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PA Development (PFLOTRAN) and the Safety Case

Glenn Hammond

Sandia National Laboratories

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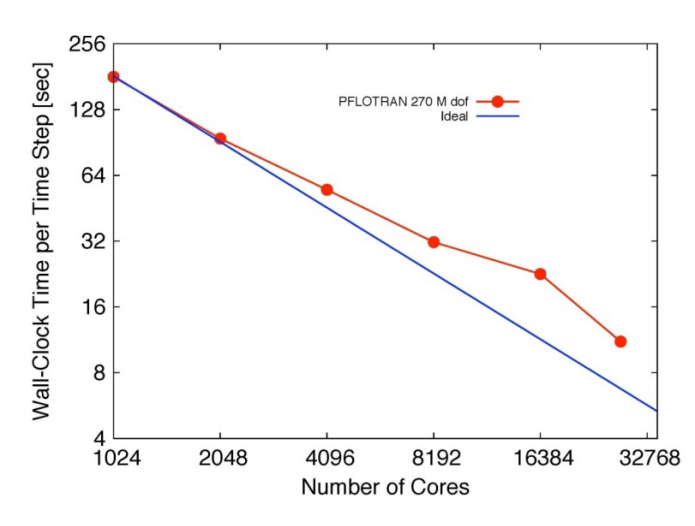
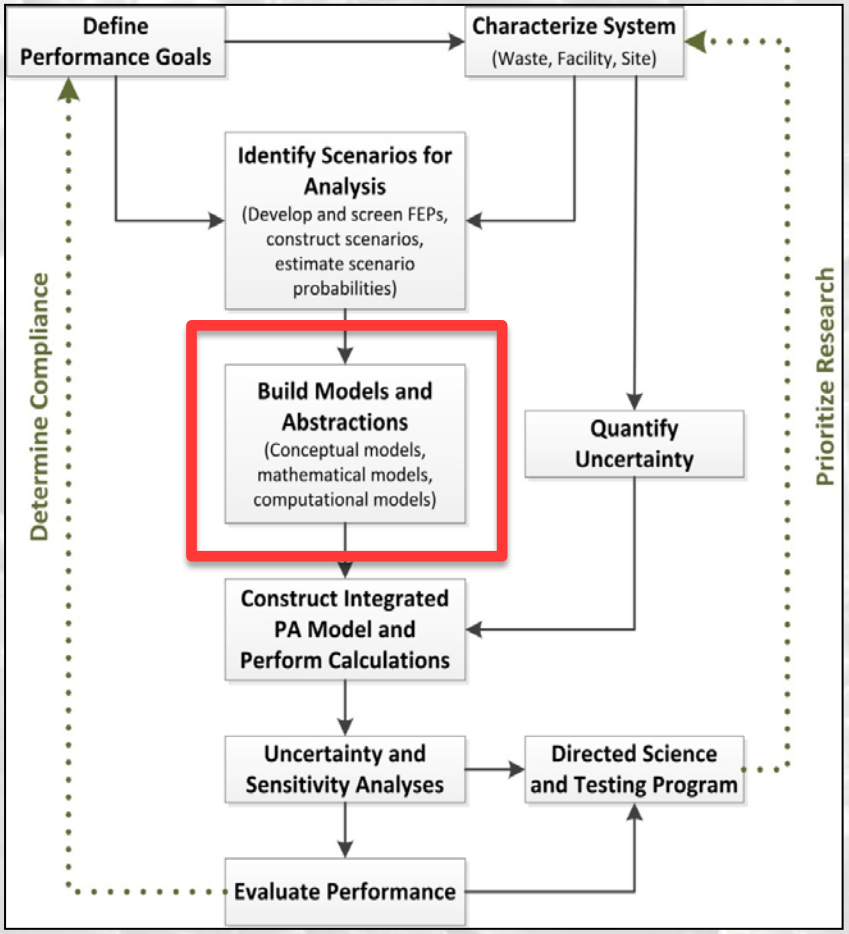
PFLOTRAN

- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 9X/2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)
- Founded upon PETSc parallel framework
  - Parallel communication through MPI
  - Parallel I/O through binary HDF5
  - Unstructured domain decomposition through METIS/ParMETIS (Cmake)
- Demonstrated performance
  - Maximum # processor cores: 262,144 (Jaguar supercomputer)
  - Maximum problem size 3.34 billion degrees of freedom
  - Scales to over 10K cores



