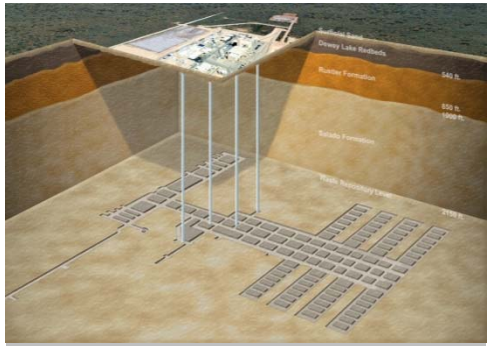
Exceptional service in the national interest

Sandia National Laboratories



Modernization of WIPP PA

Heeho Park

U.S. DEPARTMENT OF ENERGY | NNSA

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S Department of Energy.

Overview

- Introduction to WIPP
  - WIPP and WIPP PA
  - Why Modernize PA?
- Introduction to PFLOTRAN
- Current Progress
  - Integration of WIPP-specific functionality
  - Proof-of-concept 3D two-phase undisturbed scenario
  - Proof-of-concept 3D single-phase human borehole intrusion
- Advantages of Modernization
  - Consolidation into one code and single conceptual model
  - V&V testing suite and documentation

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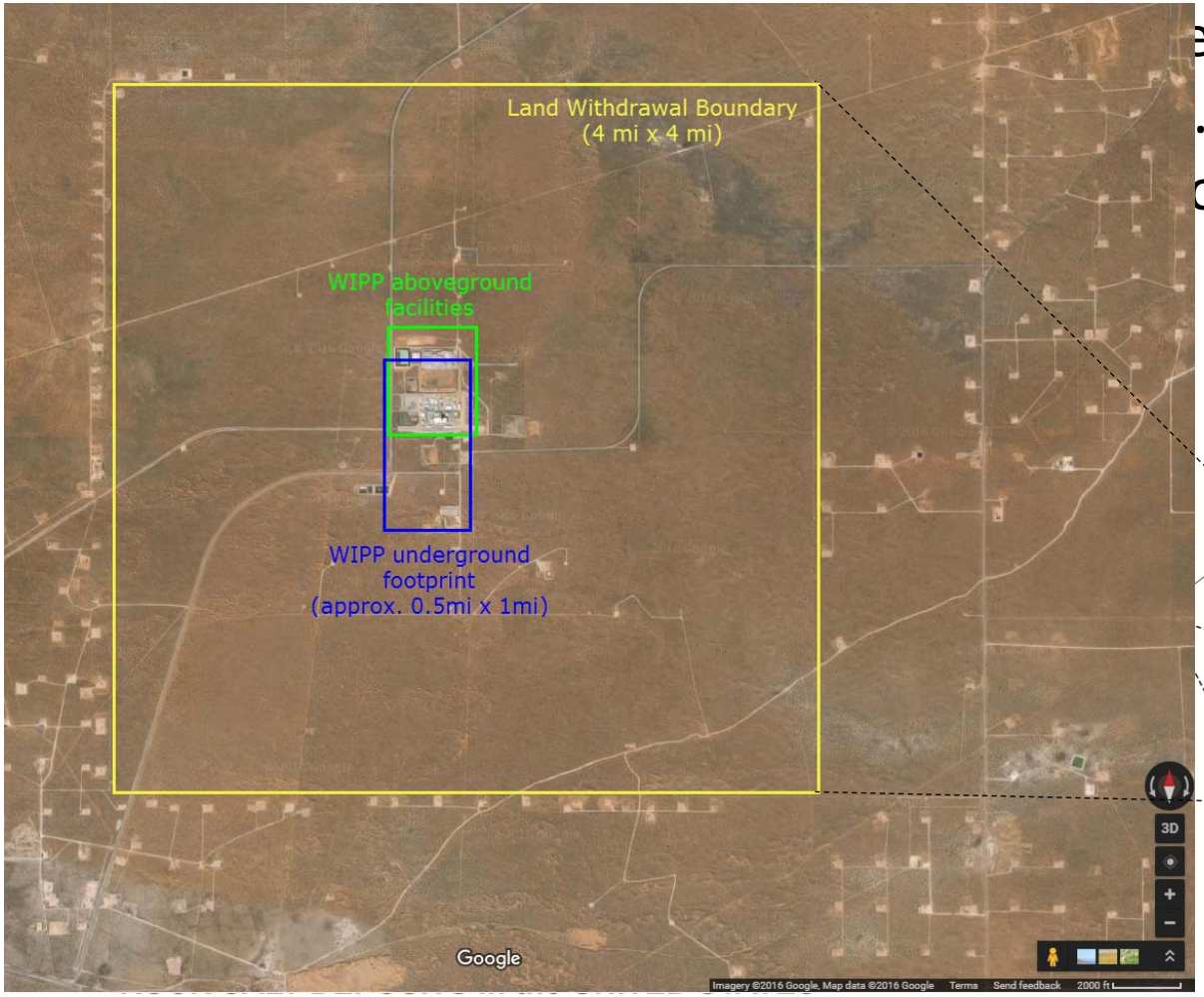
WIPP



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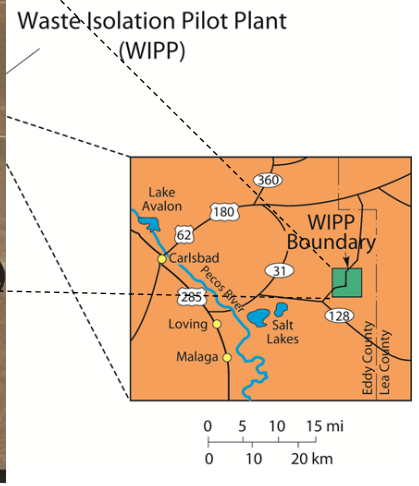
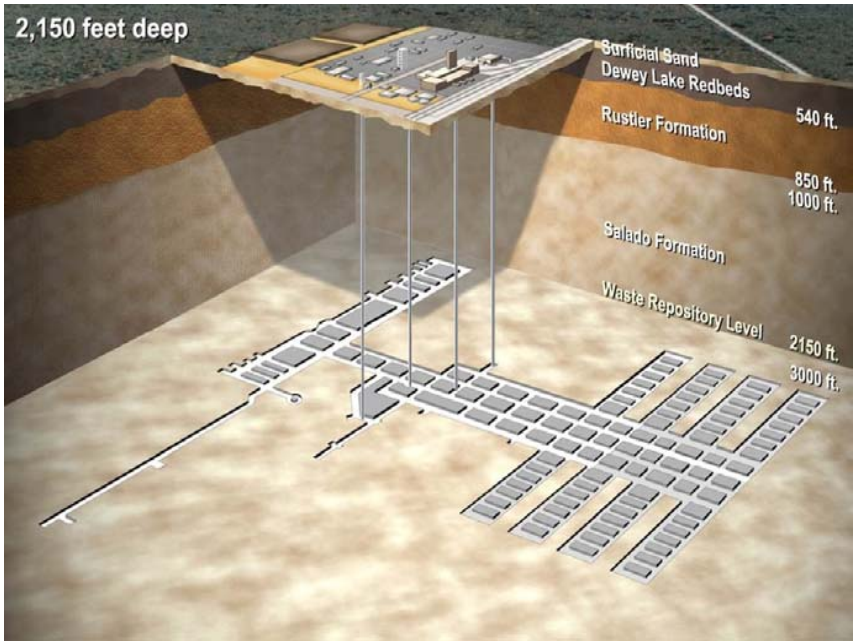


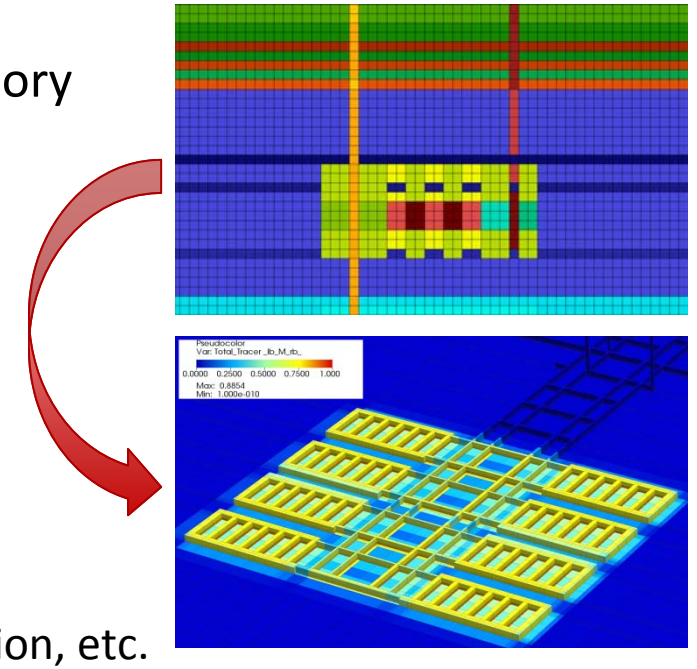
WIPP PA

- The DOE demonstrates compliance with containment requirements by means of performance assessment (PA) calculations conducted by Sandia National Laboratories (SNL) to Environmental Protection Agency (EPA)
- WIPP PA calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure.



PA Modernization

- Why?
  - 3D representation of the waste repository
    - Modifications or expansions
    - No requirement for symmetry
    - More realistic representation
  - More mechanistic process models
    - Anisothermal (heat generating wastes)
    - Miscible multiphase flow
    - Multicomponent transport
    - Radioactive decay and ingrowth, sorption, etc.
    - High-resolution mesh near repository (unstructured grid)



- How?
  - Massively parallel computing capability
    - Simulation size only depends on hardware capability

Overview

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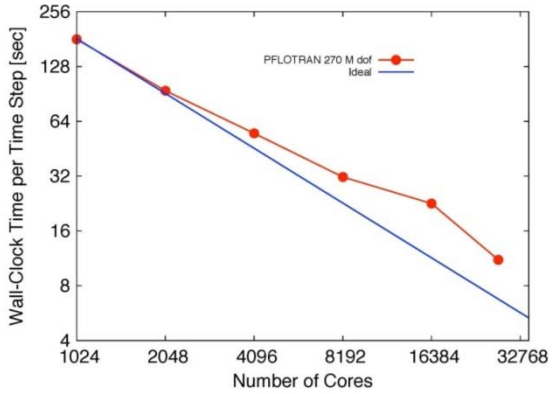
PFLOTRAN

Sandia National Laboratories

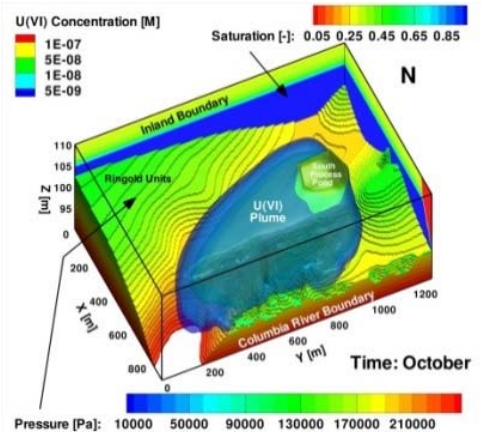
- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)



- Founded upon well-known (supported) open source libraries
  - MPI, PETSc, HDF5, METIS/ParMETIS/CMAKE
- Demonstrated performance
  - Maximum # processes: 262,144 (Jaguar supercomputer)
  - Maximum problem size: 3.34 billion degrees of freedom
  - Scales well to over 10K cores

Application of PFLOTRAN

- Nuclear waste disposal
  - **Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM**
  - DOE Used Fuel Disposition Program
  - SKB Forsmark Spent Fuel Nuclear Waste Repository (Sweden, Amphos[21])
- Climate: coupled overland/groundwater flow; CLM
  - Next Generation Ecosystem Experiments (NGEE) Arctic
  - DOE Earth System Modeling (ESM) Program
- Biogeochemical transport modeling
  - U(VI) fate and transport at Hanford 300 Area
  - Hyporheic zone biogeochemical cycling
    - Columbia River, WA, USA
    - East River, CO, USA
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers
- Colloid-facilitated transport



