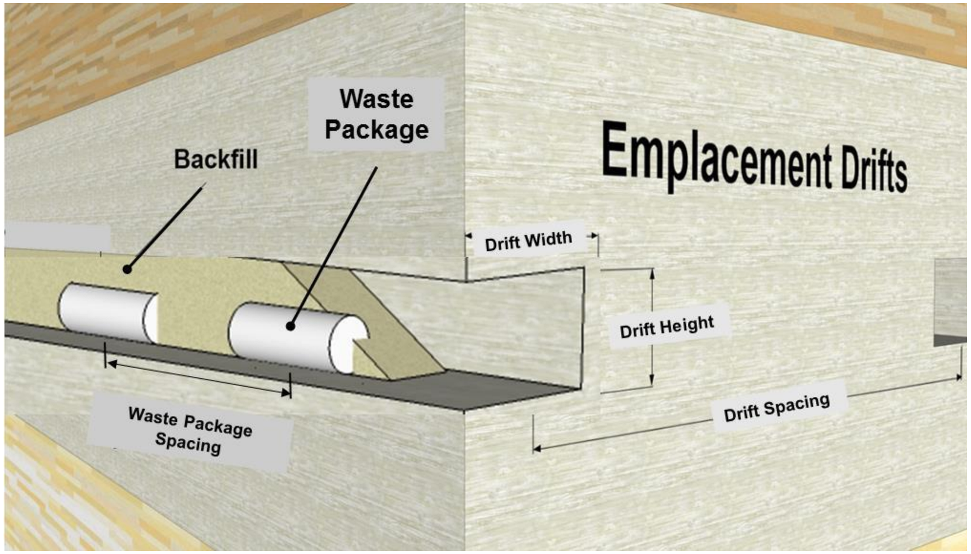


Key deterministic parameters for the clay reference case NBS:

Model Region	Permeability (m^2)	Porosity	Tortuosity	Effective Diffusion Coefficient (m^2/s)	Saturated Thermal Conductivity (W/m/K)
DRZ	3.16×10^{-19}	0.25	0.25	6.25×10^{-11}	1.7
Shale	3.16×10^{-20}	0.25	0.25	6.25×10^{-11}	1.7
Interbed	1.00×10^{-16}	0.20	0.20	4.00×10^{-11}	2.5
Aquifer	3.16×10^{-15}	0.20	0.20	4.00×10^{-11}	3.0
Sediment	1.00×10^{-15}	0.20	0.20	4.00×10^{-11}	1.7
Confining Layer	3.16×10^{-20}	0.20	0.20	4.00×10^{-11}	1.7

Generic Clay/Shale *Engineered Barrier System (EBS)* and Concept of Operations

- **Waste inventory:**
  - ~70,000 MTHM SNF
  - ~13,400 WPs
  - Burn-up = 60 GWd/MT
- **Drift spacing and WP loading based on 200°C thermal limit for clay (greater than in other programs)**
  - 100-year out-of-reactor decay cooling (required because of low clay thermal *K*)
  - 12 PWR assemblies per WP
  - 7.5 kW/WP
- **Repository depth = 500 m**
- **Repository layout**
  - 84 pairs of 805-m long drifts
    - Drift spacing = 20 m
    - 80 WPs (5-m-long) per drift with 10-m spacing
  - 1.5-m thick, bentonite/sand (70/30 wt%) buffer in drifts—sand increases thermal *K*
  - Bentonite drift/shaft seals



Key deterministic parameters for the clay reference case EBS:

Model Region	Permeability (m^2)	Porosity	Tortuosity	Effective Diffusion Coefficient (m^2/s)	Saturated Thermal Conductivity (W/m/K)
Waste Package	1.00×10^{-13}	0.30	1.00	3.00×10^{-10}	16.7
Buffer 1	1.00×10^{-16}	0.25	0.25	6.25×10^{-11}	2.5
Buffer 2	5.00×10^{-21}	0.40	0.40	1.60×10^{-10}	2.5
Shotcrete	1.00×10^{-17}	0.15	0.15	2.25×10^{-11}	1.7

Demonstration of GDSA Capabilities

1. Deterministic isothermal simulations
2. Probabilistic isothermal simulations
3. Deterministic thermal simulations
4. Probabilistic thermal simulations (in the future)