Role of PFLOTRAN in PA Methodology

PA Methodology



Input Parameter Distributions

Sensitivity Analysis and Uncertainty Quantification

DAKOTA

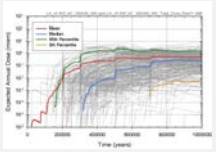
Multi-Physics Simulation and Integration

PFLOTRAN

Computational Support

- Mesh Generation - Cubit
- Visualization – ParaView, VisIt
- Parameter Database

Results



Source Term and EBS Evolution Model

- Inventory
- High resolution of spatial and temporal representation of processes and couplings:
  - WF Degradation
  - WP Degradation
  - Radionuclide Mobilization
  - Solubility Limits
  - Thermal Effects
  - Gas Generation

Flow and Transport Model

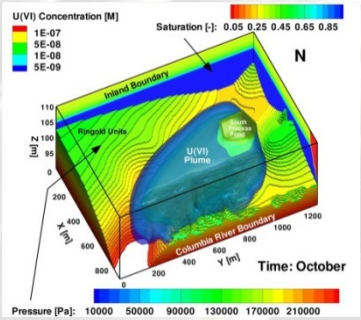
- Spatial and temporal representation of THC processes
  - Advection
  - Diffusion/dispersion
  - Sorption
  - Colloids
  - Decay and ingrowth
  - Homogeneous/heterogeneous reactions

Biosphere Model

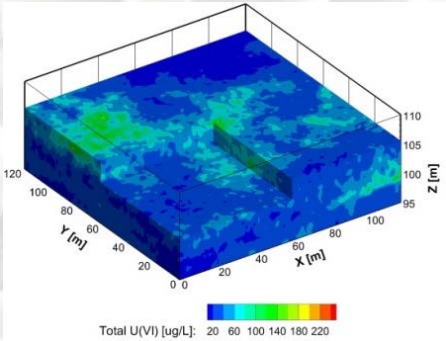
- Exposure pathways
- Uptake/transfer factors
- Radionuclide Concentrations in aquifer

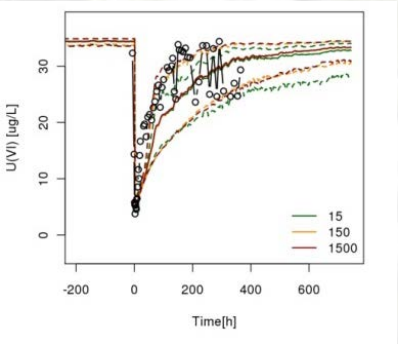
PFLOTRAN Multi-Physics Capabilities

- Flow
  - Multiphase gas-liquid
  - Interchangeable constitutive models and equations of state
- Energy
  - Thermal conduction and convection
- Multi-Component Transport
  - Advection, hydrodynamic dispersion
- Geochemical Reaction
  - Aqueous speciation (ion activity models)
  - Mineral precipitation-dissolution
  - Surface complexation, ion exchange, isotherm-based sorption
  - Radioactive decay with daughter products