Hammond and Lichtner, WRR, 2010

PFLOTRAN Multi-Physics Capability

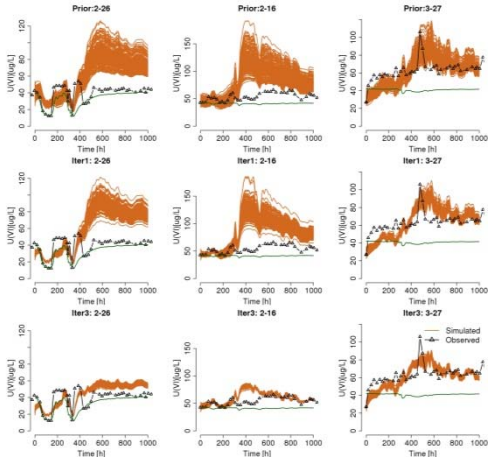
- Flow
  - Single phase, variably-saturated
  - Multiphase gas-liquid
  - Interchangeable constitutive models and equations of state
- Energy
  - Thermal conduction and convection
- Multi-Component Transport
  - Advection
  - Hydrodynamic dispersion
- Chemical Reaction
  - Aqueous speciation
  - Mineral precipitation-dissolution
  - Sorption
  - Microbiological
  - Radioactive decay with daughter products
- Geomechanics
  - Elastic deformation
- Geophysics
  - Coupling to E4D

(Tim Johnson, PNNL)

PFLOTRAN Computing Capability

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

Data Assimilation



Xingyuan Chen, PNNL, 2011

PFLOTRAN Developers

Overview

- Introduction to WIPP
  - WIPP and WIPP PA
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- Introduction to PFLOTRAN
- **Current Progress**
  - Integration of WIPP-specific functionality
  - Proof-of-concept 3D two-phase undisturbed scenario
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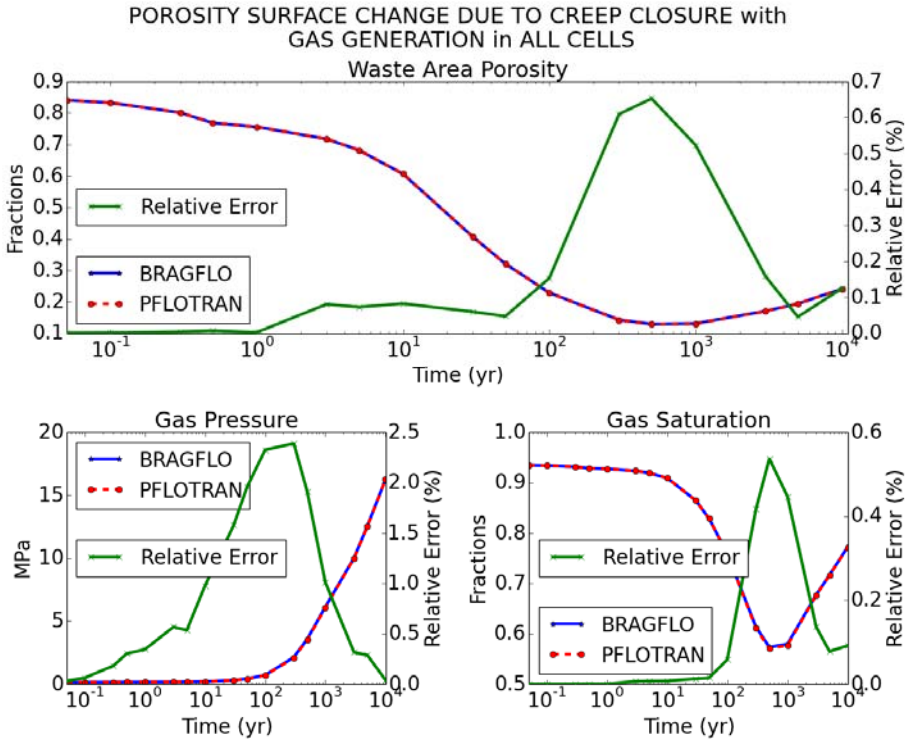
WIPP-Specific Functionality

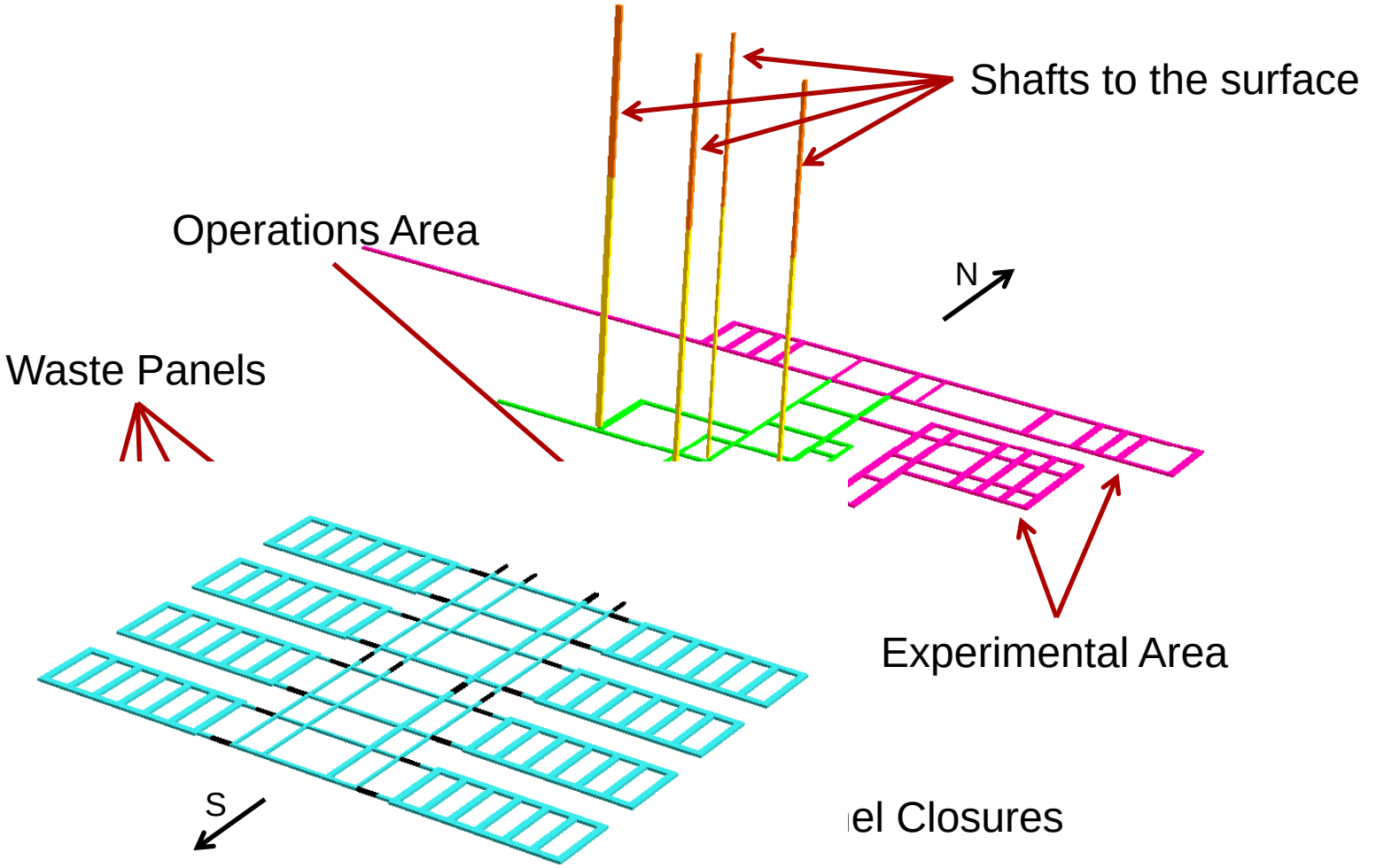
- Gas generation in two-phase flow
- Change in porosity due to creep closure
- Fractures in marker beds and disturbed rock zones (DRZ)
- Klinkenberg effect
- RKS equation of state for gas density
- Material map change due to creep closure and borehole intrusion
- Direct brine release
- LHS interface with PFLOTRAN
- Preprocessor of PFLOTRAN - PrePFLOTRAN

Verification of Functionalities

- WIPP-specific functionalities are implemented to PFLOTRAN
- The functionality is verified by comparing to the current PA code
- Verification on complex problem scenarios not possible due to key differences in process models.