PFLOTRAN Simulation Domain

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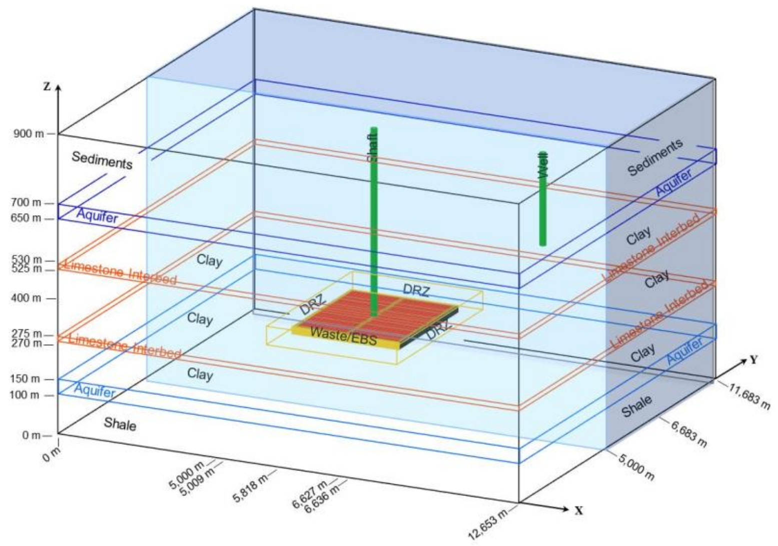
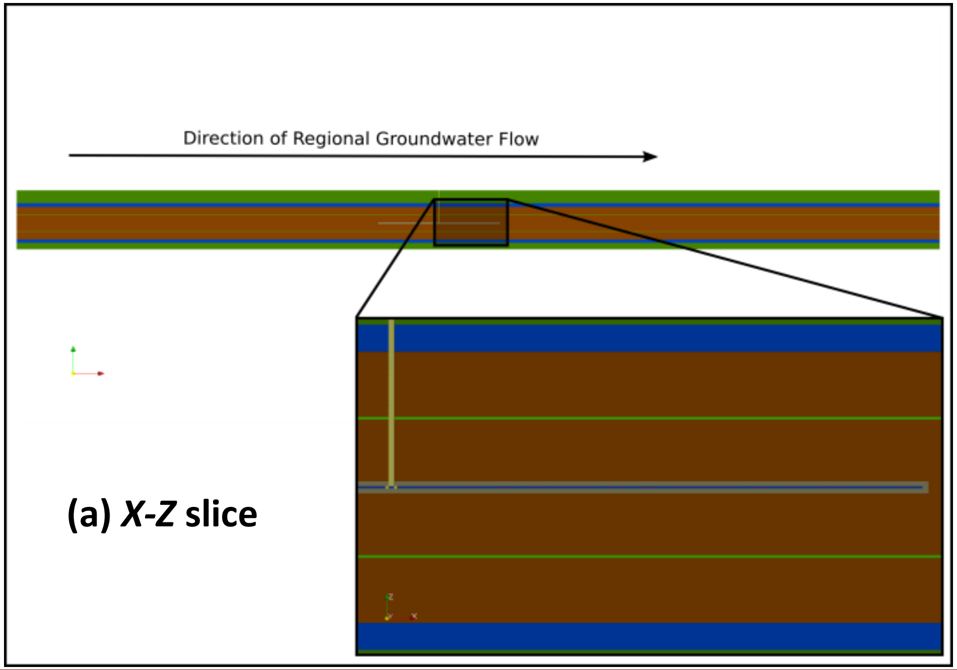
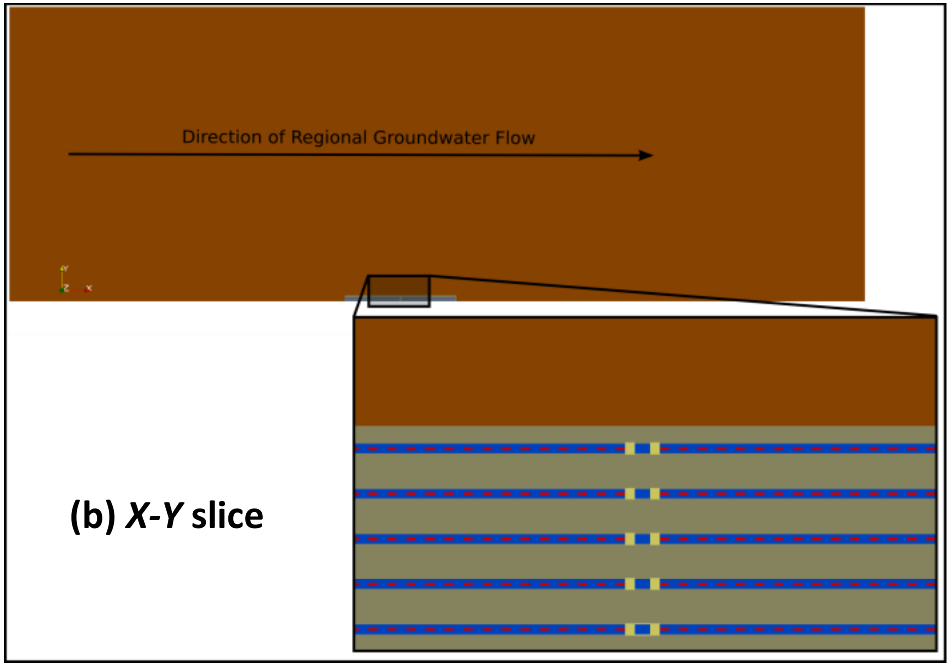


- **Half domain width in *y*-direction, but with 5 drift pairs, 800 waste packages, a central access hallway, and a shaft**
  - reflective boundary condition at *y* = 0 m implies 10 drift pairs, 1600 waste packages, and 2 shafts centered in a 10,000-m wide domain.
- **regional geothermal heat flux of 60 mW/m^2**
- **regional head gradient west to east of –0.0013 (m/m)**
- **5 km from repository to aquifer withdrawal well**
- **~ 4,000,000 total grid cells**