Hammond and Lichtner, WRR, 2010

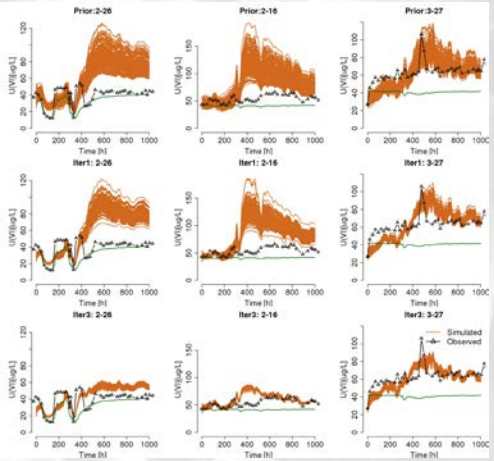




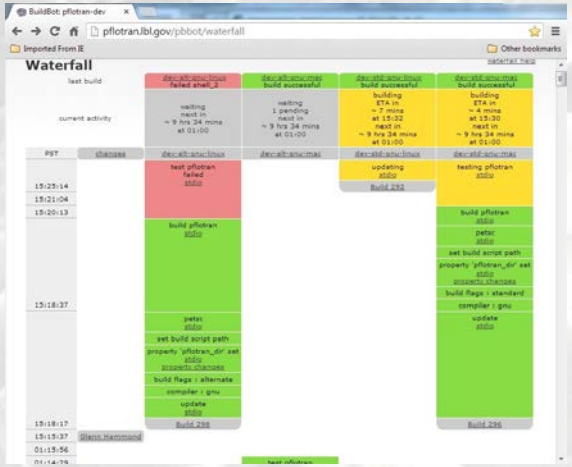
PFLOTRAN Computing Capabilities

- 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 and QA

Data Assimilation

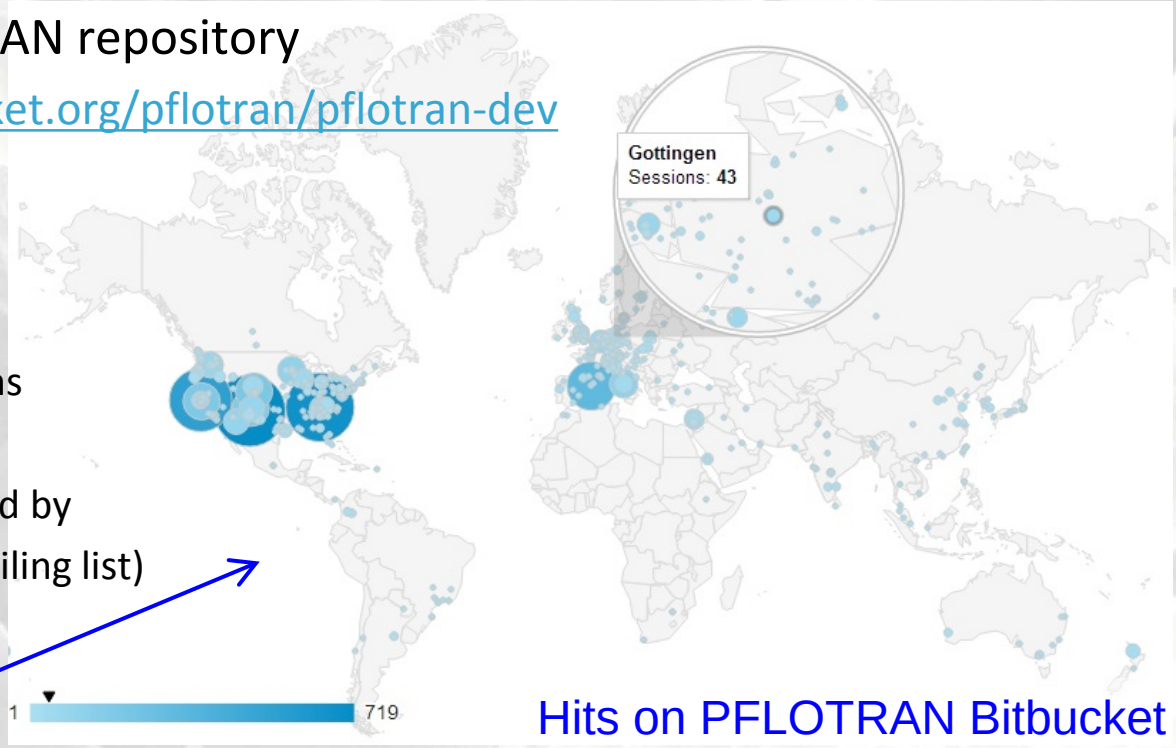


Buildbot



PFLOTRAN Support Infrastructure

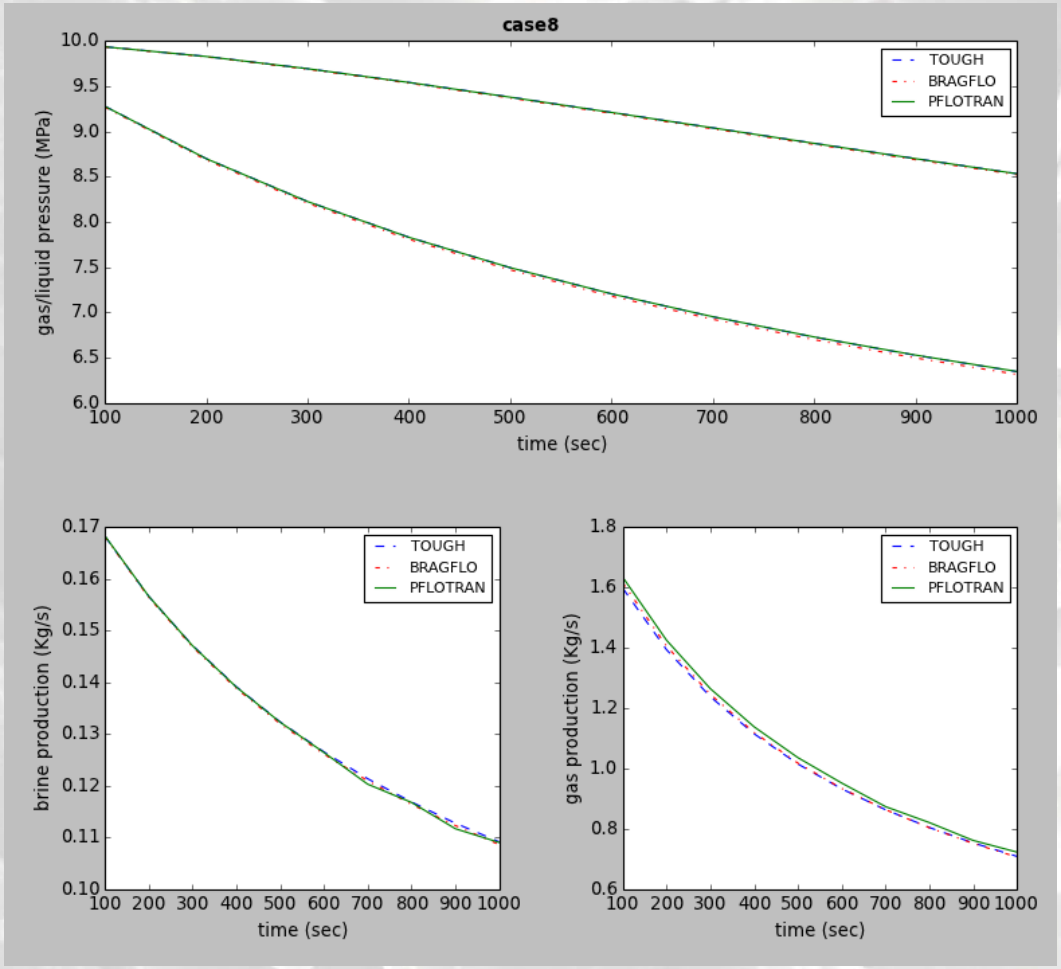
- **Mercurial:** distributed source control management tool
- **Bitbucket:** online PFLOTRAN repository
  - hg clone https://bitbucket.org/pflotran/pflotran-dev
  - Source tree
  - Commit logs
  - Wiki
    - Installation instructions
    - Quick guide
    - FAQ (entries motivated by questions on mailing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



