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PFLOTRAN:
Coupled THC Simulations

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Outline of Presentation

- PA model/code development
  - PA objectives and development philosophy
    - Conceptual and computational model guidelines
    - Model and code architecture
- Application of enhanced PA model
  - Generic salt repository reference case
  - Demonstration simulations:
    - Isothermal vs. thermal (heat-generating)
    - Single drift vs. multi-drift
- Summary and future work

Acknowledgments

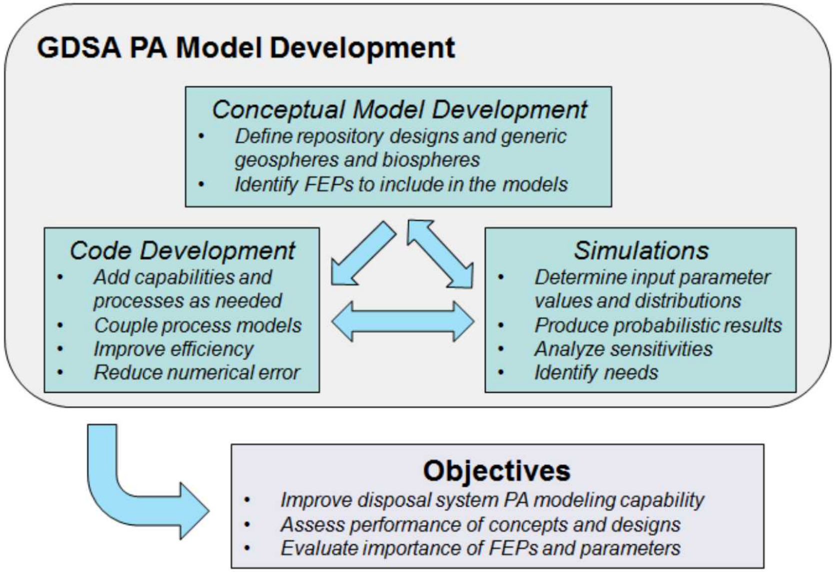
- Conceptual model development: Paul Mariner, Geoff Freeze, Emily Stein, Payton Gardner
- Code development: Glenn Hammond
- Simulations: Payton Gardner, Emily Stein

PA Model/Code Development Philosophy

- **Objective: More accurate solution to the coupled continuum field equations (mass, momentum, energy) over a large heterogeneous domain, including**
  - **Quantification and propagation of uncertainties, both aleatory and epistemic**
  - **Direct representation in PA model of significant coupled multi-physics processes in three dimensions (3-D)**
  - **Realistic spatial resolution of features and processes**
    - *Explicit representation of all waste packages*

- **Key points:**
  - **Less reliance on assumptions, simplifications, and process abstractions**
  - **Adopt 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**

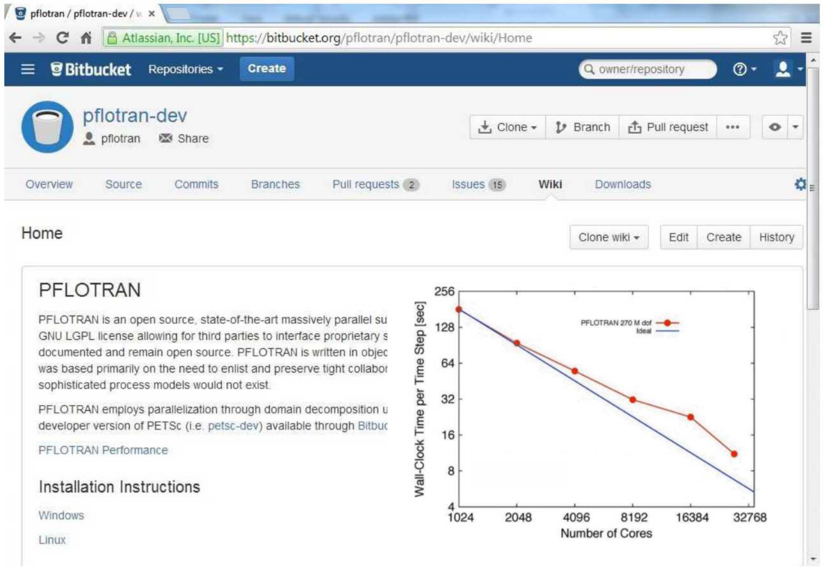
- **Goals: (1) Enhance confidence and transparency in safety case and (2) enable better decisions**



PA Computational Model Guidelines

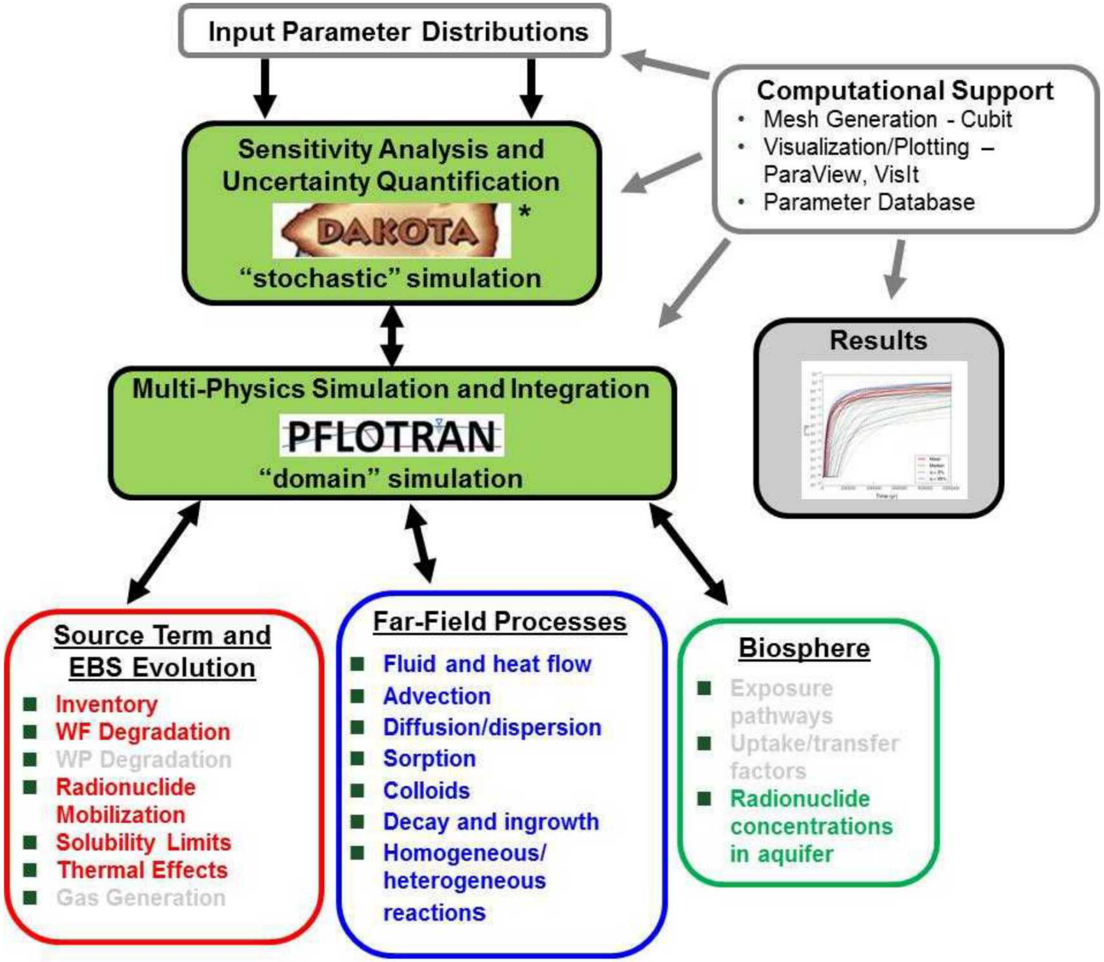
- **Required code capabilities:**
  - Parallel high-performance computing (HPC) environment
  - Open source development and distribution
    - *Transparency*
    - *Shareable among experts and stakeholders*
  - Flexible and extensible; scalable
    - *Modular implementation of simple and/or advanced PA component models and FEPs*
  - Domain scientist "friendly", e.g., Fortran 2003/2008
  - Leverage existing computational capabilities
    - *Meshing, visualization, HPC solvers, etc.*
  - Amenable to future advances in computational methods and hardware
  - Multiple realizations
  - Three-dimensional (3D) domain solvers
  - Appropriate CM and QA

PFLOTRAN



Enhanced PA Computational Model

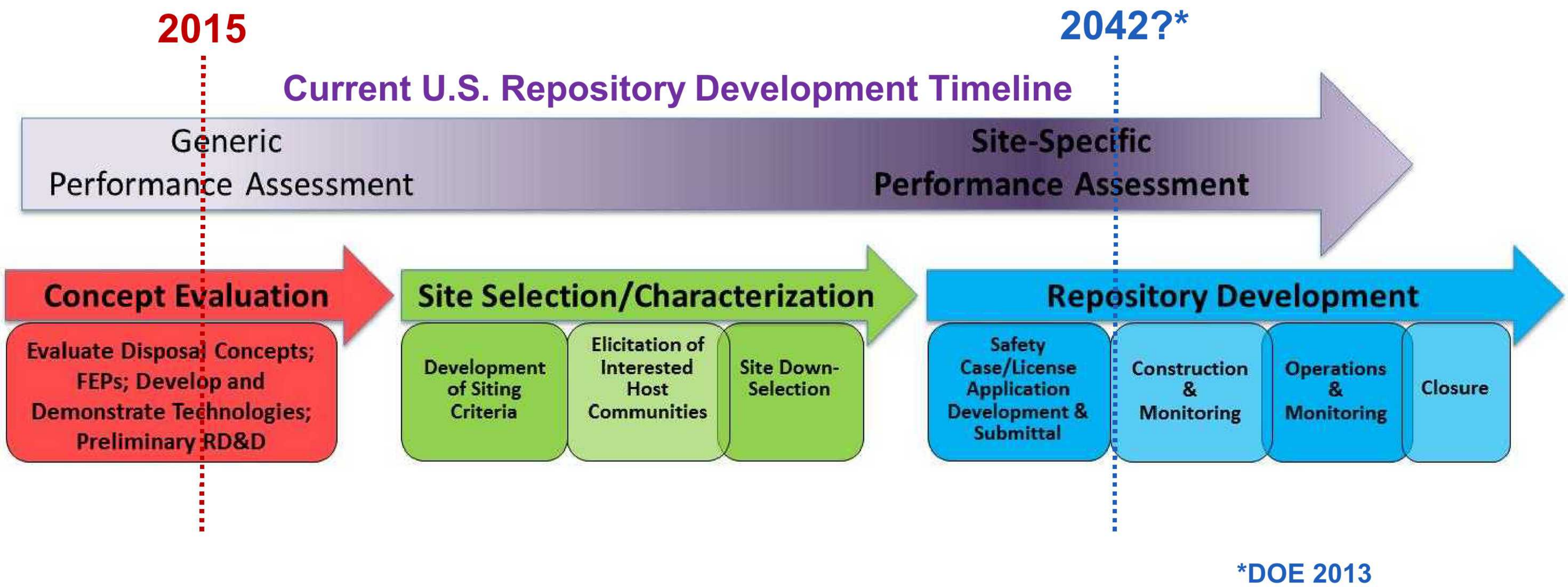
- ***Domain simulation*, PFLOTRAN**
  - Coupled processes in 3-D
  - Spatial variability in features and processes
  - *Three major components*: source term and EBS processes; far-field natural system processes; biosphere processes
- ***Stochastic simulation*, DAKOTA**
  - Uncertainty quantification (UQ) and propagation of model input parameters, both aleatory and epistemic,
  - Sensitivity analysis of output metrics (e.g., biosphere dose) versus input parameters



*Design Analysis Kit for Optimization and Terascale Applications

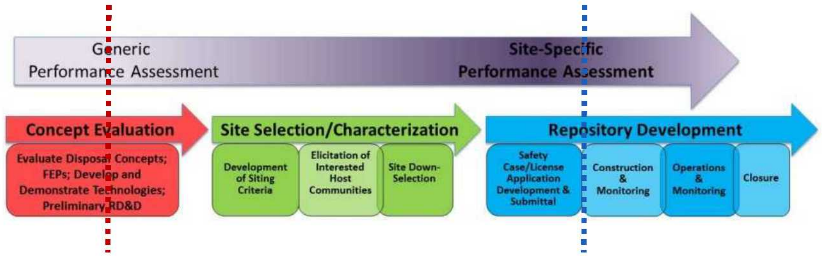
Uses of the Enhanced PA Capability

- **Use the PA model/code throughout the repository lifecycle to:**
  - Evaluate potential disposal concepts and sites in various host rock media
  - Help prioritize RD&D activities (initially *generic*; later *site-specific*)
  - Support safety case development during all phases of lifecycle



Evolution of Computing Power

- **Moore's Law: "the number of transistors in a dense integrated circuit *doubles* approximately every *two* years."**
  - **⇒ 32-fold increase in a decade**
  - **⇒ 33,000-fold in <u>three</u> decades**