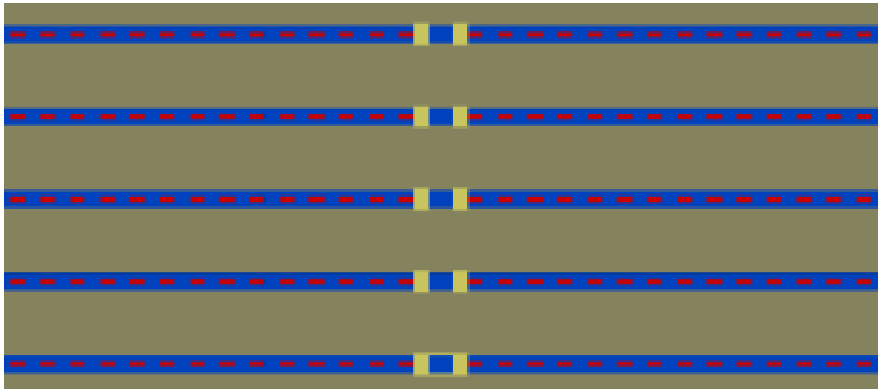
(a) *X-Z* slice



(b) *X-Y* slice

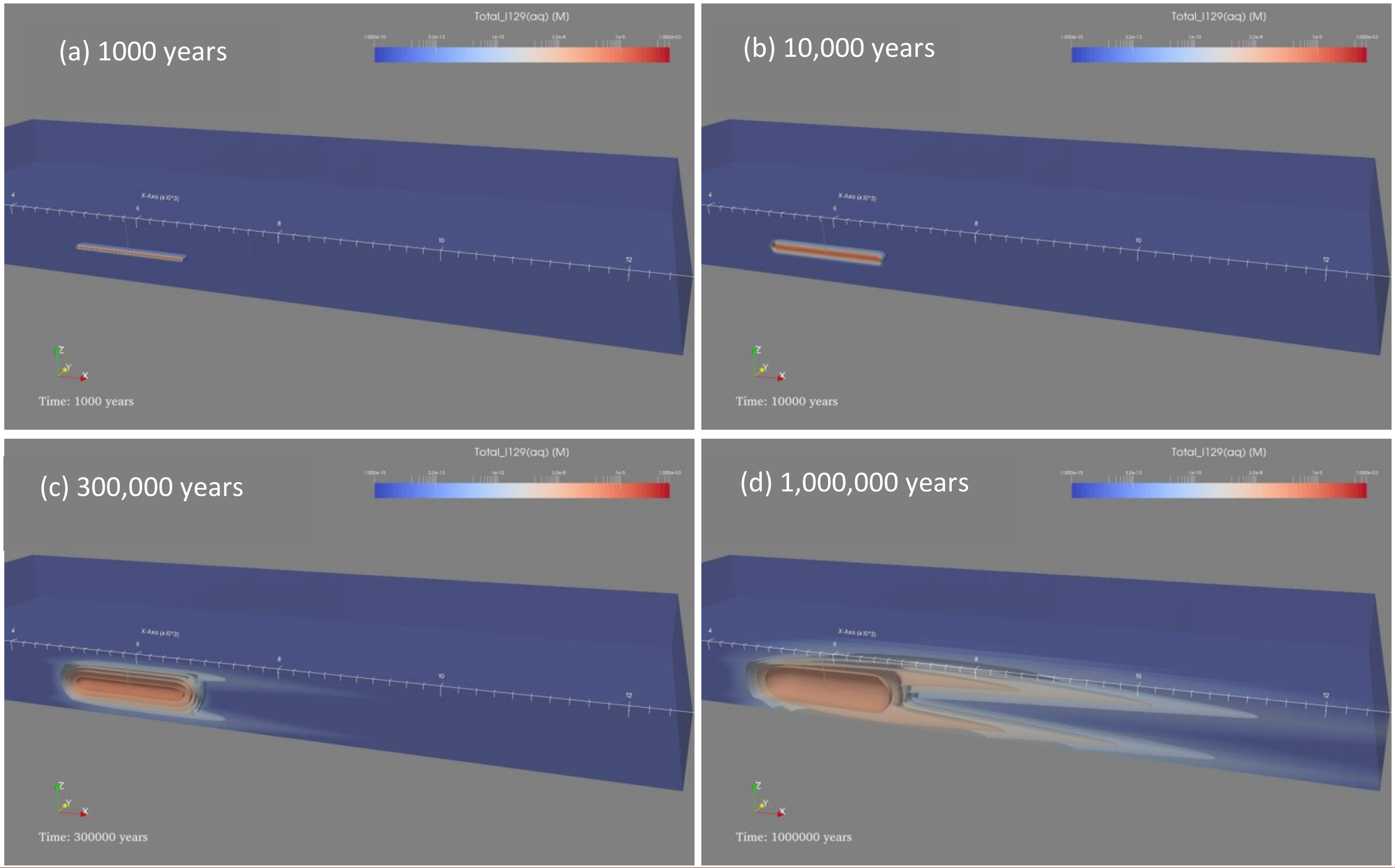
Key Aspects of Generic PA Simulations

- **Uncertainty propagation and sensitivity analyses (DAKOTA) for multi-realization, probabilistic analyses**
- **Domain processes (PFLOTRAN) include**
  - **Thermal-hydrologic coupling for fluid flow in both NBS and EBS**
  - **Radionuclide transport in NBS and EBS**
    - Diffusion through bentonite buffer, DRZ and clay host rock
    - Primarily advection through aquifer and sediments
    - Element and isotope solubility limits: dissolved radionuclides can precipitate
    - Sorption (K_d) onto bentonite buffer and clay host rock , except for ^{129}I
  - **Source term for <u>each of the 800 waste packages:</u>**
    - 5 radionuclides: ^{129}I, ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th
    - Waste packages assumed to have no performance credit (fail on emplacement)
    - Instant release fraction for ^{129}I
    - Far-from-equilibrium mineral (zero-order rate law) for SNF degradation
    - Radioactive decay in all parts of domain



Deterministic *Isothermal* Simulation

- ^{129}I dissolved concentration at various times:
  - Reaches the upper and lower aquifers via diffusion through the DRZ and clay host rock
  - Advective/dispersive transport carries it downgradient in aquifers, based on regional flow



