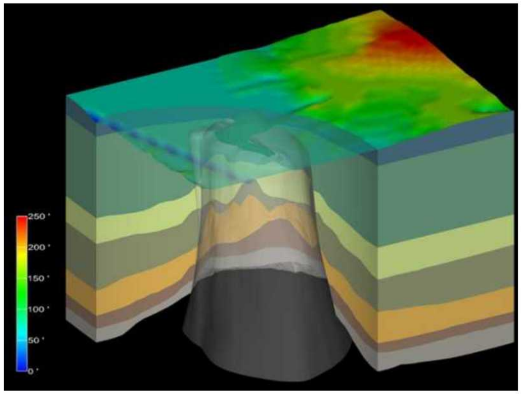
Exceptional service in the national interest

Sandia National Laboratories

SAND2019-0789PE



PFLOTRAN Overview

Robert MacKinnon and Glenn Hammond

Applied Systems Analysis and Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

Engineered Earth Systems

- Backend of the Nuclear Fuel Cycle
  - Spent Fuel and Waste Science and Technology Campaign, Office of Nuclear Energy, DOE
    - Disposal Research Mission - Develop capabilities to support implementation of the nation’s future deep geologic repository for disposal of commercial spent nuclear fuel and high-level waste
- DOE Managed Nuclear Waste
  - Waste Isolation Pilot Plant (WIPP), Carlsbad Field Office, Office Of Environmental Management, DOE
    - Develop a three-dimensional performance assessment model to support future WIPP re-certification analyses

What is a deep geologic repository?

An engineered facility sited, designed, and constructed deep (typically below 300 m) in a stable geologic environment such that the engineered and natural systems combine to provide safe, long-term, isolation and containment of the nuclear waste

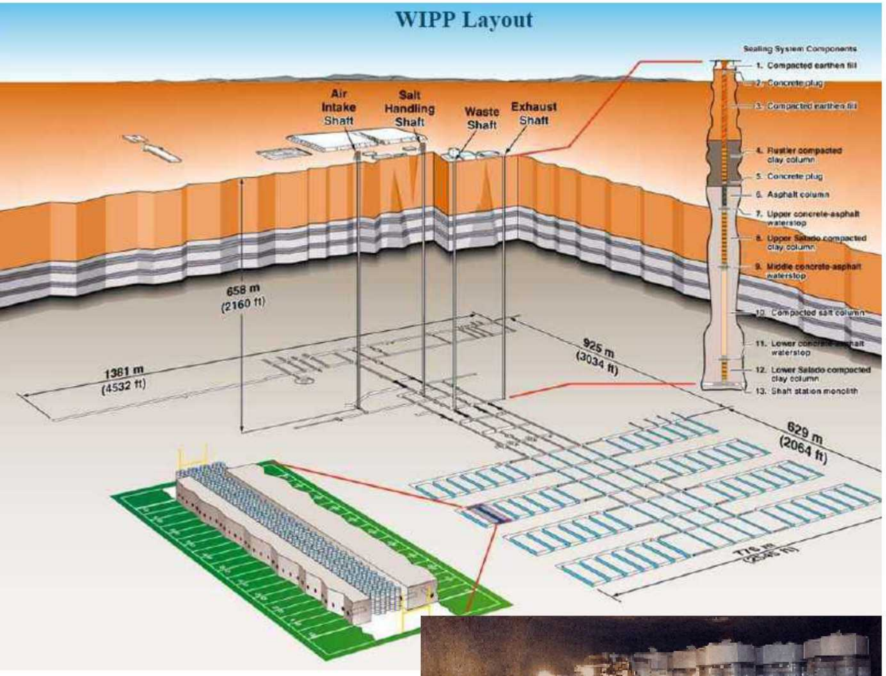
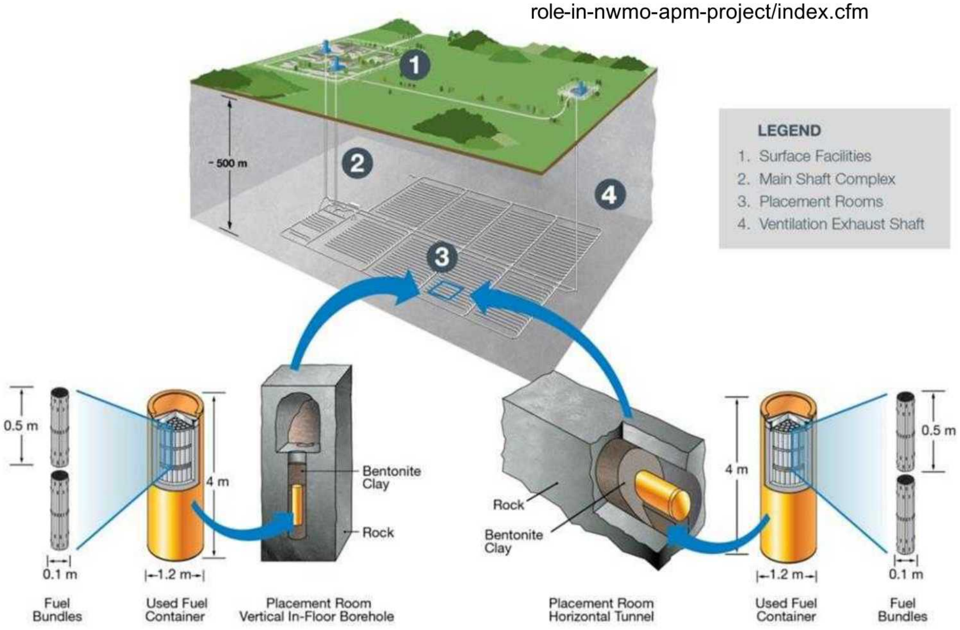
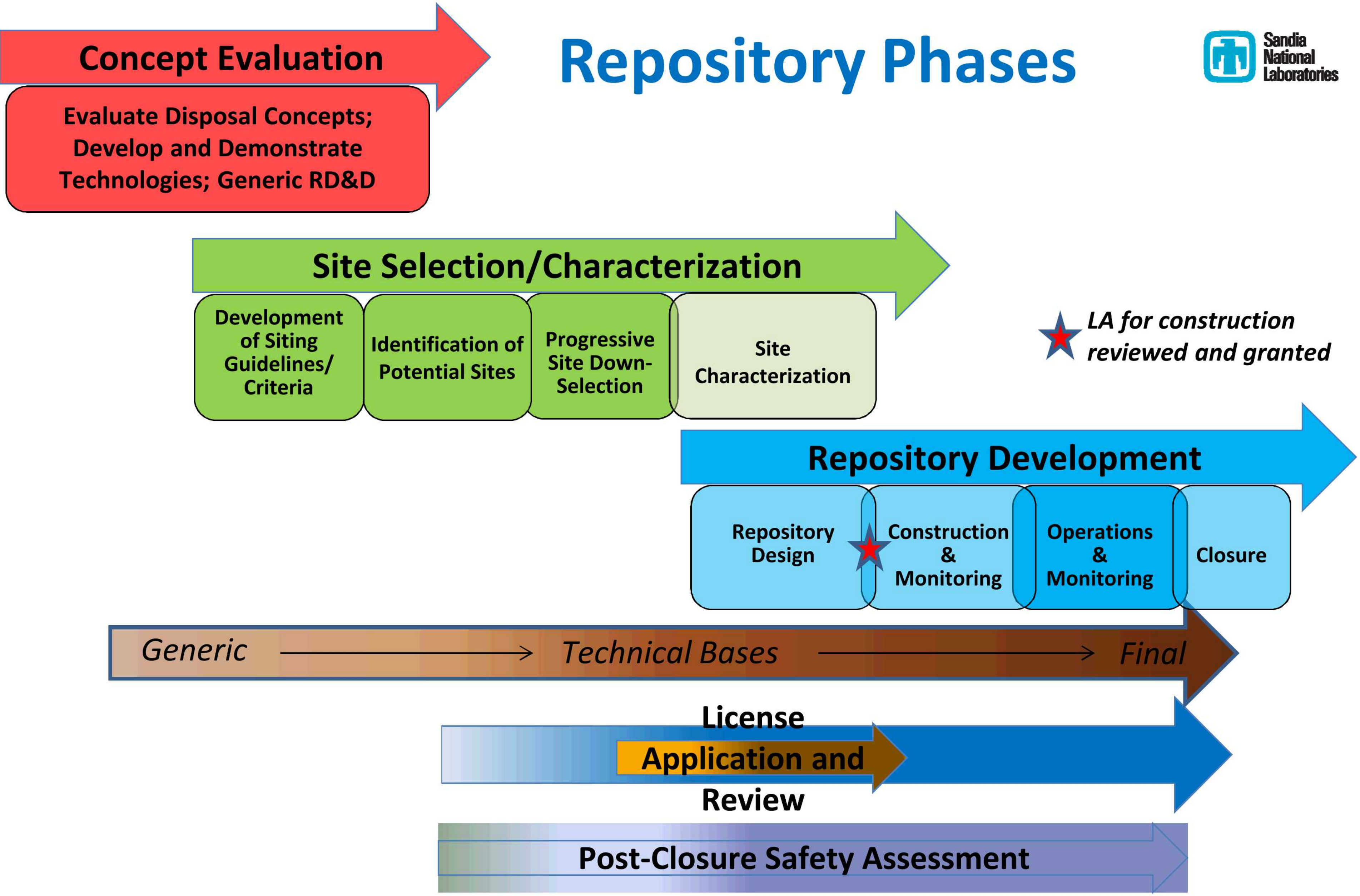