<u>1964</u>: *IBM 360/Model 30*

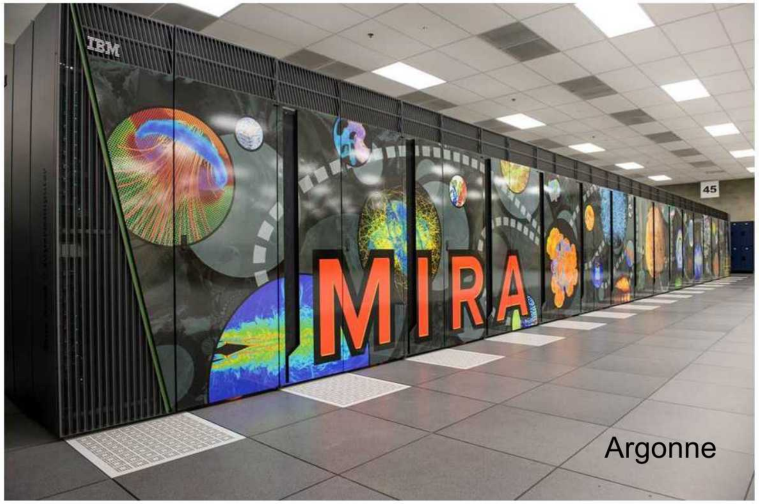
35×10^3 IPS

1 CPU, 8 KB Memory

<u>2012</u>: *IBM Blue Gene/Q*

10×10^{15} FLOPS

786,432 CPUs; 7.86×10^{11} KB DRAM



three decades

2042

IBM T-rex

$10^{??}$ 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
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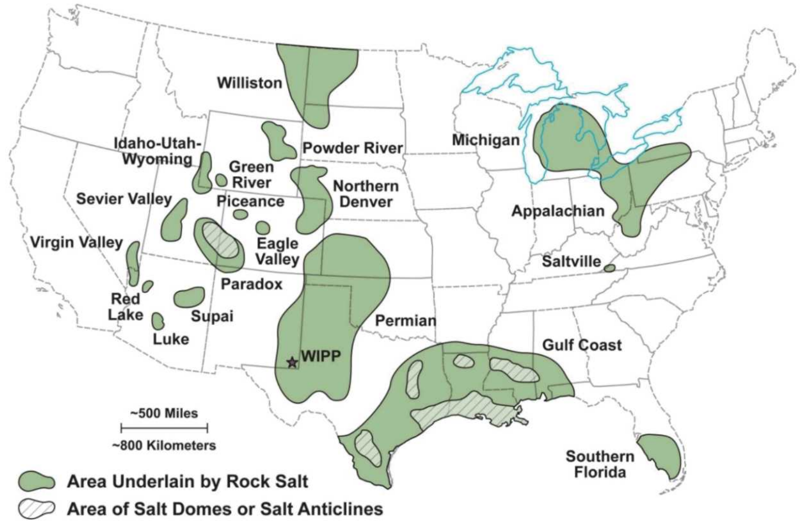
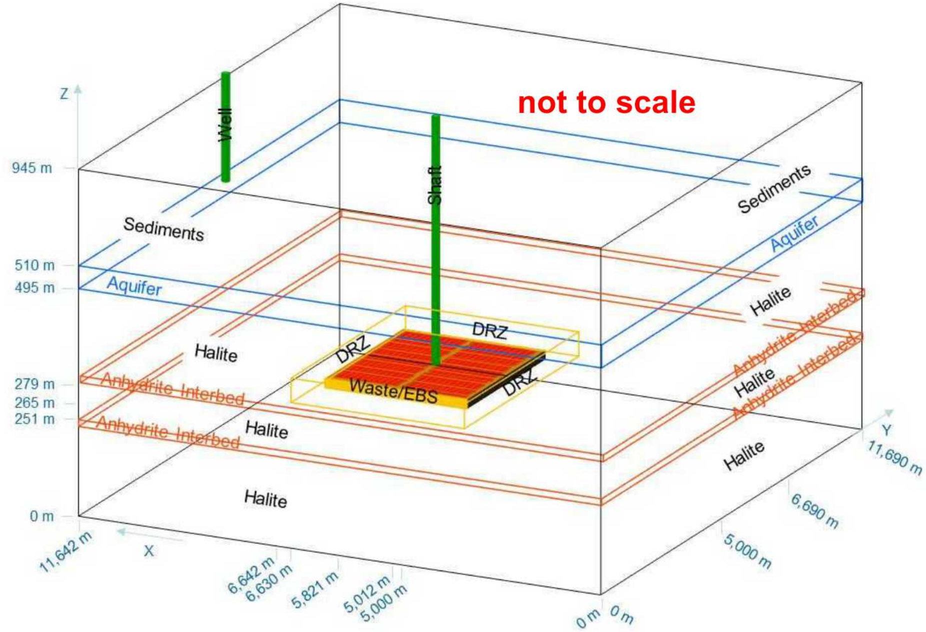
Application of Generic PA Model:

Salt Reference Case & TH Simulations

Salt Reference Case – Natural Barrier System (NBS)

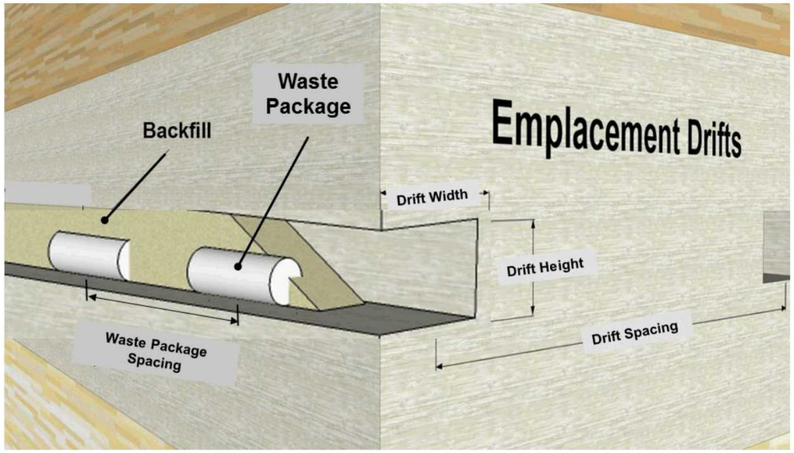
- ***Reference Case* is a surrogate for site- and design-specific information**
  - Documents information and assumptions needed for *generic* disposal system models
  - Helps ensure consistency across analyses (e.g., PA, process modeling, UA/SA)
- **Salt host rock:**
  - Use parameters representative of five major bedded salt basins in the U.S.
- **Disturbed rock zone (DRZ):**
  - Typical properties from international studies and from WIPP
- **Interbeds:**
  - Types (e.g., dolomite, anhydrite) and frequency
  - Dimensions, location (near DRZ), and properties
- **Representative aquifer:**
  - A single-porosity, saturated, sedimentary formation
  - Depth above repository, thickness, physical and chemical characteristics





Salt Reference Case – EBS and Concept of Operations

- Waste inventory
  - ~70,000 MTHM SNF
  - ~13,400 WPs
  - Burn-up = 60 GWd/MT
  - Instant release fraction = 11.25%
- Drift spacing and WP loading based on 200°C thermal limit for salt
  - 12 PWR assemblies per WP; 7.5 kW/WP
- Repository layout
  - 84 pairs of 809-m drifts
    - Drift spacing = 20 m
    - 80 WPs (5-m-long) per drift with 10-m spacing
  - Crushed salt backfill in drifts
  - Sealed shafts (similar to WIPP)



Model Region	Permeability (m^2)	Porosity	Tortuosity	Effective Diffusion Coefficient[a] (m^2/s)	Longitudinal Dispersivity (m)	Saturated Thermal Conductivity (W/m·°K)	Specific Heat Capacity (J/kg·°K)
Waste Package	1.00×10^{-13}	0.500	1.00	6.90×10^{-10}	0.5	16.7	466
Backfill	1.00×10^{-18}	0.113	0.48	1.24×10^{-10}	0.2	2.5	927
Shaft seals	1.58×10^{-20}	0.113	0.48	1.24×10^{-10}	20.0	2.5	927
DRZ	1.12×10^{-16}	0.0129	0.23	6.82×10^{-12}	1.0	4.9	927
Halite	3.16×10^{-23}	0.0182	0.01	4.19×10^{-13}	50.0	4.9	927
Interbed (anhydrite)	1.26×10^{-19}	0.011	0.22	5.57×10^{-12}	50.0	4.9	927
Aquifer	1.00×10^{-13}	0.150	0.53	1.83×10^{-10}	50.0	1.5	959
Sediments	1.00×10^{-15}	0.20	0.58	2.67×10^{-10}	50.0	1.5	927

[a] Effective diffusion coefficient = (free water diffusion coefficient) × (tortuosity) × (porosity)

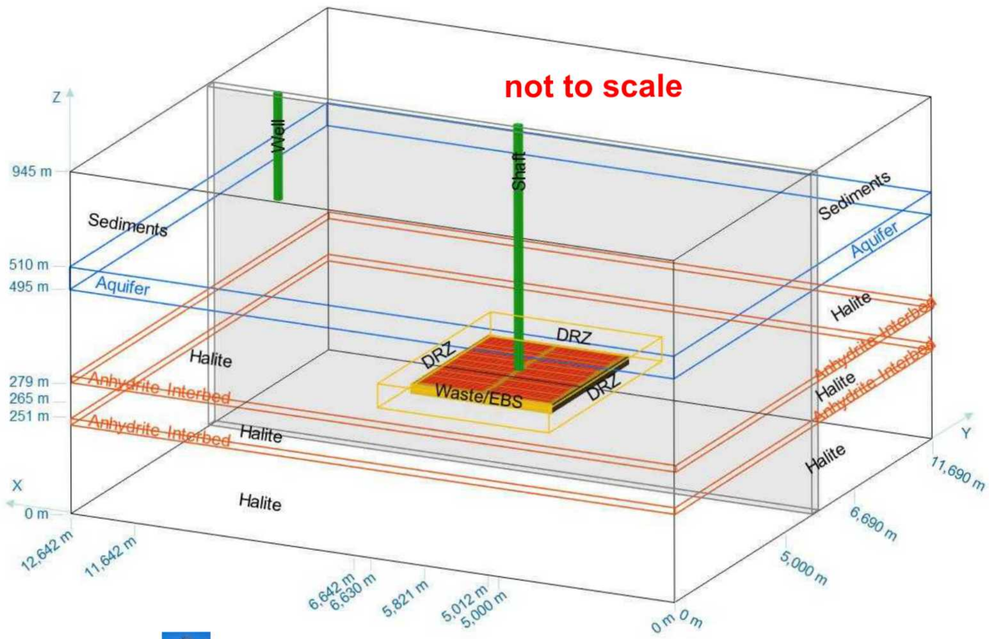
- Relatively fast SNF fractional degradation rate, $m(t)/m_0 = e^{-\lambda t}$, based on bromide-containing brines (from German program, Kienzler et al. 2012):

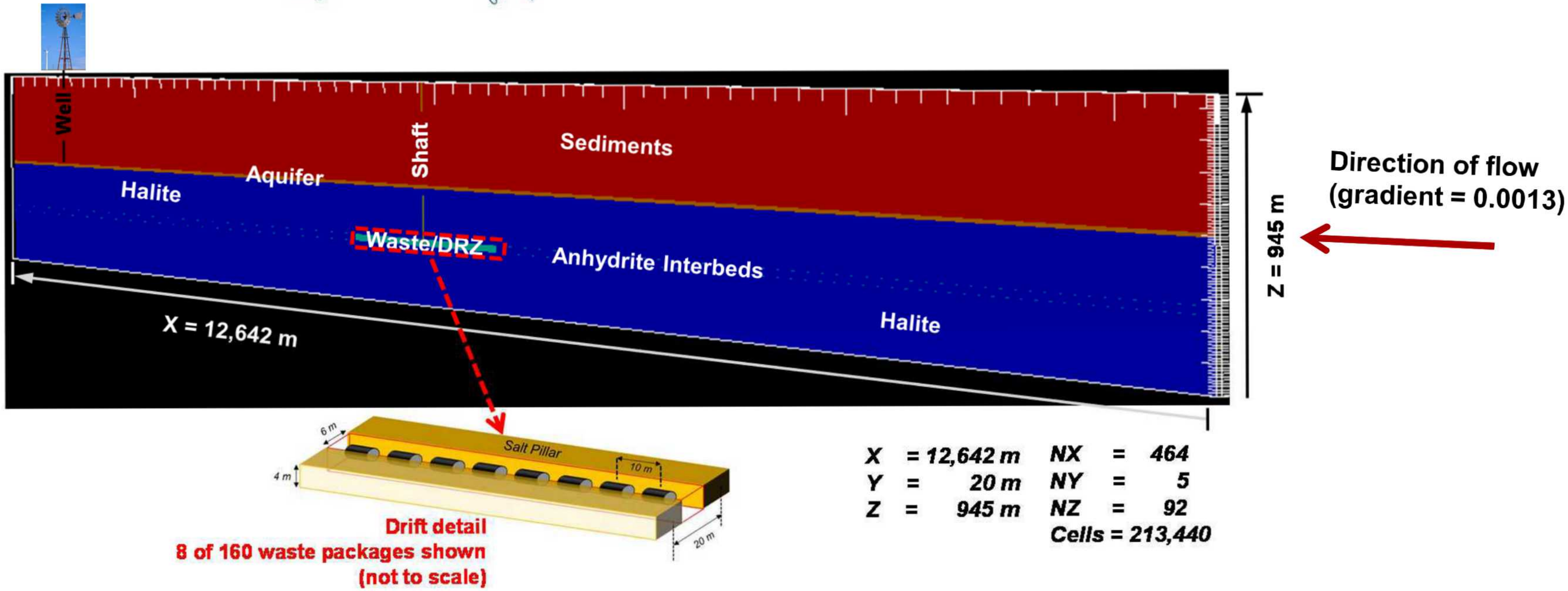
Case	λ (yr^{-1})	Time for 50% Degradation (yrs)	Time for 99% Degradation (yrs)
Deterministic	3.6525×10^{-4}	~ 1,900	~ 12,500
Probabilistic – Lower	3.6525×10^{-6}	~ 190,000	~ 1,250,000
Probabilistic – Upper	3.6525×10^{-3}	~ 190	~ 1,250

