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Enhanced Performance Assessment Models For Generic Deep Geologic Repositories for HLW and SNF

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Sandia National Laboratories

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U.S. DEPARTMENT OF ENERGY

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Outline of Presentation

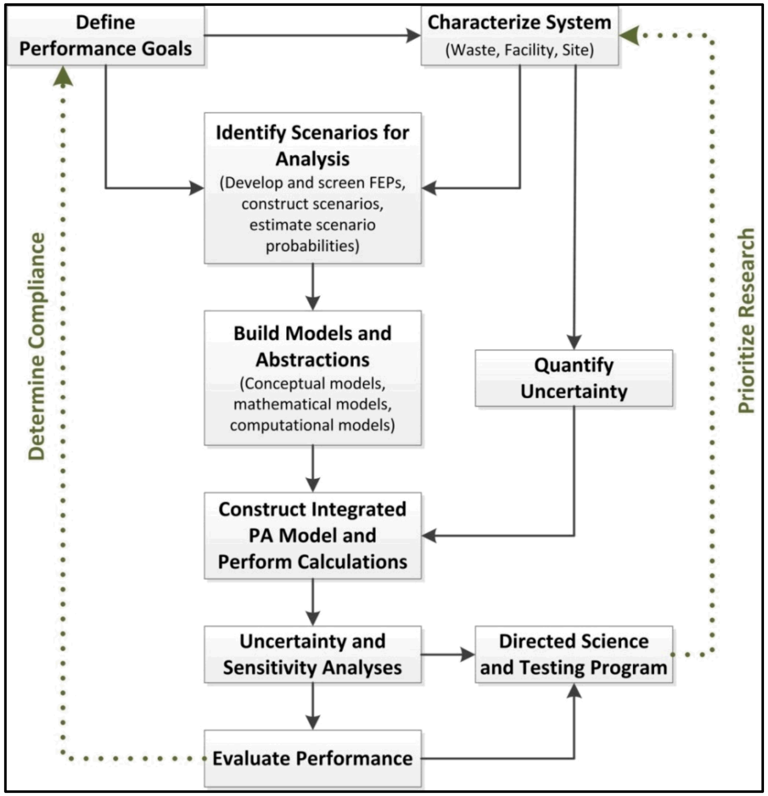
- Performance assessment (PA) model/code development philosophy and architecture
- Example application of enhanced PA model
  - Generic salt repository reference case
  - Demonstration simulations
- Summary and future work

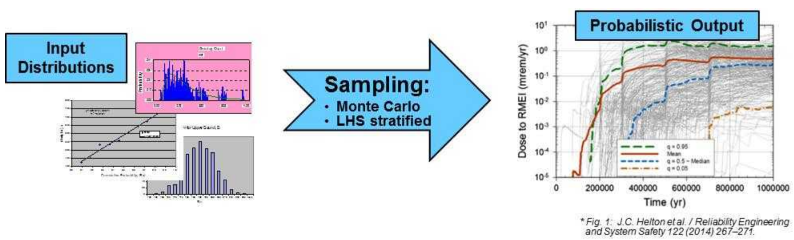
Acknowledgments

- Code development: Glenn Hammond
- Conceptual model development: Paul Mariner, Geoff Freeze, Emily Stein, Payton Gardner
- 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/Uses of the Enhanced PA Capability

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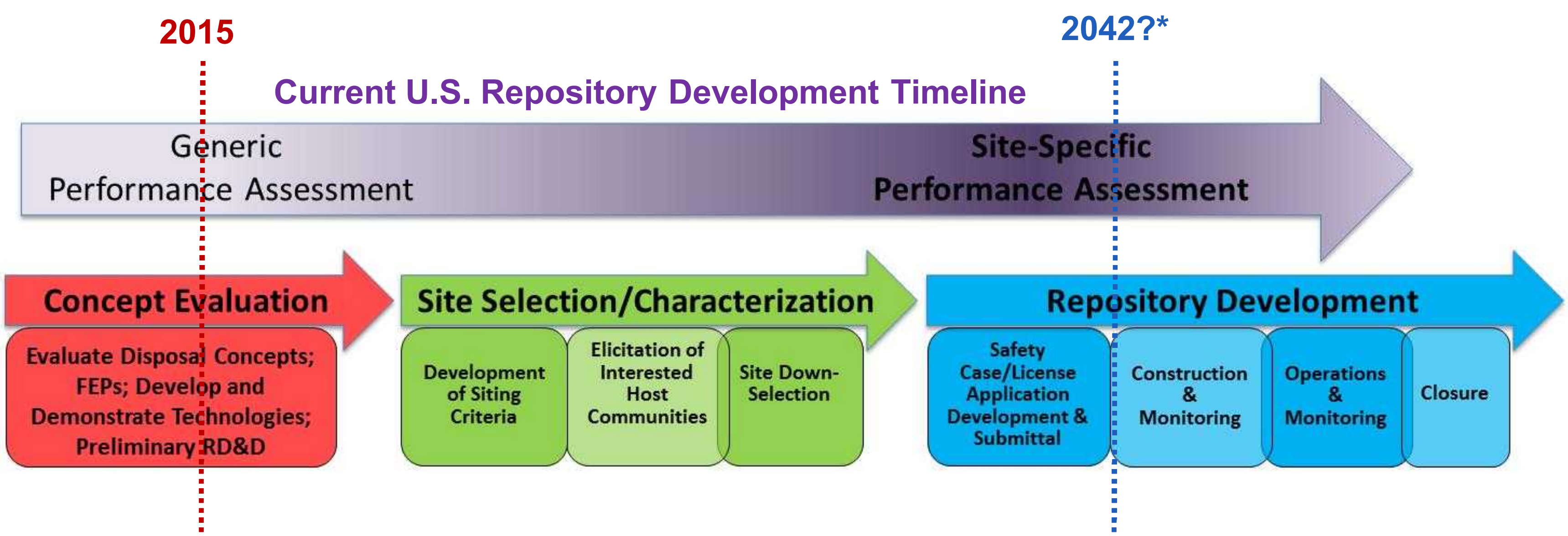
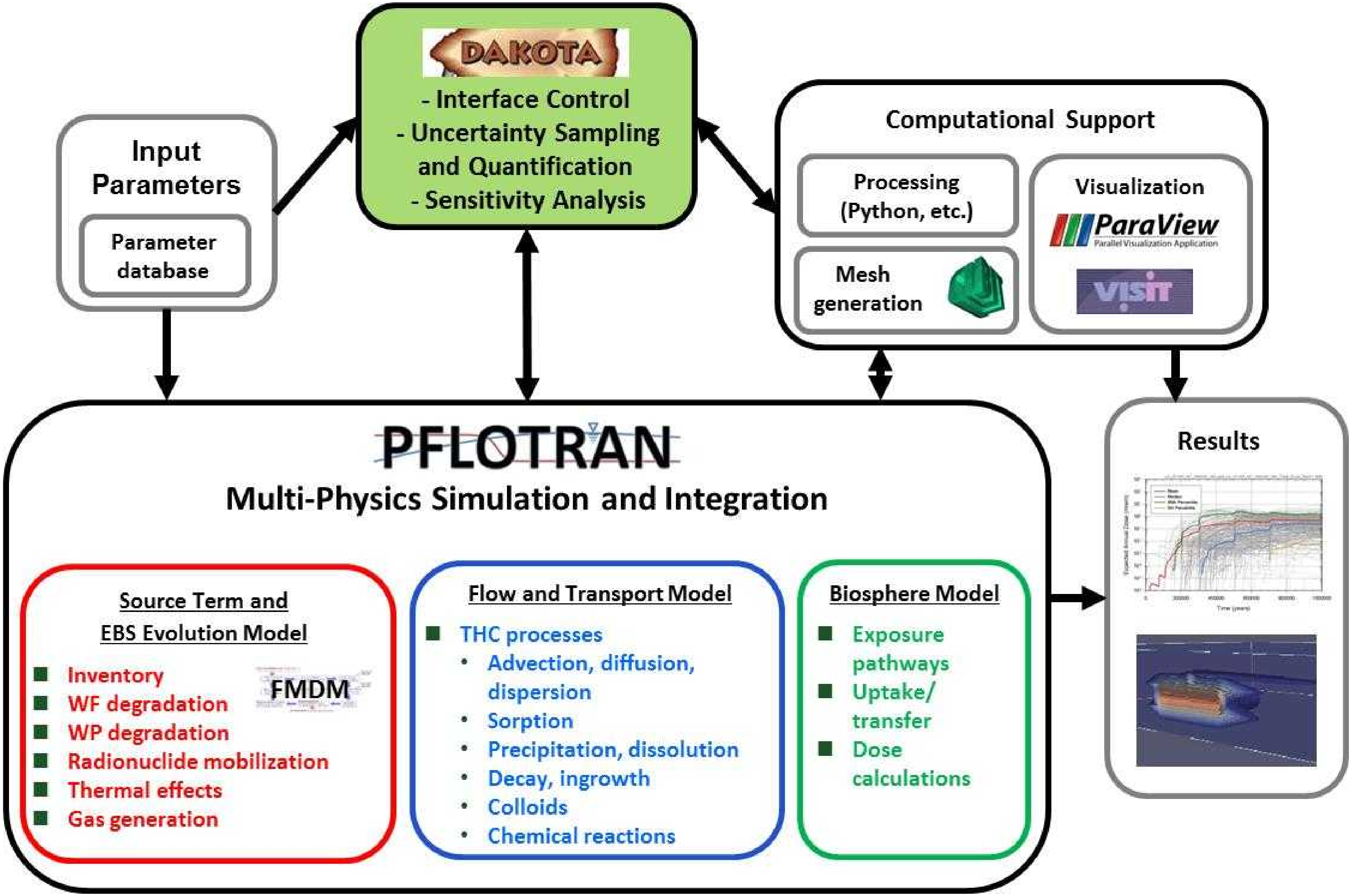
- **Goals:**
  - Enhance confidence and transparency in disposal system safety case
  - Enable better decisions (technical, political, fiscal)
- **Uses:**
  - Evaluate potential disposal concepts and sites in various host rock media
  - Help prioritize RD&D activities (initially *generic*; later *site-specific*)
  - Support safety case development during all phases of lifecycle