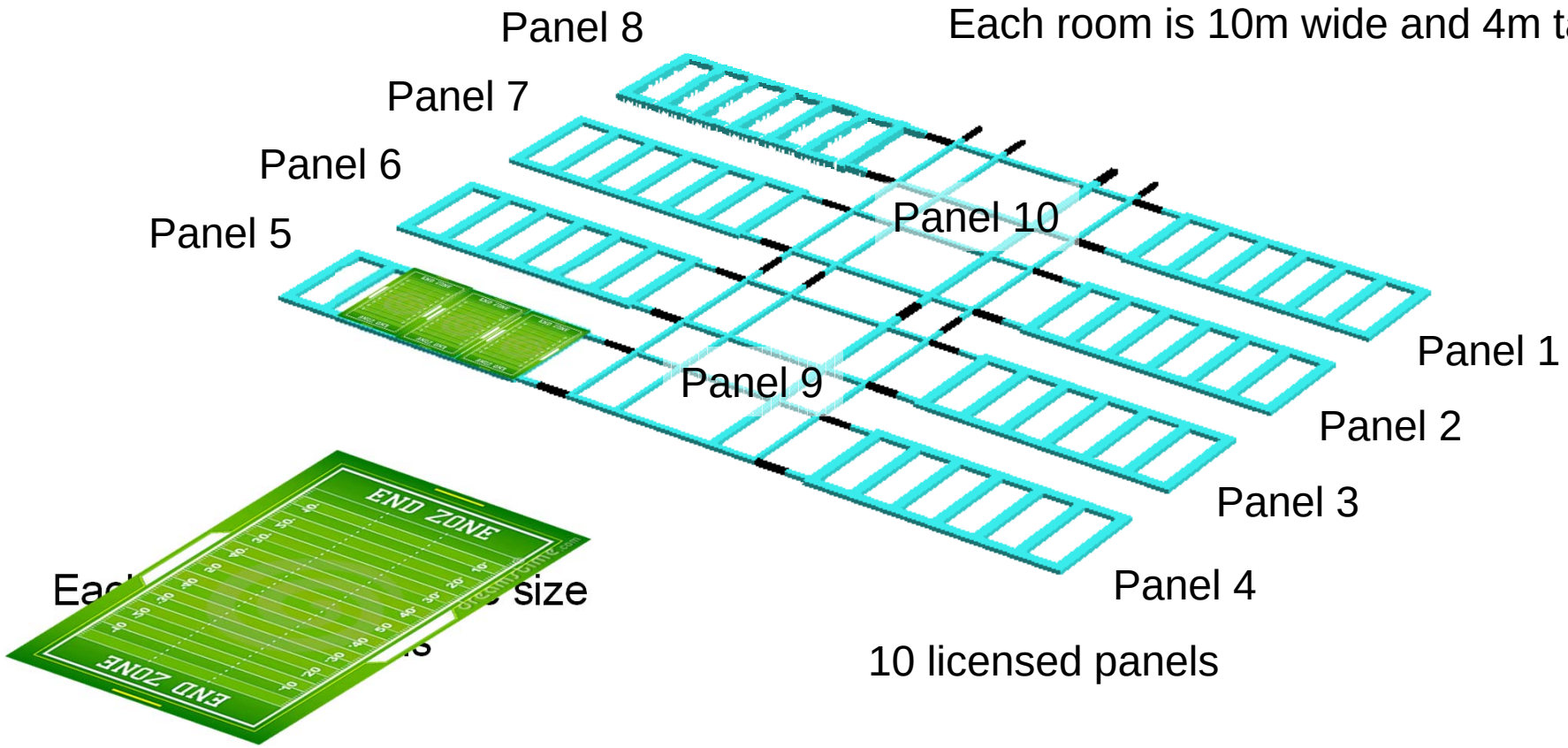


WIPP Underground Structures



Panels and Rooms

Room 7 Room 6 Room 5 Room 4 Room 3 Room 2 Room 1



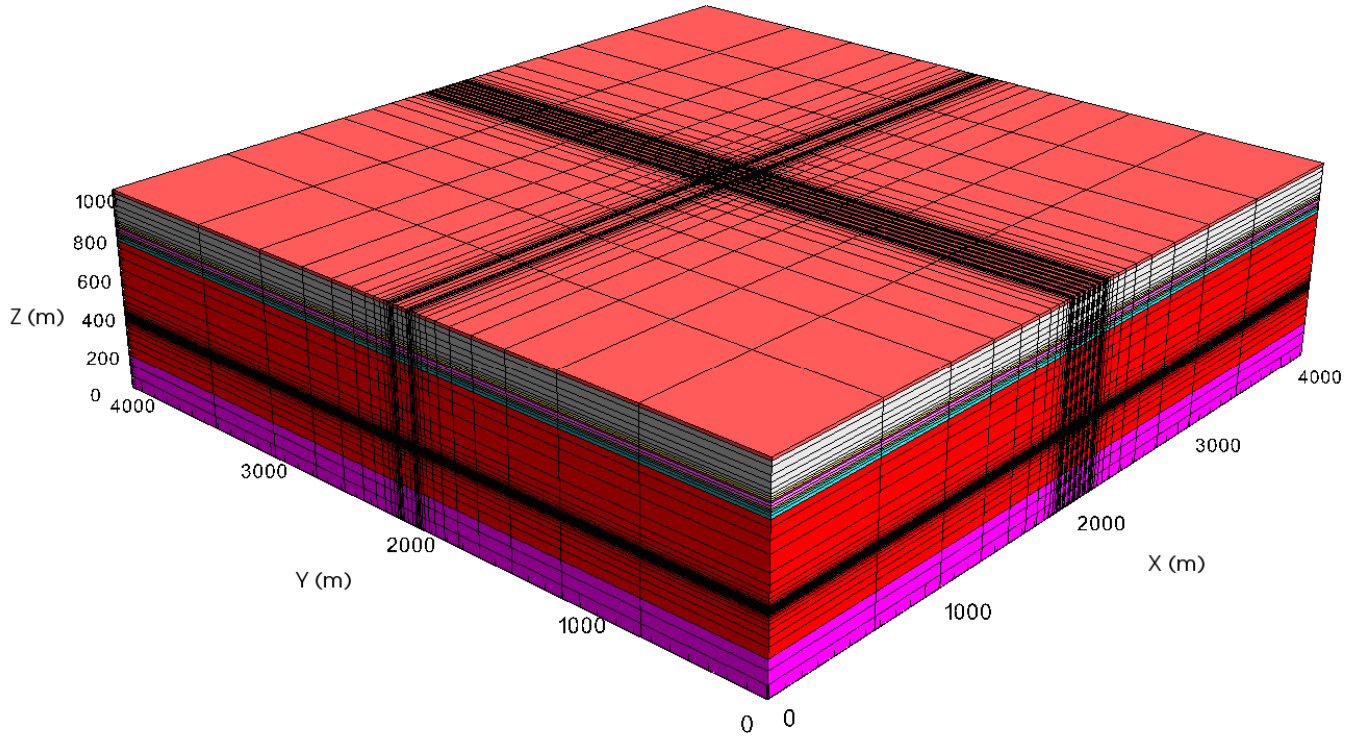
Waste Rooms

3D two-phase flow and transport

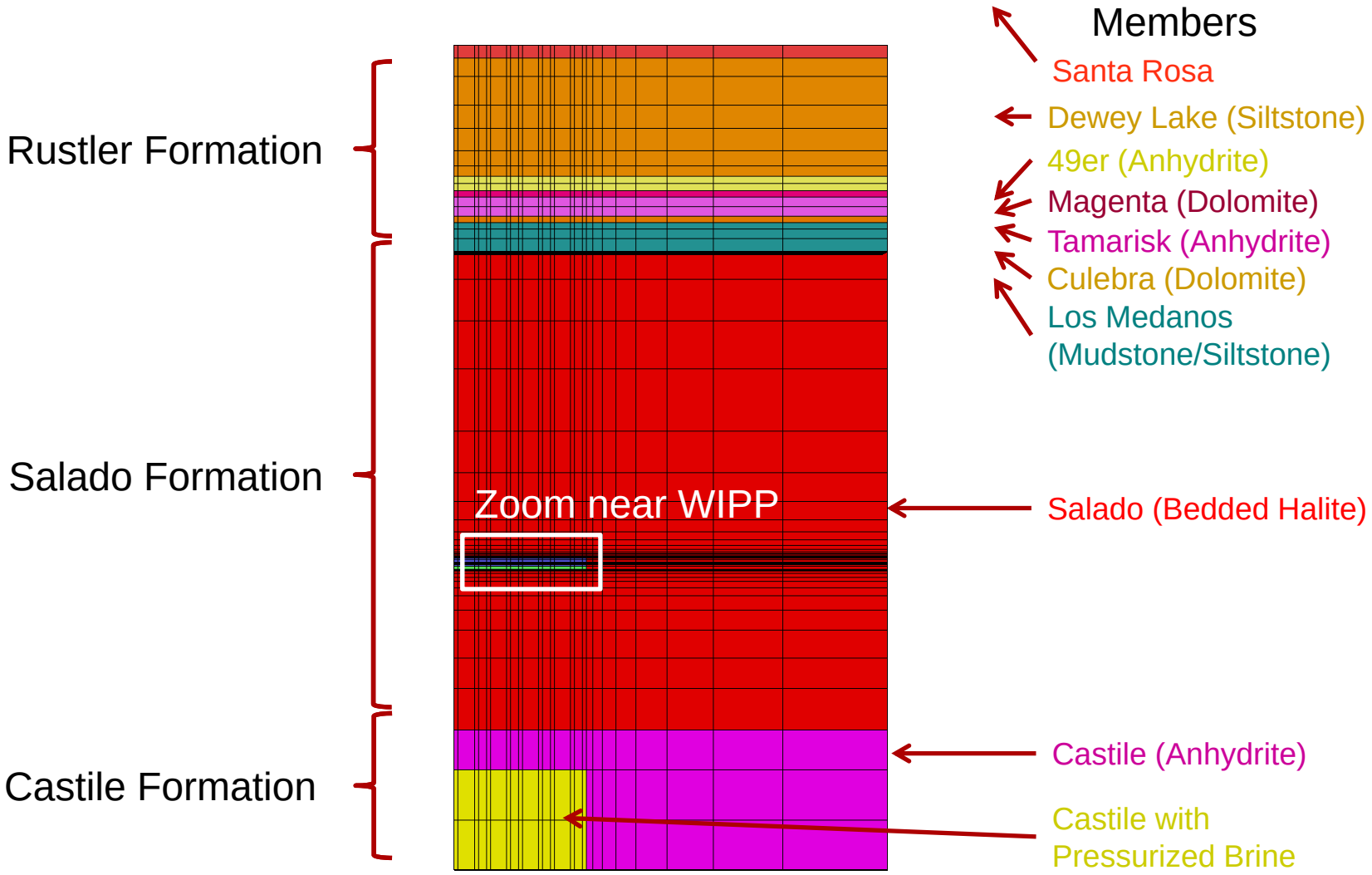
- 3D single panel model
- Designed for proof of concept
- Flow model
  - Two-phase involving gas-liquid-energy (hydrogen, brine)
  - Initial Conditions
    - Excavated waste panel is unsaturated
    - Disturbed rock zone (DRZ) is 40% saturated due to mechanical opening
    - Rest of the domain is saturated up to the water table
  - Boundary Condition
    - No-flow boundary condition at 2 km away
  - Waste area generates gas (hydrogen) for 10,000 years as a function of saturation
  - Isothermal, Creep Closure, Fracture
- Transport model
  - Tracking tracer; Am-241, Pu-239, Pu-238, U-234, and Th-230;
  - Radioactive decay reactions
    - Pu-238 ($t_{1/2}$=84yr) → U-234 ($t_{1/2}$=2.46E5yr) → Th-230
  - Sorption

Single Panel Model Domain

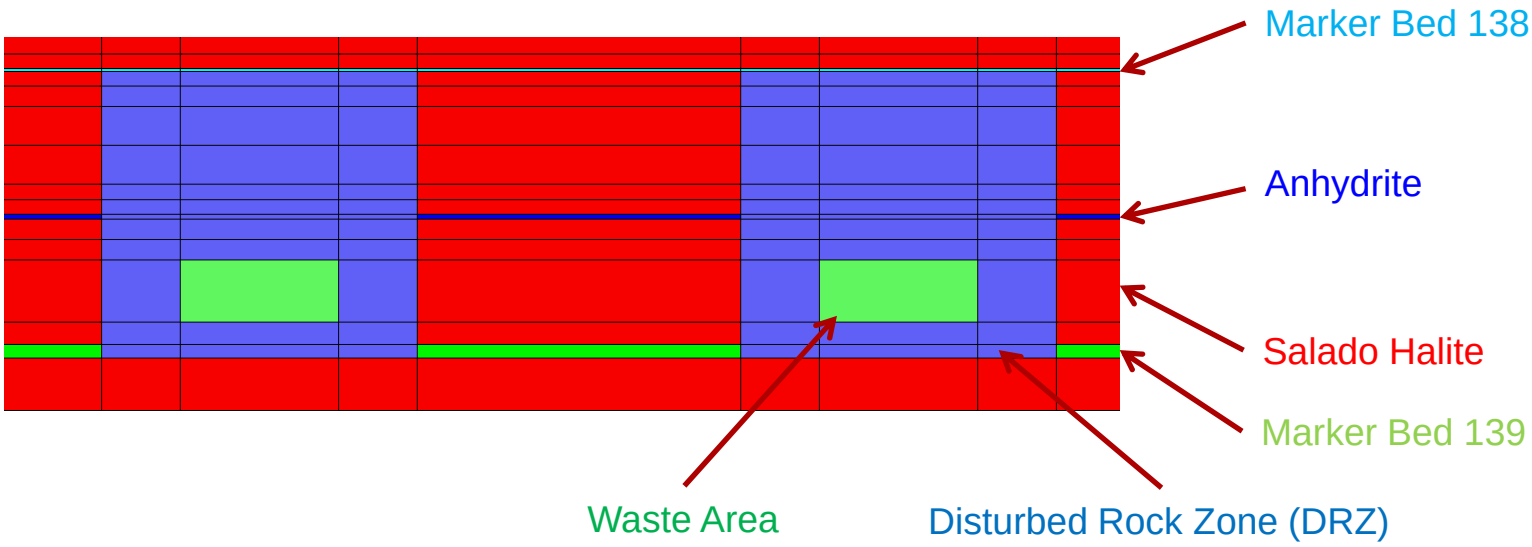
- 97,614 elements
- Domain spans out 2 km from the panel in x and y directions