Hits on PFLOTRAN Bitbucket site over past year

PFLOTRAN Verification

- Test cases for WIPP codes (BRAGFLO and NUTS) set up and executed with PFLOTRAN
  - E.g., BRAGFLO Case #8 “Well production at a specified bottom hole pressure”



PFLOTRAN results compared to BRAGFLO and WIPP version of TOUGH2 (TOUGH28W)

Generic Salt Repository PA Model – Simulation Summary

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

Stochastic Simulation

DAKOTA

Uncertainty quantification, LHS stratified sampling, sensitivity analysis

Deterministic Simulation

PFLOTRAN

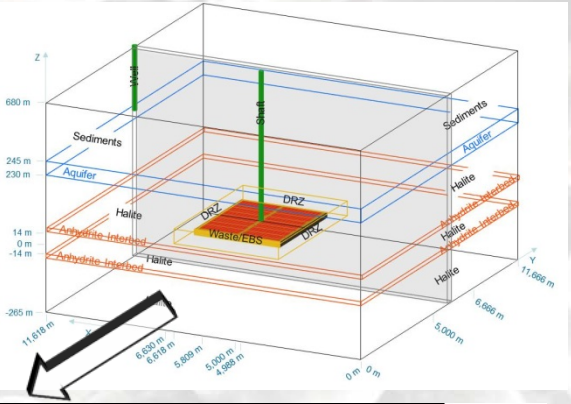
Integrated multi-physics simulations for EBS & NBS