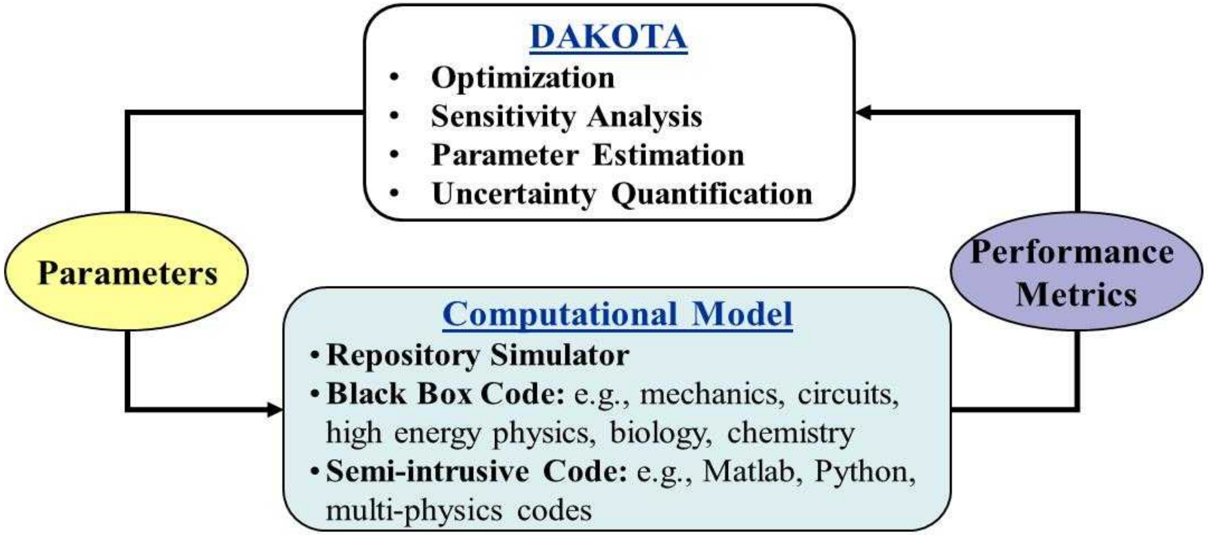
*DOE 2013

Enhanced PA Computational Model Architecture



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

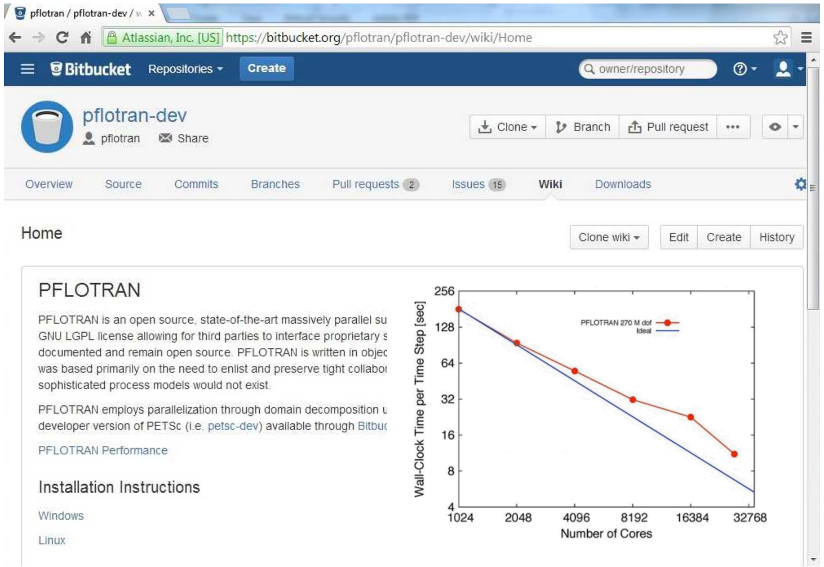


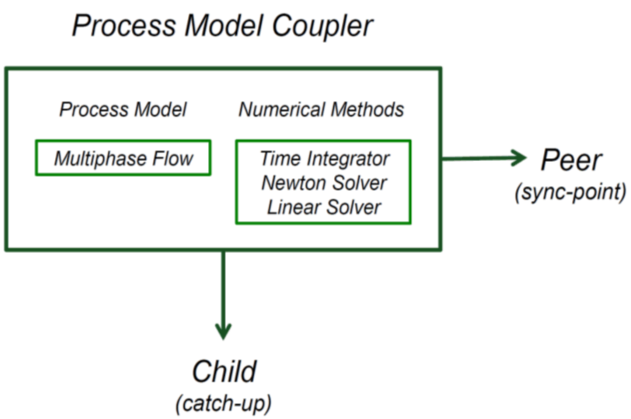
http://dakota.sandia.gov/

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 (petascale)
- 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*
- 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

PFLOTRAN





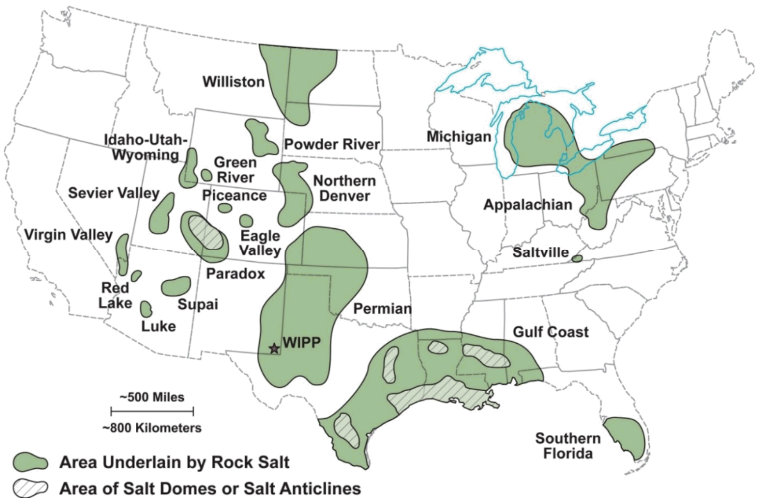
Application of Generic PA Model:

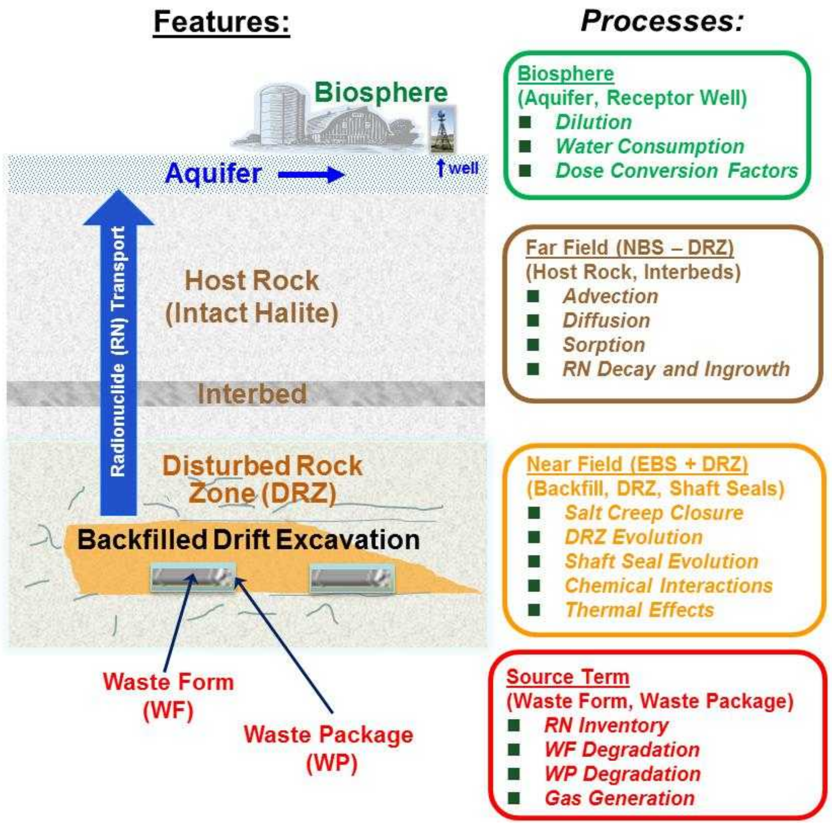
Salt Reference Case & TH Simulations

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)

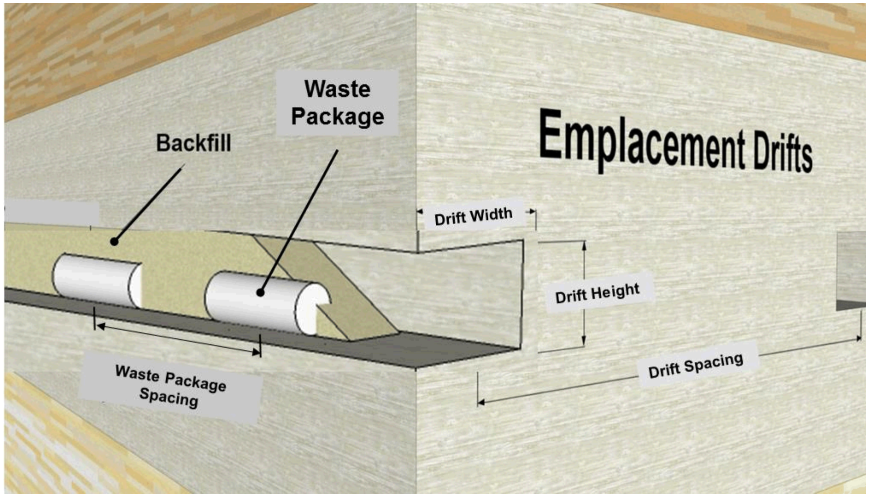
- **Salt host rock:**
  - Use parameters representative of five major bedded salt basins in the U.S.
- **Disturbed rock zone (DRZ), interbeds, representative aquifer:**
  - Typical properties from international studies and from WIPP





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%
  - Relatively fast SNF fractional degradation rate, based on bromide-containing brines (Kienzler et al. 2012)
- 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)

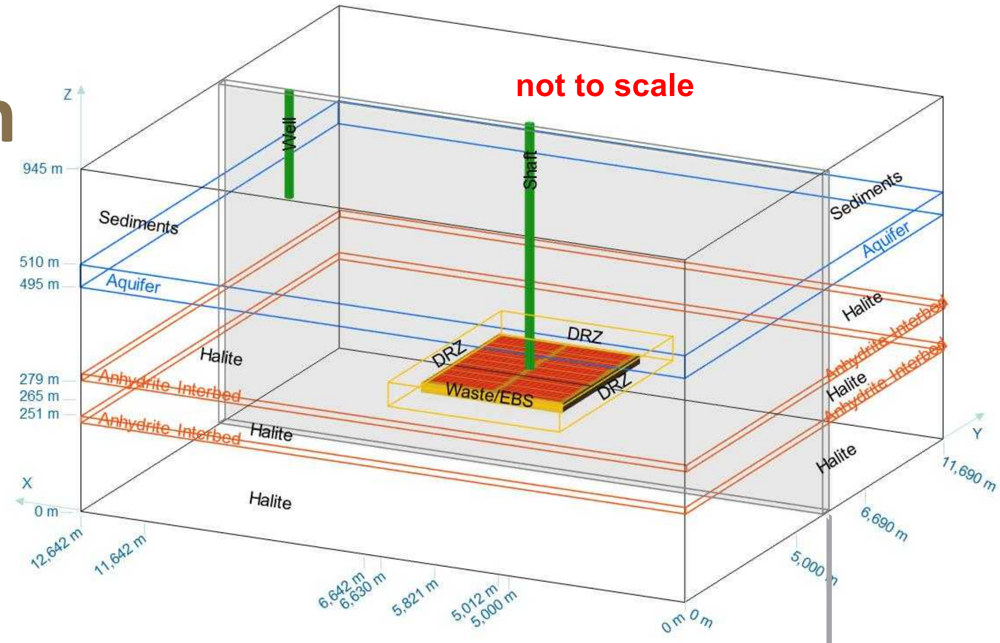
Model Region	Permeability (m^2)	Porosity	Tortuosity	Effective Diffusion Coefficient[a] (m^2/s)	Longitudinal Dispersivity (m)	Saturated Thermal Conductivity (W/m·°K)	Specific Heat Capacity (J/kg·°K)
Waste Package	1.00×10^{-13}	0.500	1.00	6.90×10^{-10}	0.5	16.7	466
Backfill	1.00×10^{-18}	0.113	0.48	1.24×10^{-10}	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