Figure Source: https://www.cnsc-ccsn.gc.ca/eng/waste/high-level-waste/cnsc-role-in-nwmo-apm-project/index.cfm



Repository Phases



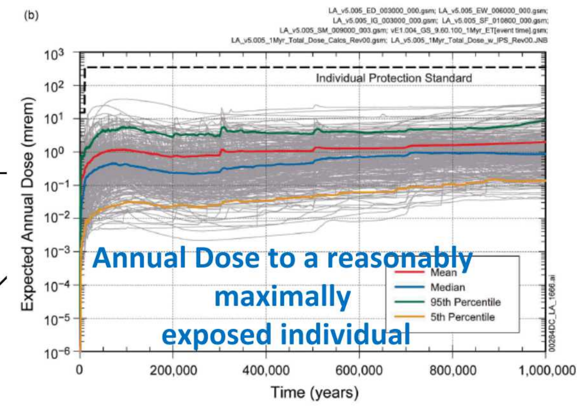
Elements of Performance Assessment

Biosphere
- Dilution
- Irrigation
- Water Consumption
- Dose Conversion Factors

Repository Design
- Location and layout
- No. and type of WPs
- EBS and Seals
- Thermal Loading and Ventilation

Near Field (EBS + DRZ)
- EBS Evolution
- DRZ Evolution
- Chemical Interactions
- Thermal Effects
- Mechanical Effects
- Flow and Transport

Performance Goal



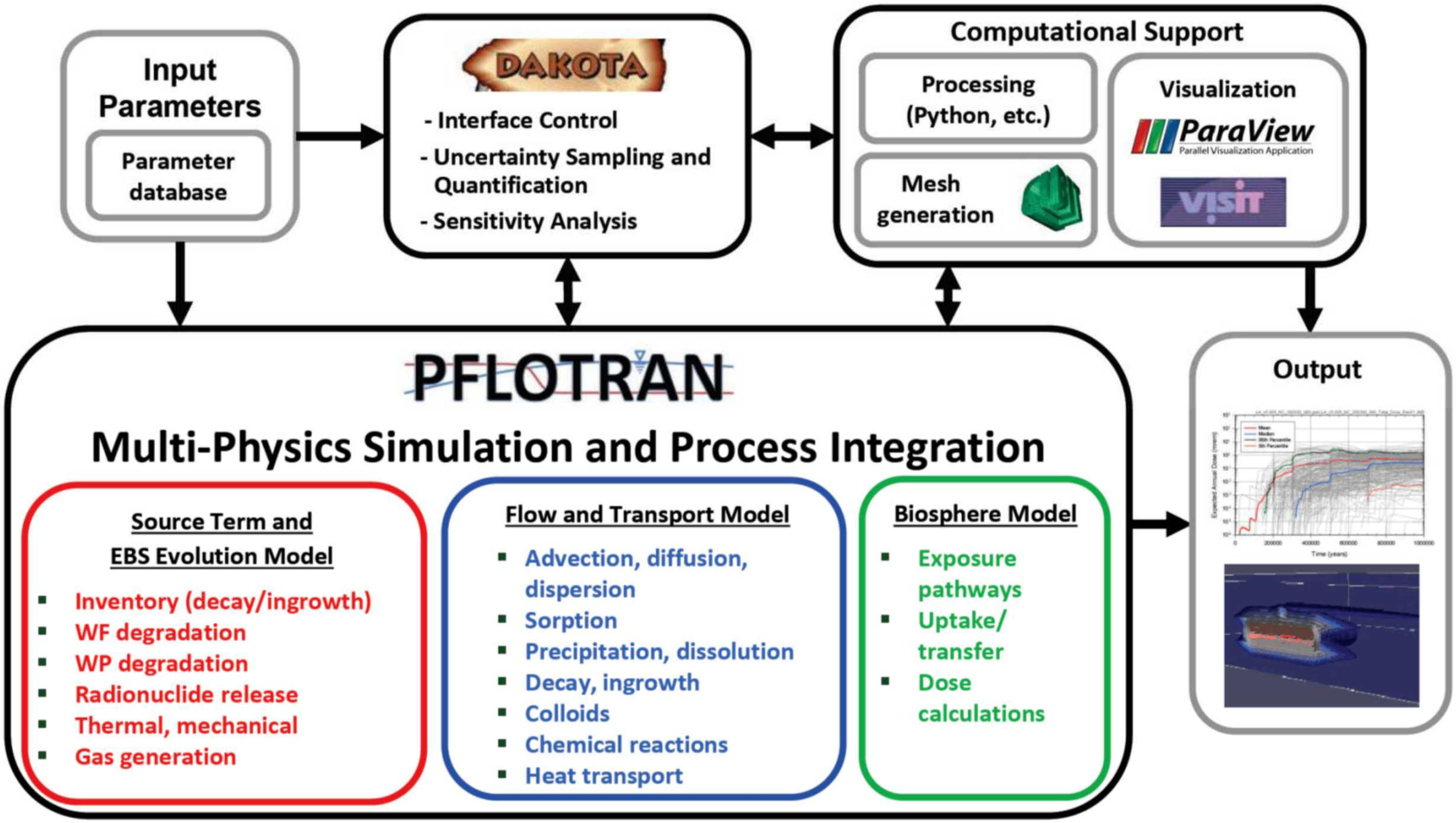
Source Term
- RN Inventory
- WF Degradation
- WP Degradation
- Gas Generation
- RN Release

Far Field
- Flow and Transport
- Sorption
- RN Decay and Ingrowth

Natural System
- Climate
- Stratigraphy
- Hydrogeology
- Geochemistry
- Material properties
- Disruptive events

Engineered Barrier System (EBS)
Radionuclide (RN)
Waste Form (WF)
Waste Package (WP)
Disturbed Rock Zone (DRZ)