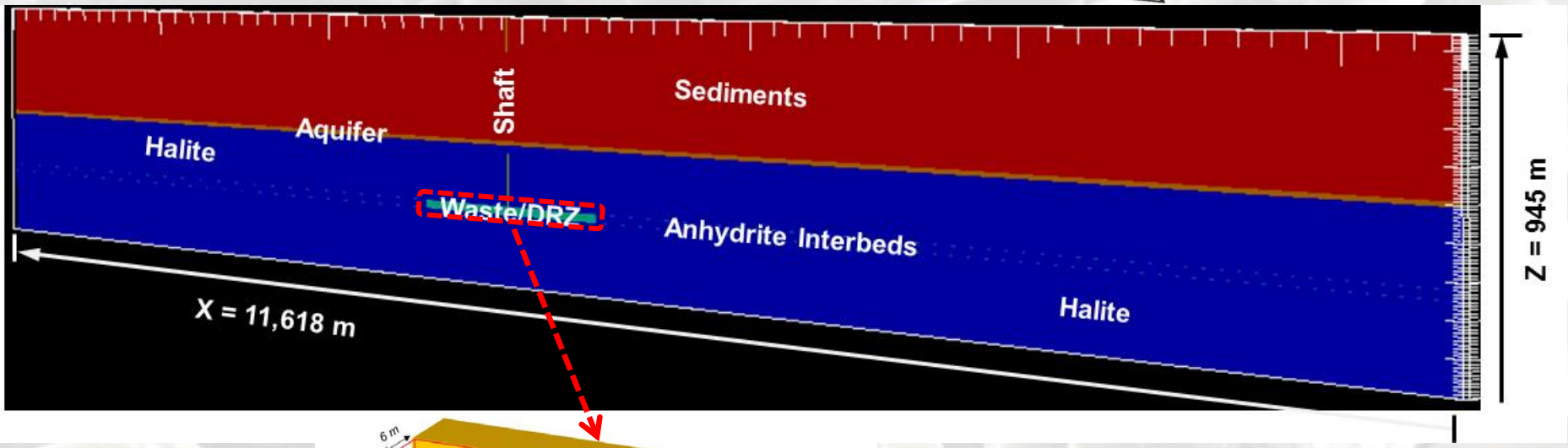
RED SKY

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

Generic Salt Repository PA Model – 3D Model Domain

- Simulation domain
  - 3D vertical slice
  - 20-m wide pillar to pillar
  - 1 drift pair (2 800-m long drifts)
    - 160 waste packages and backfill