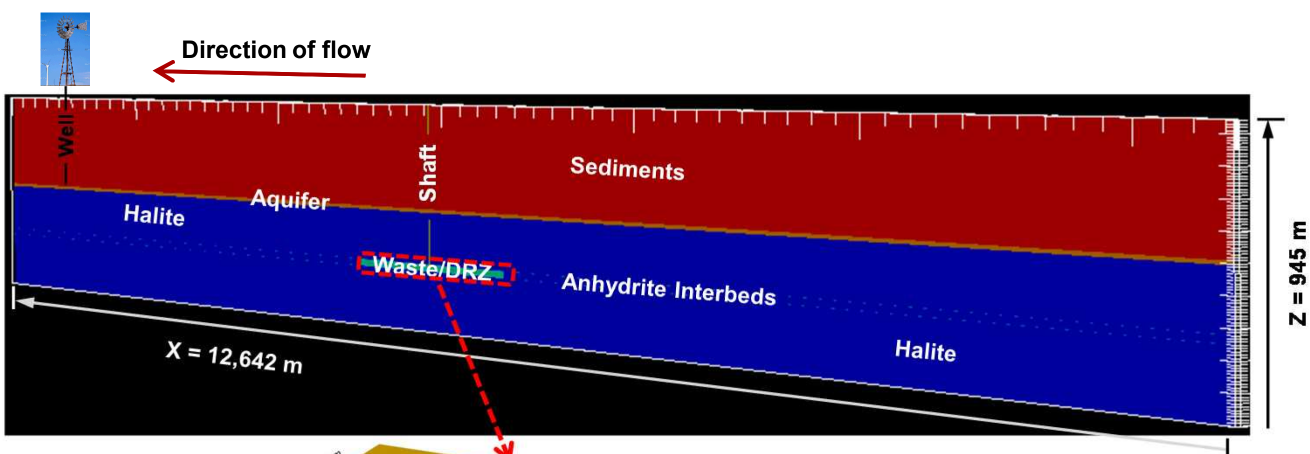
[a] Effective diffusion coefficient = (free water diffusion coefficient) × (tortuosity) × (porosity)

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





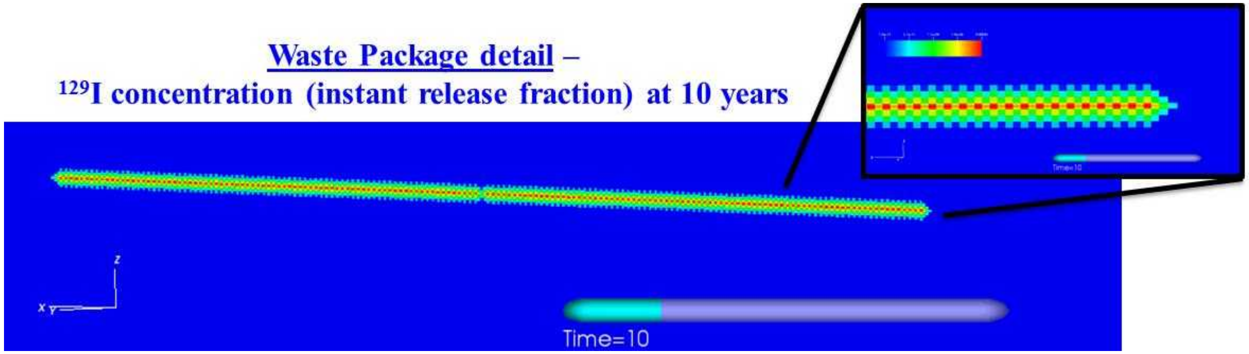
Drift detail
8 of 160 waste packages shown
(not to scale)

X = 12,642 m		NX = 464	
Y = 20 m		NY = 5	
Z = 945 m		NZ = 92	
		Cells = 213,440	

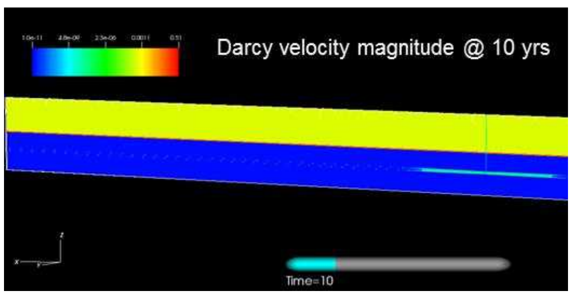
Salt Repository, Single-Drift
→ Deterministic *Isothermal** Simulation

***non-heat generating waste**

Waste Package detail – ^{129}I concentration (instant release fraction) at 10 years



– **EBS:** source term for each waste package
  - *5 radionuclides: ^{129}I, ^{241}Am, ^{237}Np, ^{233}U, ^{229}Th*



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

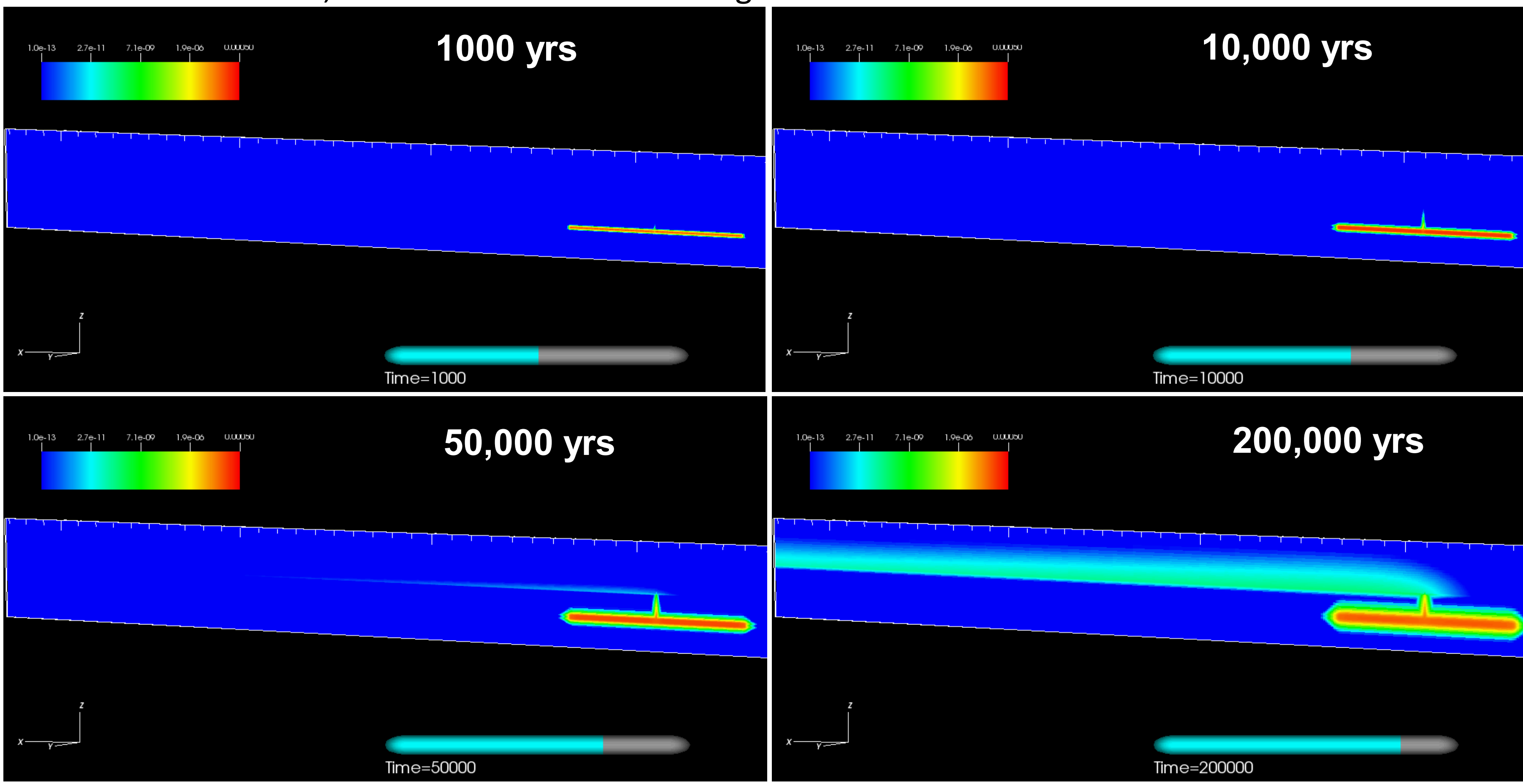
- Diffusion-dominated when N_{Pe} ~<10

– **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, $D_{eff} = \phi\tau D_w$ (m^2/s)	Longitudinal Dispersivity (m)	Longitudinal dispersion coefficient, $D_L = \alpha_L u$ (m^2/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