Probabilistic *Isothermal* Simulations

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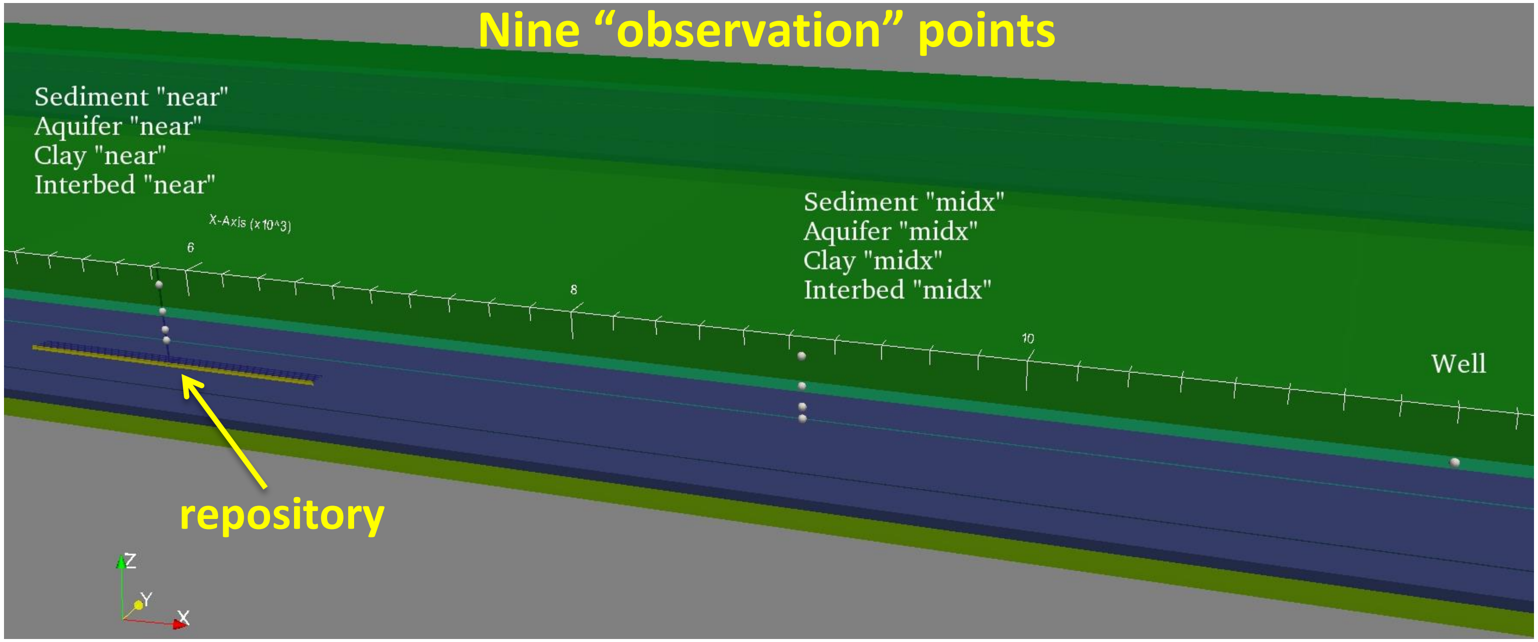
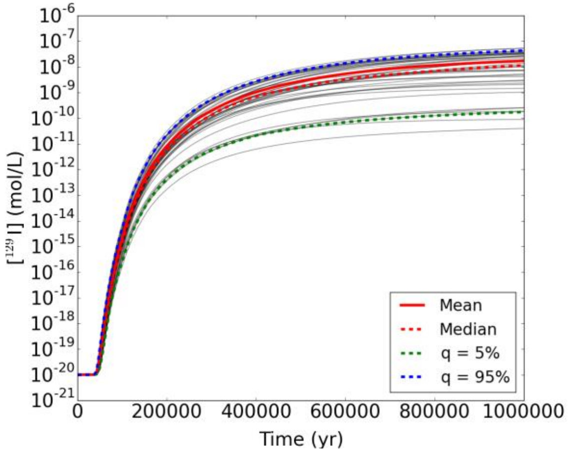
- **9 sampled parameters**
- **50 realizations**
- **Sensitivity analyses with DAKOTA:**
  - Spearman Rank Correlation Coefficient (SRCC), i.e., local sensitivity analyses, for max ^{129}I concentration over 1,000,000 years vs. sampled input parameter(s)

Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste form degradation rate constant (mol/m^2/s)	4.8×10^{-8}	$10^{-10} - 10^{-7}$	Log uniform
^{129}I K_d (ml/g)	0.0	$9.28 \times 10^{-7} - 7.84 \times 10^{-3}$	Log uniform
^{237}Np K_d (ml/g)	173	30 – 1000	Log uniform
Bentonite/Quartz Buffer Porosity	0.25	0.1 – 0.4	Uniform
Shaft Porosity	0.4	0.1 – 0.4	Uniform
DRZ Porosity	0.25	0.1 – 0.4	Uniform
Shale Porosity	0.25	0.1 – 0.4	Uniform
Interbed Permeability (m^2)	1.0×10^{-16}	$10^{-18} - 10^{-14}$	Log uniform
Aquifer Permeability (m^2)	3.2×10^{-15}	$10^{-16} - 10^{-13}$	Log uniform

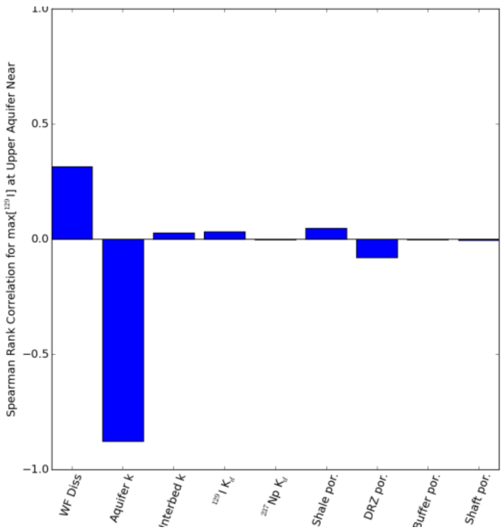


Probabilistic *Isothermal** Simulation – Example Sensitivity at "Aquifer" Observation Points

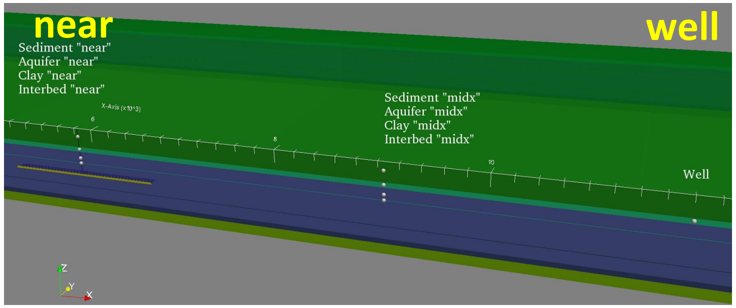
[129I] histories at aquifer "near"



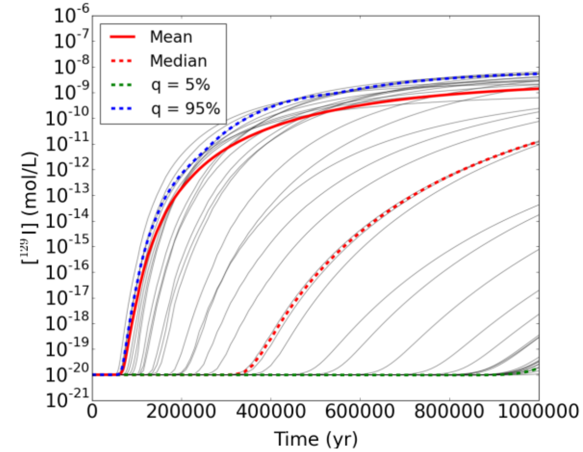
SRCCs for max [129I] at aquifer "near"