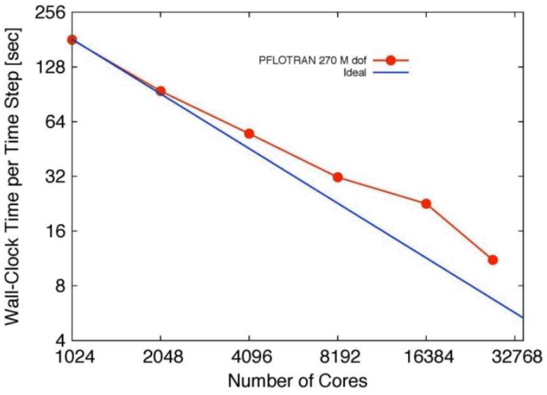
GDSA Framework



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

PFLOTRAN Development Timeline

2000 2002 2004 2006 2008 2010 2012 2014 2016 2018 2020

First release

SciDAC-funded rewrite

Process model refactor

Peter Lichtner

Glenn Hammond

Richard Mills

Chuan Lu

Jitu Kumar

Gautam Bisht

Satish Karra

Ben Andre

Nate Collier

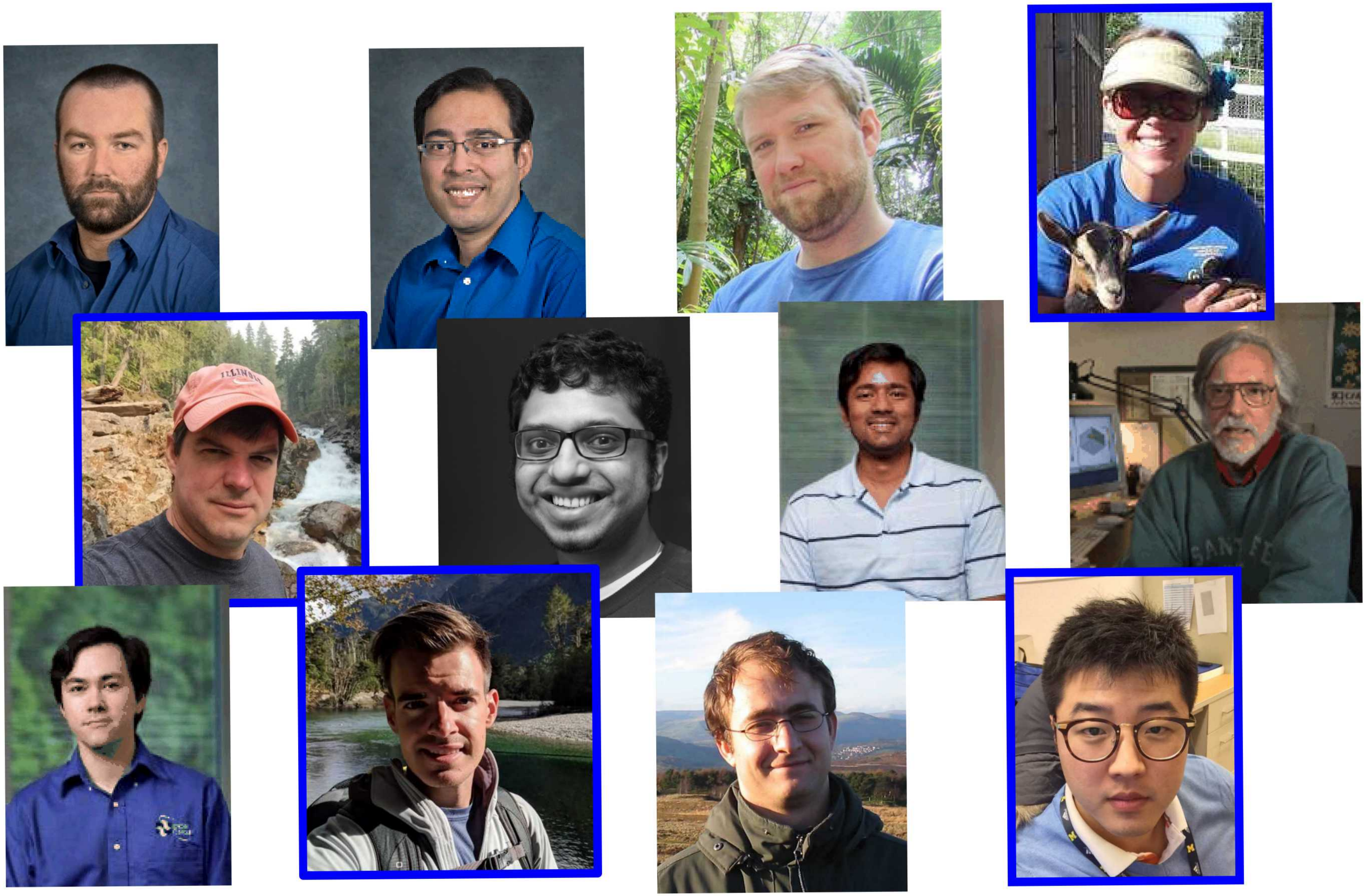
Heeho Park

Paolo Orsini

Jennifer Frederick

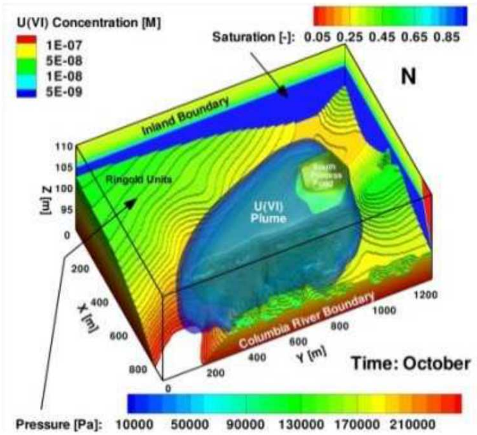
Michael Nole

PFLOTRAN Developers



Application of PFLOTRAN

- Nuclear waste disposal
  - Waste Isolation Pilot Plant (WIPP) in Carlsbad, NM
  - US DOE NE Spent Fuel and Waste Science and Technology (SFWST)
  - 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
- Oil & Gas (OpenGoSim.com)
- CO_2 sequestration
- Enhanced geothermal energy
- Radioisotope tracers

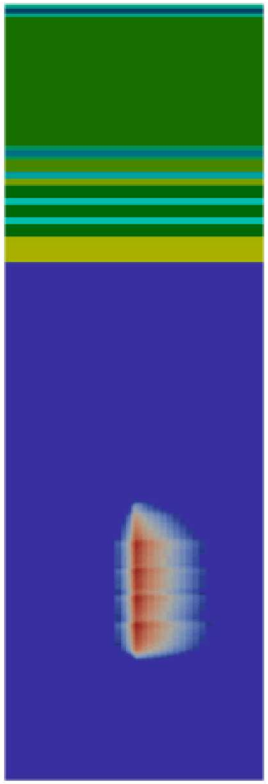


Hammond and Lichtner, WRR, 2010

Discretization and Numerical Methods

- Spatial discretization
  - Finite volume (2-point flux default)
  - Structured and unstructured grids
- Time discretization: fully-implicit backward Euler
- Nonlinear solver
  - Newton-Raphson
  - Line search/damping with custom convergence criteria
- Linear solver: direct (LU) or iterative (BiCGStab)
- Multi-physics coupling
  - Flow and transport/reaction: sequential
  - Transport and reaction: global implicit
  - Geomechanics and flow/transport: sequential

Deep Borehole Waste Disposal

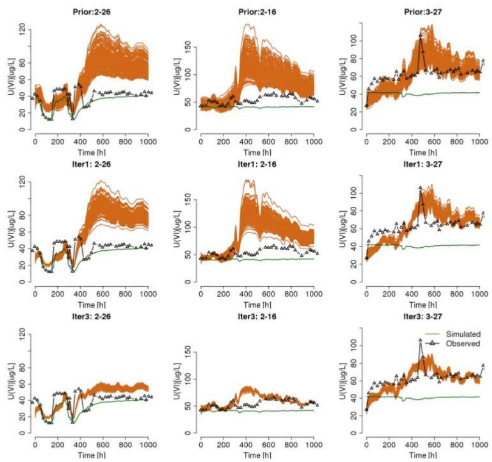


Emily Stein, SNL, 2015

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



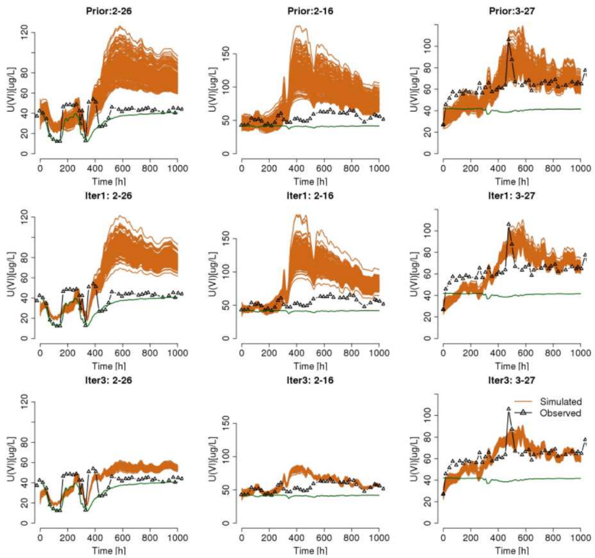
Xingyuan Chen, PNNL, 2011

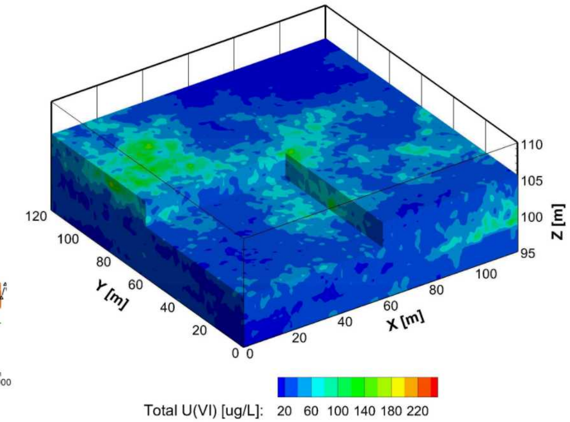
Benefits of Massively Parallel HPC

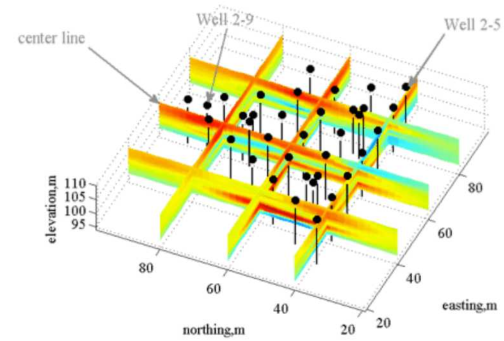
Sandia National Laboratories

Data Assimilation at the Hanford 300 Area (Xingyuan Chen, 2011)

- Problem domain:
  - 120×120×15m
  - $\Delta x, \Delta y, \Delta z$ = 1,1,0.5 m
  - 432K grid cells
  - 15 chemical species
  - 6.48M dofs total
- 1-2 month simulation:
  - Δt = 1 hour
- Computing, e.g.
  - 128 cores (single realization)
  - 64,000 cores (500 realizations)
  - 1 hour wallclock runtime
  - ~7 cpu years







Open Source Development

- Open source software refers to code that:
  - Free
  - Publicly available
  - Legally modified
  - Legally shared with anyone
- PFLOTRAN: GNU Lesser General Public License (LGPL).
  - The original or modified source may not be sold for profit.
  - Third-party software linked to or wrapped around PFLOTRAN (e.g. graphical user interfaces [GUIs], pre-/post-processing tools, etc.) may be proprietary.