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

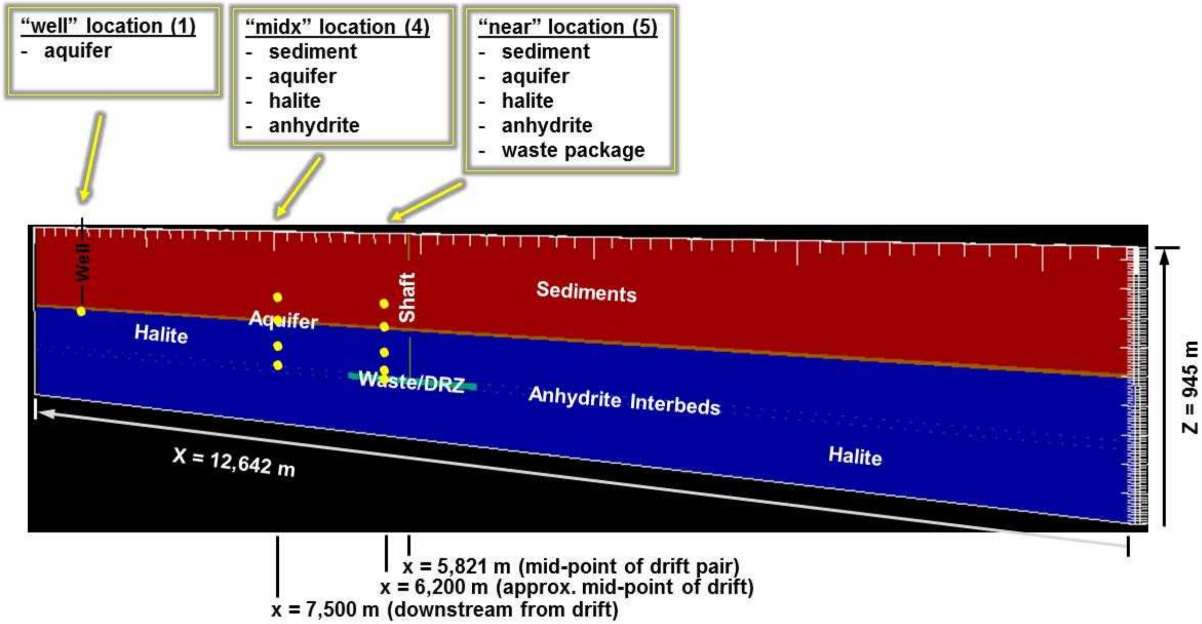


Salt Repository, Single-Drift → *Probabilistic* ***Isothermal**** Simulation

- **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}	$1.00\times10^{-10} – 1.00\times10^{-7}$	Log uniform
^{129}I K_d^P (ml/g)	0.0	$9.28\times10^{-7} – 7.84\times10^{-3}$	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}	$1.00\times10^{-21} – 1.00\times10^{-17}$	Log uniform[b]
Aquifer Permeability (m^2)	1.00×10^{-13}	$1.00\times10^{-14} – 1.00\times10^{-12}$	Log uniform

- **Ten observation points:**



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

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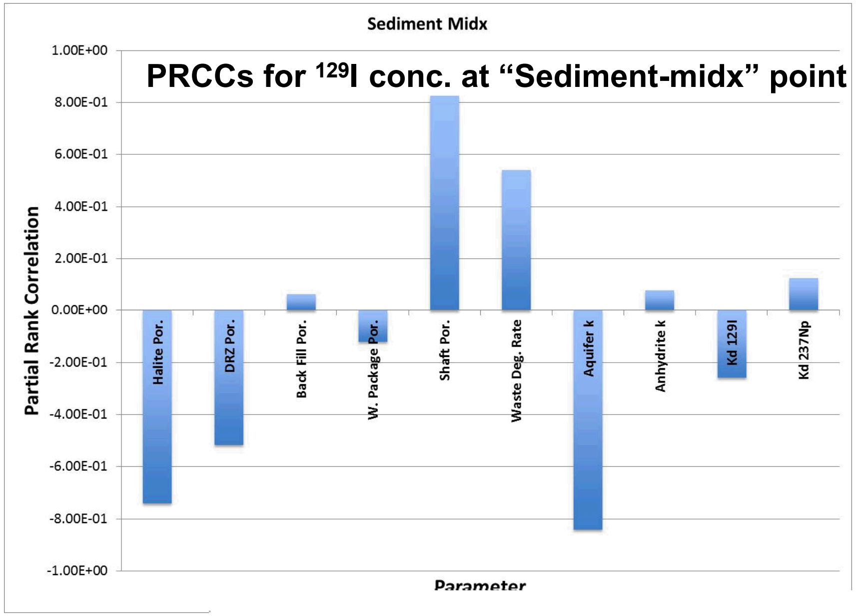
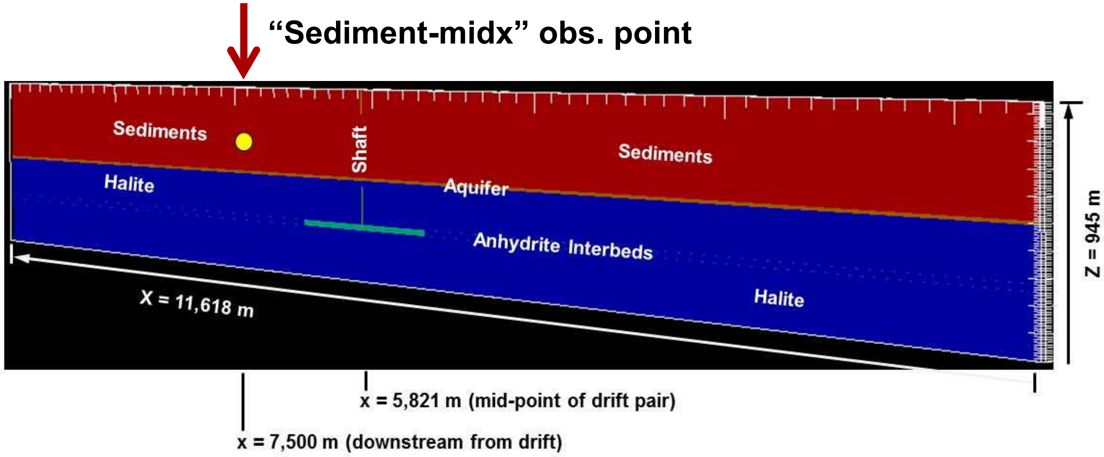
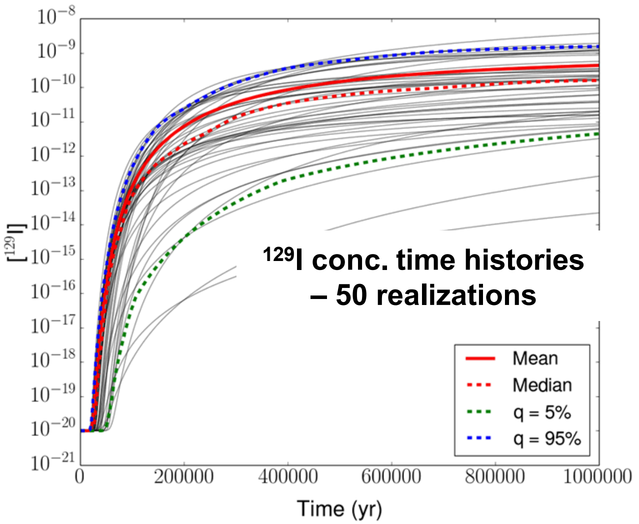
- **Strong positive PRCC for shaft seal porosity – higher ϕ_{shaft} increases effective diffusion coefficient for transport to the aquifer:**

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

- **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**







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**

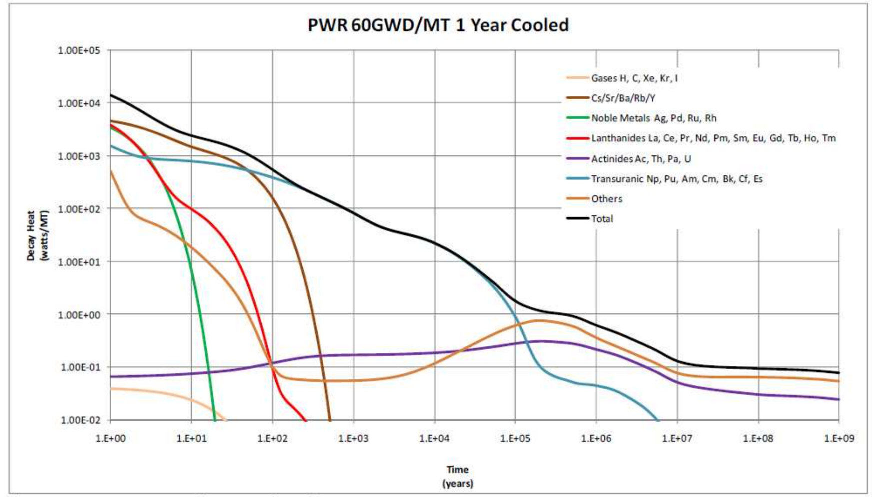
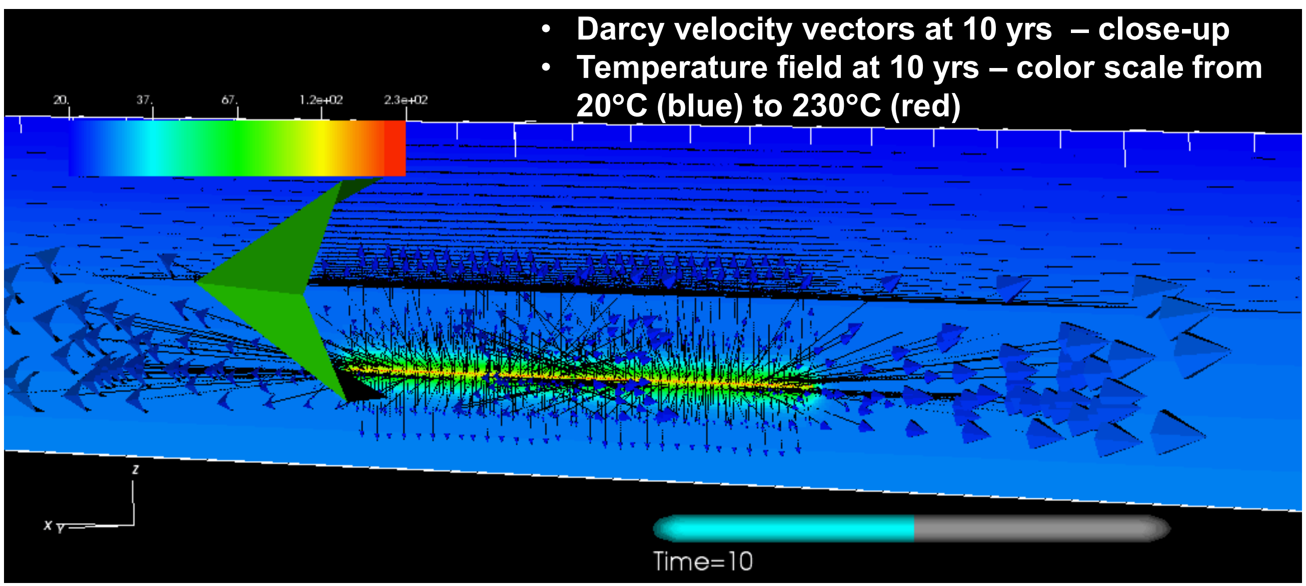


Figure 3-11 PWR 60 GWd/MT Used Fuel Decay Heat



- **Outward fluid velocity from repository region at 10 years — due to *thermal expansion* of fluid**