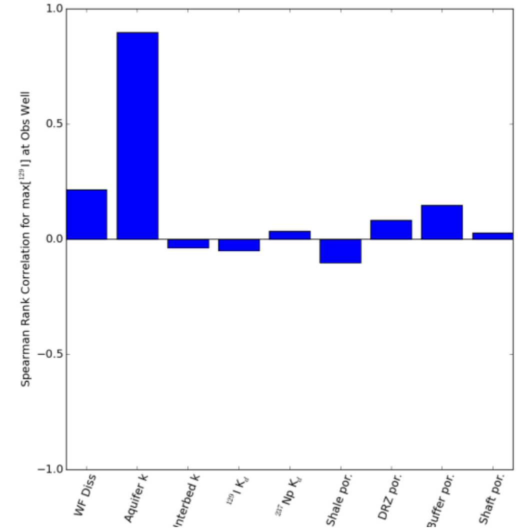
- **Small variation in max [129I] across time histories for aquifer observation point close to repository, relative to large variation in max [129I] at aquifer well location (5 km from repository):**
  - Because of shorter travel distance—less time for concentration spreading
  - Negative correlation to aquifer permeability at near point (effect of dilution); positive correlation to aquifer permeability at well point (effect of spreading over time)
  - Positive correlation to WF degradation rate at all observation points (increases source cell concentration)