Simulations

“Quasi 2-D”, Single-Drift Simulation Domain

- 1 “drift pair” (80 WPs upstream and 80 WPs downstream of access shaft)
- 20-m wide pillar to pillar
- “3-D vertical slice”
- Reflection BCs at y = 0 and y = 20 m





Salt Repository, Single-Drift
→ Deterministic *Isothermal** Simulation

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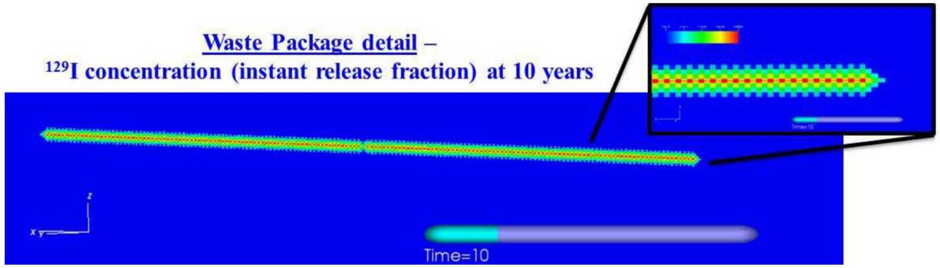
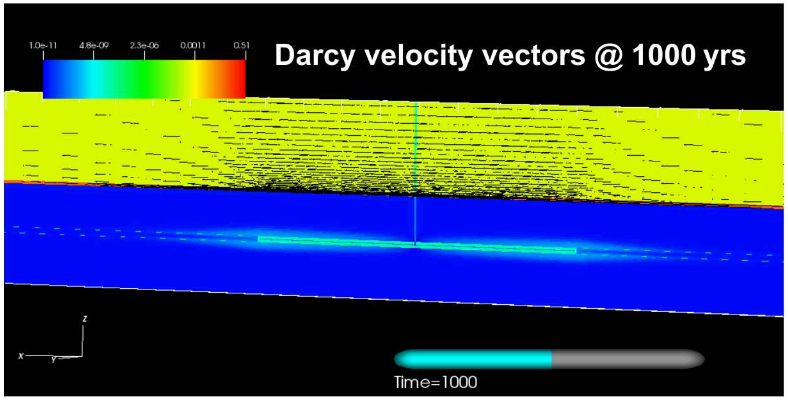
***non-heat generating waste**

– **EBS:** source term for <u>each waste package</u> →
  - *5 radionuclides: ^{129}I, ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th*
  - *Waste form (SNF) degradation rate controlled by kinetics*
  - C: *solubility limits, dissolved radionuclides can precipitate*



– **NBS:** 3-D flow and transport
  - *Primarily diffusion through DRZ and bedded salt*
  - *Primarily advection through aquifer and sediments*



– **Peclet Number**, N_{Pe}, in various layers:

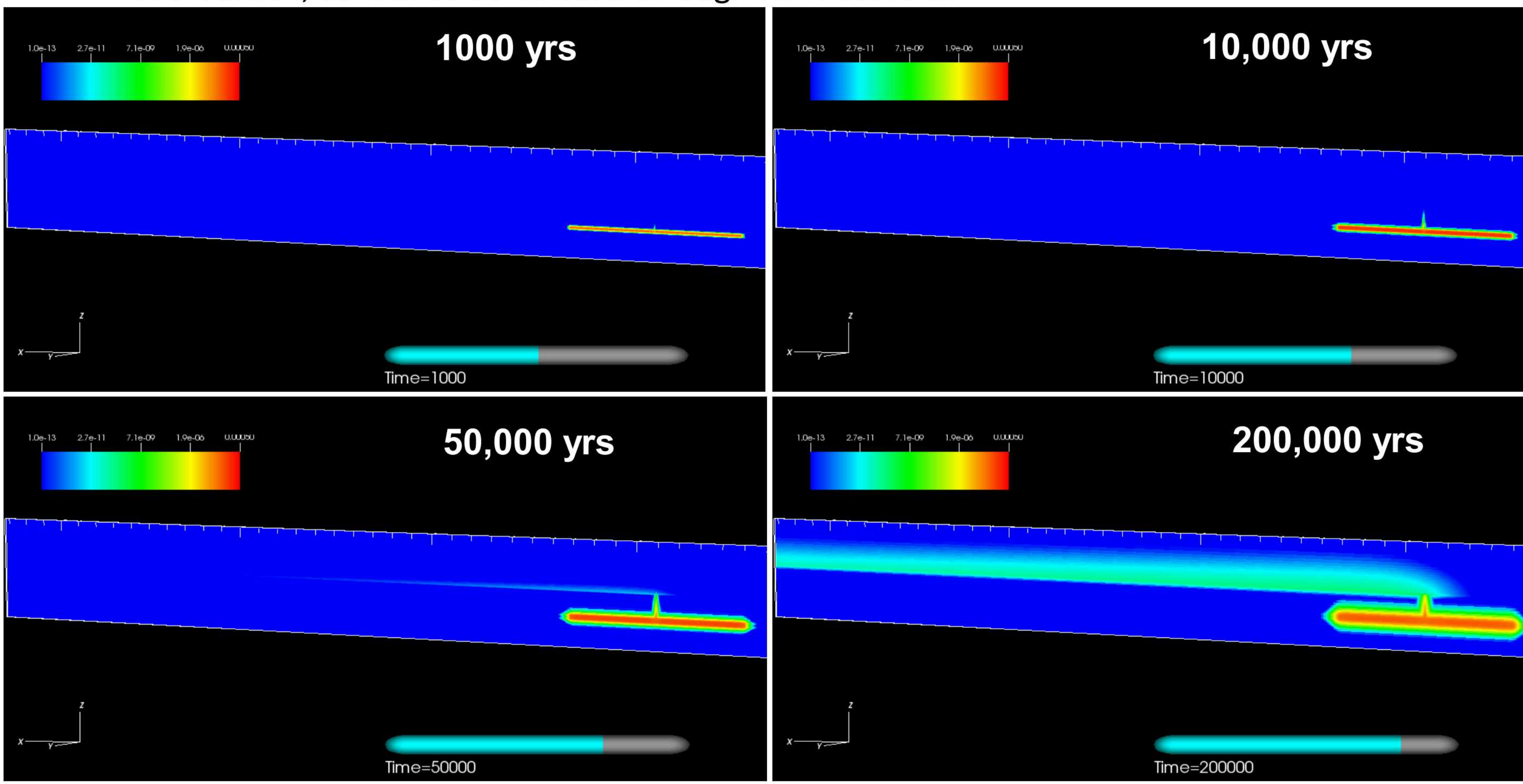
Region	Darcy velocity, u (m/s)[1]	Effective Diffusion Coefficent, $D_{eff} = \phi\tau D_w$ (m²/s)	Longitudinal Dispersivity (m)	Longitudinal dispersion coefficient, $D_L = \alpha_L u$ (m²/s)	Peclet Number, N_{Pe}
Halite	3.17×10^{-19}	4.19×10^{-13}	50.0	1.585×10^{-17}	0.0038
Interbed (anhydrite)	1.90×10^{-15}	5.57×10^{-12}	50.0	9.5×10^{-14}	1.7
Aquifer	1.58×10^{-9}	1.83×10^{-10}	50.0	7.9×10^{-8}	98
Sediments	1.58×10^{-11}	2.67×10^{-10}	50.0	7.9×10^{-10}	75

$$N_{Pe} = \frac{uL_{sys}}{D_{eff} + \alpha_L u}$$

- Diffusion-dominated when N_{Pe} ~<10
  – Halite and anhydrite

Salt Repository, Single-Drift → Deterministic *Isothermal** Simulation

- **^{129}I dissolved concentration at various simulation times:**
  - reaches the aquifer and overburden sediments via upward diffusion through the shaft seals
  - advects downgradient through aquifer and overburden; diffuses upward from aquifer to overburden, as well as downward through salt host rock



Salt Repository, Single-Drift → Deterministic *Thermal* Simulation

- **Decay heat flux for 60 GWd/MT PWR SNF (Carter et al. 2012)**
- **Geothermal gradient of 8°C/km – similar to WIPP**

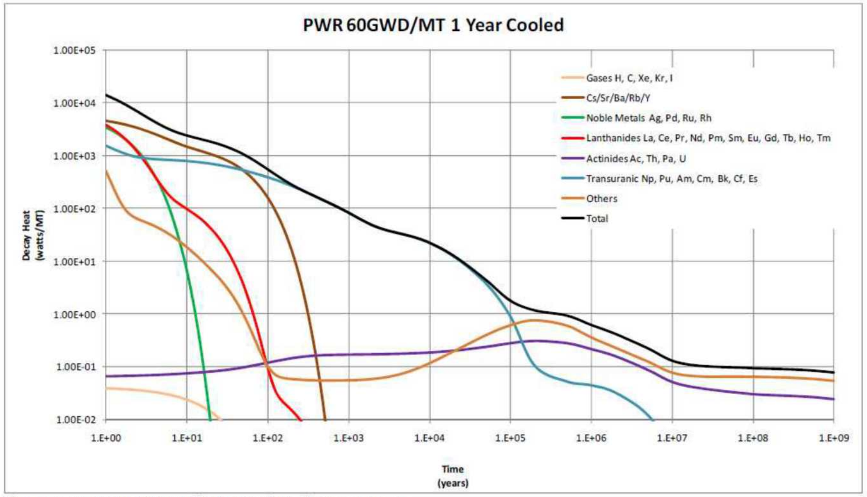
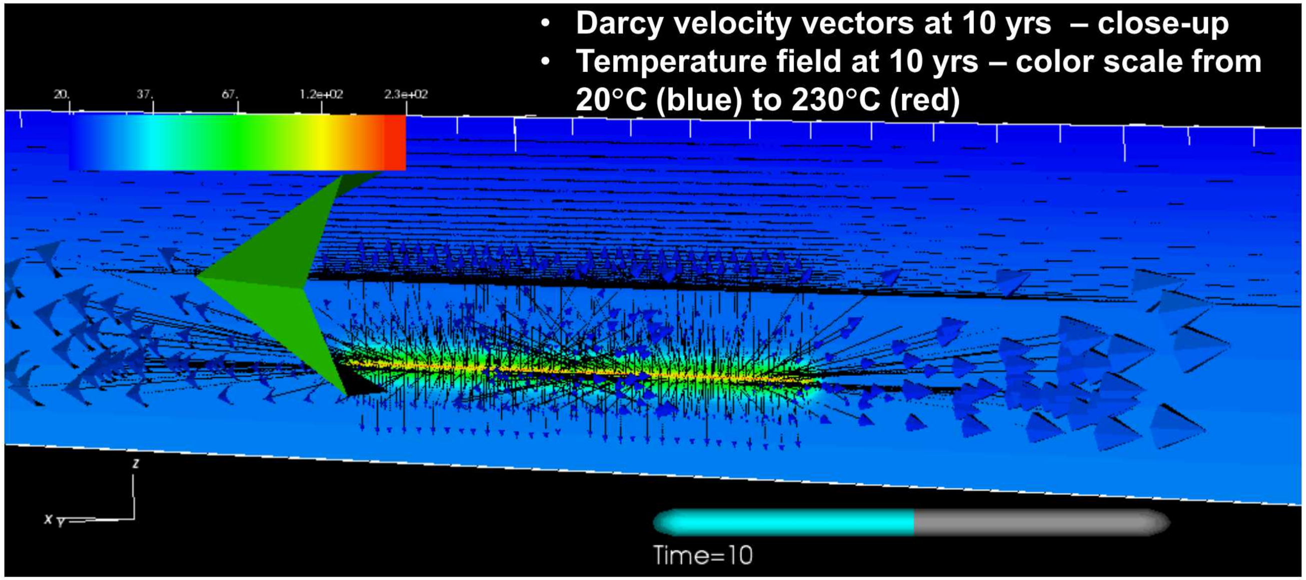