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

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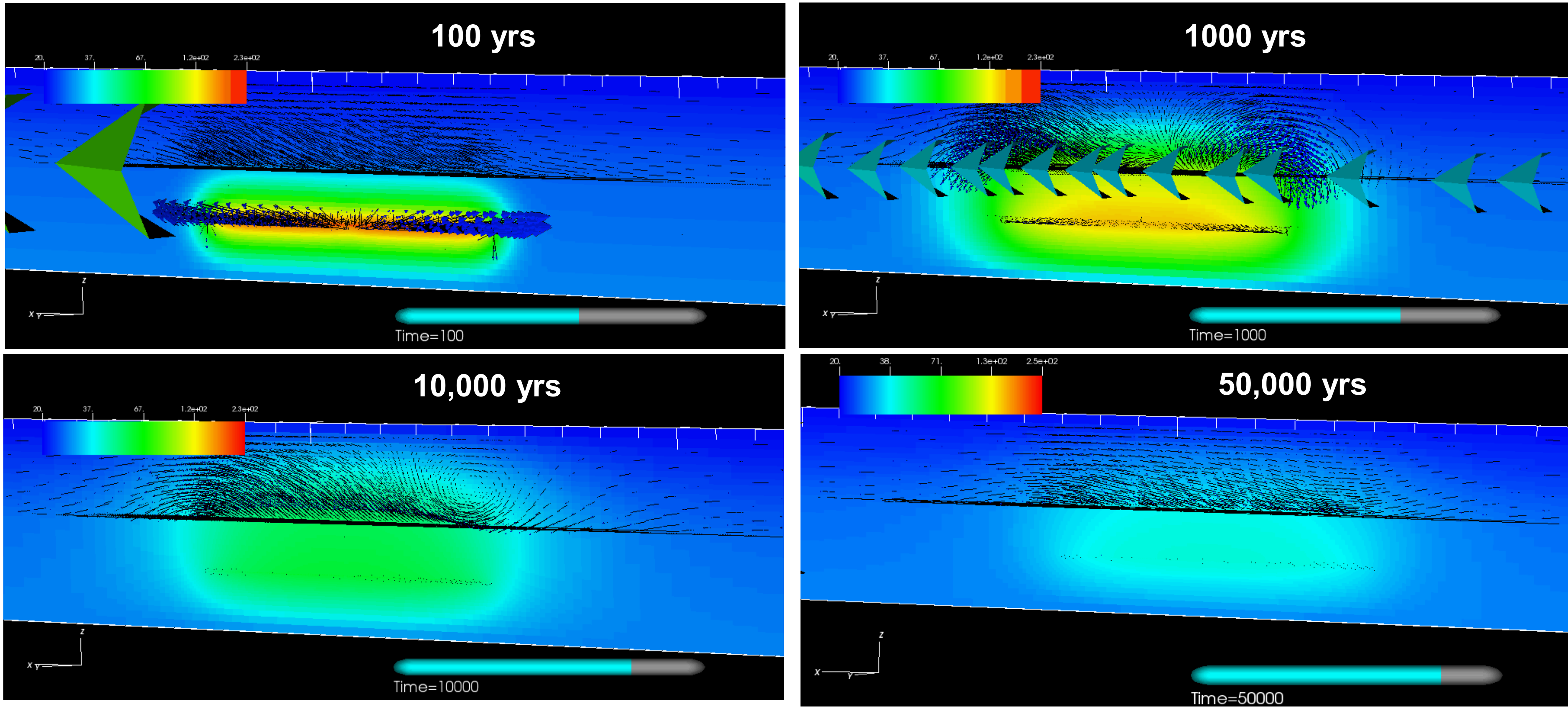
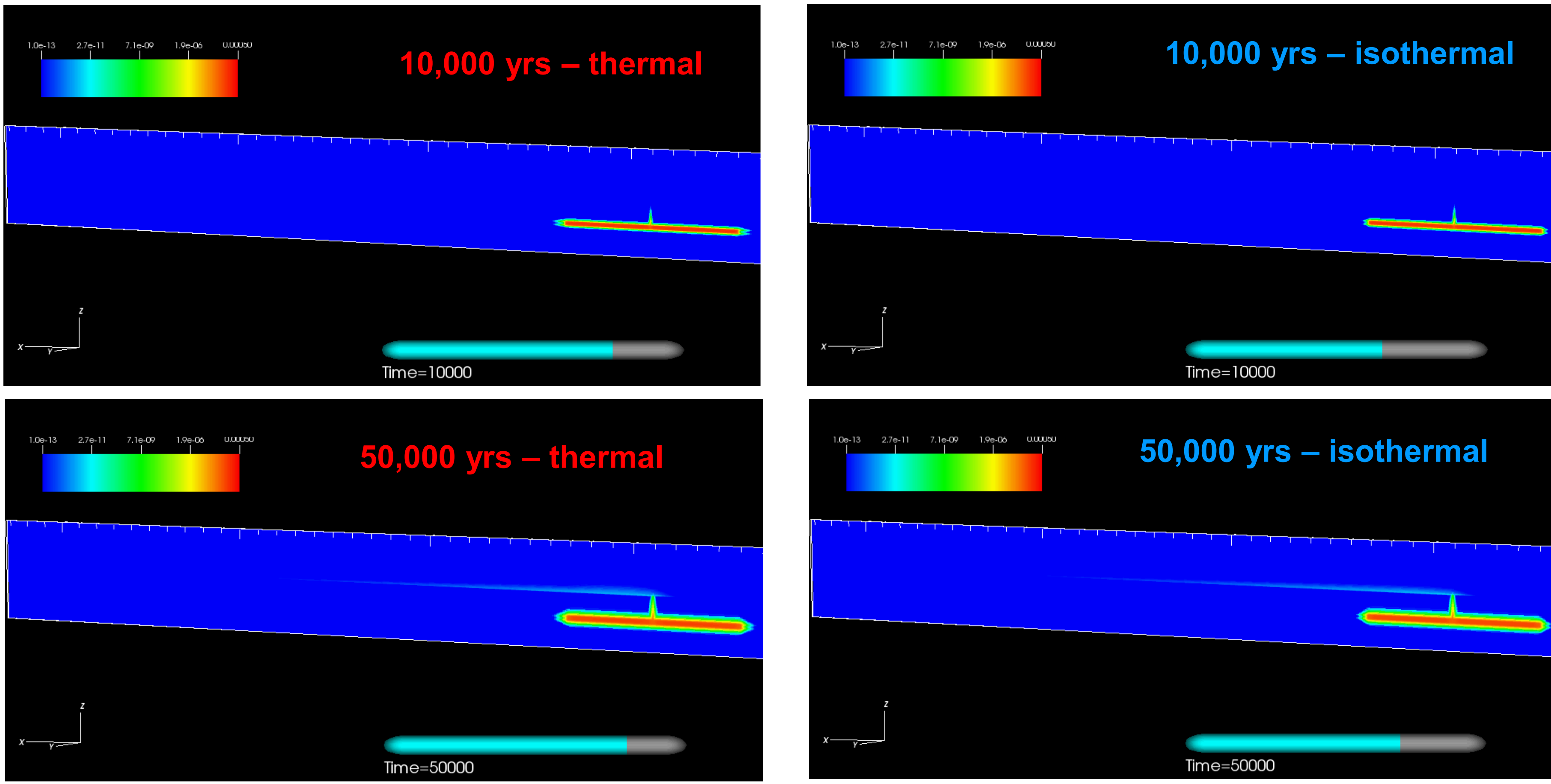
- **Thermally-driven (buoyancy) fluid convection cells for more than 10,000 yrs:**
  - **Darcy velocity vectors at various times**
  - **Temperature field at various times – color scale from 20°C (blue) to 230°C (red)**



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

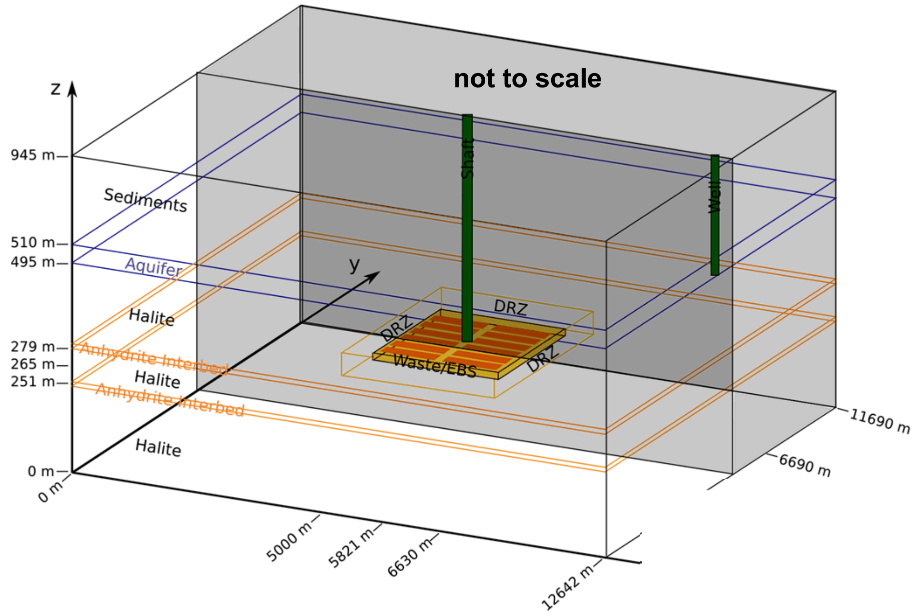
- **^{129}I Concentration at 10,000 years and 50,000 years (thermal vs. isothermal)**
  - **Only small effect from heat pulse (at early times due to thermal expansion of fluid)**
  - **Convection cells gone before 50,000 years, which is the transport time up the shaft seal**