[129I] histories at aquifer well

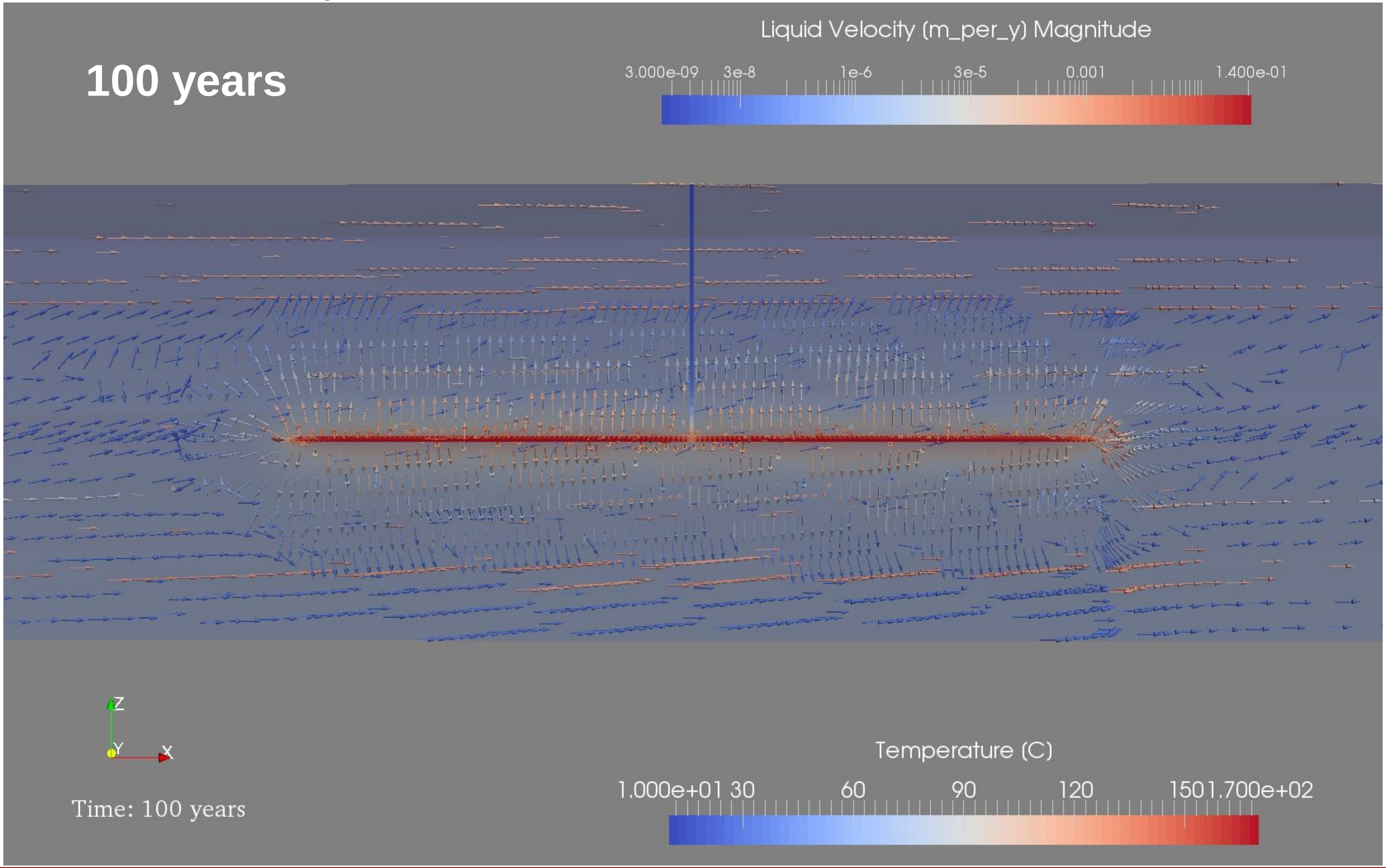


SRCCs for max [129I] at aquifer well



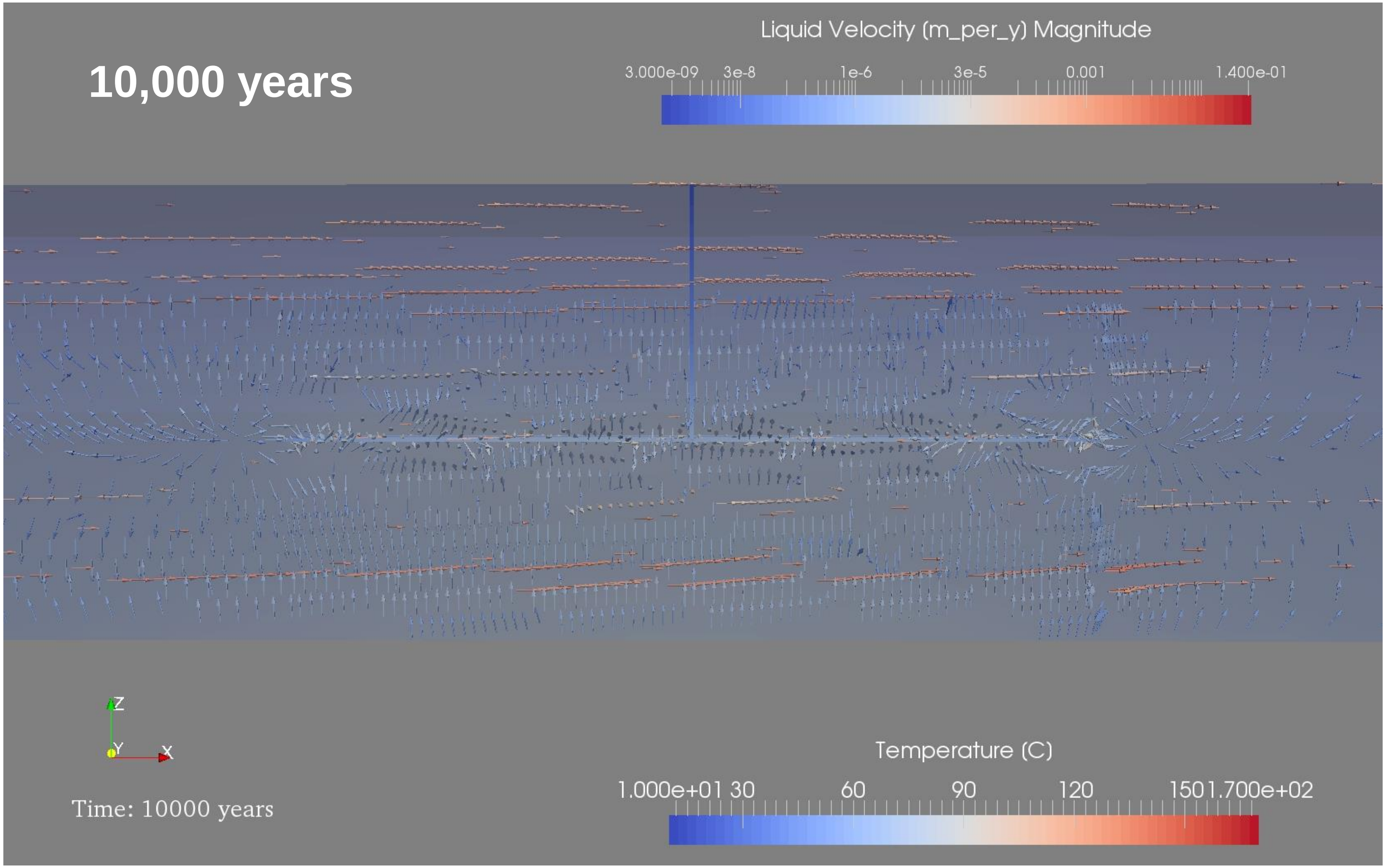
Deterministic *Thermal* Simulation
(energy equation included)

- **Outward fluid flow from repository region — due to *thermal expansion* of fluid at early times:**



Deterministic *Thermal* Simulation

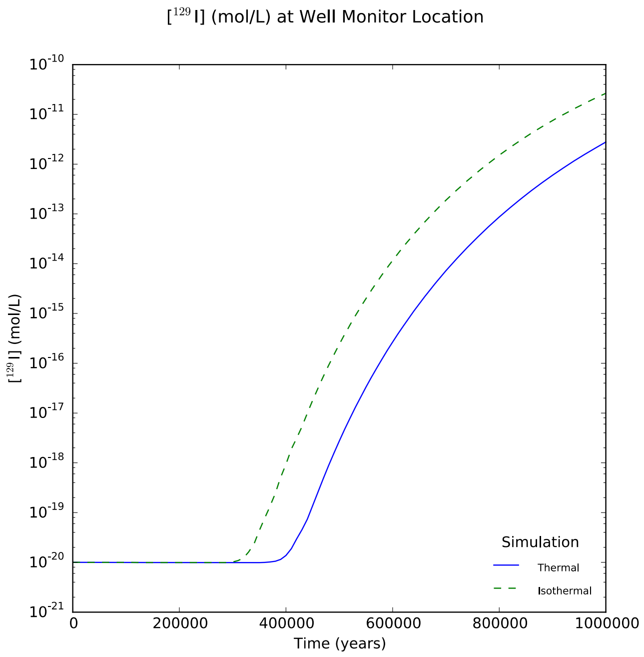
- **Inward fluid flow to repository region at later times — during cooling period after peak temperature, due to fluid contraction:**



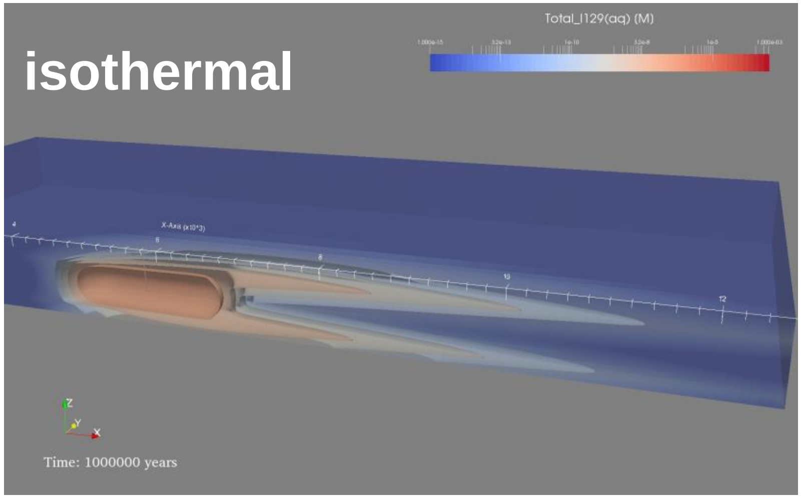
Deterministic *Thermal* Simulation

- **Cooling repository has the effect of drawing fluid inward, and therefore inhibits radionuclide transport outward, and thus decreases ^{129}I concentrations in the far field (upper aquifer) by about an order-of-magnitude compared to concentrations in the isothermal simulation:**