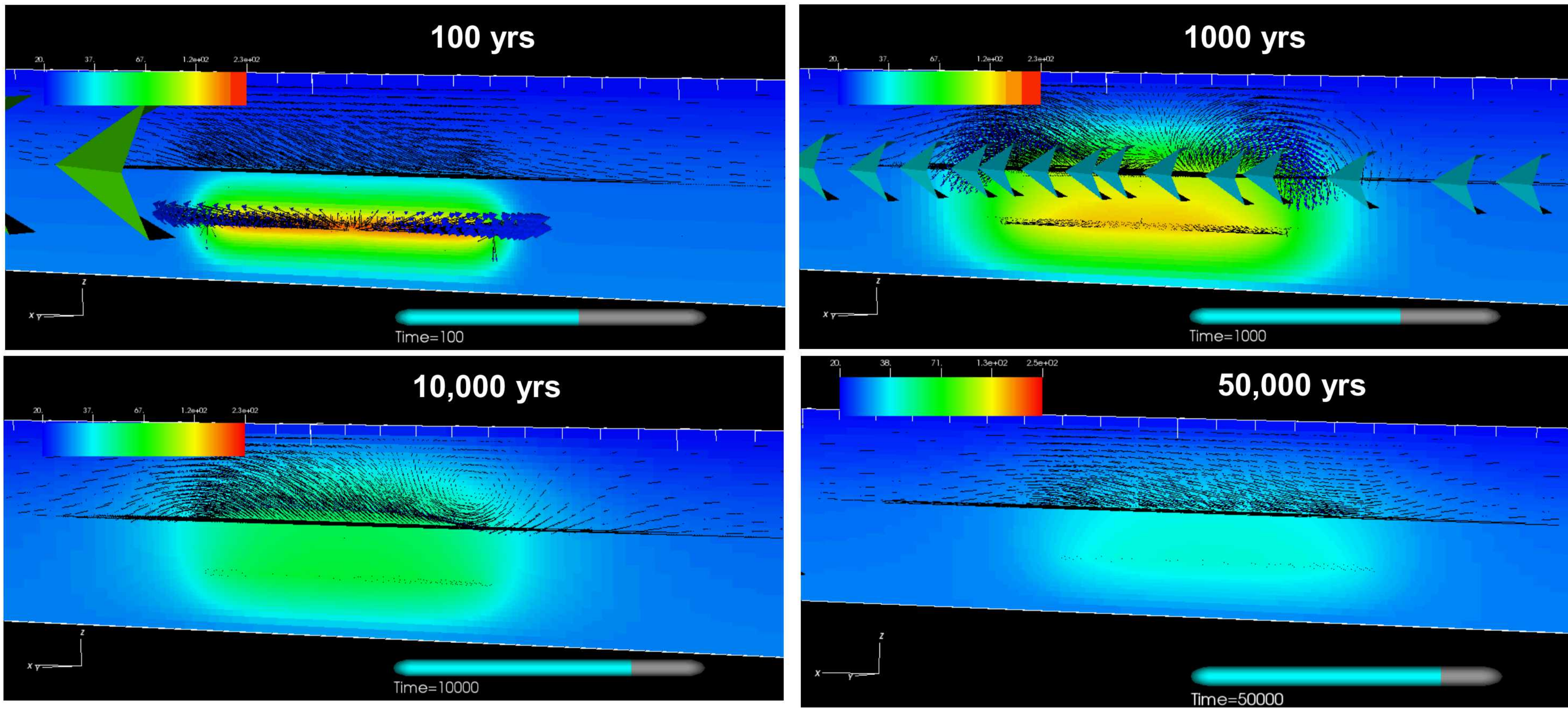
Figure 3-11 PWR 60 GWd/MT Used Fuel Decay Heat



- **Outward fluid velocity from repository region — due to *thermal expansion* of fluid**

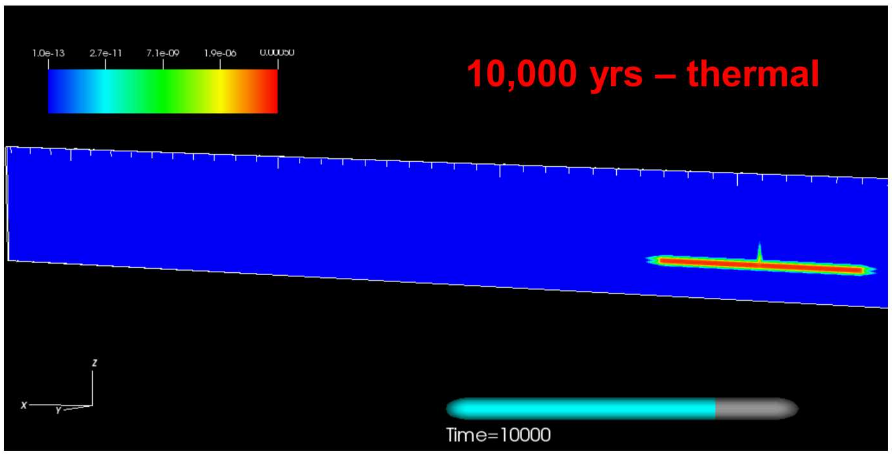
Salt Repository, Single-Drift → Deterministic *Thermal* Simulation

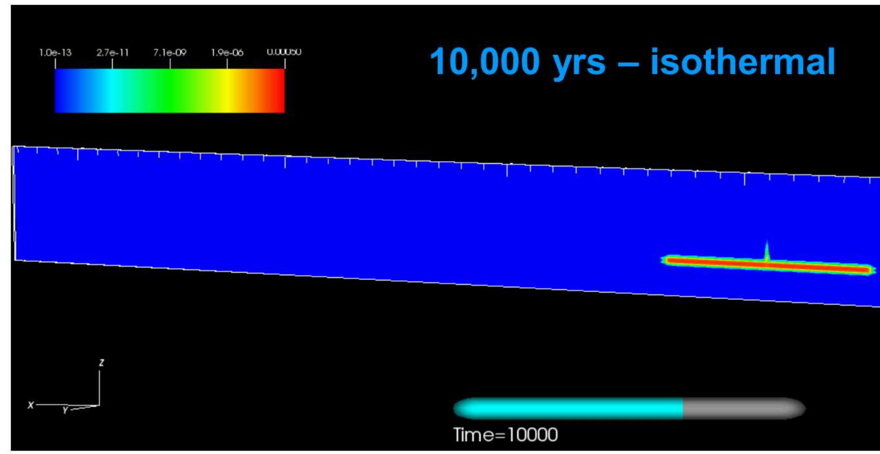
- **Thermally-driven (buoyancy) fluid convection cells for more than 10,000 yrs:**
  - **Darcy velocity vectors at various times**
  - **Temperature field at various times – color scale from 20°C (blue) to 230°C (red)**

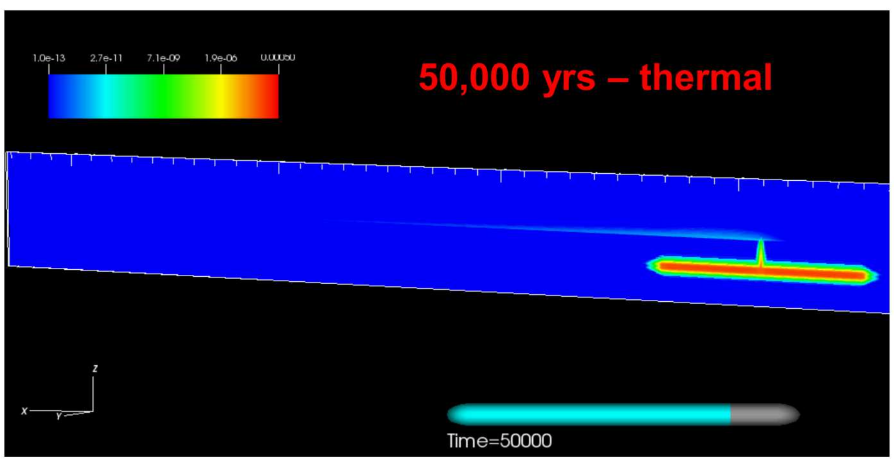


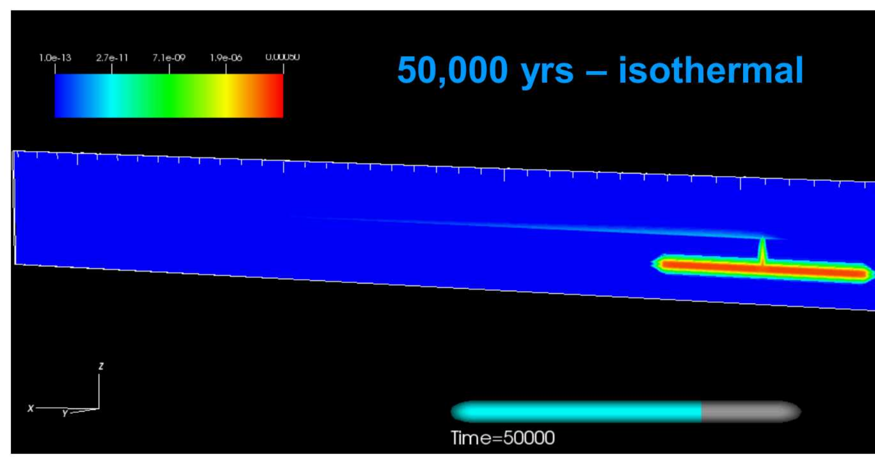
Salt Repository, Single-Drift
→ Deterministic *Thermal* vs. *Isothermal*

- **^{129}I Concentration at 10,000 years and 50,000 years (thermal vs. isothermal)**
  - **Only small effect from heat pulse (at early times due to thermal expansion of fluid)**
  - **Convection cells gone before 50,000 years, which is the transport time up the shaft seal**







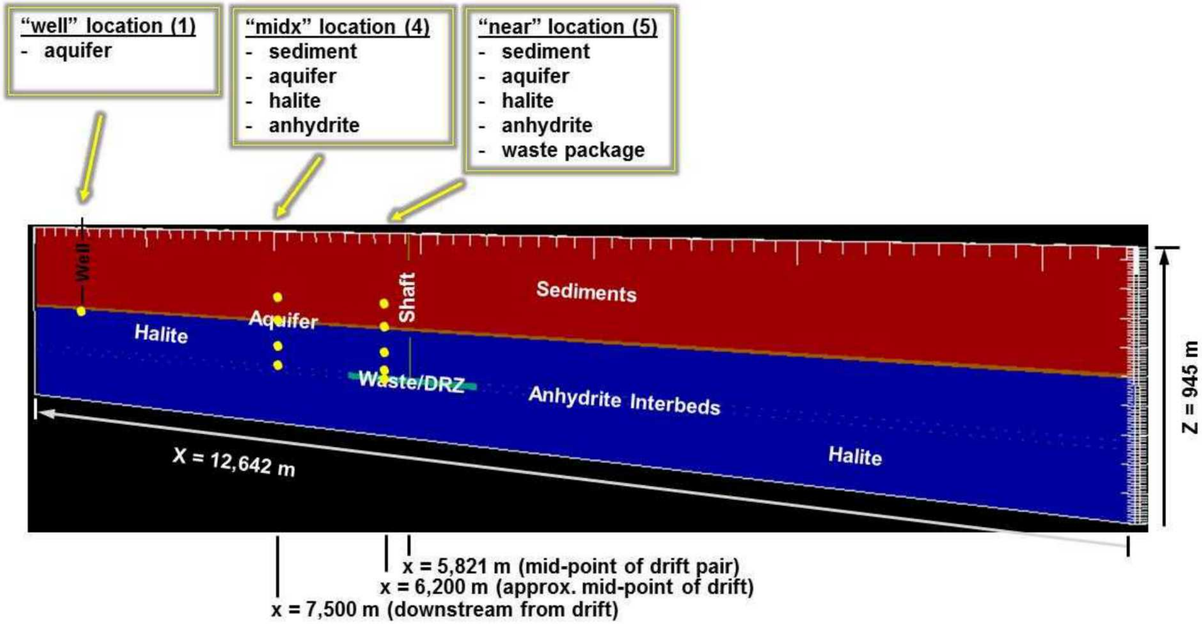


Salt Repository, Single-Drift → *Probabilistic* ***Isothermal**** Simulation

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

Model Parameter	Deterministic Value	Probability Range	Distribution Type
Waste form degradation rate constant (mol/m^2/s)	4.8×10^{-8}	1.00×10^{-10} – 1.00×10^{-7}	Log uniform
^{129}I K_d^P (ml/g)	0.0	9.28×10^{-7} – 7.84×10^{-3}	Log uniform
^{237}Np K_d^P (ml/g)	5.5	1.0 – 10.0	Log uniform
Waste Package Porosity	0.30	0.05 – 0.50	Uniform
Backfill Porosity	0.113	0.010 – 0.200	Uniform
Shaft Porosity	0.113	0.010 – 0.200	Uniform
DRZ Porosity	0.0129	0.0010 – 0.1000	Uniform
Halite Porosity	0.0182	0.0010 – 0.0519	Uniform[a]
Anhydrite Interbed Permeability (m^2)	1.26×10^{-19}	1.00×10^{-21} – 1.00×10^{-17}	Log uniform[b]
Aquifer Permeability (m^2)	1.00×10^{-13}	1.00×10^{-14} – 1.00×10^{-12}	Log uniform