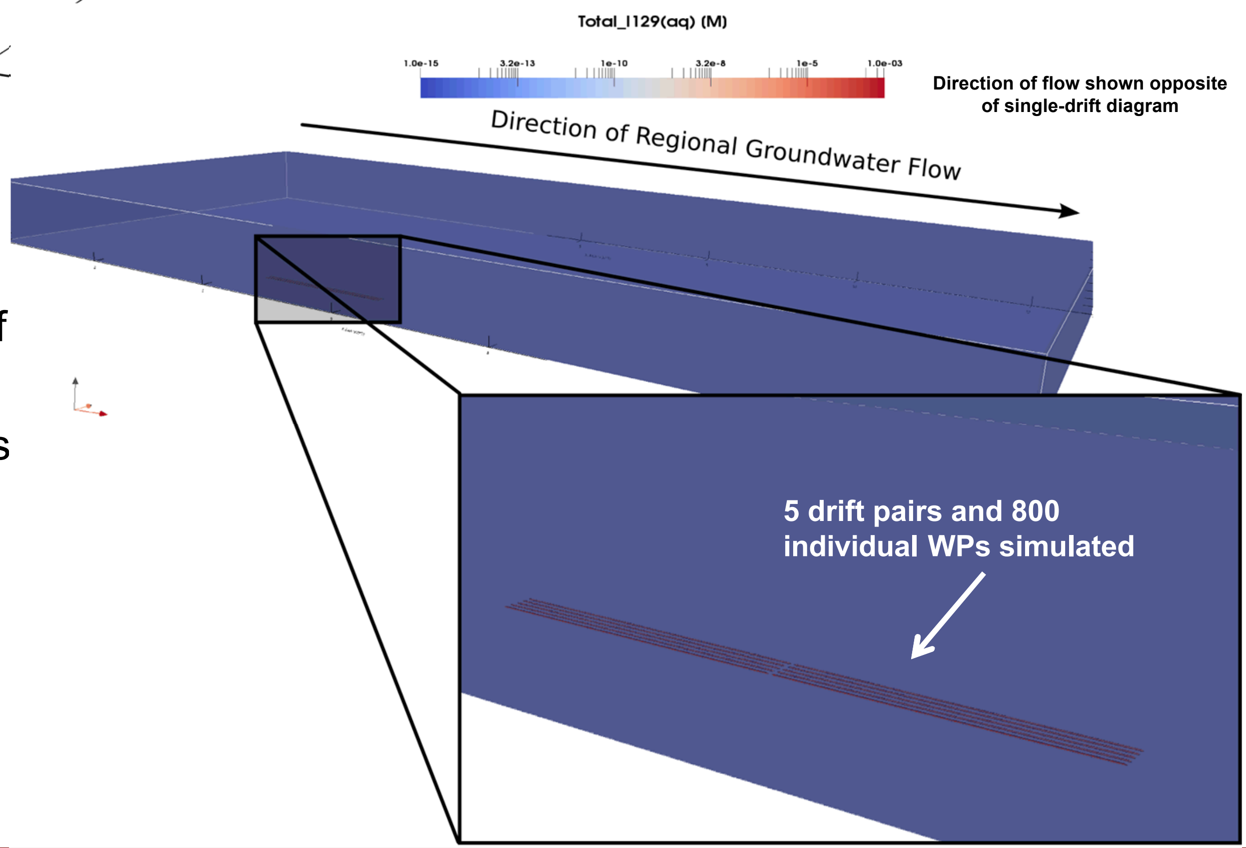
Single-Drift Simulation "Caveats"

- 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



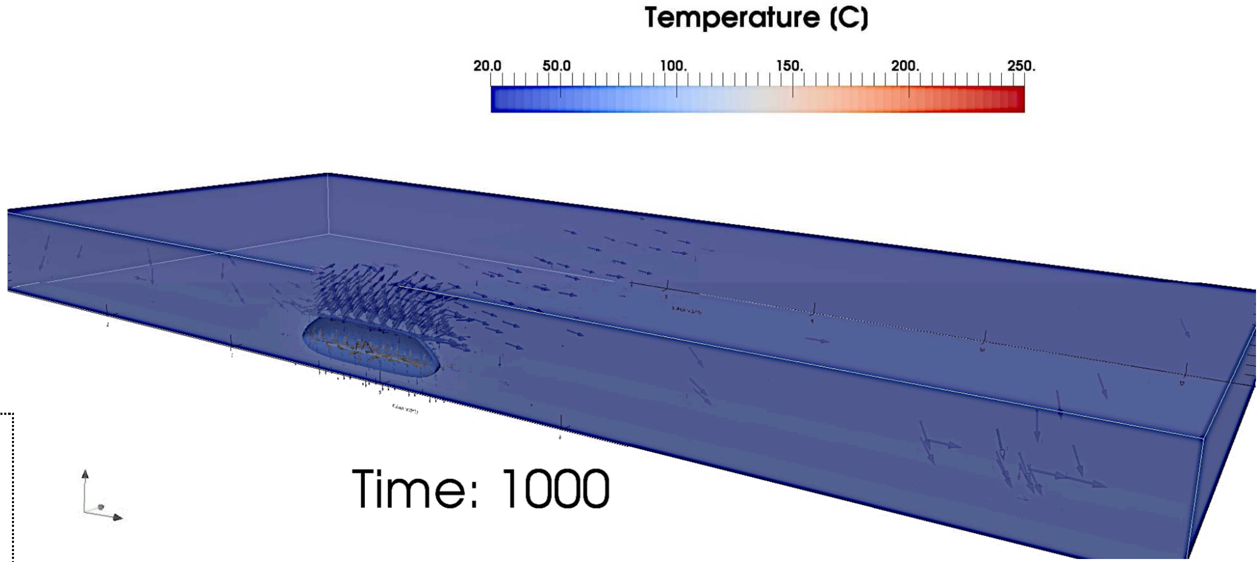
X	=	12,642 m	*NX*	=	387
Y	=	5100 m	*NY*	=	39
Z	=	945 m	*NZ*	=	71
			Cells	=	1,071,603



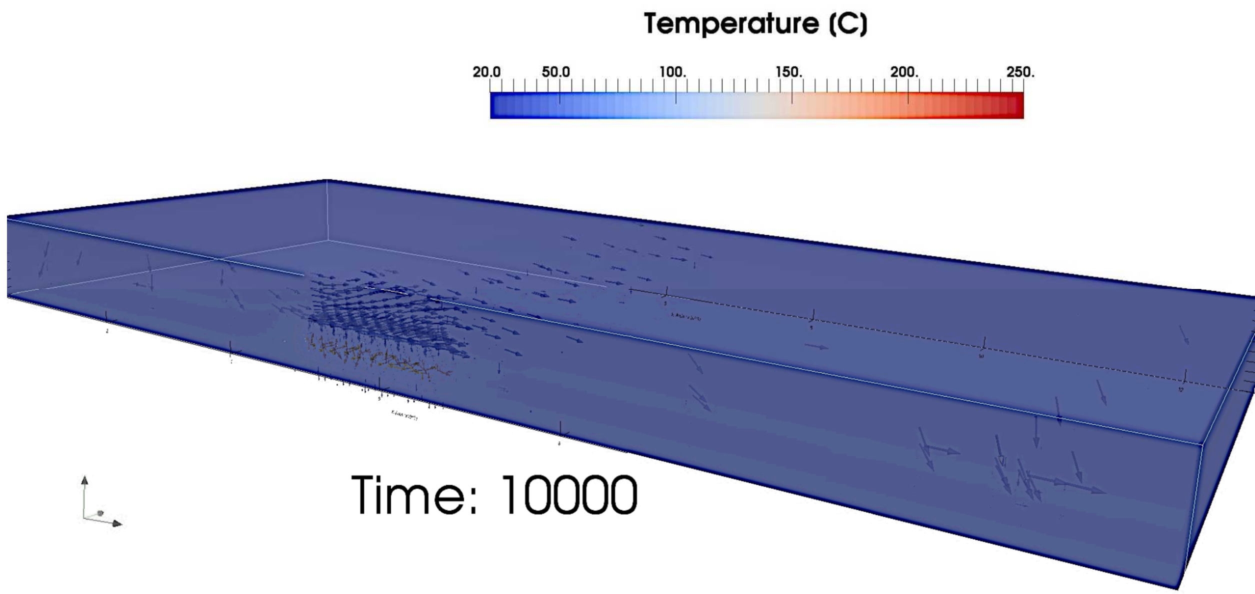
- 5 “drift pairs”
- 3-D half-domain in *y*-direction (100 m of drifts and 5000 m of undisturbed host rock
- Reflection BC at y = 0 (implies 10 drift pairs by symmetry)

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

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

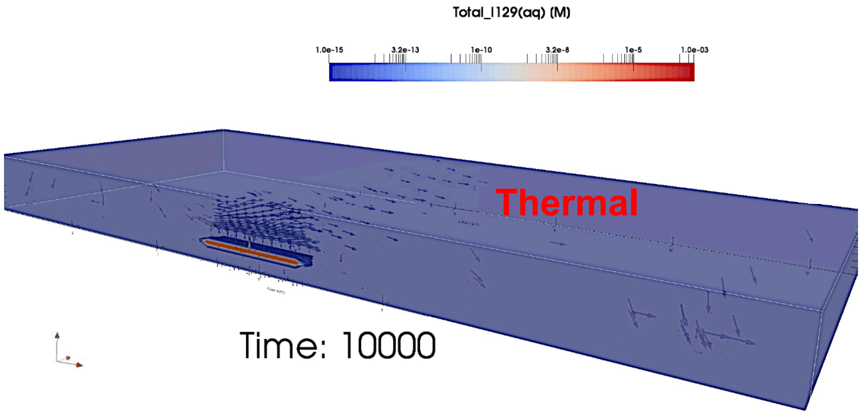


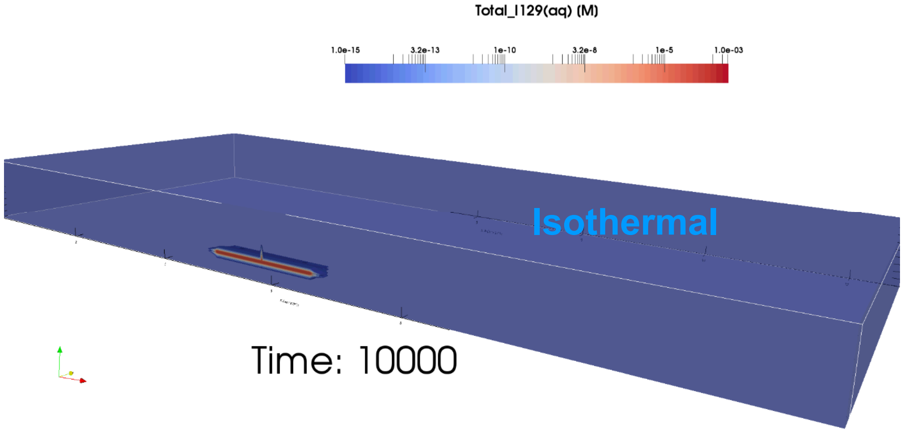
- *Thermally-driven, buoyant flow for more than 10,000 years*
- *Convection cells not obvious compared to single-drift simulation – perhaps dissipated in y-direction*