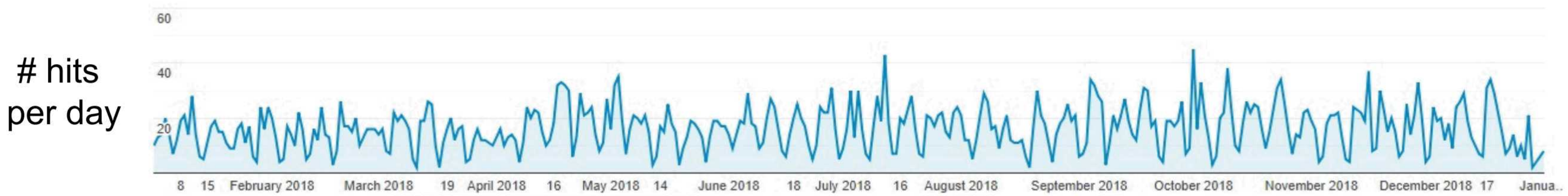
Benefits of Open Source

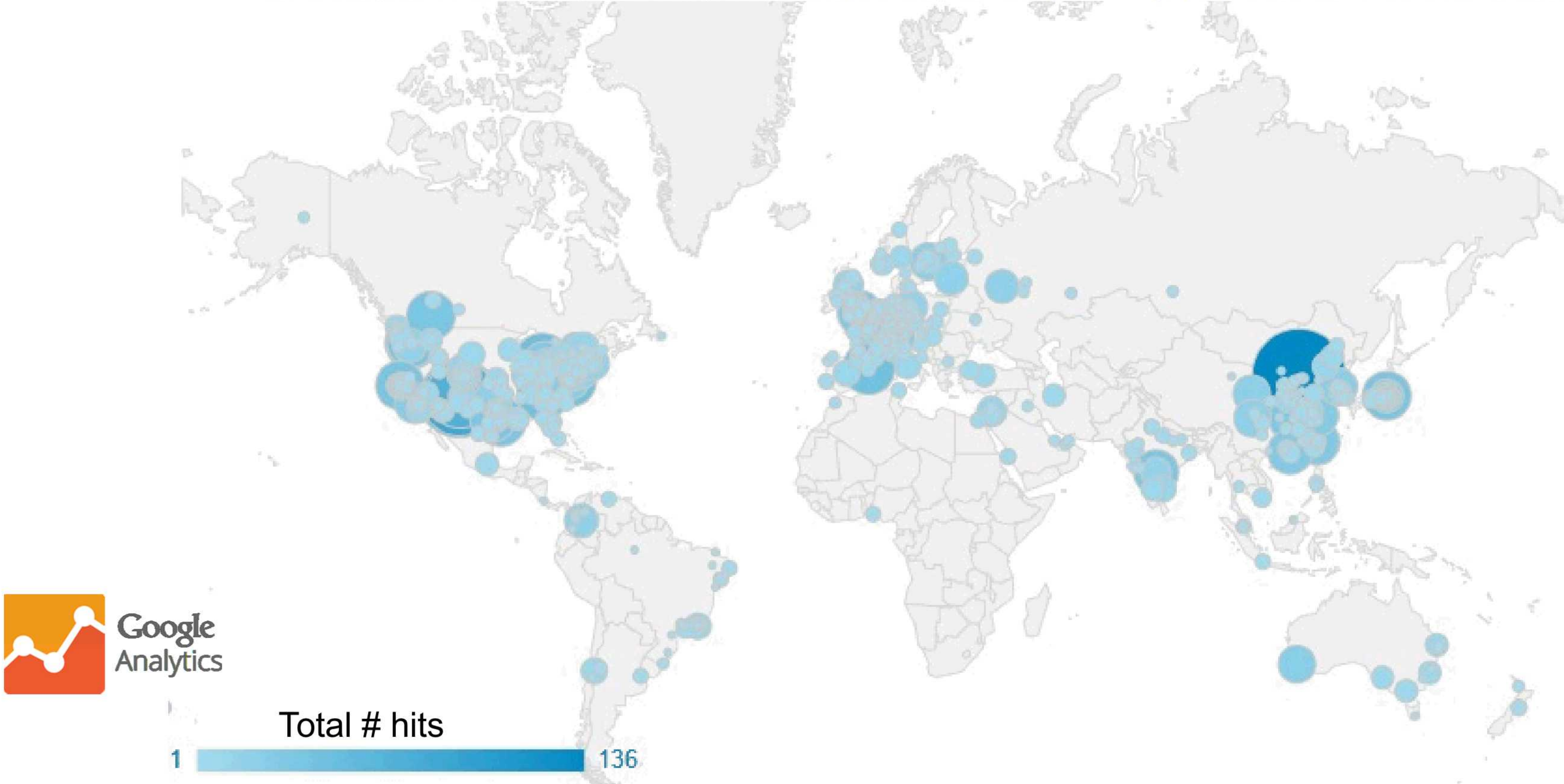
- Encourages collaboration
  - Development
  - Testing
  - Debugging
- Transparency exposes implementation details critical to scientific reproducibility, but excluded by journal publications.
- More optimal use of funding
  - Funding pooled across diverse set of projects/budgets.
  - What would have been spent on licensing fees can be redirected toward development.
  - Infinite benefit to those unfunded
- The most fit codes tend to survive (natural selection)
- The open source community can drive the code to evolve beyond the original vision (evolution).

PFLOTRAN Support Infrastructure

- www.pflotran.org: documentation and overview
- Git: distributed source control management tool
- Bitbucket: online PFLOTRAN repository
  - git clone https://bitbucket.org/pflotran/pflotran
  - Source tree
  - Commit logs
  - Pull requests
  - Issue tracker
  - Wiki
    - Link to documentation.pflotran.org
      - Developer/Theory/User guides/QA/FAQ
- Quality Assurance is in progress
- Travis CI: automated building and testing (regression and unit)
- Google Groups: pflotran-users and pflotran-dev mailing lists
- Google Analytics: tracks behavior on Bitbucket