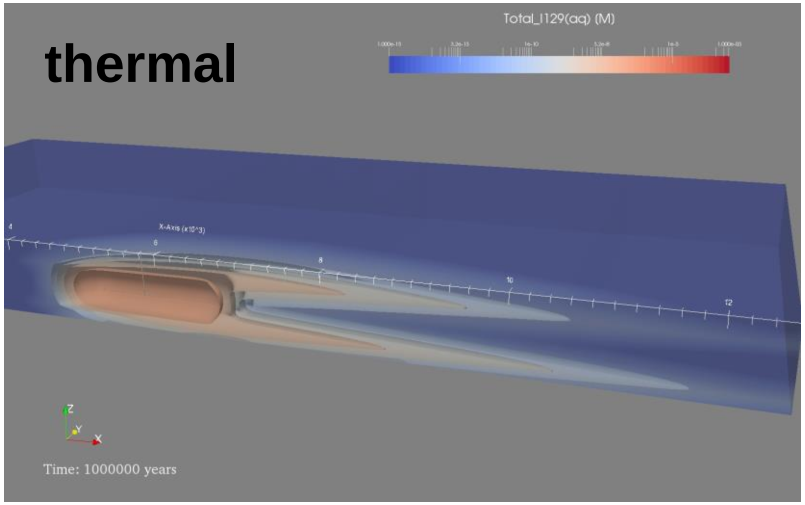
Thermal (blue solid) vs. isothermal (green dash) [^{129}I] time histories at well location:



[^{129}I] plume at 10^6 years (heat or energy equation ignored)



[^{129}I] plume at 10^6 years (heat or energy equation included)



Summary and Future Work

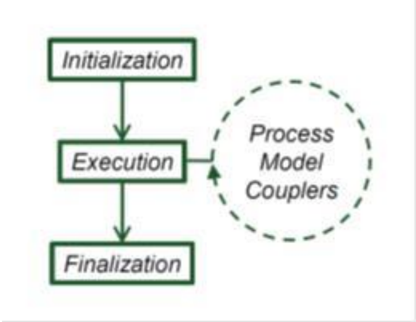
- **An enhanced PA modeling capability has been developed to:**
  - Evaluate generic and/or specific disposal sites in various geologic media
  - Support prioritization of UFD RD&D activities
  - Enhance confidence and transparency in the safety case
- **Application to a generic clay/shale repository reference case:**
  - Generic reference cases important during Concept Evaluation Phase
  - Demonstrate the capabilities of the GDSA multi-physics, high-performance computing, parallel architecture, open-source PA framework
  - Effect on radionuclide transport from coupled T-H processes
- **Ongoing and future work includes**
  - Simulations in other media/concepts, e.g., mined granite, deep borehole
  - Coupling with additional process models, e.g., discrete fracture networks
  - Defense waste repository simulations (DOE-managed HLW and SNF)
  - Application to WIPP PA

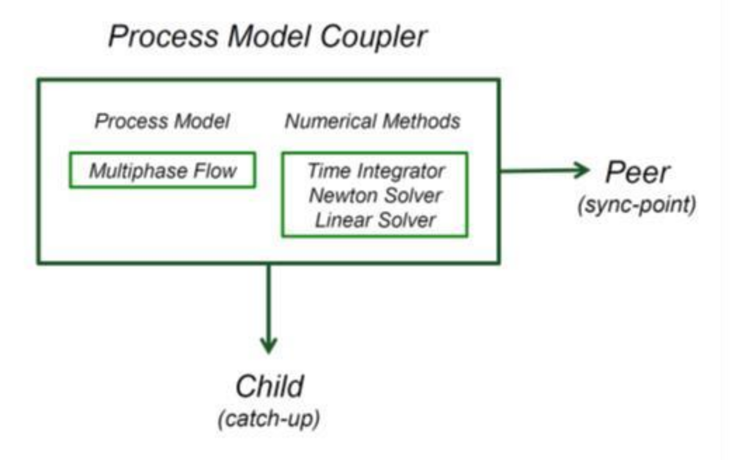
Questions?

Backup Slides

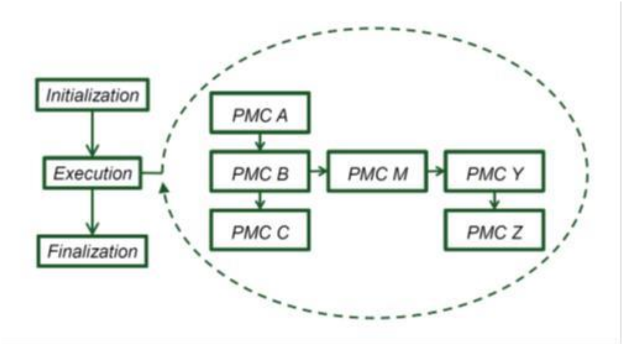
PFLOTRAN Capabilities (cont.)

- PFLOTRAN provides "factories" (code that constructs and destroys data structures, linkages, etc.) to integrate a custom set of process models and time integrators for simulating multi-physics processes
- The "Process Model Coupler" or PMC is a Fortran class that encapsulates a process model (in this case, multiphase flow), providing numerical methods (time integrators and solvers) for solution
  - Each PMC has two pointers to other process models, one to a peer and the other to a child.
  - After each parent PMC time step, the child PMC immediately takes as many time steps as necessary to catch up
  - Necessary information (e.g. state and secondary variables) is transferred between peer and child



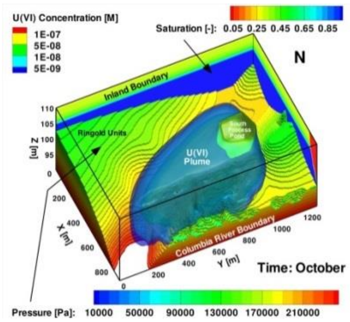


- PFLOTRAN's PMCs can be nested in sophisticated trees or graphs to accommodate any number of processes coupled across varying time scales