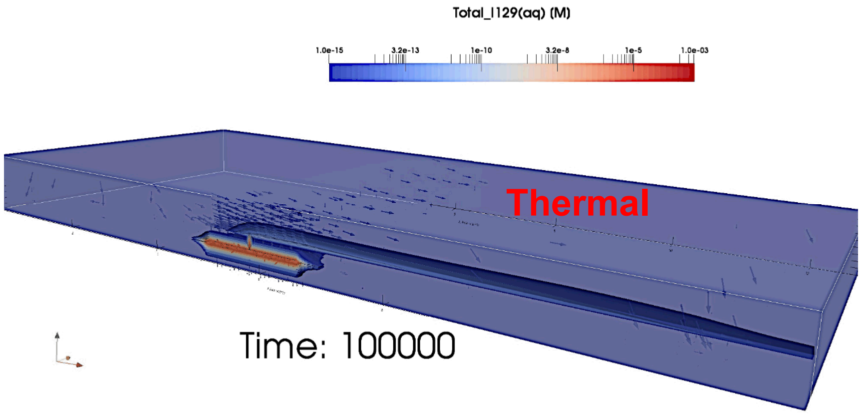


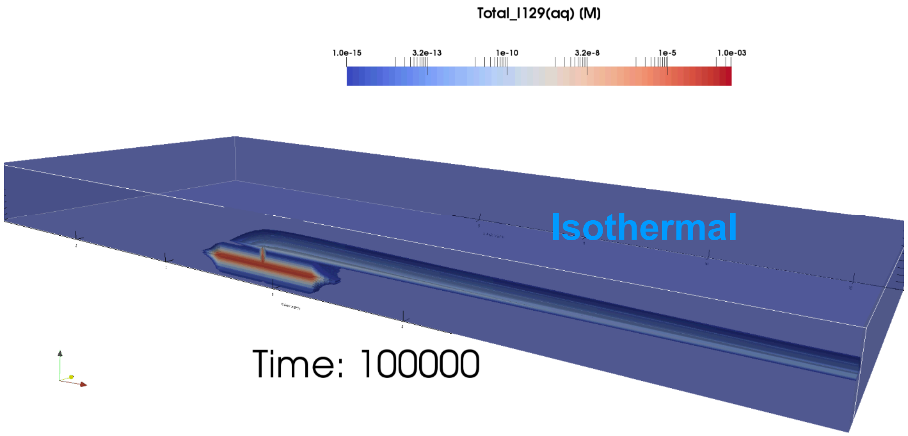
Salt Repository, Multi-Drift
→ Deterministic *Thermal* vs. *Isothermal*

- ***129I dissolved 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, seems to reduce the upward diffusive spread of 129I into the sediments**



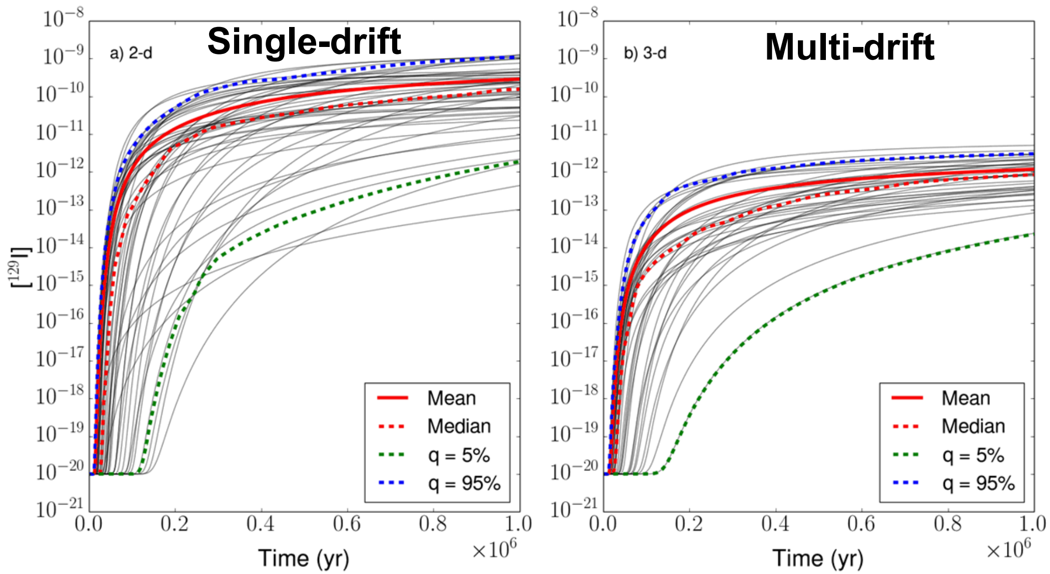




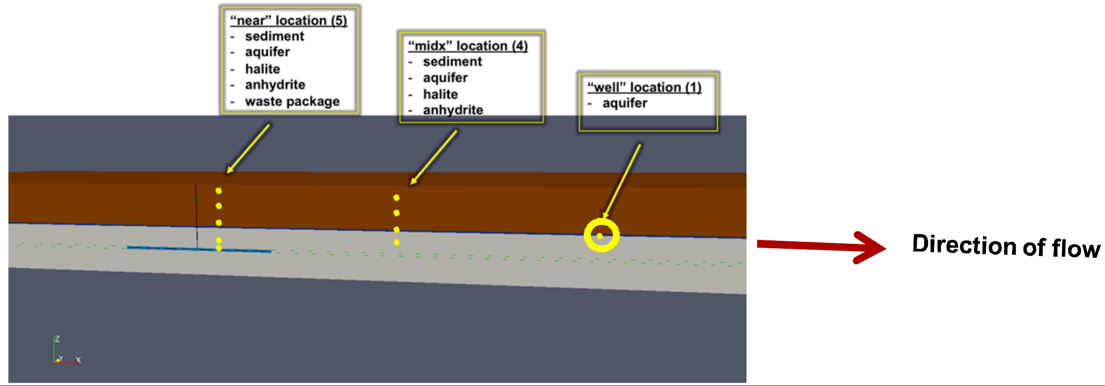


Multi-Drift vs. Single-Drift Comparison
→ *Probabilistic **Thermal***

- **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:**

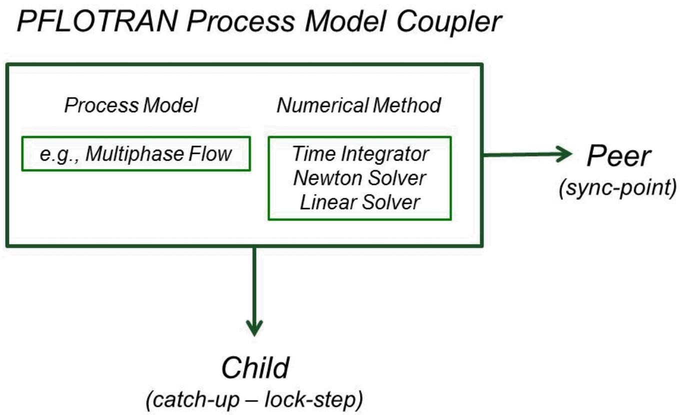


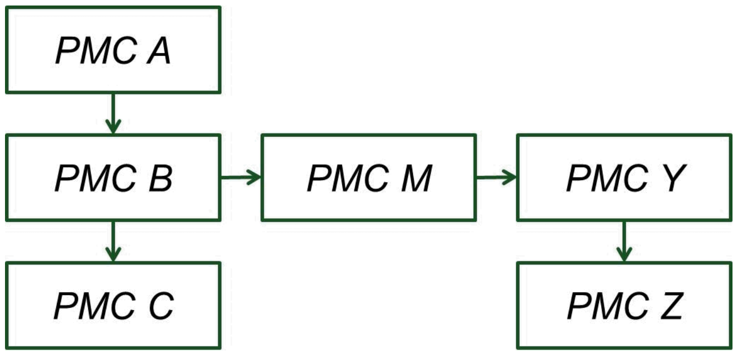
[129]I conc. time histories – 50 realizations at "Well" obs. point



Future Work

- **Application to other media and concepts:**
  - 3-D simulations of a clay/shale reference case (recently completed)
  - 3-D simulations of DOE-managed HLW in bedded salt (recently completed)
  - Application to deep borehole disposal in crystalline basement rock
  - Application to WIPP performance assessment
  - Simulations in fractured crystalline rock (to be started next fiscal year)
- **Incorporation of additional processes, models, and domain resolution, e.g.,**
  - Grid refinement studies (begun already)
  - Inclusion of all drifts/WPs in a half repository
  - Nested architecture





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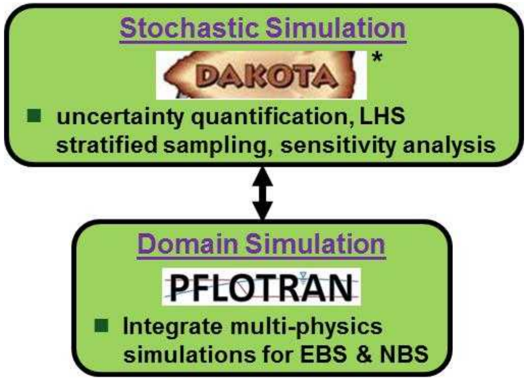
Questions?

Backup Slides

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

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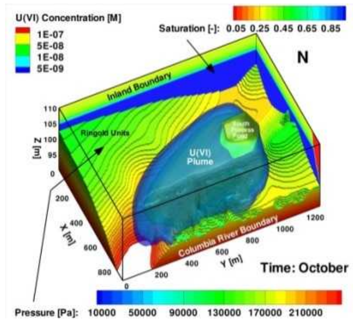
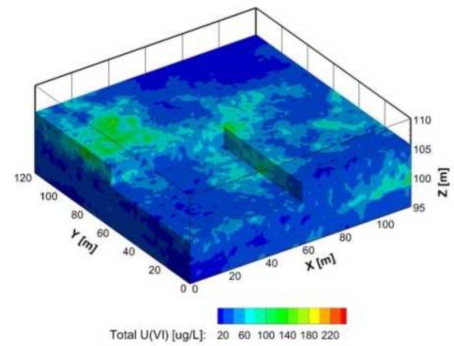
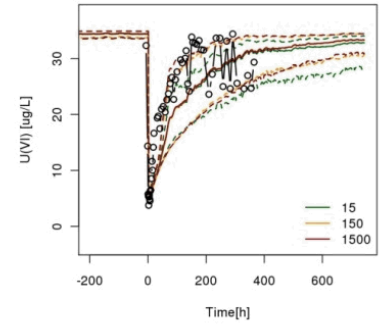
PFLOTRAN Process Modeling