Geologic Structures at WIPP

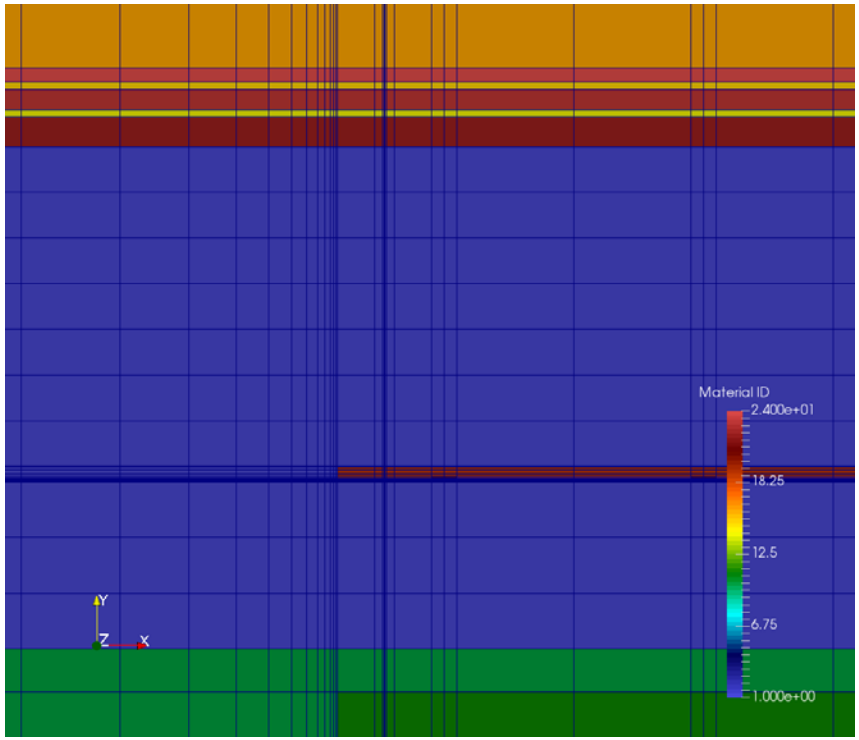


WIPP Surroundings

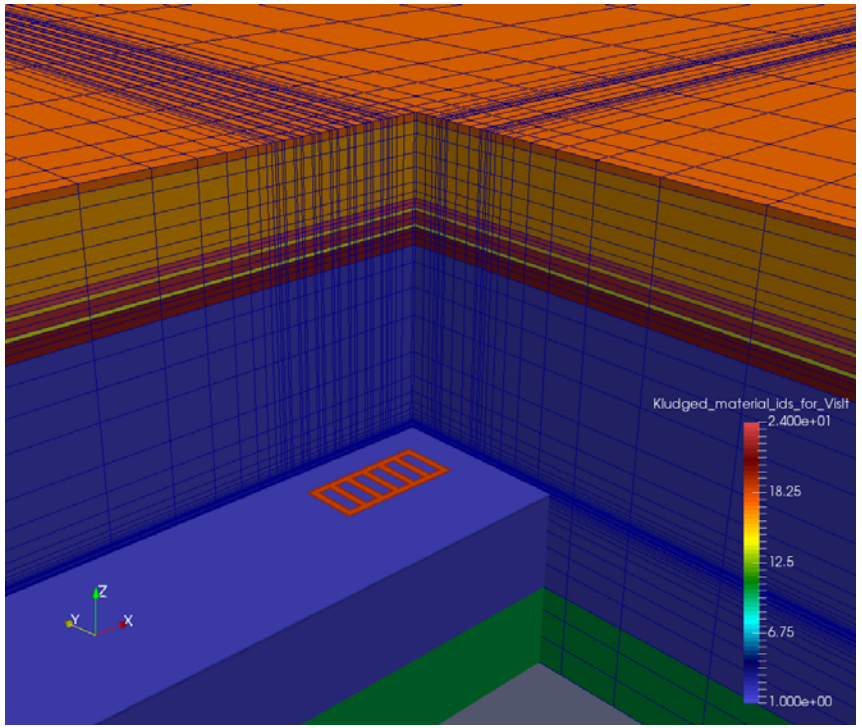


3D two-phase flow and transport

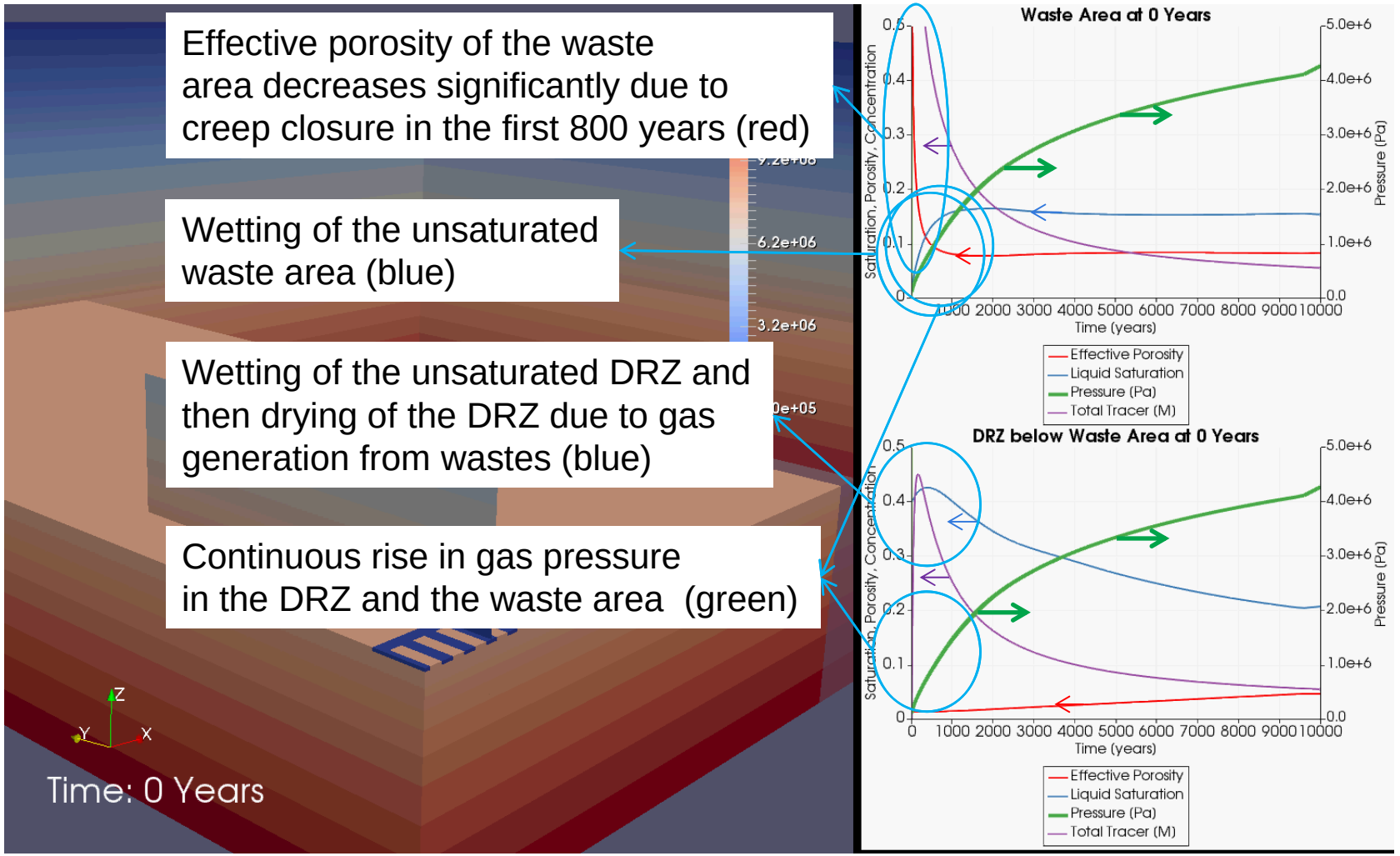
BRAGFLO



PFLOTRAN



WIPP Specific Functions



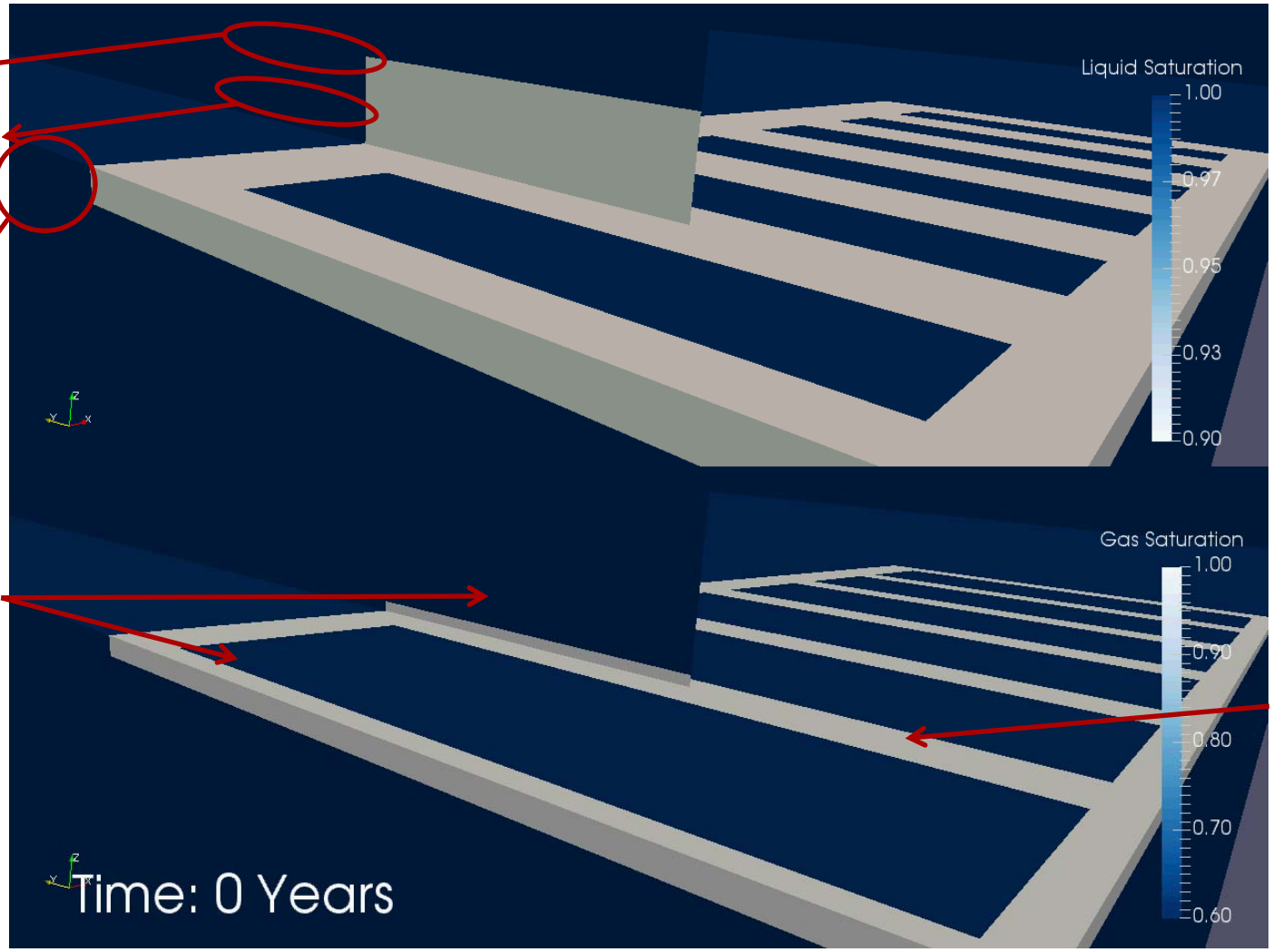
3D two-phase flow and transport

MB 138

Anhydrite

MB 139

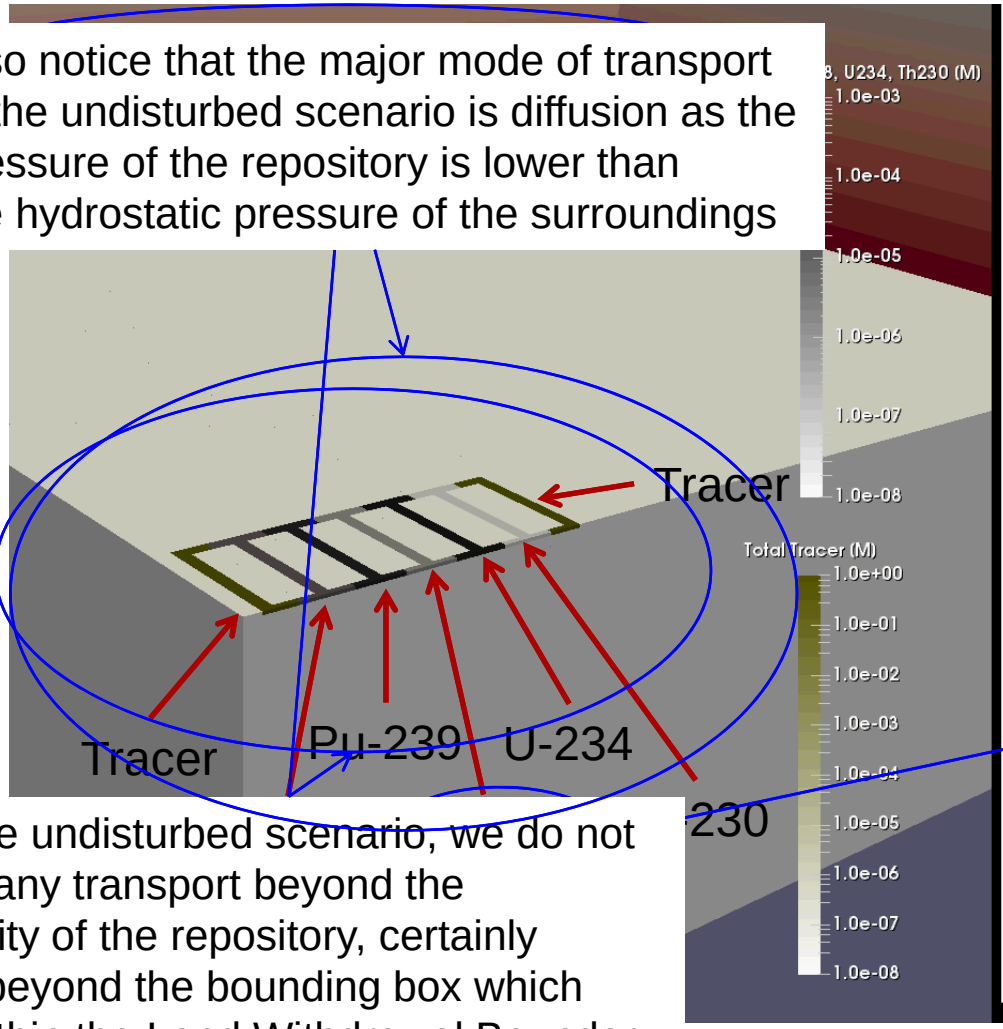
Liquid saturation decrease in the disturbed rock zone