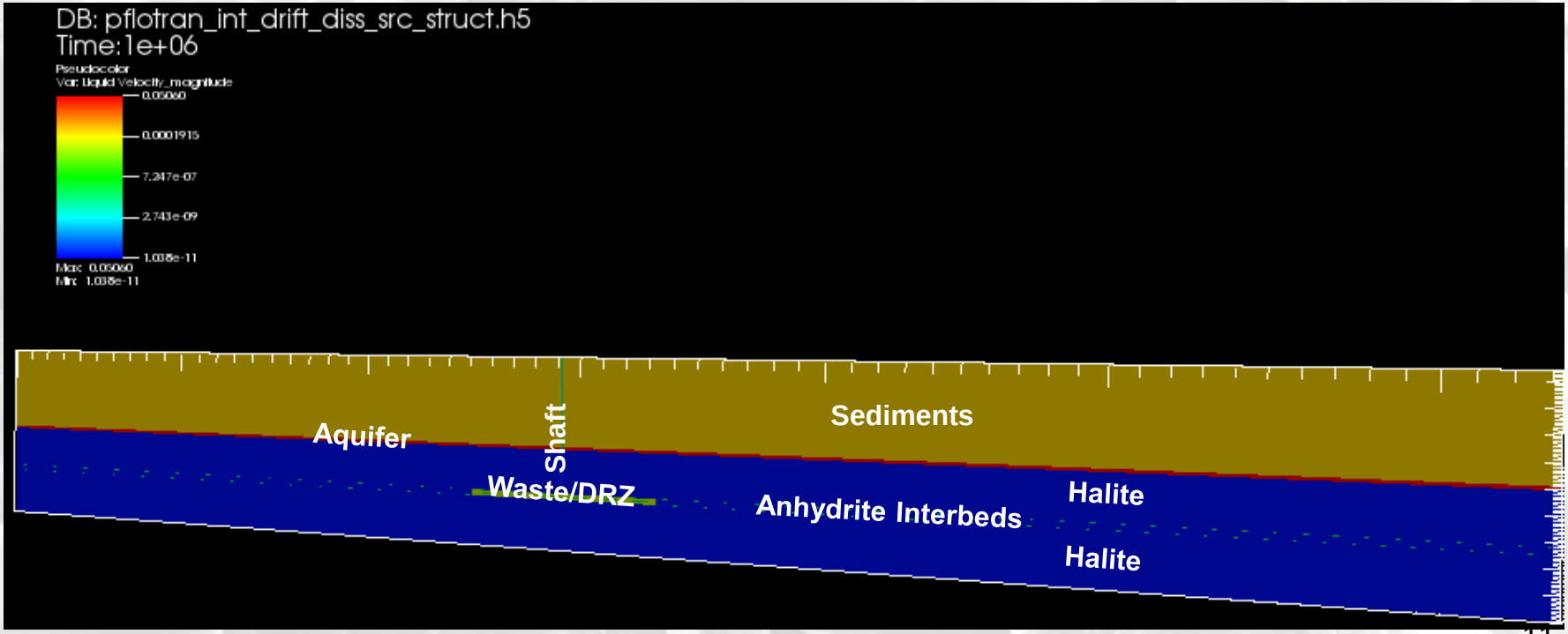


1 of 2 drifts shown
8 of 160 waste packages shown

X	=	11,618 m	NX	=	455
Y	=	20 m	NY	=	5
Z	=	945 m	NZ	=	92
			Cells = 209,300		

Generic Salt Repository PA Model – Deterministic Simulation Results

- Horizontal Darcy velocity (m/yr)
  - Diffusion through DRZ, bedded salt, and shaft
  - Advection (horizontal) through aquifer
  - Diffusion (vertical) and advection (horizontal) through sediments



Payton Gardner, SNL 6224, Albuquerque NM

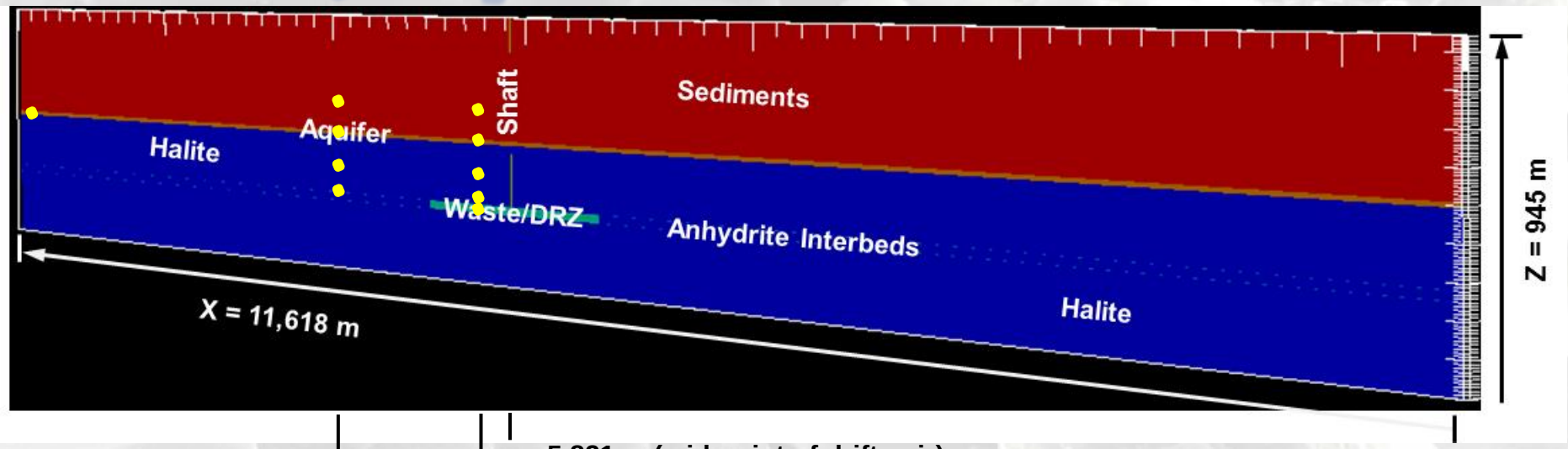
Generic Salt Repository PA Model – Probabilistic Simulations