- **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



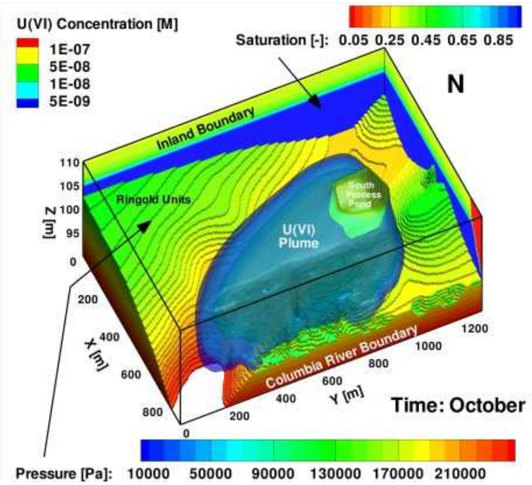
Hammond and Lichtner, WRR, 2010





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

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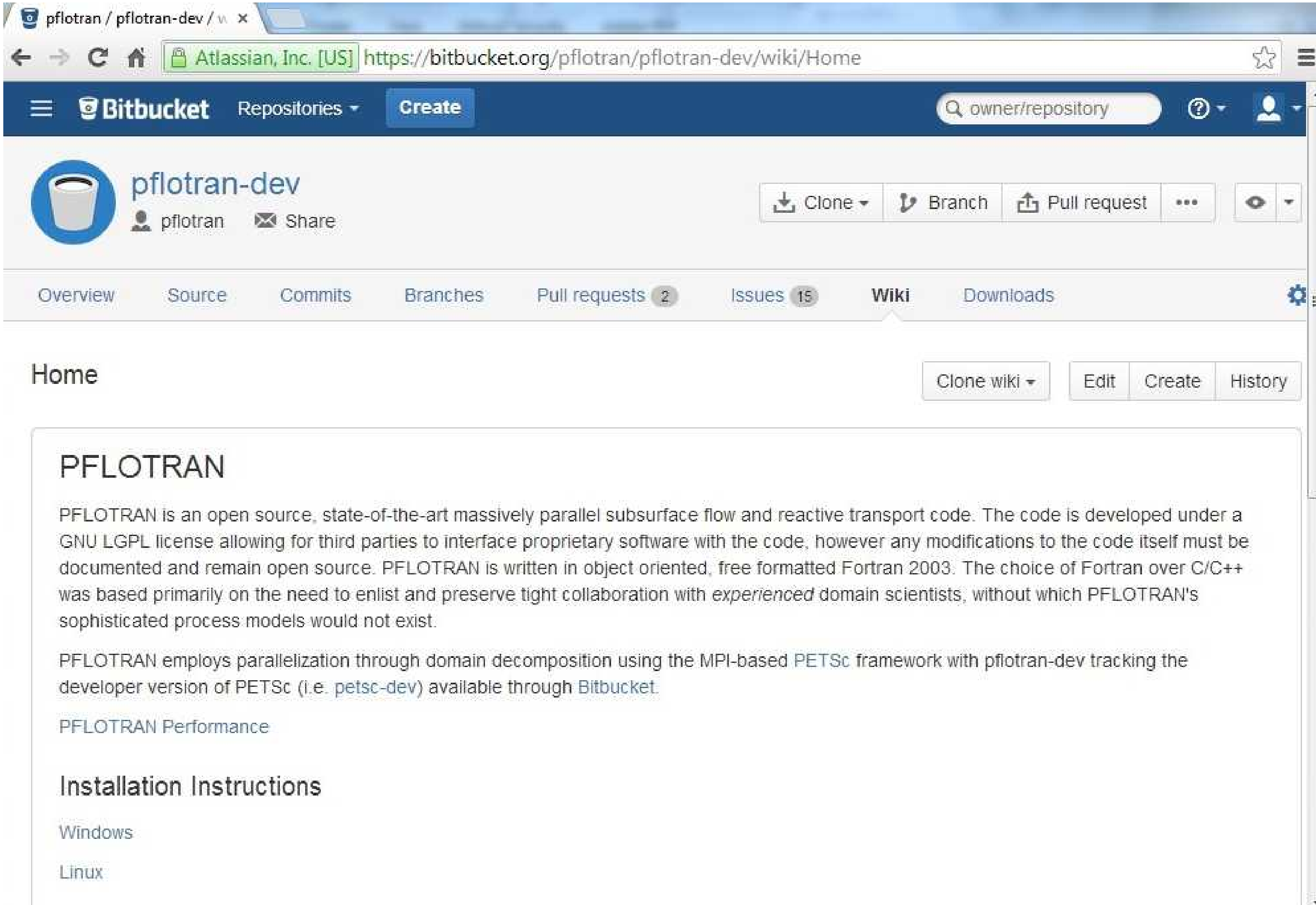
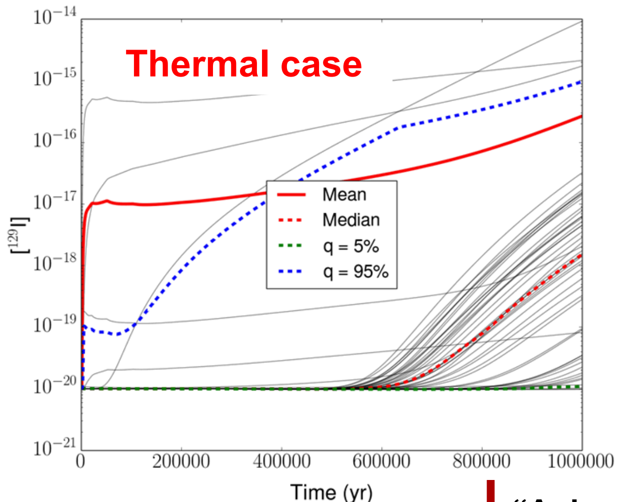


PFLOTRAN Support Infrastructure

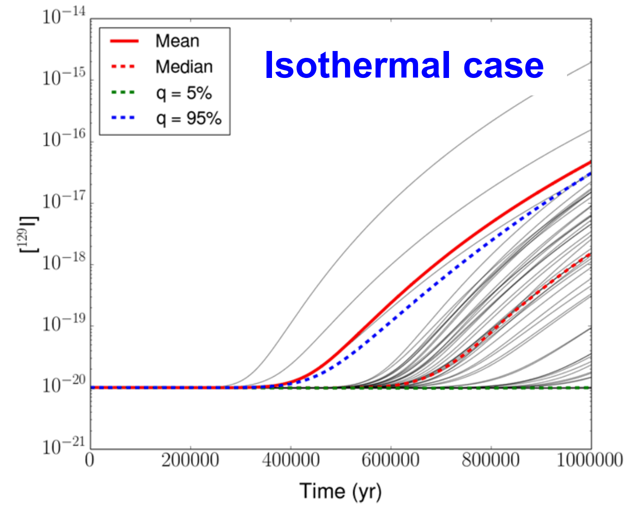
- Mercurial: distributed source control management tool
- Bitbucket: online PFLOTRAN repository
  - `hg clone https://bitbucket.org/pflotran/pflotran-dev`
  - Source tree
  - Commit logs
  - Wiki
    - Installation Instuctions
    - Quick Guide
    - FAQ (entries motivated by questions on mailing list)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

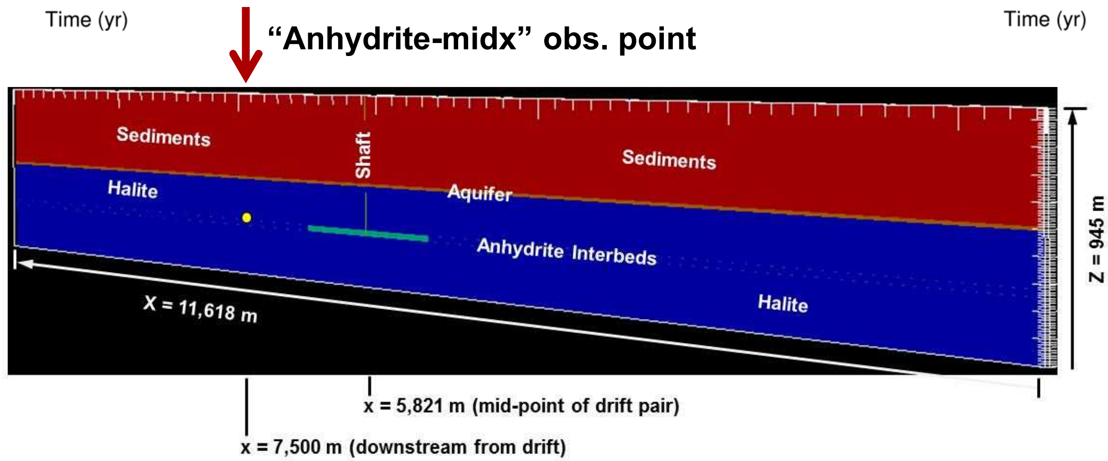
Probabilistic ***Thermal*** **Simulation, Single-Drift – Results at "Anhydrite-Midx" Observation Pt.**

- **^{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

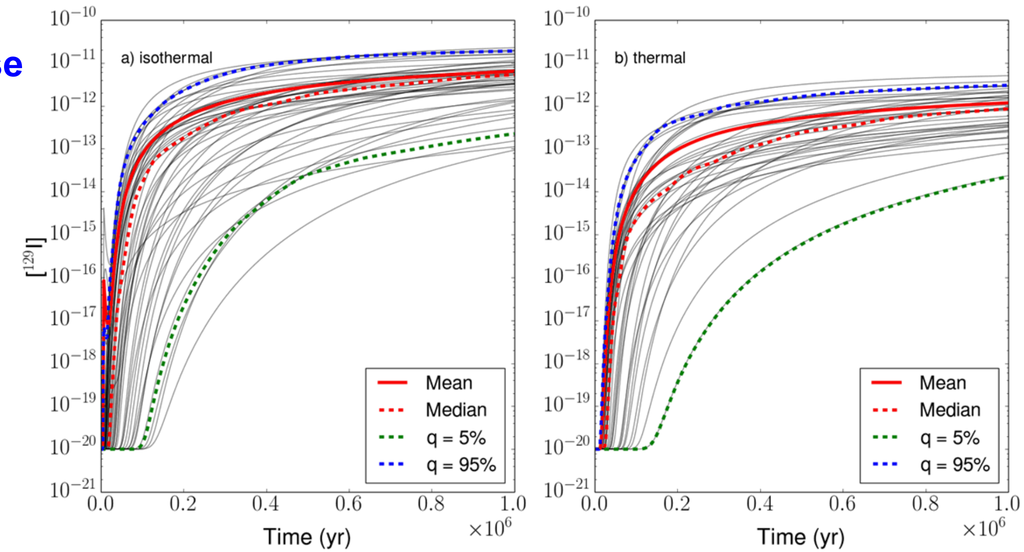




Salt Repository, Multi-Drift
→ *Probabilistic Thermal vs. Isothermal*

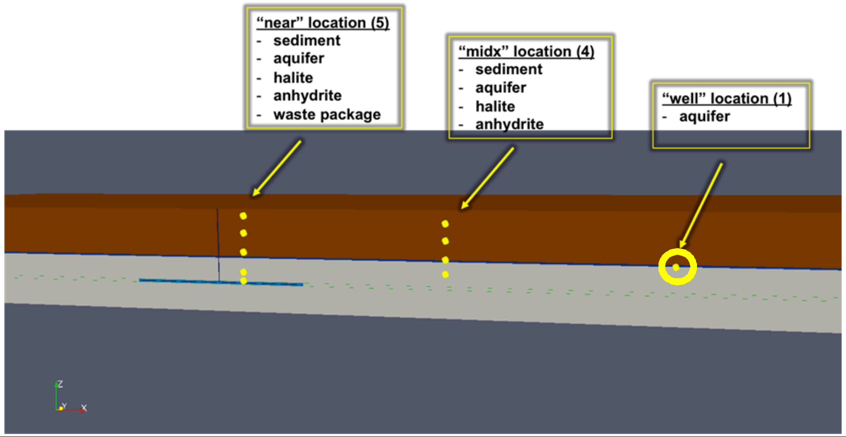
- **Downward vertical component of regional flow in thermal case reduces ^{129}I concentrations at aquifer withdrawal well – effect needs further investigation**

Isothermal case



Thermal case

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



Direction of flow