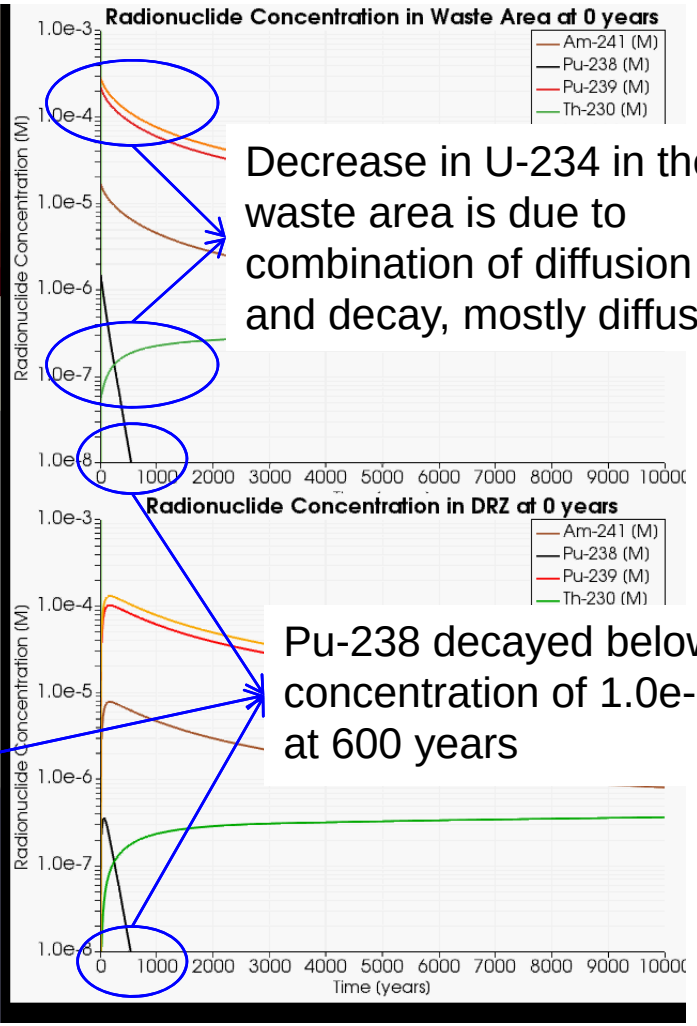


Liquid saturation increase in the waste area

3D two-phase flow and transport

Also notice that the major mode of transport in the undisturbed scenario is diffusion as the pressure of the repository is lower than the hydrostatic pressure of the surroundings





Decrease in U-234 in the waste area is due to combination of diffusion and decay, mostly diffusion

Pu-238 decayed below concentration of 1.0e-8 at 600 years

In the undisturbed scenario, we do not see any transport beyond the vicinity of the repository, certainly not beyond the bounding box which is within the Land Withdrawal Boundary

ParaView animation

Borehole intrusion to brine pocket

- 3D single room with very large pressurized brine pocket model
- Designed for proof of concept
- Flow model
  - Single-phase with brine only
  - Initial Conditions
    - The domain is fully saturated even in excavated zone
    - Most extreme brine pocket pressure (15 MPa)
  - Boundary Condition
    - No-flow boundary condition at 600 m away from the room
- Transport model
  - Tracking tracer; Am-241, Pu-239, Pu-238, U-234, and Th-230;
  - Radioactive decay reactions
    - Pu-238 ($t_{1/2}$=84yr) → U-234 ($t_{1/2}$=2.46E5yr) → Th-230
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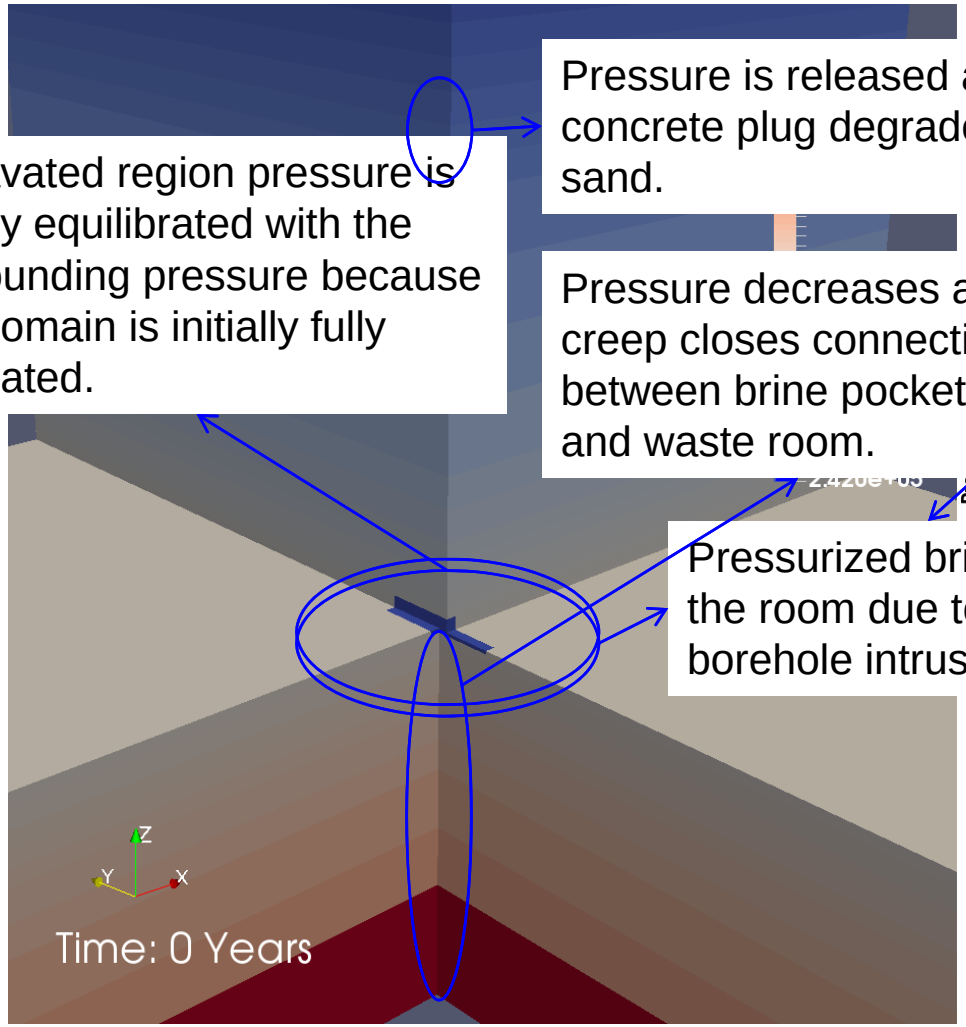
Borehole intrusion to brine pocket

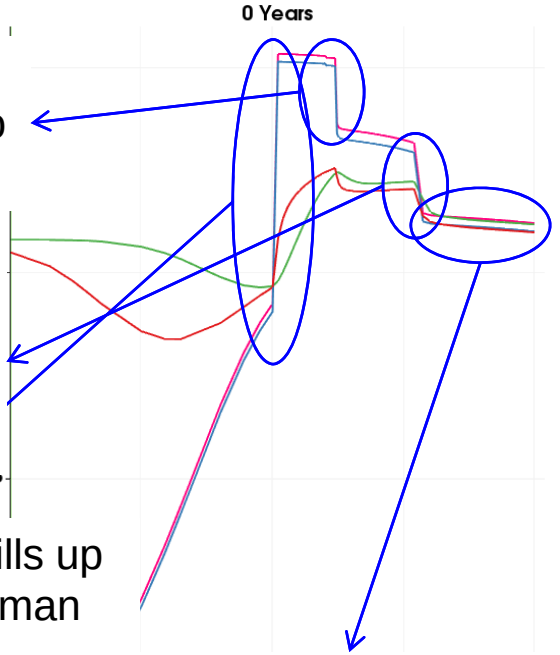


Excavated region pressure is nearly equilibrated with the surrounding pressure because the domain is initially fully saturated.

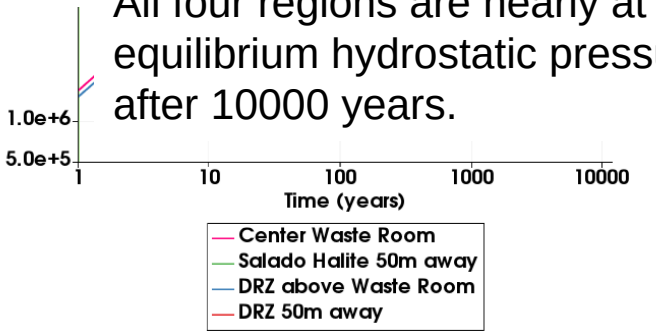
Pressure is released as concrete plug degrades to sand.

Pressure decreases as creep closes connection between brine pocket and waste room.

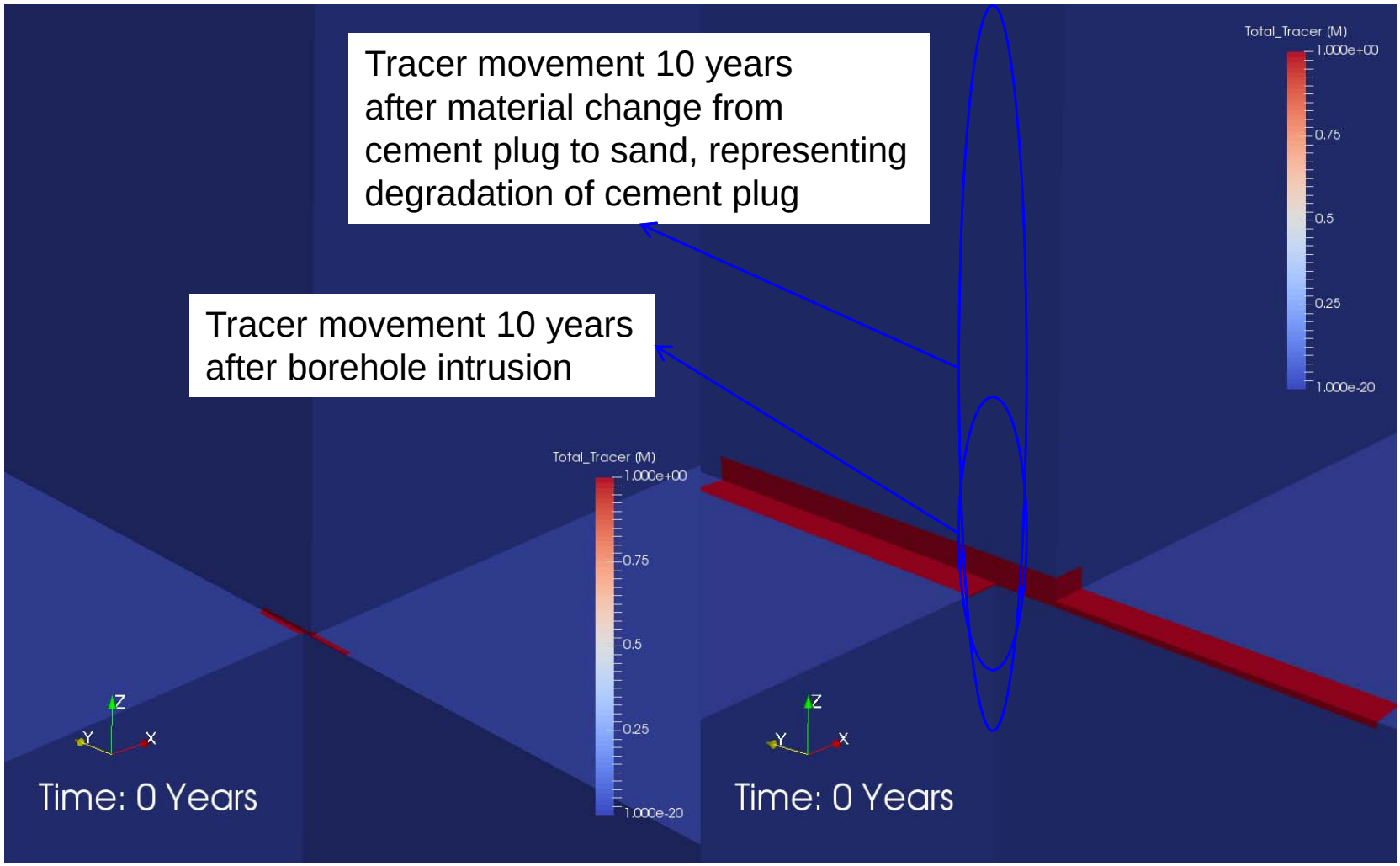
Pressurized brine fills up the room due to human borehole intrusion.