- Sensitivity analysis (partial rank correlation) at 10 locations

“well” location (1)
- aquifer

“midx” location (4)
- sediment
- aquifer
- halite
- anhydrite

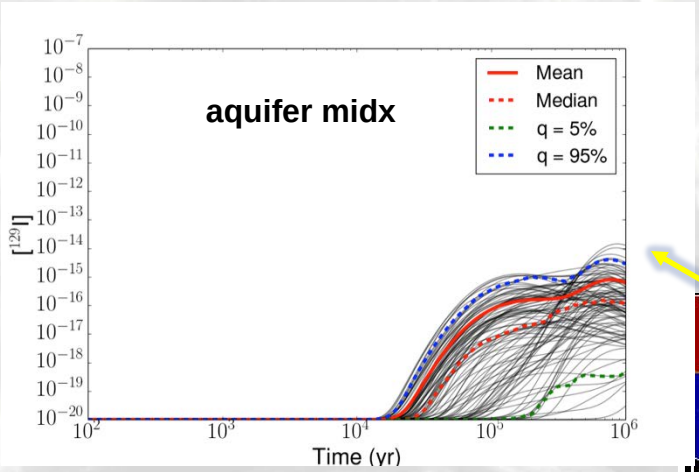
“near” location (5)
- sediment
- aquifer
- halite
- anhydrite
- waste package

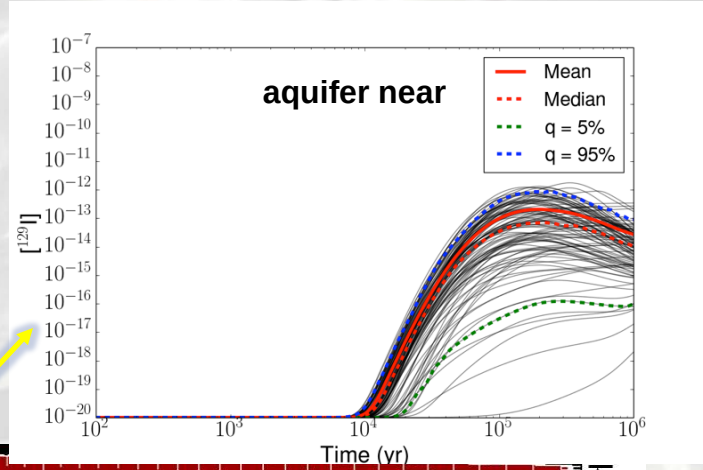


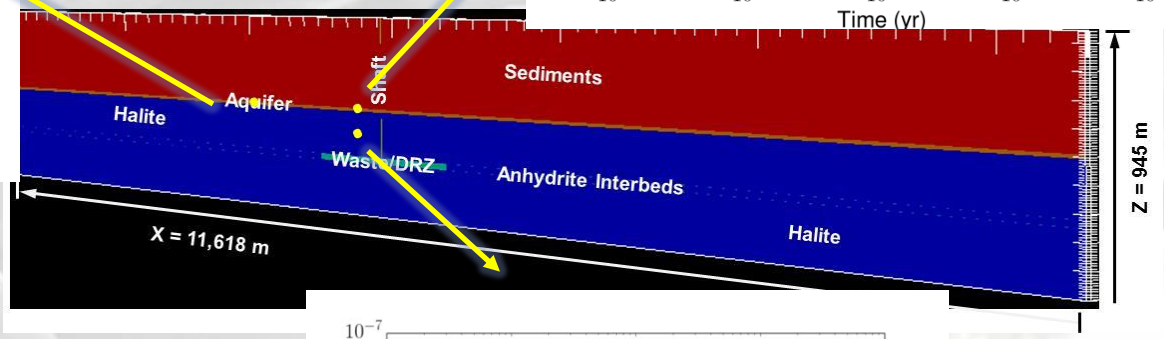
x = 5,821 m (mid-point of drift pair)
x = 6,200 m (approx. mid-point of drift)
x = 7,500 m (downstream from drift)

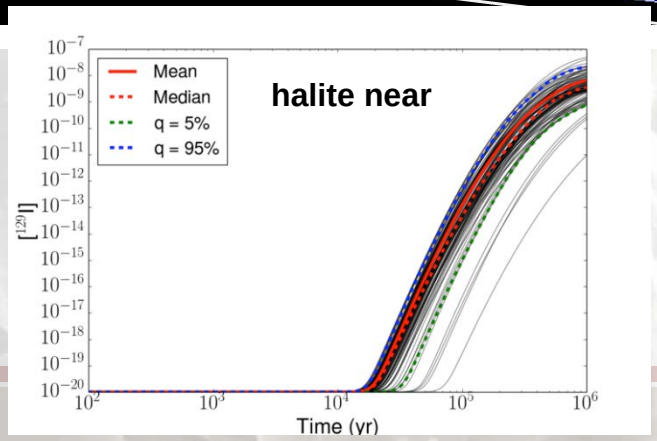
Generic Salt Repository PA Model – Multi-Realization Analysis