Hits on PFLOTRAN site in 2018



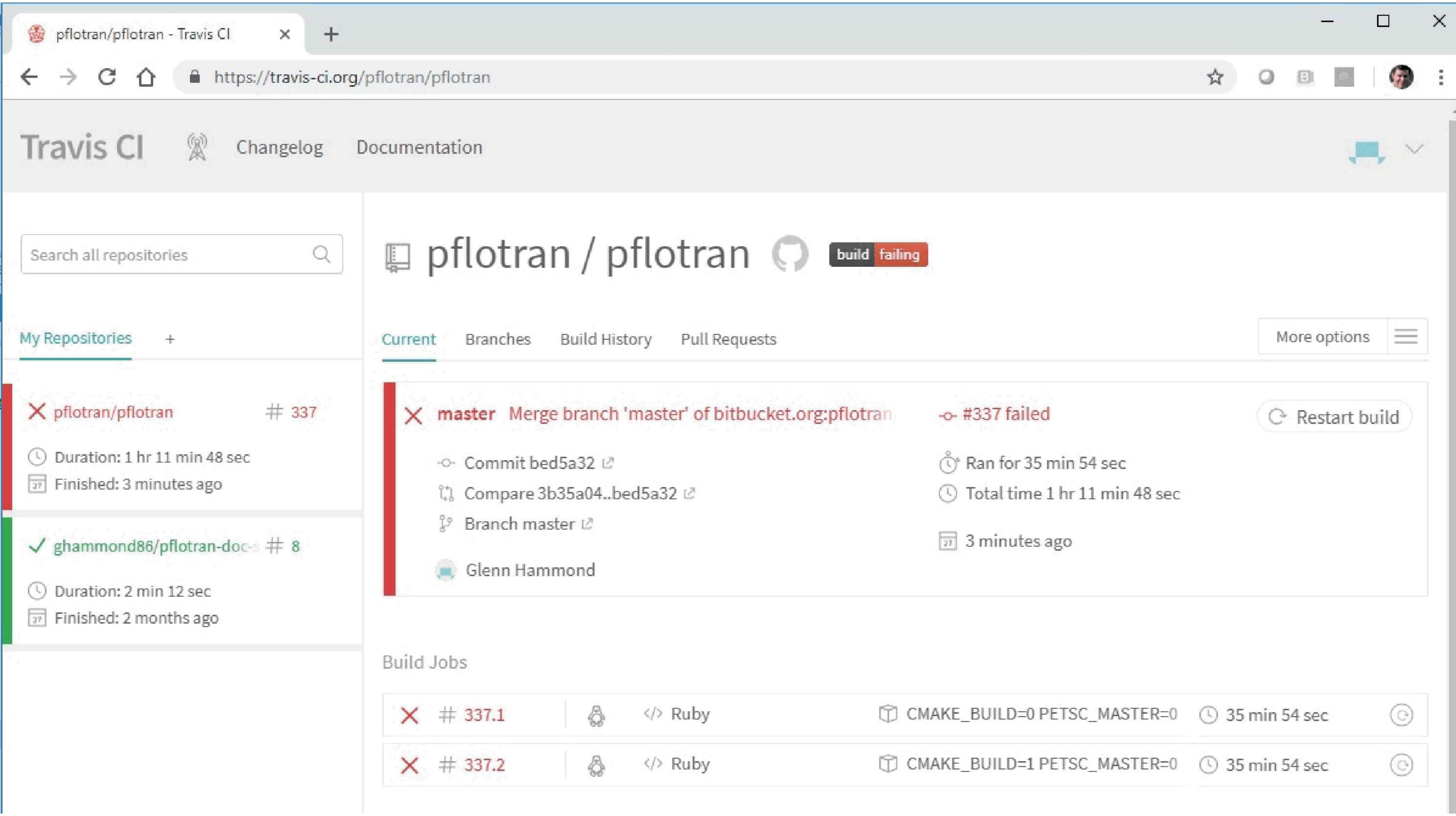


Travis CI Automated Build/Test

- Example test failure
  - Perturb critical pressure for water equation of state by 10 billionths of a percent

```
diff -r f9f01bbf557a src/pflotran/eos_water.F90
--- a/src/pflotran/eos_water.F90     Thu Jul 28 18:59:00 2016 -0700
+++ b/src/pflotran/eos_water.F90     Fri Jul 29 10:31:57 2016 -0700
@@ -893,6 +893,7 @@

   tc1 = H2O_CRITICAL_TEMPERATURE    ! K
   pc1 = H2O_CRITICAL_PRESSURE       ! Pa
+  pc1 = pc1 + 1.d-10*H2O_CRITICAL_PRESSURE ! perturb by 1e-10
   vc1 = 0.00317d0  ! m^3/kg
   utc1 = one/tc1   ! 1/C
   upc1 = one/pc1   ! 1/Pa
```

Travis CI: Build/Test Failed



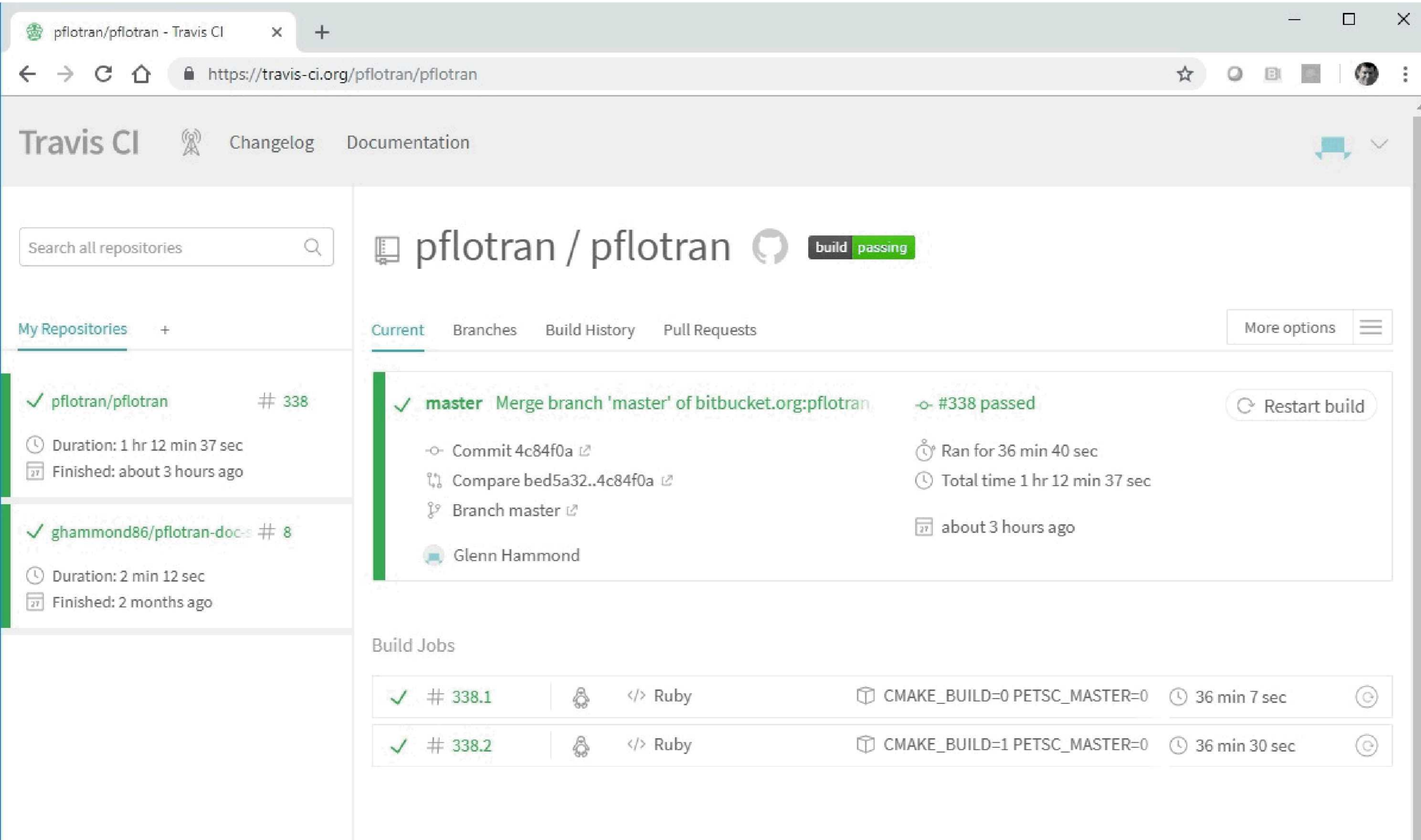
PFLOTRAN Unit/Regression Test Output

```
Running pflotran unit tests :
....................................F.......................
Time:         0.006 seconds

 Failure in: testEOSWater_DensitySTP
   Location: [test_eos_water.pf:157]
expected: +998.3234 but found: +998.3234;     difference: |+0.4774847E-11| >
tolerance:+0.1000000E-15.

 FAILURES!!!
Tests run: 60, Failures: 1, Errors: 0
----------------------------------------------------------------------


  Test log file : pflotran-tests-2018-09-25_17-01-20.testlog
Running pflotran regression tests :
.................F.F....FFFFF.....F...........F........F..FF.FFF.FF......FF......
F........................F...FFFF....FFFFFF................F.F.F...FF............
.F...............FF.............F..F.............................................
............FF..F........FF...........................
----------------------------------------------------------------------
Regression test summary:
    Total run time: 279.741 [s]
    Total tests : 297
    Tests run : 297
    Failed : 46
```

pflotran-tests-2018-09-25_17-01-20.testlog

```
543_hanford_srfcplx_param...
    cd /home/travis/build/pflotran/pflotran/regression_tests/default/543
    /home/travis/build/pflotran/pflotran/src/pflotran/pflotran -malloc 0
      -successful_exit_code 86 -input_prefix 543_hanford_srfcplx_param
    # 543_hanford_srfcplx_param : run time : 3.11 seconds
    diff 543_hanford_srfcplx_param.regression.gold
543_hanford_srfcplx_param.regression
    FAIL: LIQUID VELOCITY [m/d]:1 : 1.084136795e-11 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:31 : 7.3779567027e-12 > 1e-12 [relative]
    FAIL: LIQUID VELOCITY [m/d]:29 : 2.25552127701e-12 > 1e-12 [relative]
    ...
    FAIL: UO3.2H2O SI:Min : 4.38503889665e-12 > 1e-12 [relative]
    FAIL: UO2(PO3)2 SI:Min : 4.39851271218e-12 > 1e-12 [relative]
    FAIL: UO2SO4 SI:Min : 4.38535476851e-12 > 1e-12 [relative]
    FAIL: Torbernite SI:Min : 8.80326710311e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2.4H2O SI:Min : 1.31617137493e-11 > 1e-12 [relative]
    FAIL: UO2CO3 SI:Min : 4.38491638053e-12 > 1e-12 [relative]
    FAIL: UO3.0.9H2O(alpha) SI:Min : 4.37498338731e-12 > 1e-12 [relative]
    FAIL: Metatorbernite SI:Min : 8.79872832628e-12 > 1e-12 [relative]
    FAIL: CaUO4 SI:Min : 4.36268114141e-12 > 1e-12 [relative]
    FAIL: (UO2)3(PO4)2 SI:Min : 1.31646122221e-11 > 1e-12 [relative]
    FAIL: UOF4 SI:Min : 4.40415950876e-12 > 1e-12 [relative]
    FAIL: Saleeite SI:Min : 8.8055591192e-12 > 1e-12 [relative]
    FAIL: Schoepite SI:Min : 4.38503889665e-12 > 1e-12 [relative]
543_hanford_srfcplx_param... failed.
```

Travis CI: Build/Test Success



PFLOTRAN Unit/Regression Test Output

```
Running pflotran unit tests :
............................................................
Time:         0.007 seconds

 OK
 (60 tests)
----------------------------------------------------------------------

Test log file : pflotran-tests-2018-09-25_17-52-05.testlog
Running pflotran regression tests :
.................................................................................
.................................................................................
.................................................................................
......................................................
----------------------------------------------------------------------
Regression test summary:
    Total run time: 266.636 [s]
    Total tests : 297
    Tests run : 297
    All tests passed.
```