All four regions are nearly at equilibrium hydrostatic pressure after 10000 years.



Borehole intrusion to brine pocket



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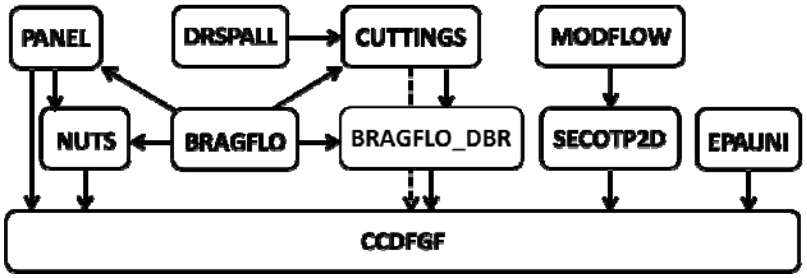
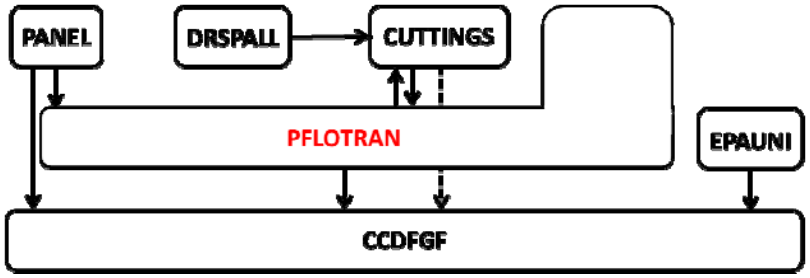
  - Consolidation into one code and single conceptual model
  - PrePFLOTRAN “run control” system
  - V&V testing suite and documentation

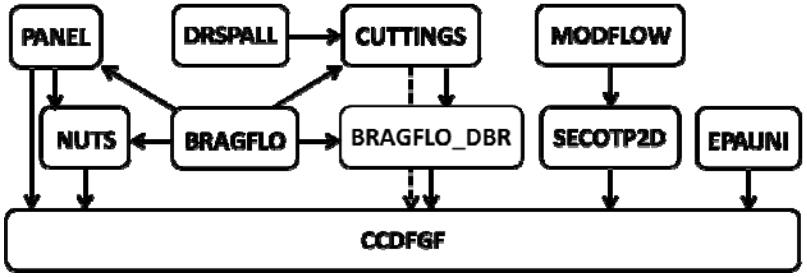
Consolidation into one code

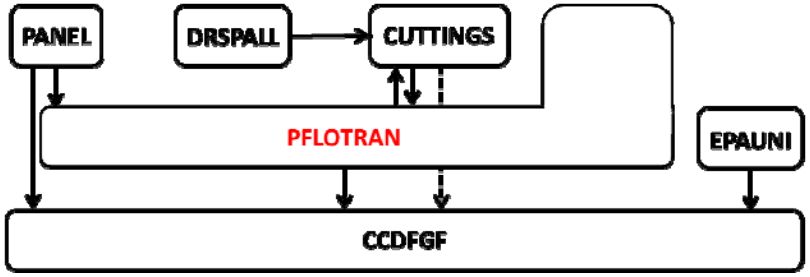




Current PA	PFLOTRAN
- **Decoupled 2D** - Structured grid - **Decoupled flow and transport calculations** - **Single core simulations** - Limitations on simulation size - **Many I/O interfaces required** - **Simplified process models and coarse mesh**	- **3D** - Unstructured/structured grid - **Coupled flow and transport calculations** - **Massively parallel** - Simulation size only depends on hardware capability - **Mechanistic process models and high mesh resolution**

One conceptual model for Culebra and Halite





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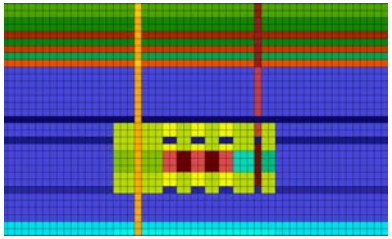
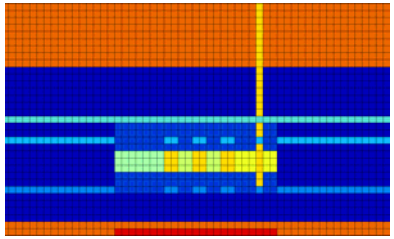
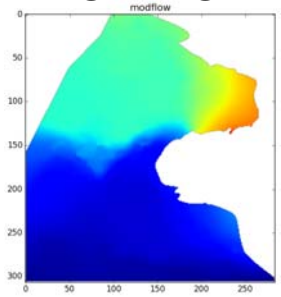


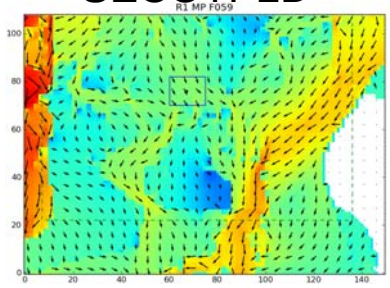
NUTS



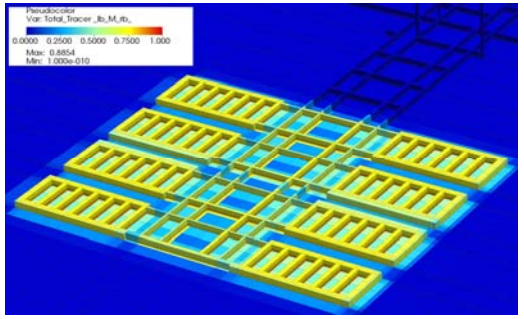
MODFLOW

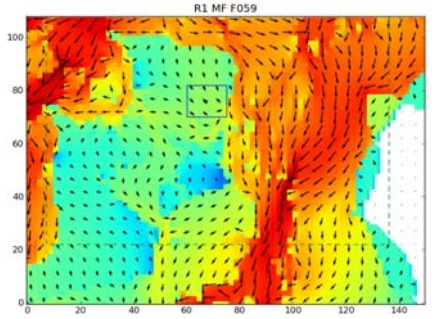


SECOTP2D



PFLOTRAN





Advantages of Modernization

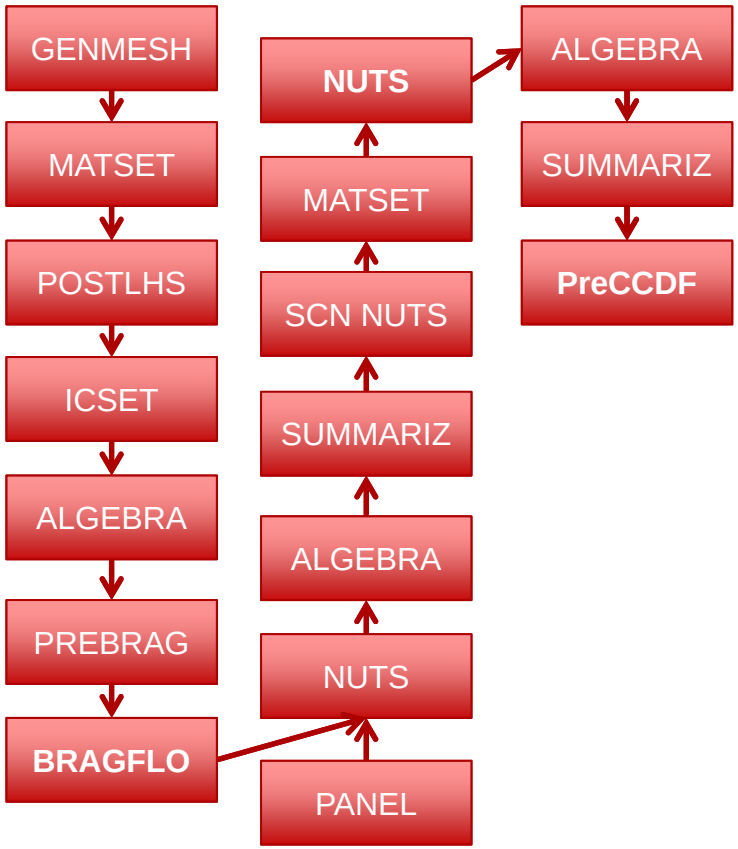
- Offers easier peer review process in support of upgrades
  - A single governing equation for all flow
  - A single governing equation for all transport
  - Peer review of a single code when a new process model is introduced
- In-house code development expertise
- Every code modification is tracked and verified through automated regression, unit, and QA testing
- Easy to change grid if necessary (less bookkeeping required)
- Direct brine release simulation will use the same domain or a subset of the full domain (no need to read and assign artificial initial conditions).