- **Ten observation points:**

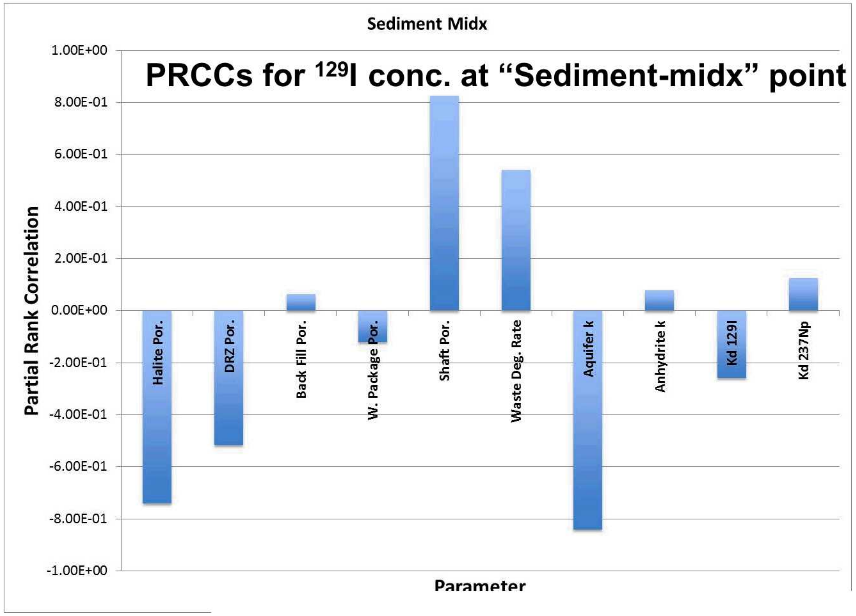


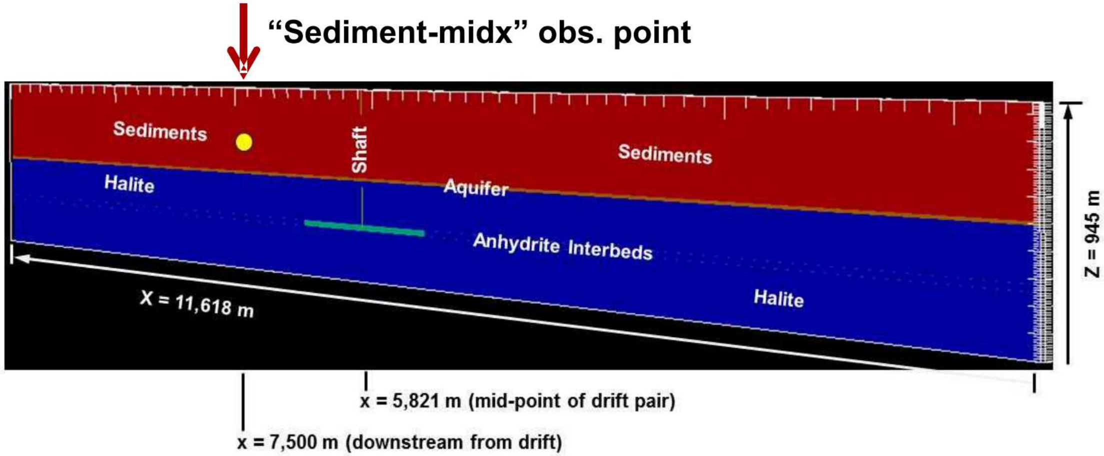
Probabilistic ***Isothermal**** **Simulation – Results at "Sediment-Midx" Observation Pt.**

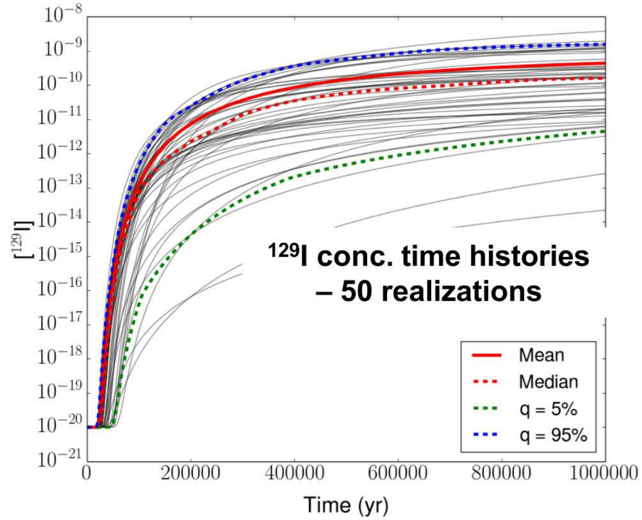
- **Strong positive PRCC for shaft seal porosity – higher ϕ_{shaft} increases effective diffusion coefficient for transport to the aquifer:**

$$(D_{eff})_{shaft} = (\phi\tau)_{shaft} D_w$$

- **Strong negative PRCC for aquifer permeability – higher $k_{aquifer}$ increases dilution and lowers concentration gradient into overburden sediments**
- **Positive PRCC for WF degradation rate – higher rate increases source cell conc.**
- **Negative PRCC for DRZ porosity – higher porosity decreases source concentration**



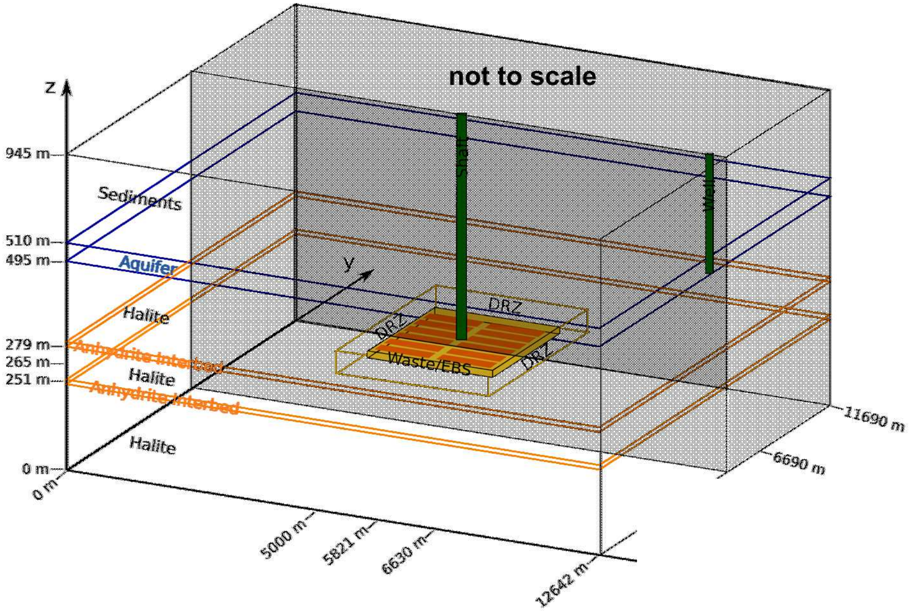




Single-Drift Simulation "Caveats"

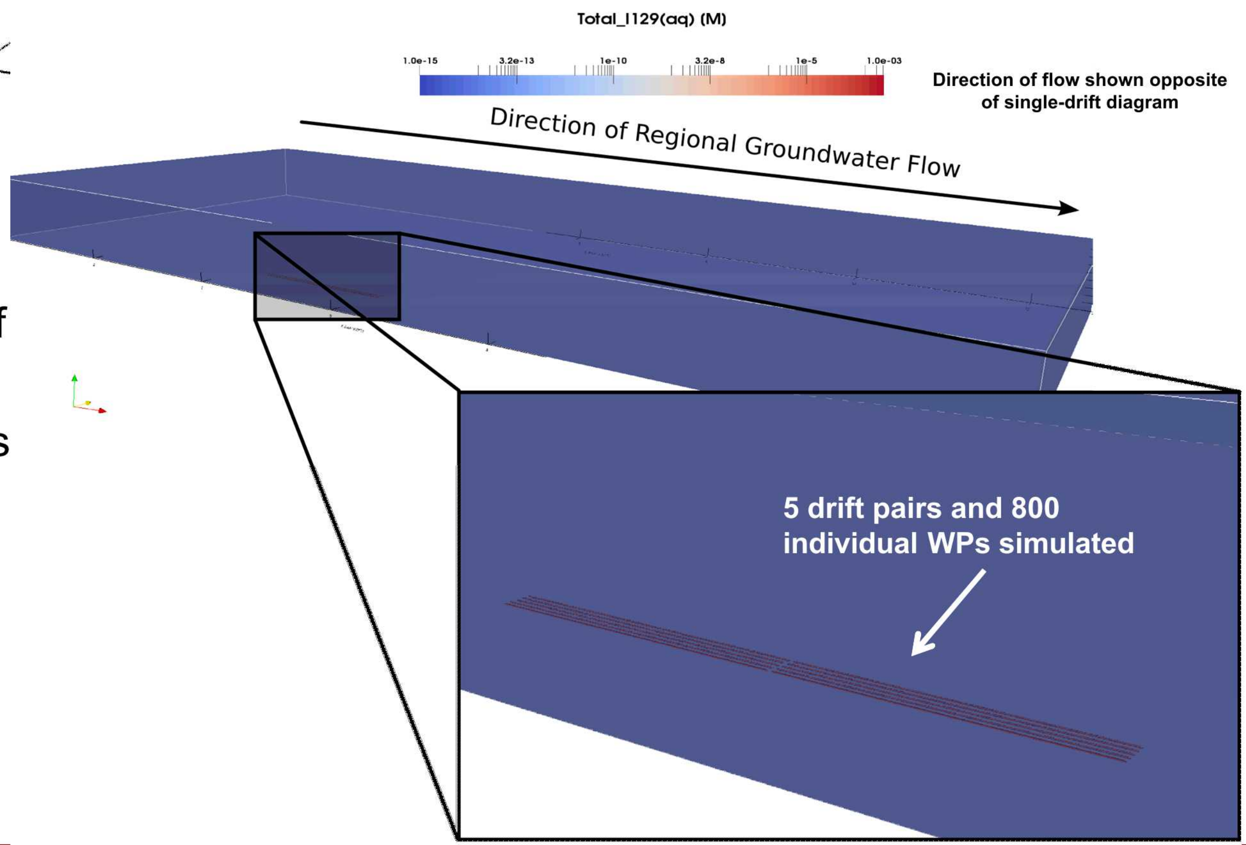
- Main purpose is to demonstrate the capabilities of the enhanced multi-physics HPC performance assessment framework
- Transport behavior of ^{129}I is a result of the assumed material properties in the various regions – may or may not occur at a potential repository site
- ^{129}I concentrations are conservatively high because the lateral boundary conditions in the *y*-direction (i.e., at the sides of the 20-m-wide, 3-D slice) are zero-gradient, no-flow:
  - Would only be true of a repository with an "infinite" number of parallel drifts and, thus, does not account for dilution from lateral mass loss
  - Also implies one access shaft per drift (results in greater diffusive transport to aquifer)
- Additional "conservative" factor:
  - No meteoric infiltration flux at the surface

3-D, Multi-Drift Simulation Domain



X	= 12,642 m		*NX*	=	387
Y	=	5100 m	*NY*	=	39
Z	=	945 m	*NZ*	=	71
			Cells =		1,071,603

- 5 “drift pairs”
- 3-D half-domain in *y*-direction (100 m of drifts and 5000 m of undisturbed host rock
- Reflection BC at y = 0 (implies 10 drift pairs by symmetry)