PFLOTRAN Flow Modes

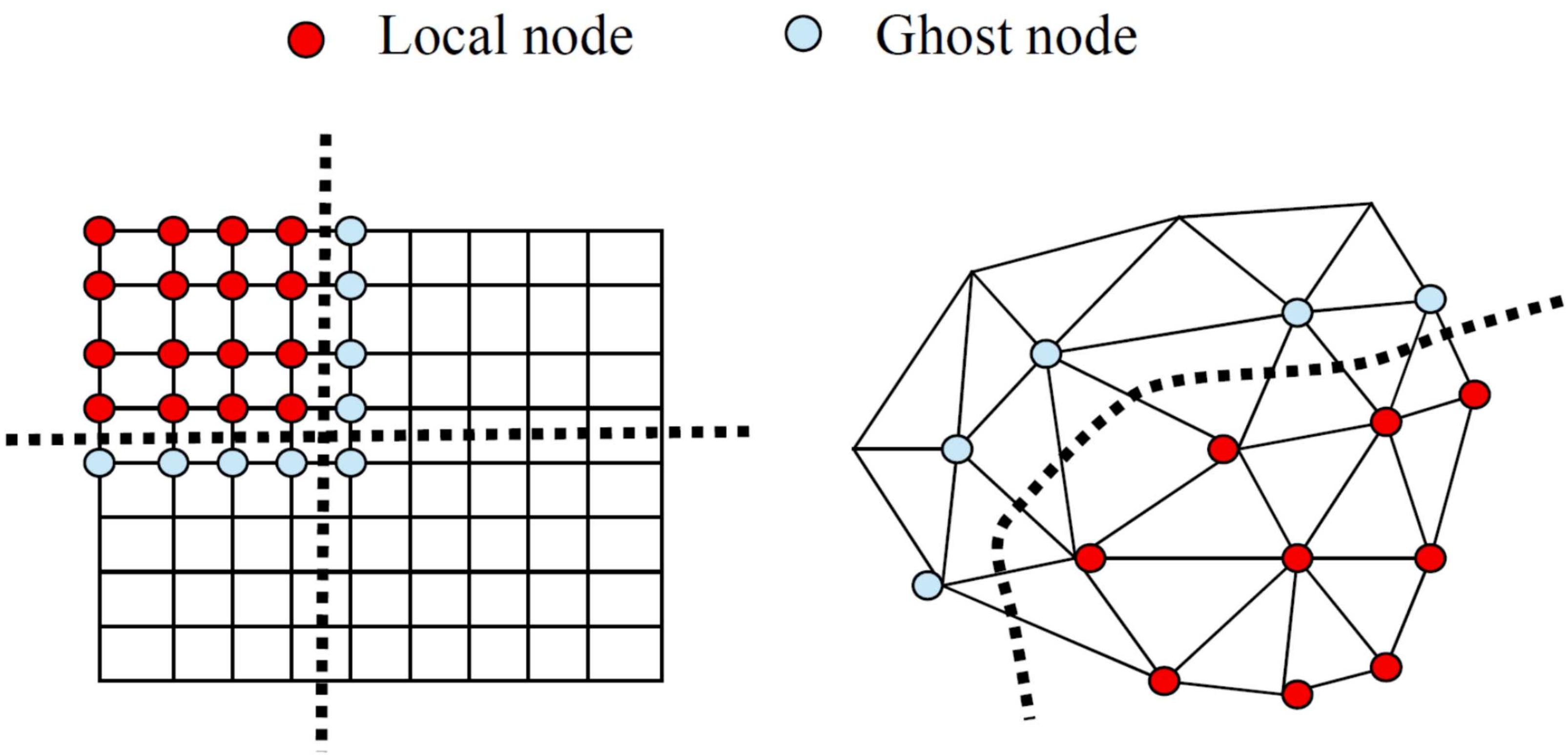
- RICHARDS: variably-saturated water
- TH: variably-saturated water-energy
- GENERAL: multiphase air-water-energy
- WIPP_FLOW: immiscible air-water
- MPHASE: supercritical CO2-water-energy
- FLASH2: supercritical CO2-water-energy (experimental)
- IMMIS: air-water (experimental)
- MISCIBLE: X-water-energy (experimental)
- TOIL_IMS: oil-water-energy (experimental)

PFLOTRAN Reactive Transport

- Transport
  - Multicomponent
  - Mobile/immobile primary species
  - Advection (upwinding)
  - Hydrodynamic dispersion
- Reaction
  - Aqueous speciation
    - Ion activity models
  - General (A + B ↔ C)
    - N^{th} order kinetics
    - Reversible
  - Mineral precipitation-dissolution
    - Prefactors
- Microbiological
  - Michaelis–Menten kinetics
  - Biomass
  - Inhibition
- Radioactive decay with daughter products
- Sorption
  - Isotherm-based: linear, Langmuir, Freundlich
  - Ion exchange
  - Surface complexation
    - Equilibrium
    - Kinetic / multirate kinetic
- Reaction Sandbox

Approach to Parallelization

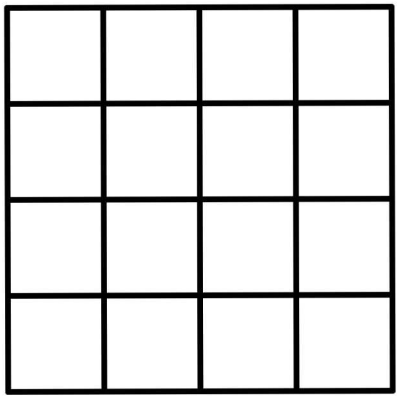
Domain Decomposition



Ghost node information used only in flux calculations.