PrePFLOTRAN

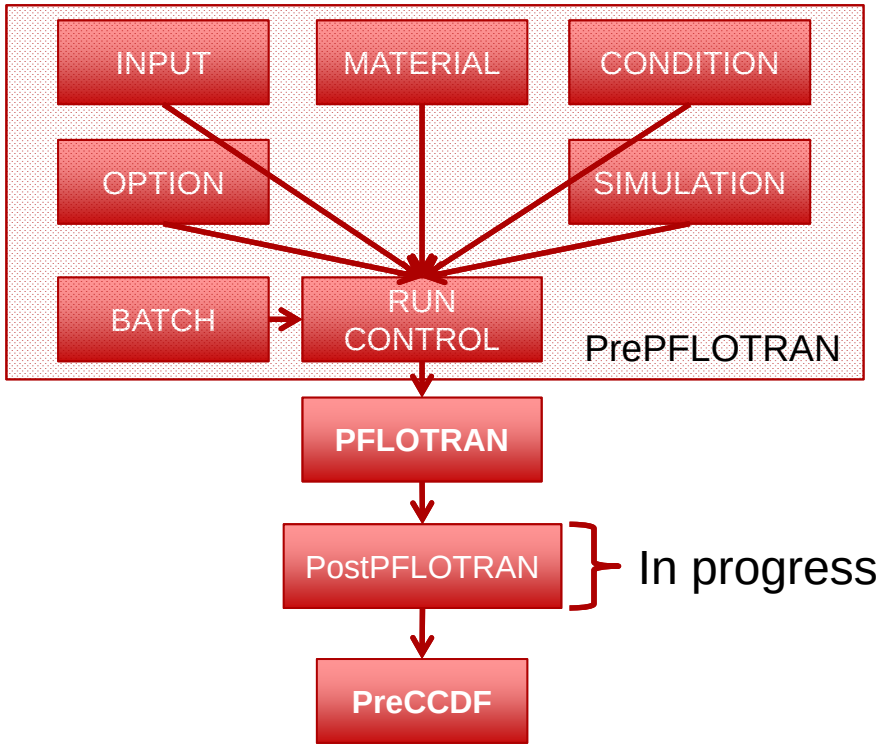
- Written in Python (ubiquitous and free)
- Documented with Sphinx
- Provides centralized “run control” for WIPP PA
  - Imports parameters from WIPP PA database
  - Converts parameters to PFLOTRAN-consistent format
  - Exports PFLOTRAN input decks (all files to execute a simulation) for all simulations (i.e. all vectors, scenarios, replicates)