Salt Repository, Multi-Drift → Deterministic *Isothermal** Simulation

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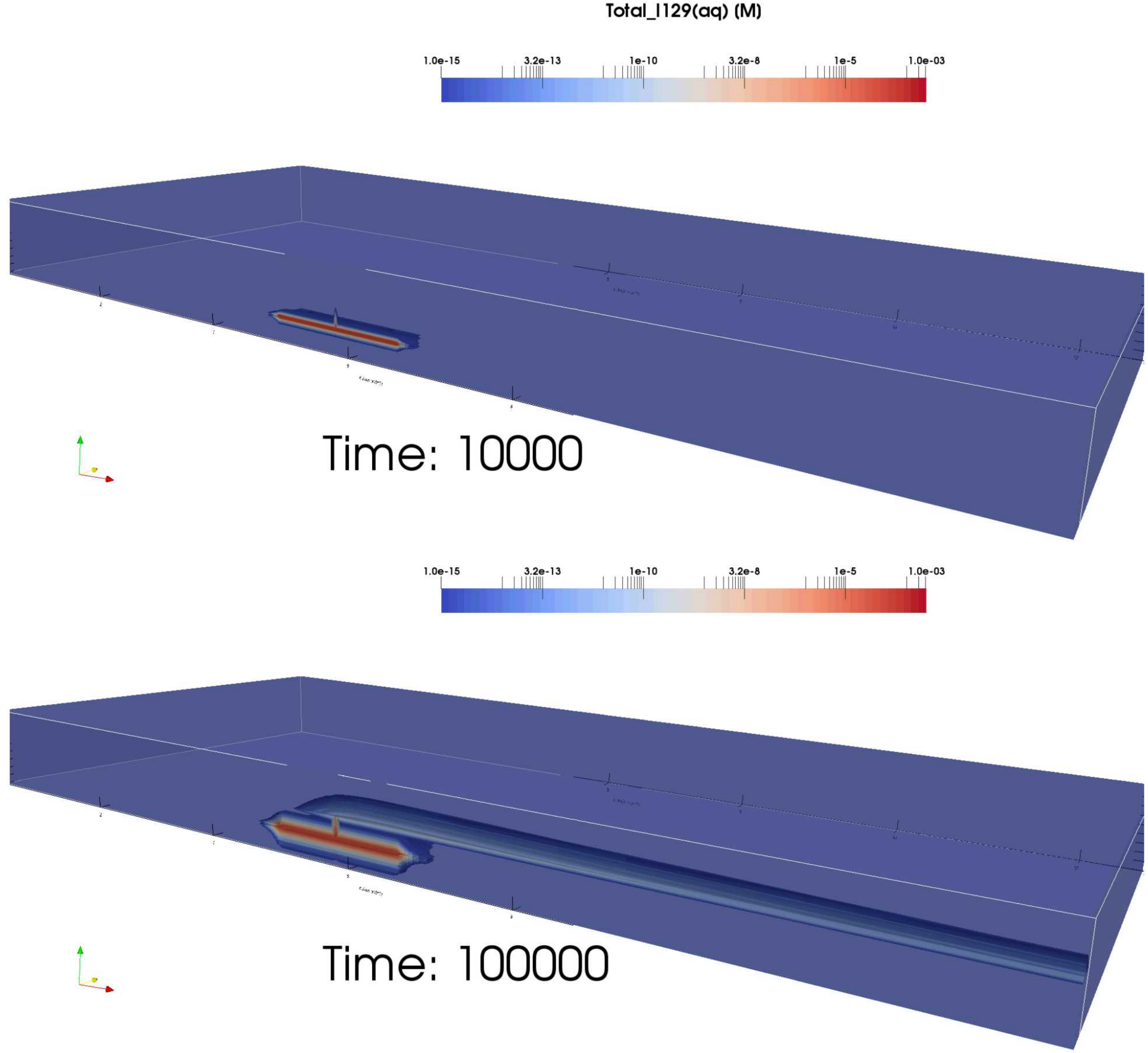
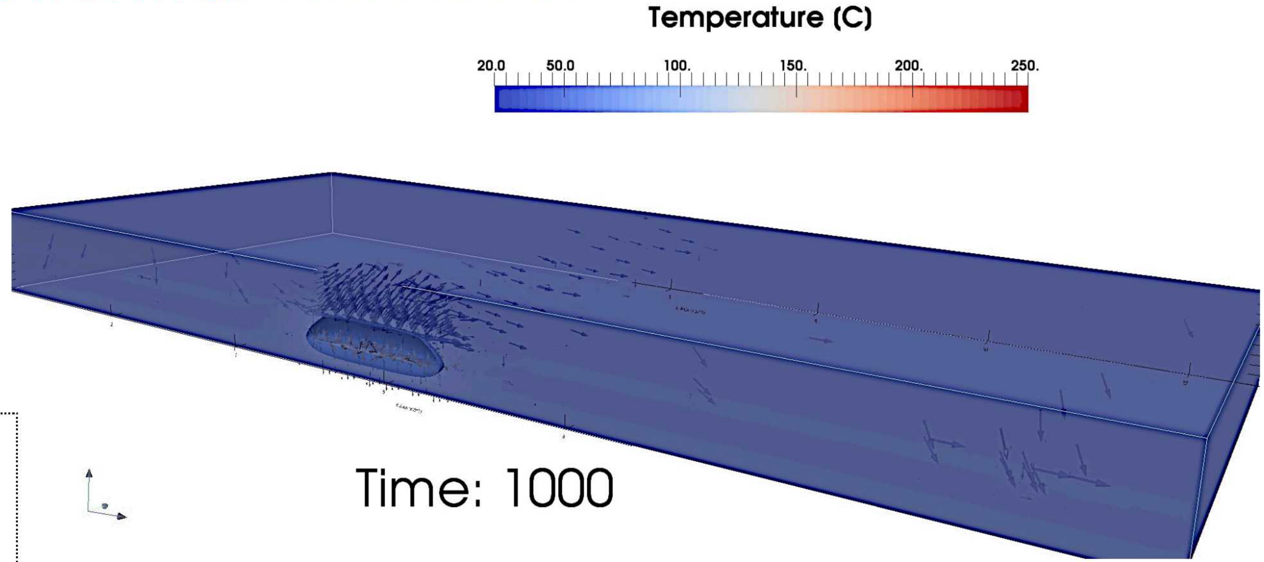
- **^{129}I dissolved concentration at various simulation times:**
  - reaches the aquifer and overburden sediments via upward diffusion through the shaft seals
  - advects downgradient through aquifer and overburden; diffuses upward from aquifer to overburden

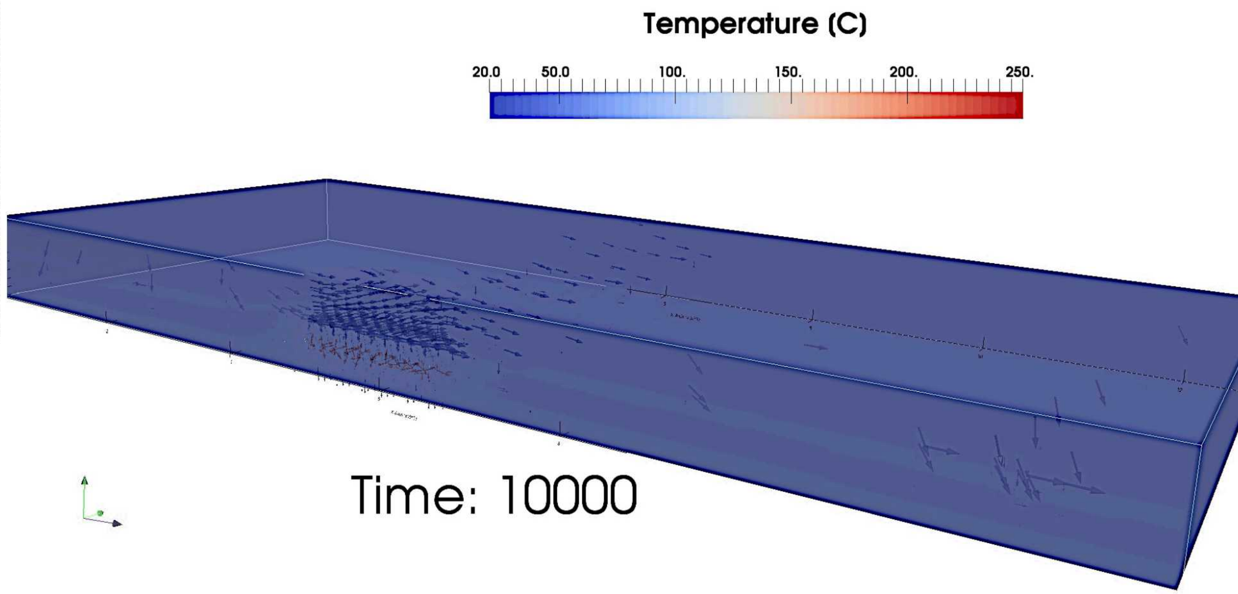


Salt Repository, Multi-Drift
→ Deterministic *Thermal* Simulation

- **Darcy velocity vectors at various times, and**
- **Temperature field at various times**

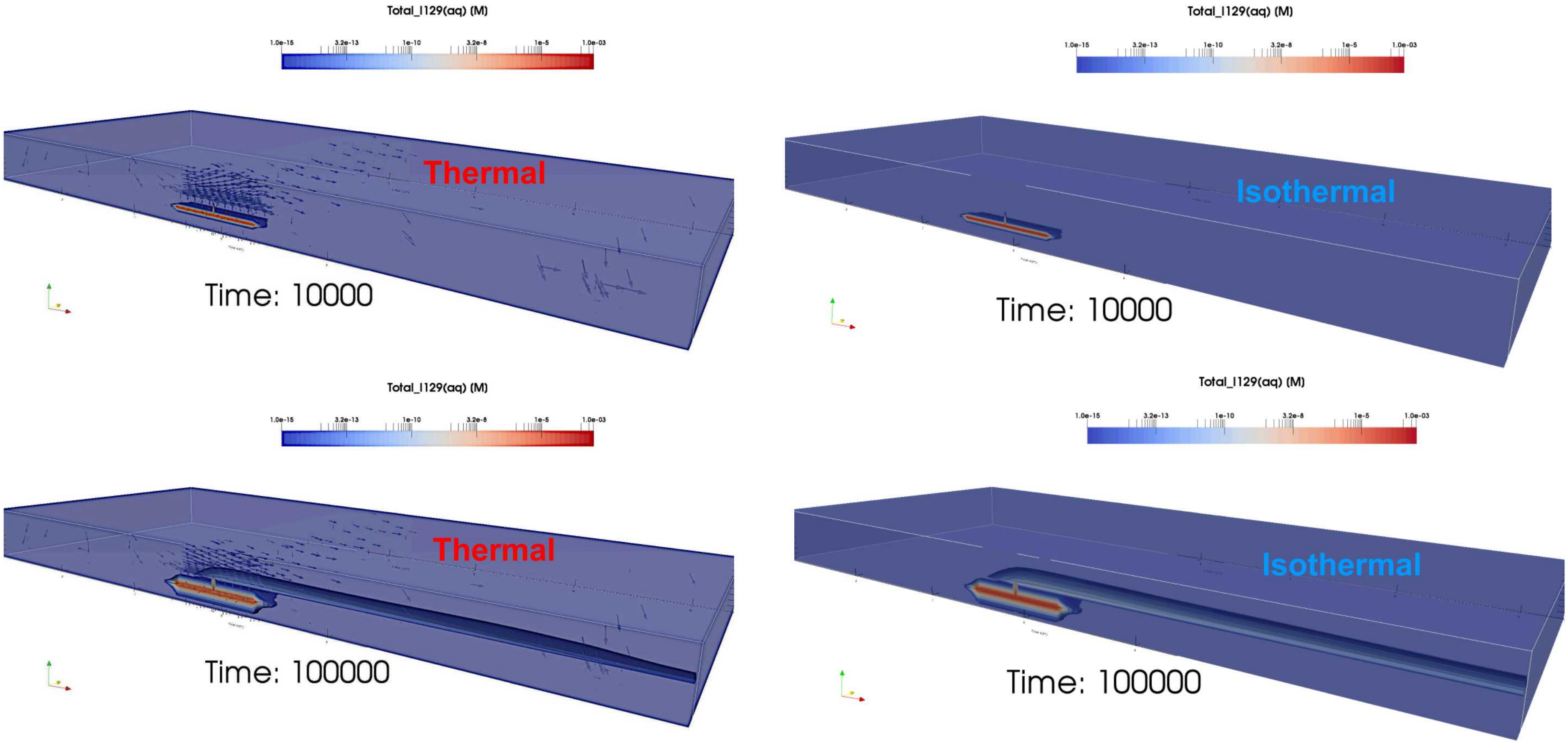
- *Thermally-driven, buoyant flow for more than 10,000 years*
- *Convection cells not obvious compared to single-drift simulation – perhaps dissipated in y-direction*





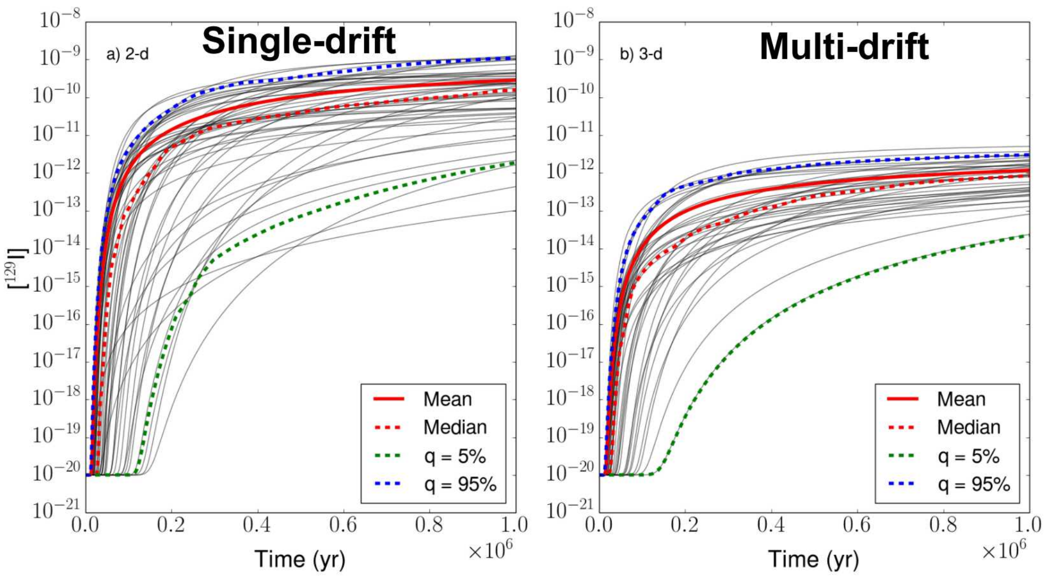
Salt Repository, Multi-Drift
→ Deterministic *Thermal* vs. *Isothermal*

- **^{129}I Concentration at 10,000 years and 100,000 years**
  - **Little effect from heat pulse at early times, prior to releases reaching the aquifer, via diffusion up the access shaft**
  - **Downwelling fluid flow in overburden sediments from heat pulse effects, downgradient of repository, reduces the upward diffusive spread of ^{129}I into the sediments**