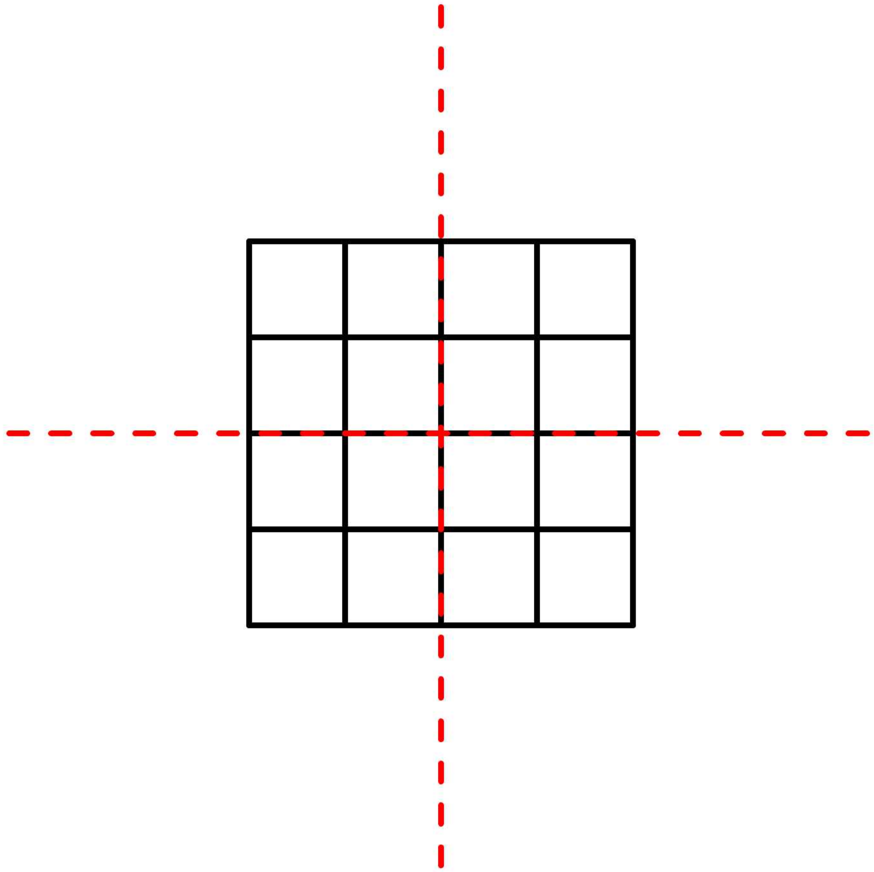
Domain Decomposition

Structured Grid Example



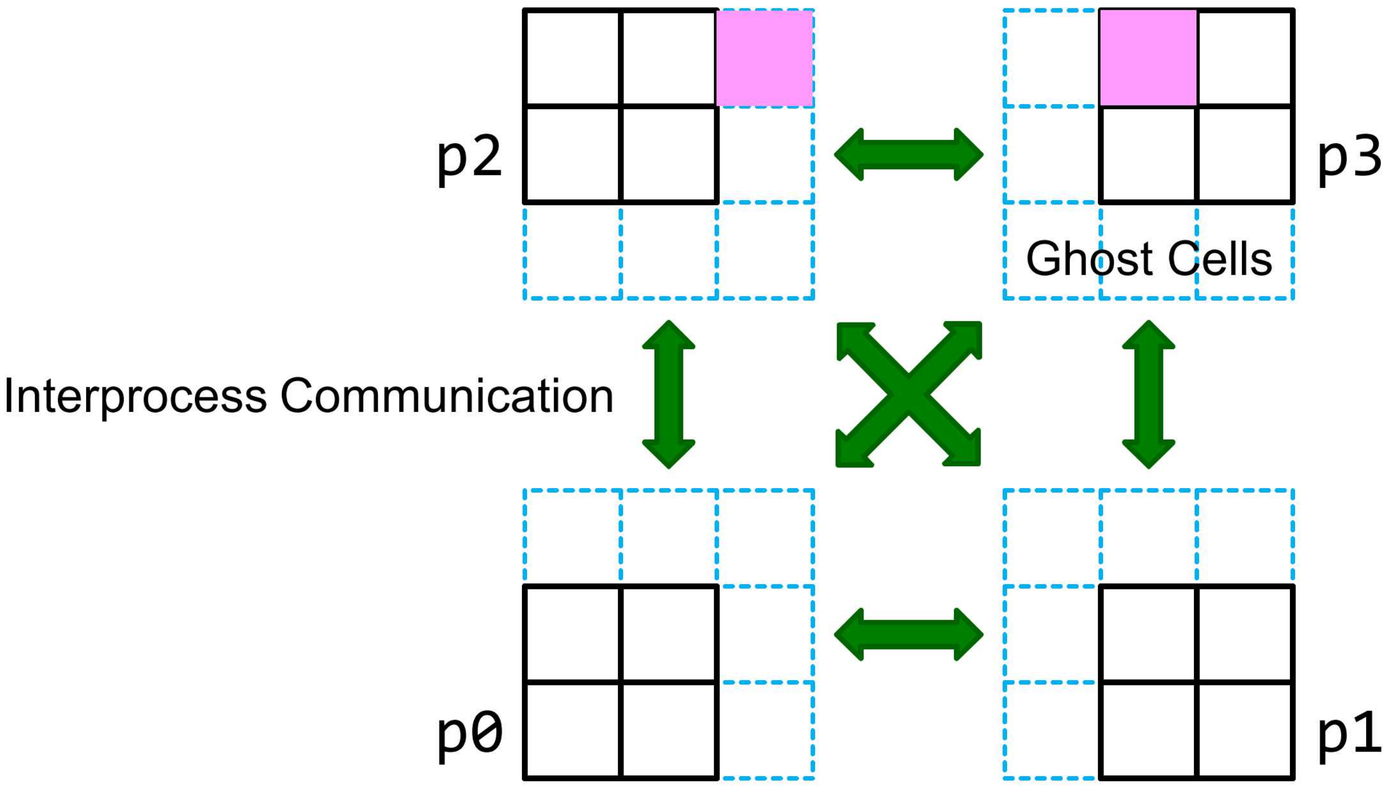
Domain Decomposition

Structured Grid Example



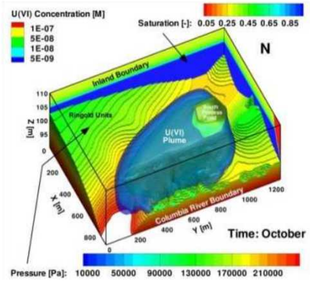
Domain Decomposition

Structured Grid Example

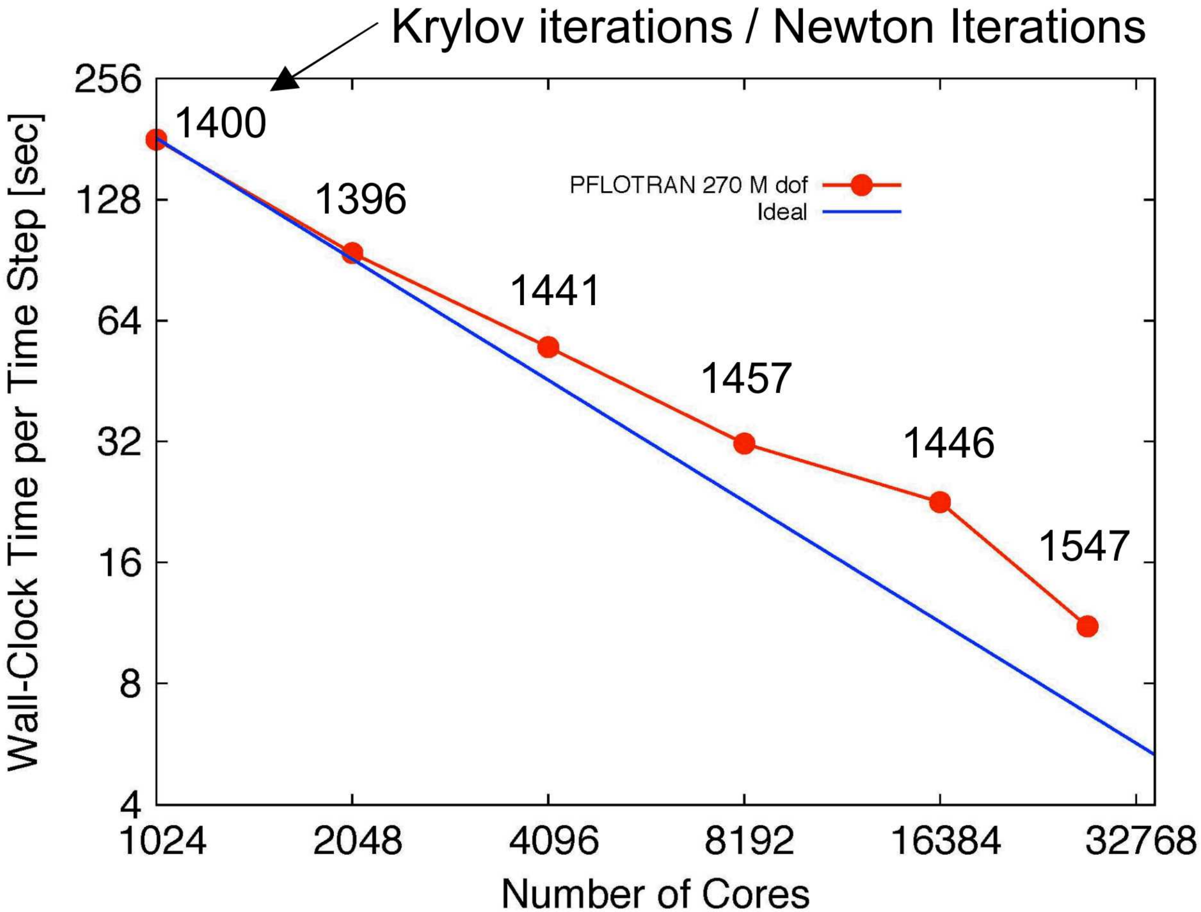


PFLOTRAN Parallel Performance

Hanford 300 Area



Hammond and Lichtner, WRR, 2010



Overall 60% efficient

Science

(1-2% of overall time)

- 75% efficient (wall clock)