- **^{129}I dissolved concentration vs. time**
  - (DAKOTA probabilistic output of 100 realizations)



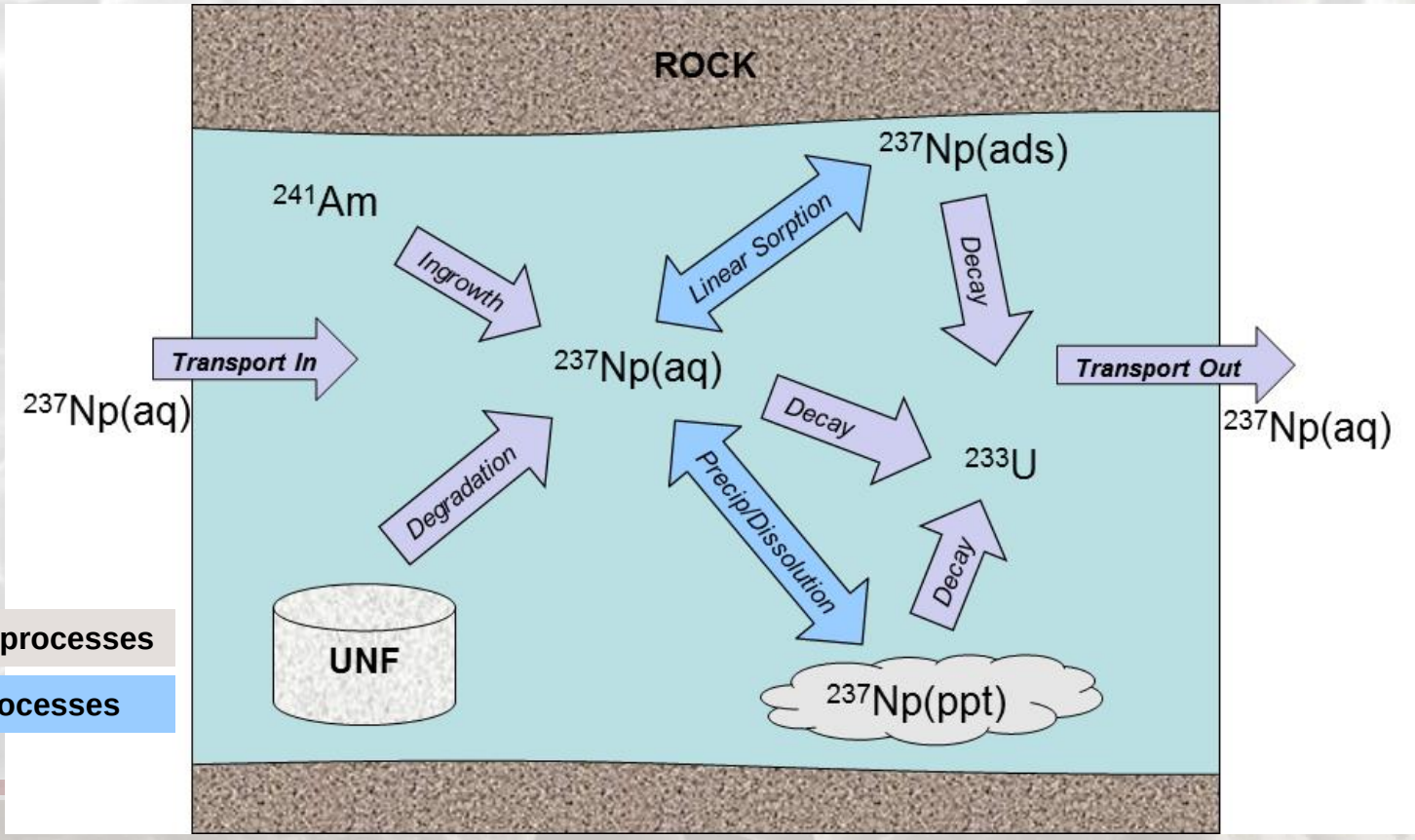






Future Directions – Coupled Radionuclide Mobilization and Transport Processes

- **Waste Form Degradation (IRF and matrix dissolution)**
- **Transport (advection, diffusion, linear sorption (K_d))**
- **Decay and Ingrowth**
- **Precipitation/Dissolution**
- **Solution Chemistry and Temperature**



Time-dependent processes

Equilibrium processes