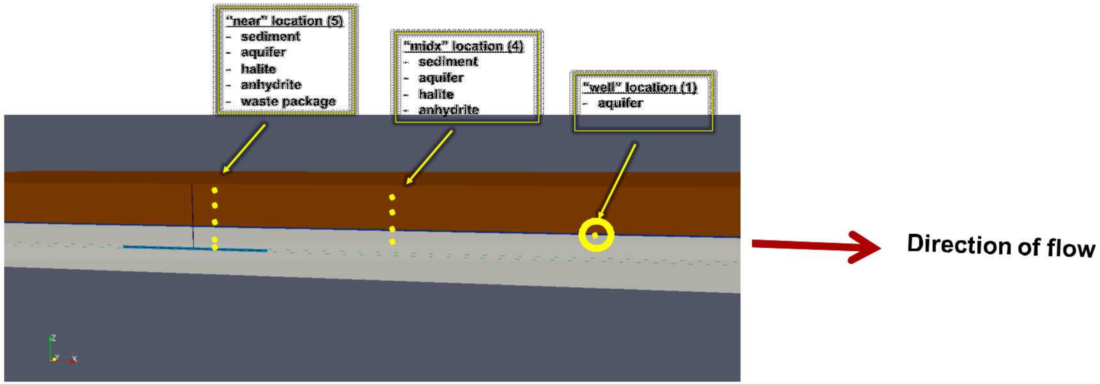


Multi-Drift vs. Single-Drift Comparison → *Probabilistic* ***Thermal***

- **The single-drift (20-m wide) reflection BC case (with effectively one shaft per drift-pair) and the five-drift half-domain (5100-m wide) represent two "bounds" for the effect of lateral dispersion/diffusion on peak concentration:**



^{129}I conc. time histories – 50 realizations at "Well" obs. point



Summary and Future Work

- **An enhanced PA modeling capability has been developed to:**
  - Evaluate generic and/or specific disposal sites in various geologic media
    - High-fidelity representation of coupled processes in 3-D, using parallel HPC architecture and software
    - Including uncertainty and heterogeneity
  - Support prioritization of UFD RD&D activities
  - Enhance confidence and transparency in the safety case
- **Application to a generic salt repository reference case**
  - Some differences in PA results based on coupled T-H process effects on fluid flow, and based on the number of drifts simulated
- **Ongoing and future work includes**
  - 3-D simulations of a clay/shale reference case (recently completed)
  - 3-D simulations of the defense-only HLW in bedded salt (recently completed)
  - Grid refinement studies (begun already)
  - Application to deep borehole disposal in crystalline basement rock
  - Application to WIPP PA
  - Inclusion of all drifts/WPs in a half repository
  - Simulations in fractured crystalline rock to be started next fiscal year

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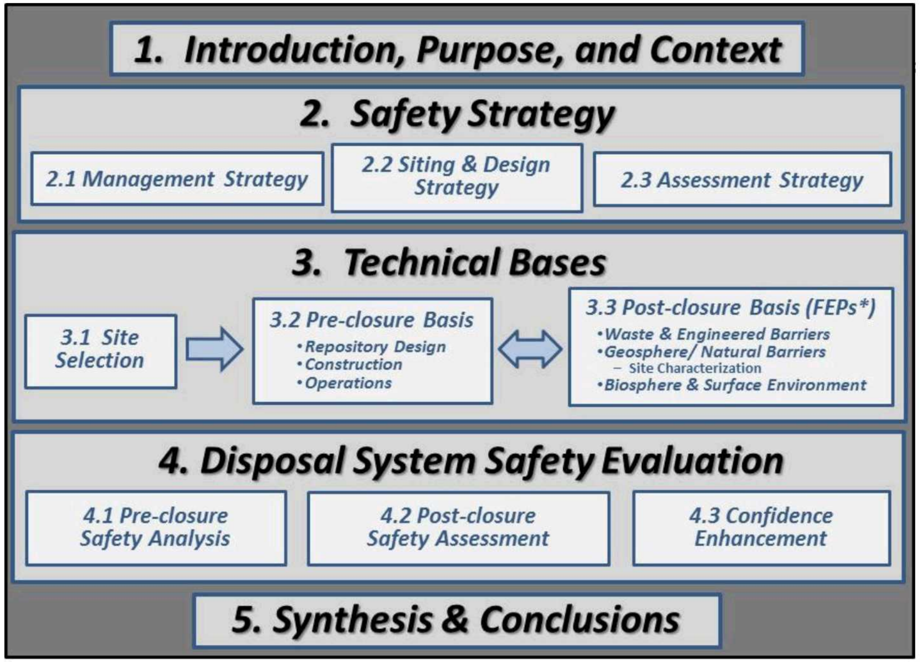
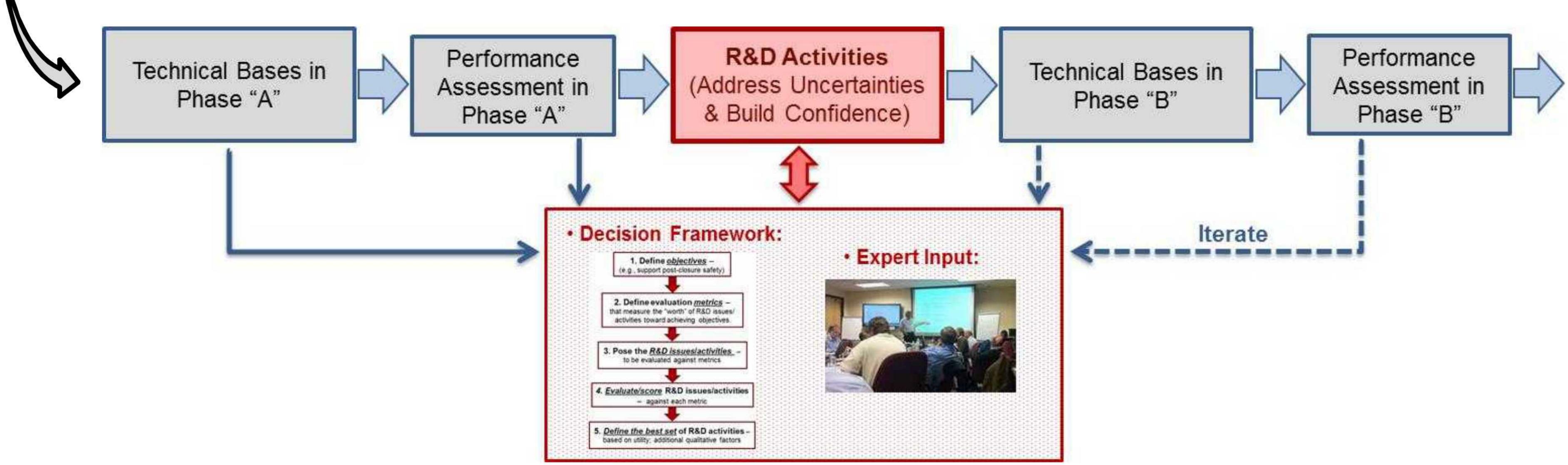
Questions?

Backup Slides

Evolution and Iteration of the Safety Case

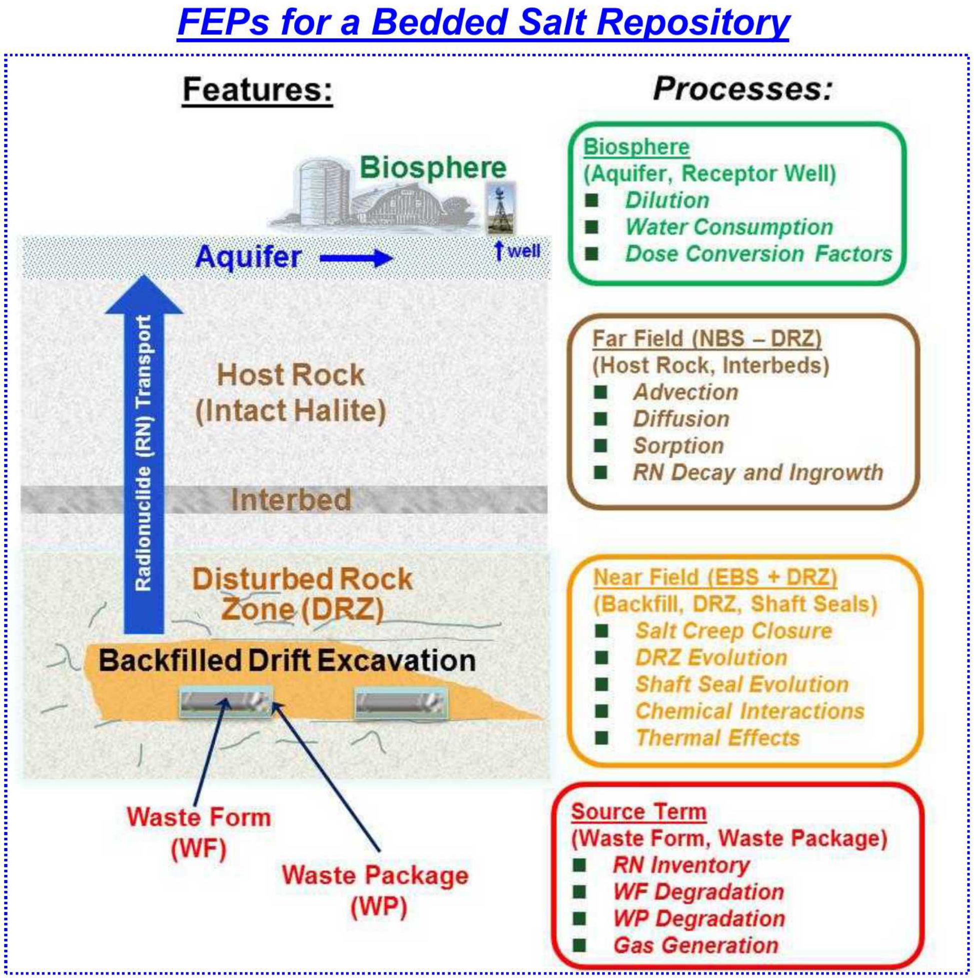
- How does safety confidence improve through time?
  - *Iteration* of two major elements of the safety case—***technical bases*** and ***performance assessment***:





PA Methodology: *Conceptual Model*

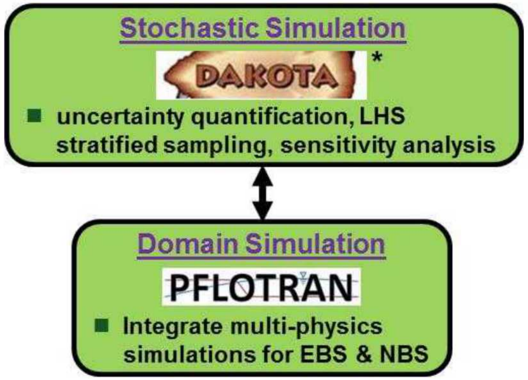
- **PA Conceptual Model Development:**
  1. *System Characterization* – characterization of the regions and features of the disposal system, including property values and quantification of uncertainty
  2. *System Design* – specification of a disposal concept, repository, layout, and engineered design features
  3. *FEPs* and Scenario Analysis* – identification and screening of potentially relevant FEPs and scenarios, for inclusion (exclusion) in PA model
  4. *PA Model Construction* – conceptual and mathematical representation of the FEPs and scenarios in the PA model/code



* Features, events, and processes

Generic Salt Repository PA Demonstration – Multi-Realization Simulations

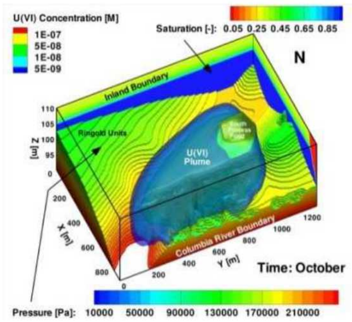
- **DAKOTA / PFLOTRAN simulations**:
  - Deterministic simulation with mean or representative values
  - 50-realization probabilistic simulation with 10 sampled parameters
  - Run on SNL Red Sky HPC cluster
    - *Nested parallelism*
    - *Many concurrent realizations*
    - *Each realization distributed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



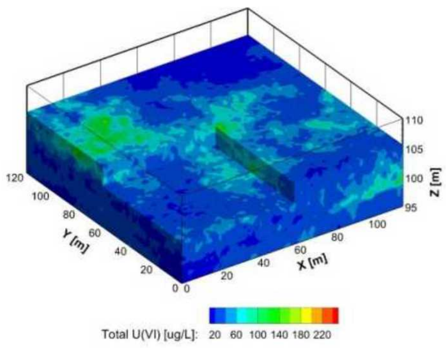
- Total nodes: 2,816 nodes / 22,528 cores
- 505 TeraFlops peak