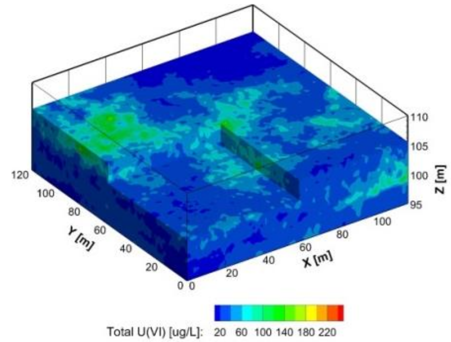


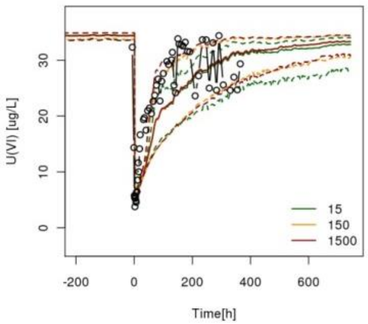
PFLOTRAN Process Modeling

- **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



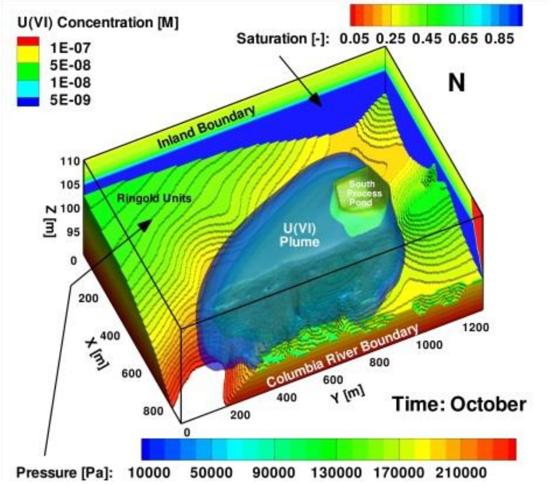
Hammond and Lichtner, WRR, 2010





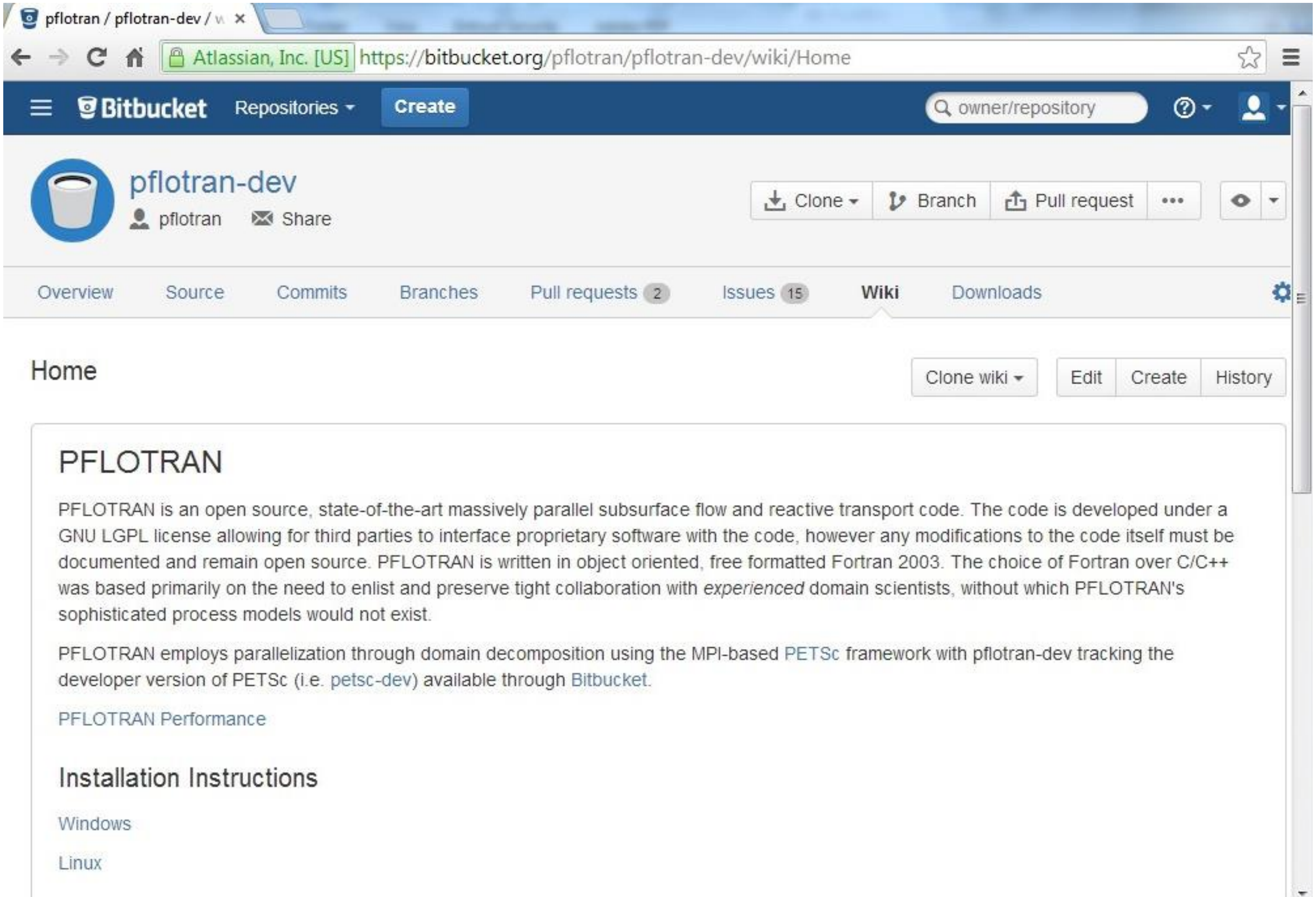
Major Projects Leveraging PFLOTRAN

- **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

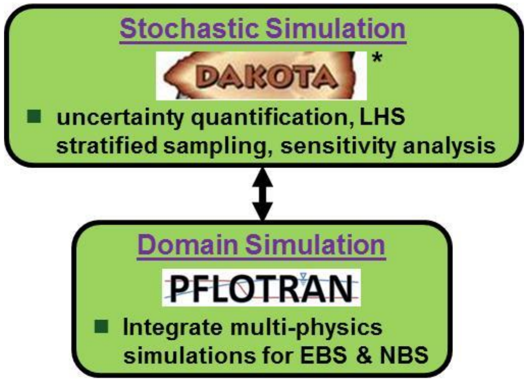
Linux

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

Generic Salt Repository PA Demonstration – Multi-Realization Simulations

- **DAKOTA / PFLOTRAN simulations**:
  - Run on SNL Red Sky HPC cluster
    - *Nested parallelism*
    - *Many concurrent realizations*
    - *Each realization distributed across many processors*
  - Deterministic simulation with mean or representative values
  - 50-realization probabilistic simulation with 10 sampled parameters



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

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