Execution process

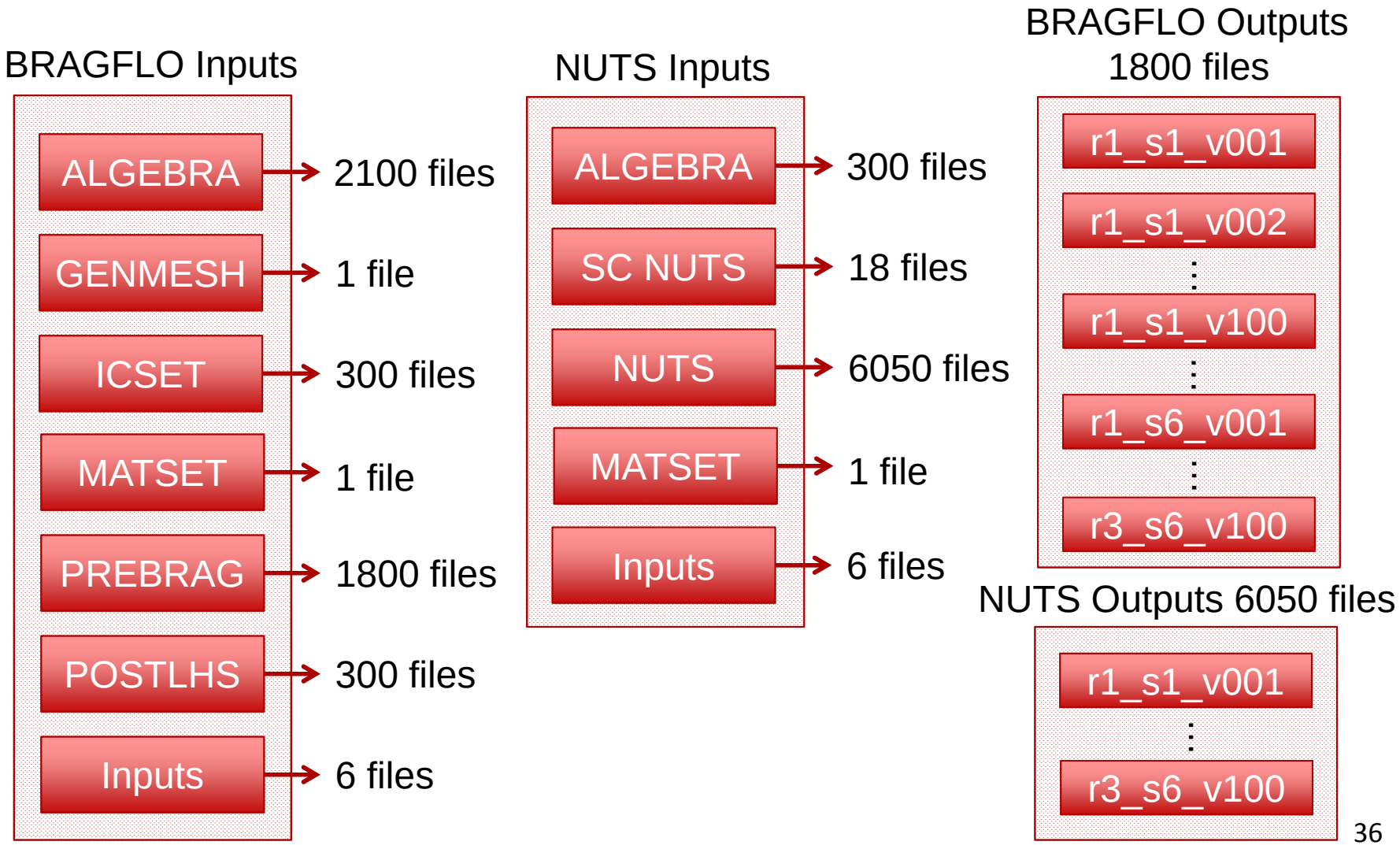
BRAGFLO



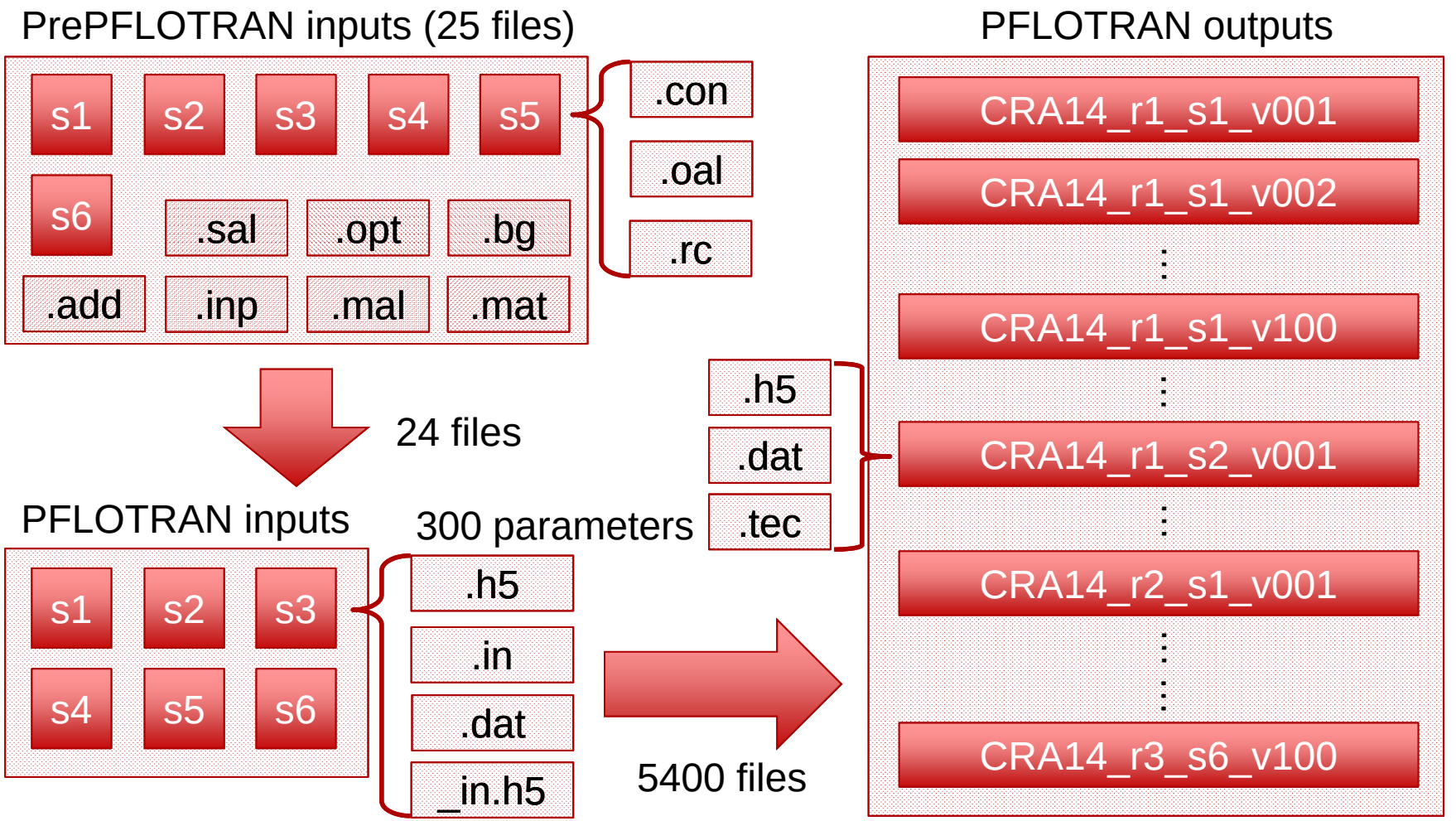
PFLOTRAN



Current file management

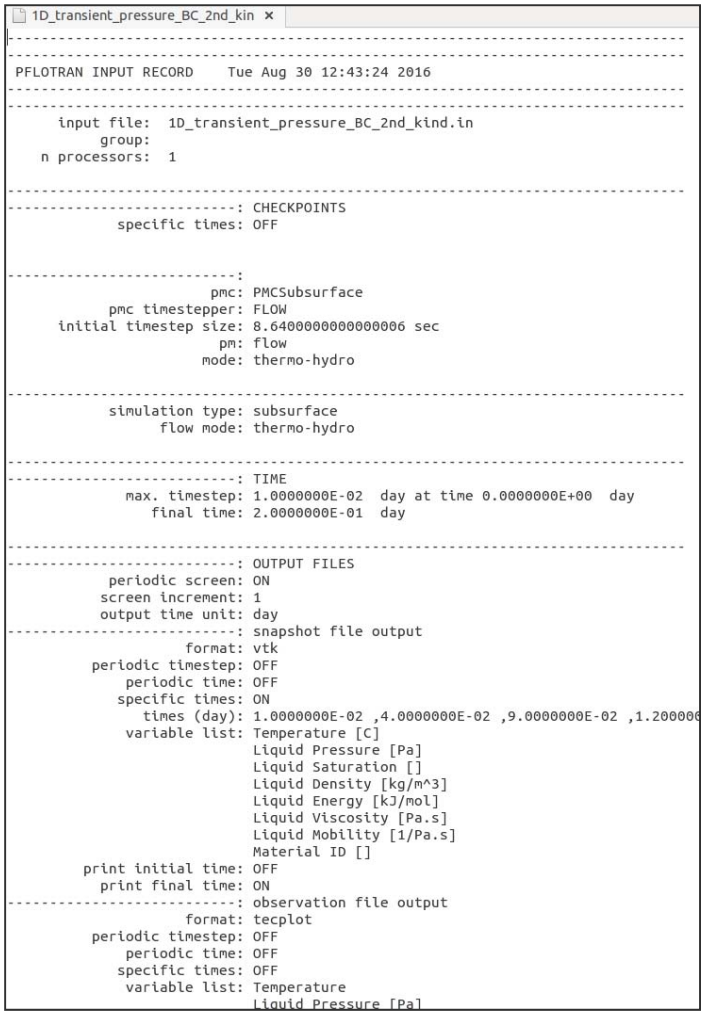


New file management



The *Input Record File*

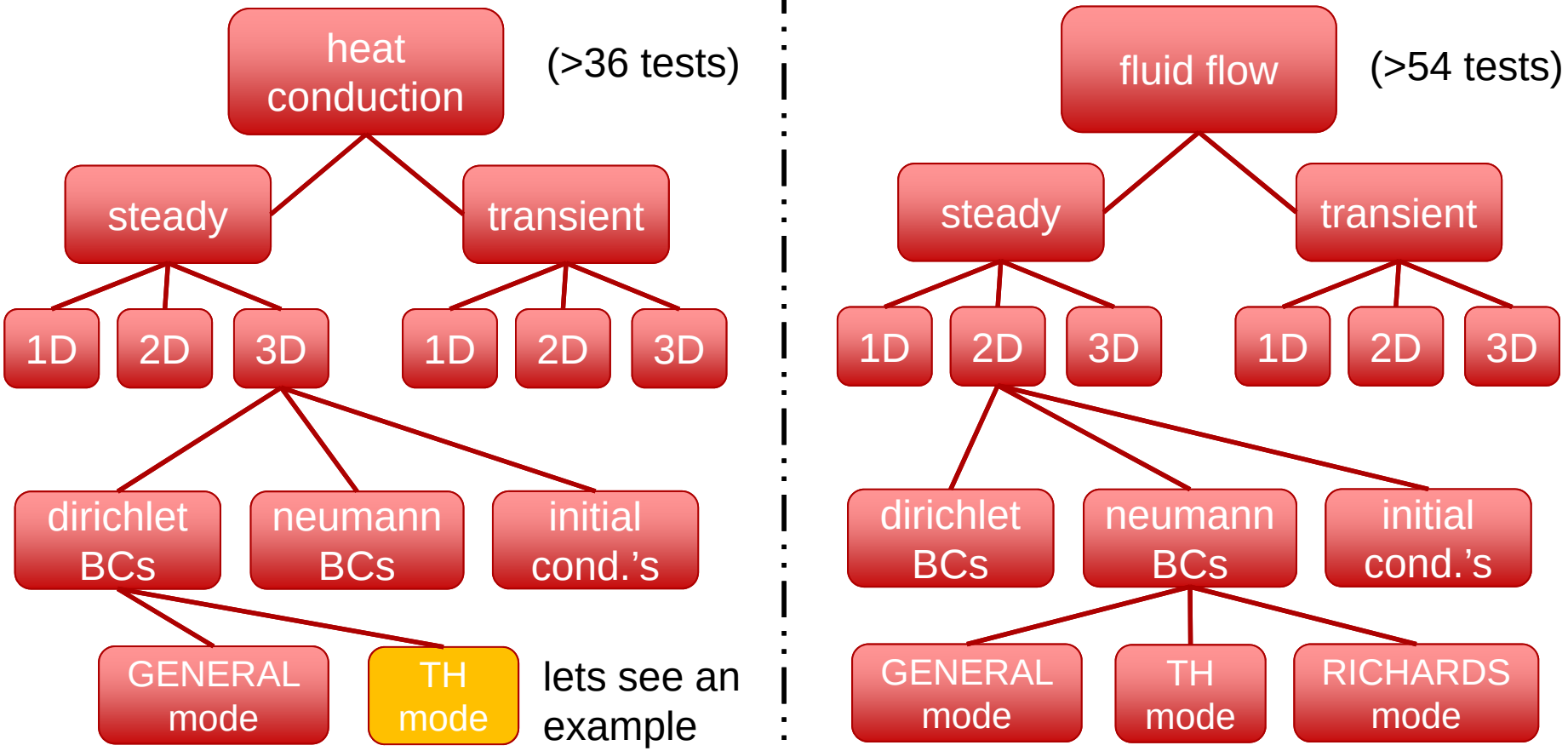
- A text file which prints out all of the "ingested information" from the input file (parameter values, options, etc.)
- Can help catch mistakes a user makes in the input file
  - Parameters that are commented out or defined multiple times
- Can act as a stand-alone document which describes the specifics of a simulation
  - Anyone should be able to re-create the simulation with this file alone
- More reader-friendly
  - It's a less cryptic description of the simulation



```
1D_transient_pressure_BC_2nd_kin ×
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
 PFLOTRAN INPUT RECORD    Tue Aug 30 12:43:24 2016
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
      input file:  1D_transient_pressure_BC_2nd_kind.in
           group:
   n processors:  1

--------------------------------------------------------------------------------
---------------------------: CHECKPOINTS
            specific times: OFF


---------------------------:
                       pmc: PMCSubsurface
          pmc timestepper: FLOW
     initial timestep size: 8.6400000000000006 sec
                        pm: flow
                      mode: thermo-hydro

--------------------------------------------------------------------------------
            simulation type: subsurface
                  flow mode: thermo-hydro

--------------------------------------------------------------------------------
---------------------------: TIME
              max. timestep: 1.0000000E-02  day at time 0.0000000E+00  day
                 final time: 2.0000000E-01  day


--------------------------------------------------------------------------------
---------------------------: OUTPUT FILES
            periodic screen: ON
           screen increment: 1
           output time unit: day
---------------------------: snapshot file output
                     format: vtk
          periodic timestep: OFF
             periodic time: OFF
            specific times: ON
               times (day): 1.0000000E-02 ,4.0000000E-02 ,9.0000000E-02 ,1.200000
             variable list: Temperature [C]
                            Liquid Pressure [Pa]
                            Liquid Saturation []
                            Liquid Density [kg/m^3]
                            Liquid Energy [kJ/mol]
                            Liquid Viscosity [Pa.s]
                            Liquid Mobility [1/Pa.s]
                            Material ID []
         print initial time: OFF
           print final time: ON
---------------------------: observation file output
                     format: tecplot
          periodic timestep: OFF
             periodic time: OFF
            specific times: OFF
             variable list: Temperature
                            Liquid Pressure [Pa]
```

Software Verification Testing Suite

- Test problems must remain simple (analytical solutions must exist)!

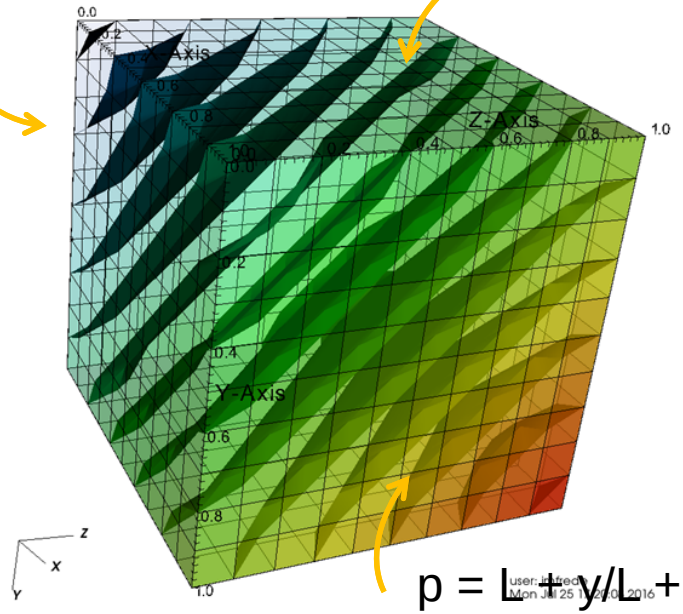


Software Verification Testing Suite

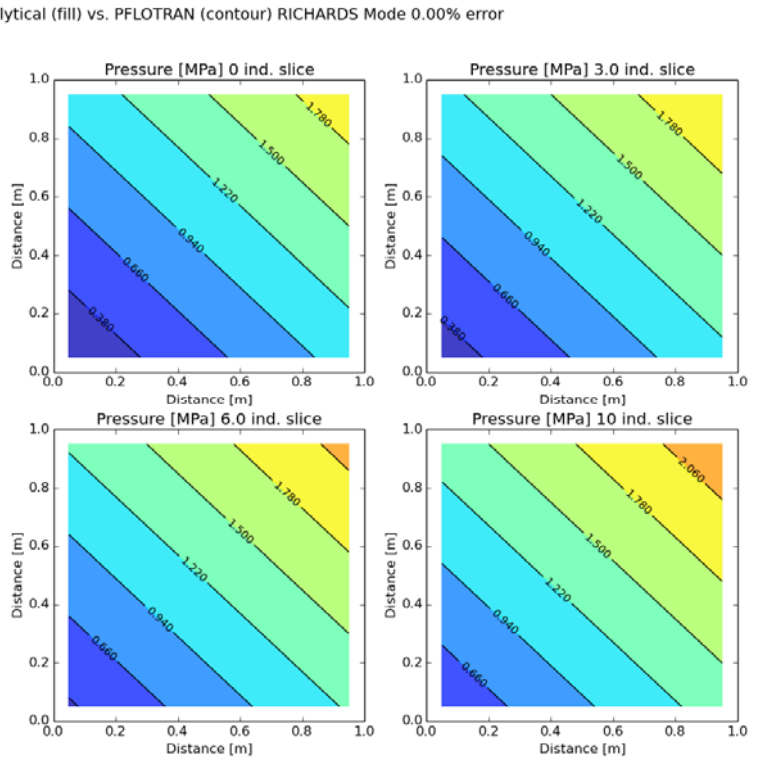
- Example test:
  - 3D domain
  - steady fluid flow/pressure field (steady-state solution)
  - dirichlet pressure boundary conditions

p = x/L + y/L MPa
east face

p = x/L + z/L MPa
top face

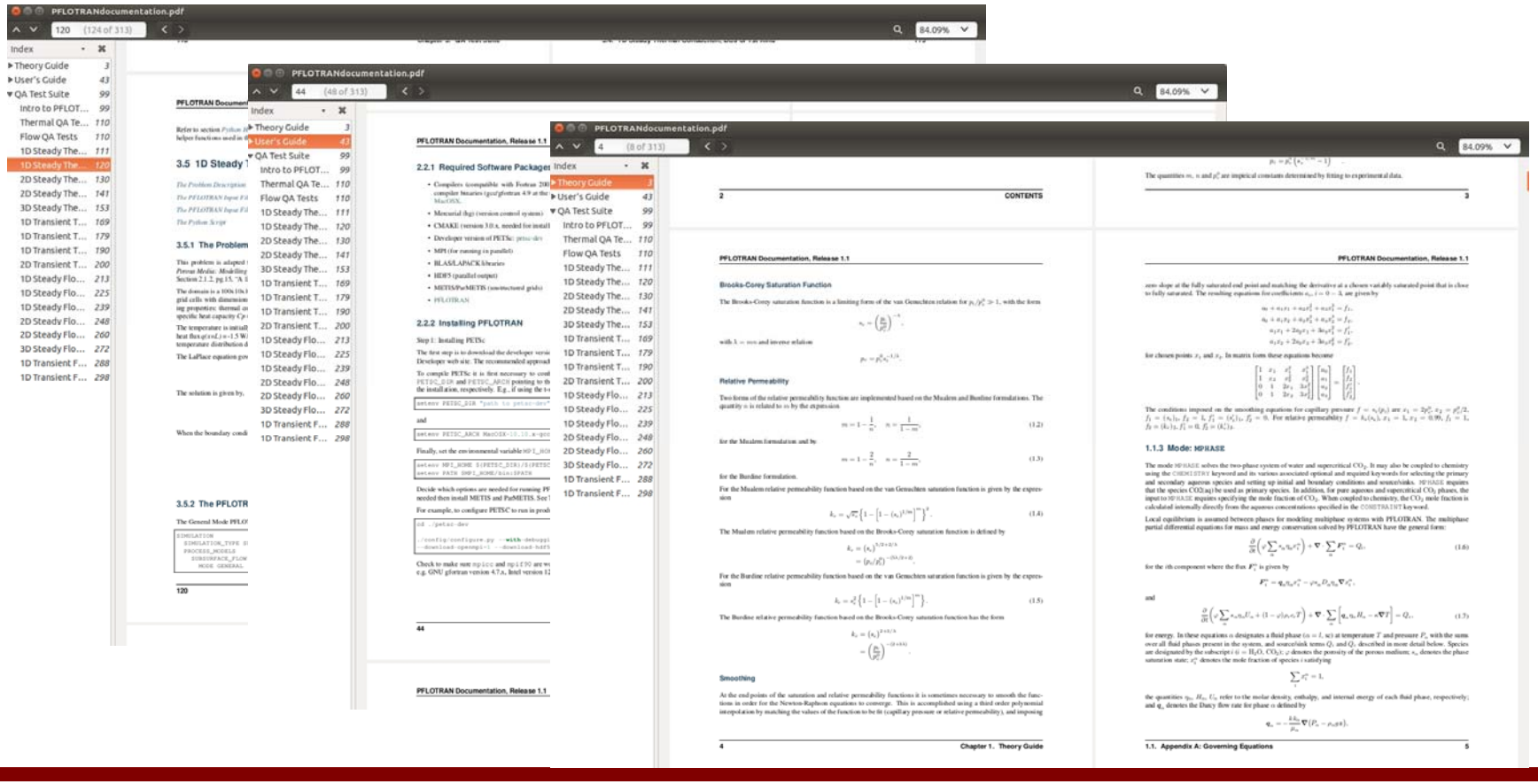


p = L + y/L + z/L MPa
south face



PFLOTRAN Documentation Overhaul

- Overhaul approach:
  - Use a documentation generator program, such as Sphinx, to generate both the website and the PDF versions of the documentation:



Questions?

- Thanks to Glenn Hammond for Introduction to PFLOTRAN slides, and Jennifer Frederick for V&V suite and documentation slides