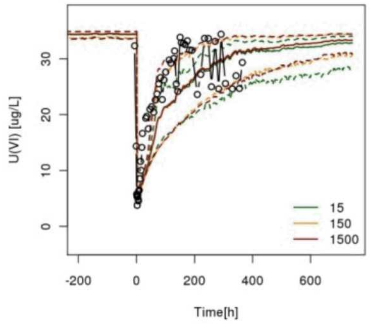
PFLOTRAN Process Modeling

- **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



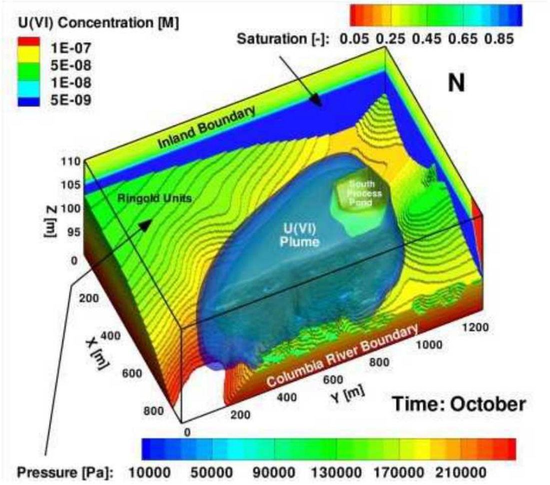
Hammond and Lichtner, WRR, 2010





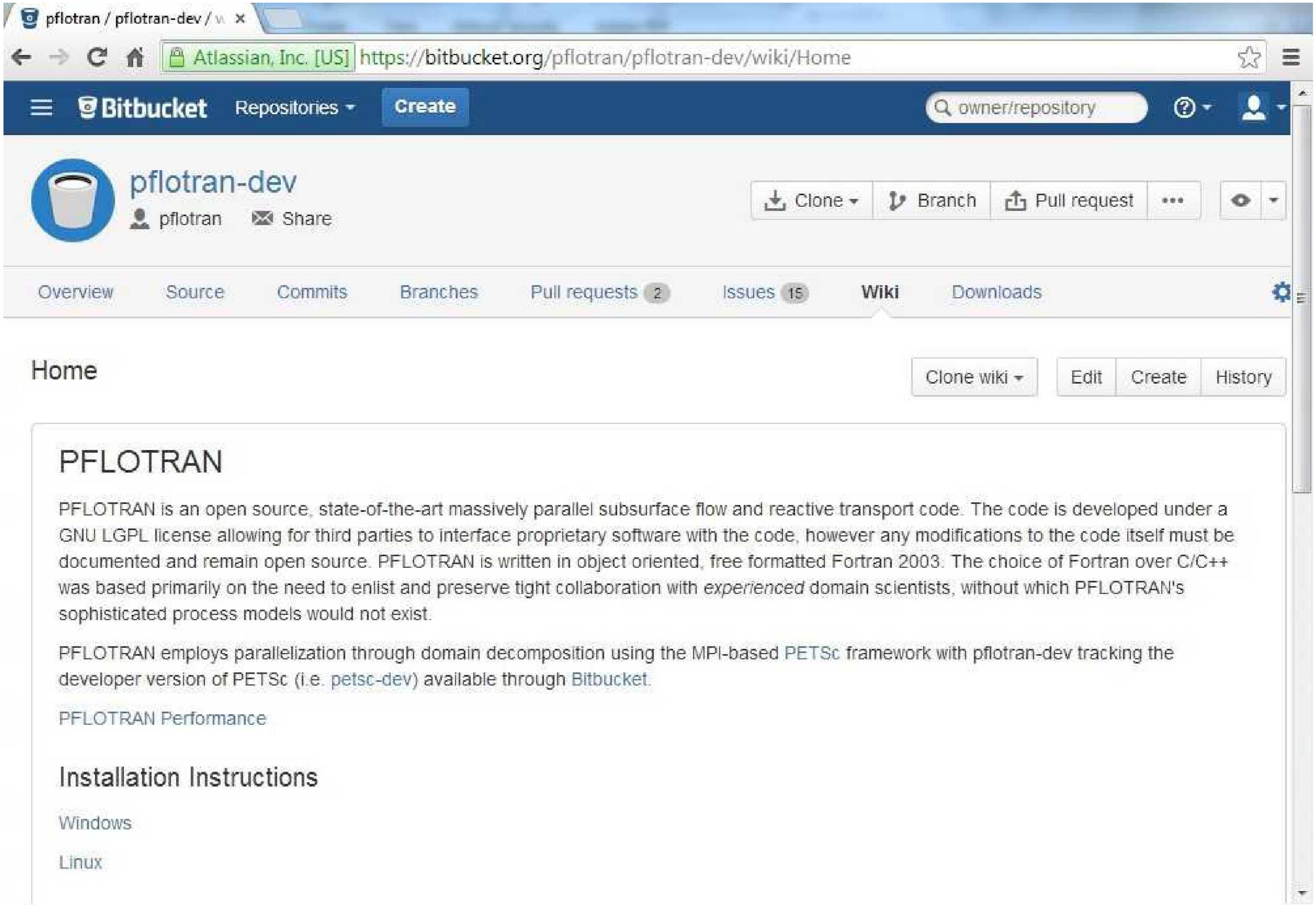
Major Projects Leveraging PFLOTRAN

- **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

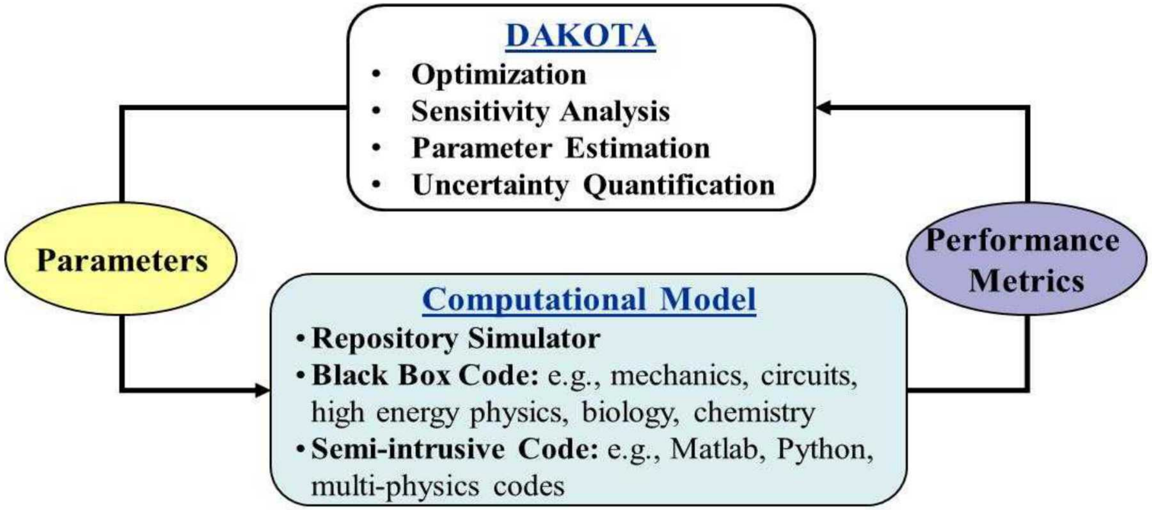
Linux

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

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

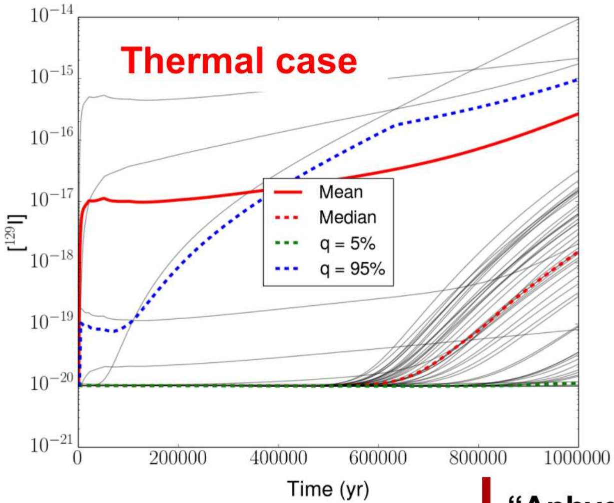


http://dakota.sandia.gov/

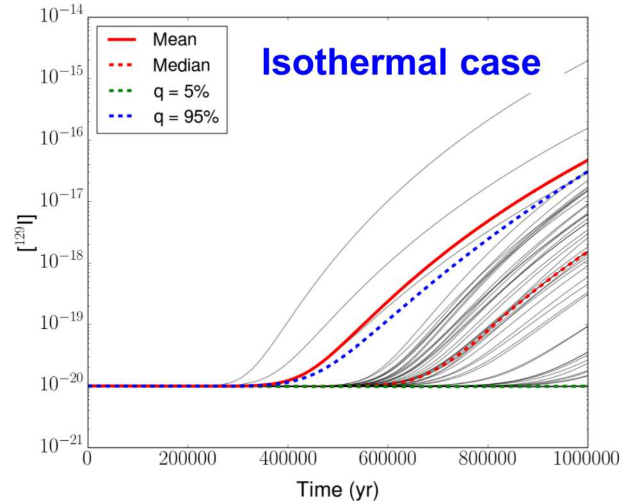
Probabilistic *Thermal* Simulation – Results at "Anhydrite-Midx" Observation Pt.

Sandia National Laboratories

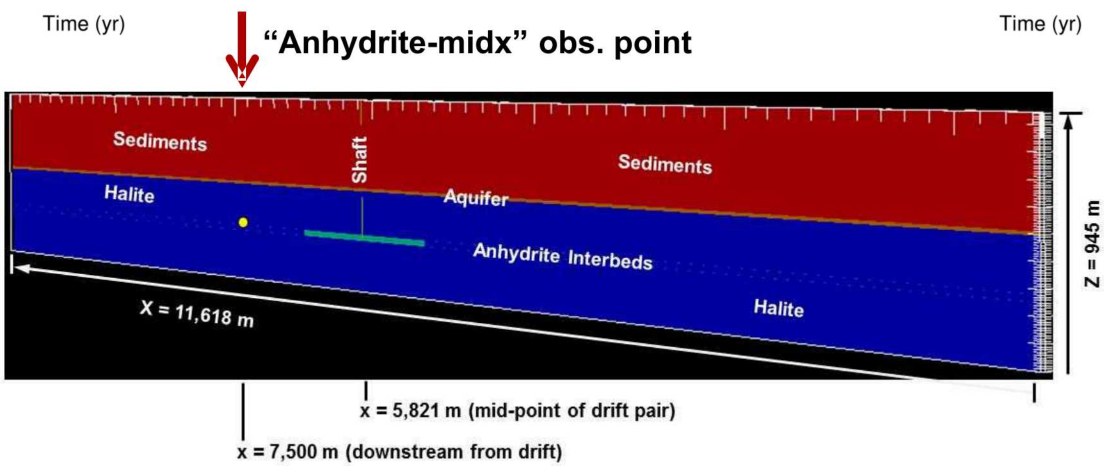
- ^{129}I concentration time histories:
  - Only small effect on 6 out of 50 realizations at a single observation point, at very low concentration levels, due to early-time thermal fluid expansion around repository
  - Caused by some high values of anhydrite permeability in the sampling



^{129}I conc. time histories – 50 realizations at "Anhydrite-midx" obs. point



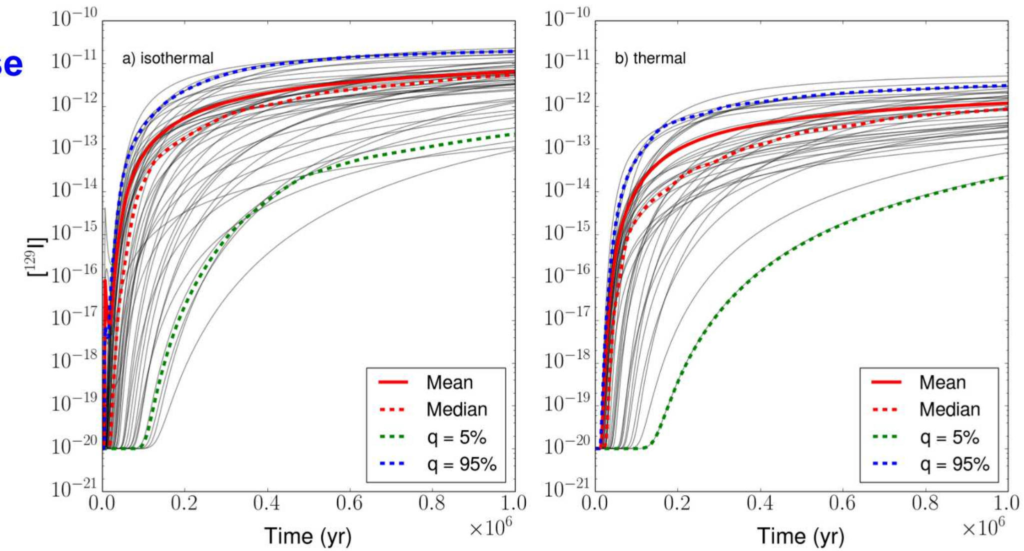
"Anhydrite-midx" obs. point



Salt Repository, Multi-Drift
→ *Probabilistic* ***Thermal*** **vs.** ***Isothermal***

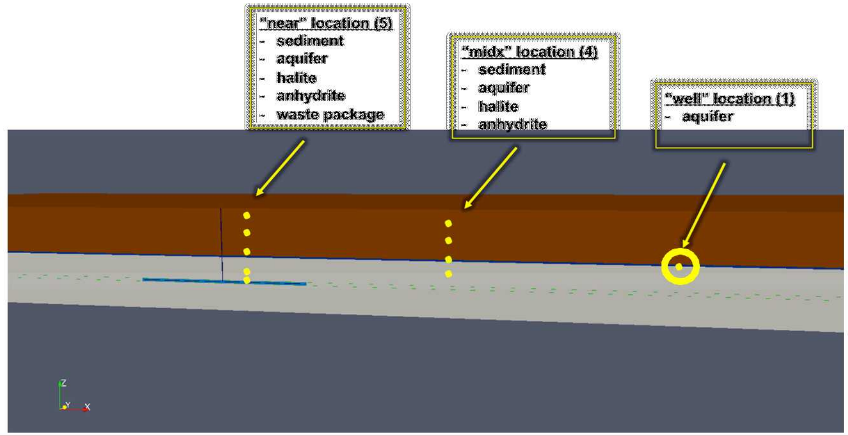
- **Downward vertical component of regional flow in thermal case reduces ^{129}I concentrations at aquifer withdrawal well – effect needs further investigation**

Isothermal case



Thermal case

^{129}I conc. time histories – 50 realizations at "Well" obs. point



Direction of flow