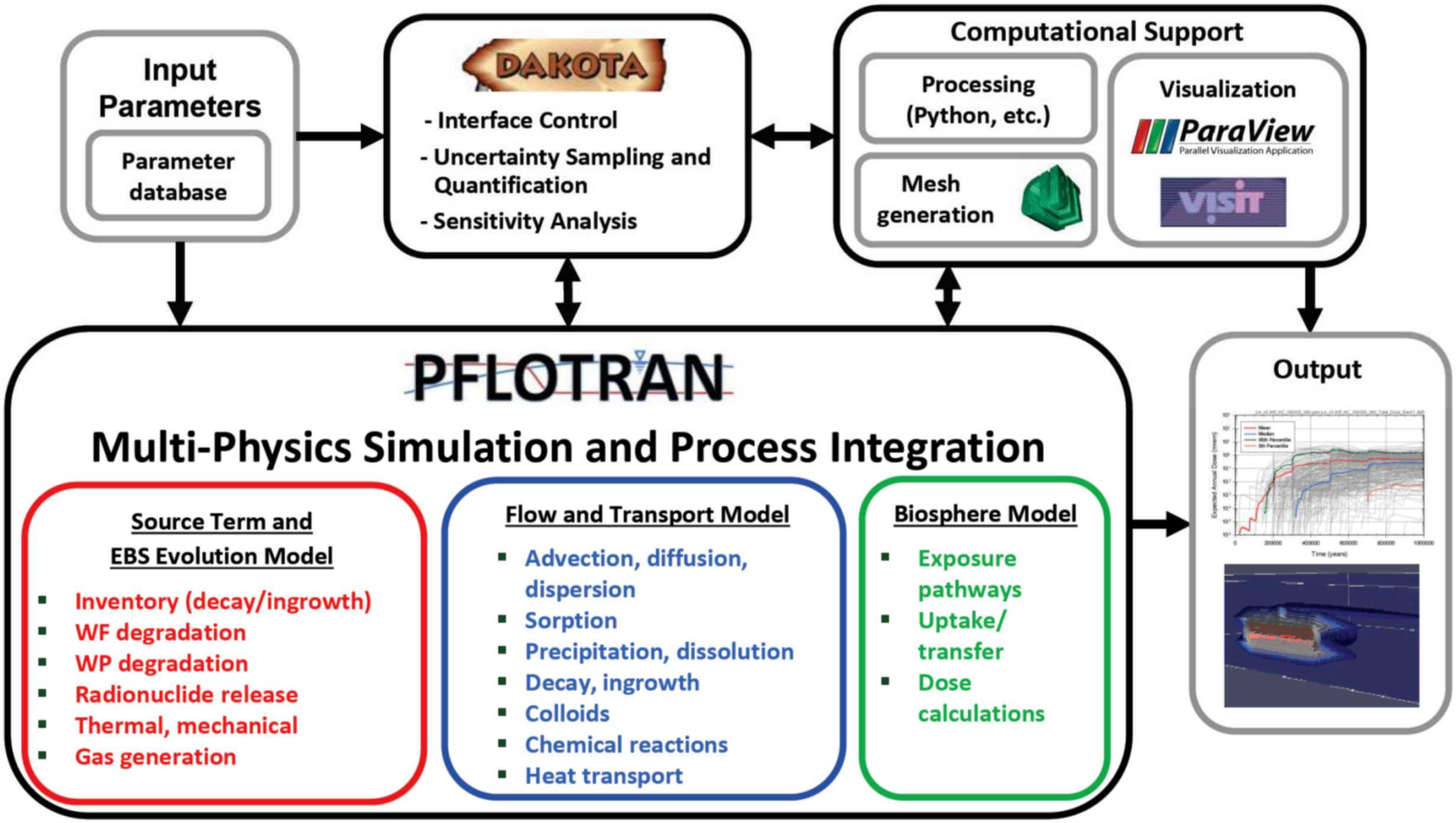
Solvers

(96% of overall time)

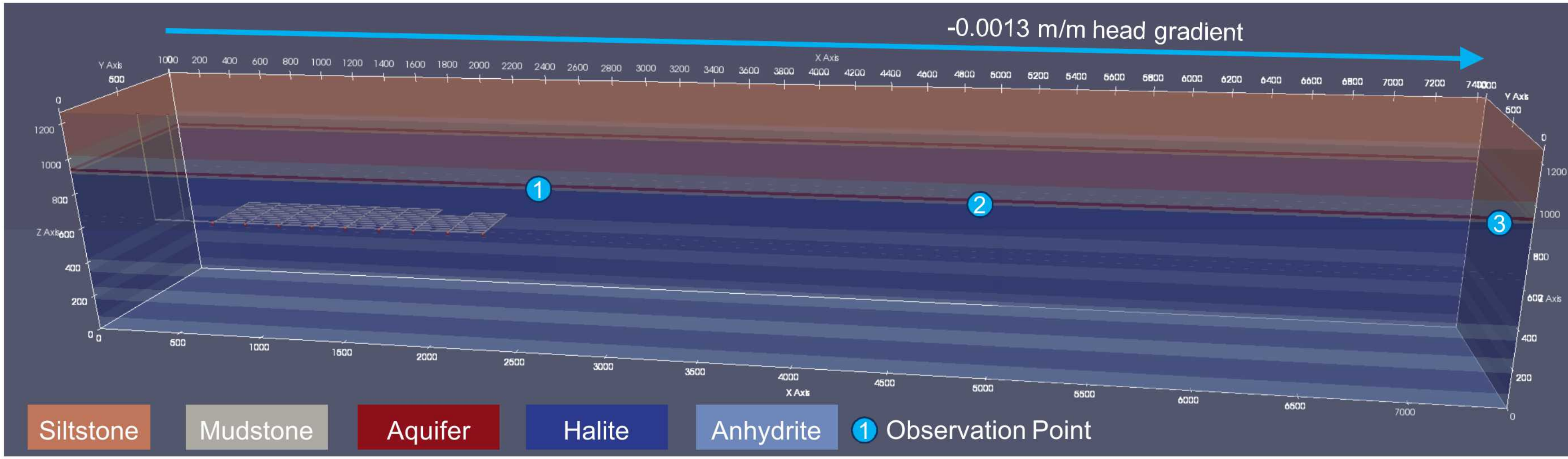
- 90% efficient (iteration count)
- 64% efficient (wall clock)

GDSA Framework

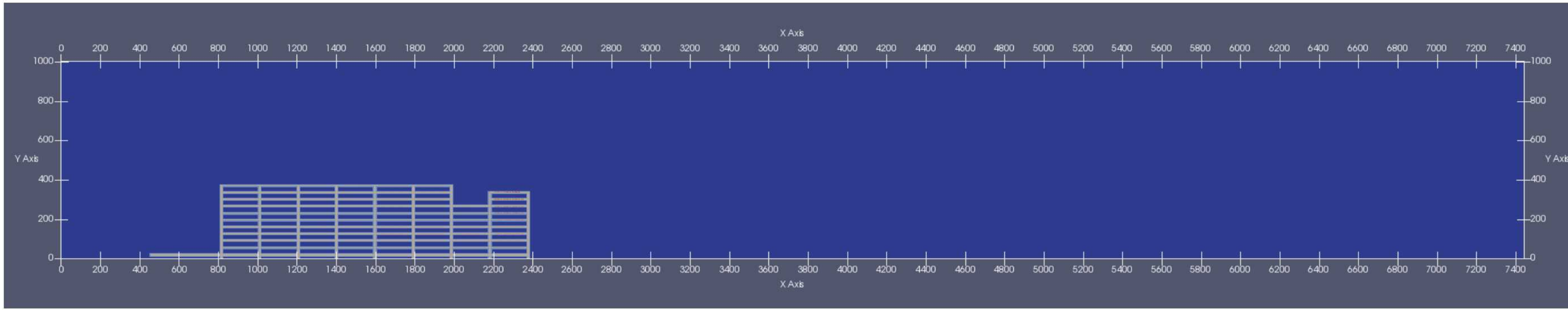
Geologic Disposal Safety Assessment – pa.sandia.gov



Generic Salt Repository



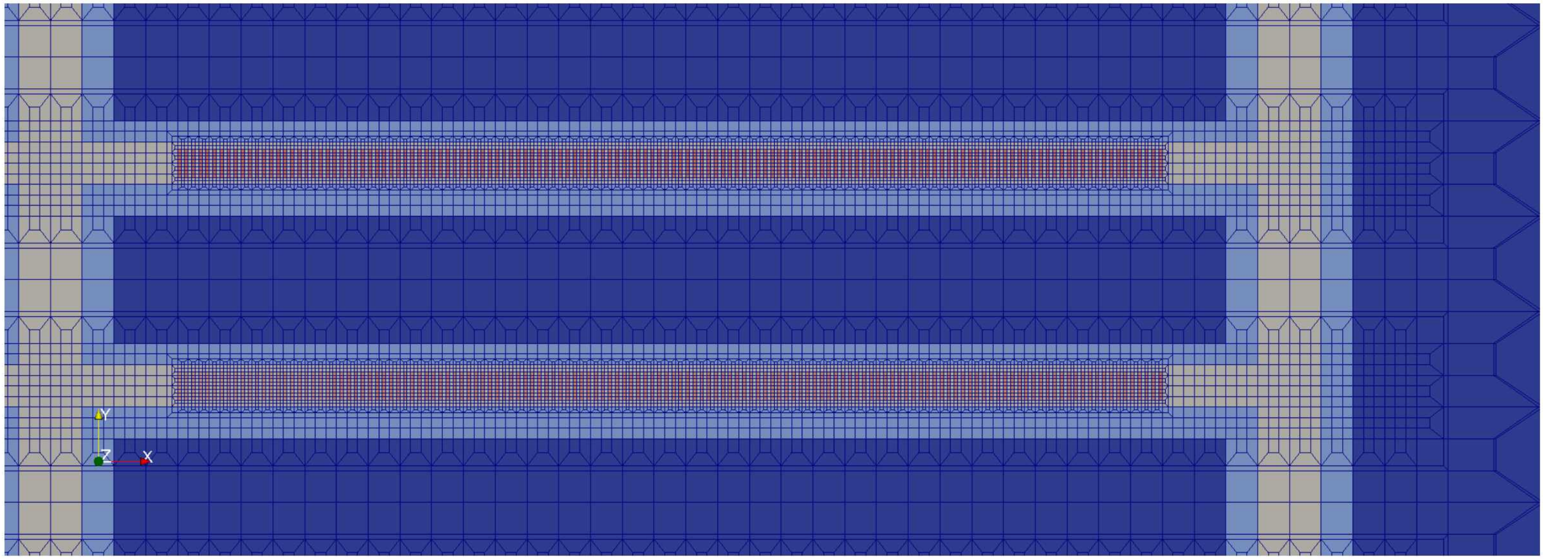
Horizontal Cross Section



Stein, E.R., S.D. Sevougian, G.E. Hammond, J.M. Frederick and P.E. Mariner, (2016) *Performance Assessment of a Generic Repository in Bedded Salt, AGU Fall Meeting, San Francisco CA. SAND2016-12457C*

Grid Refinement in Repository Rooms

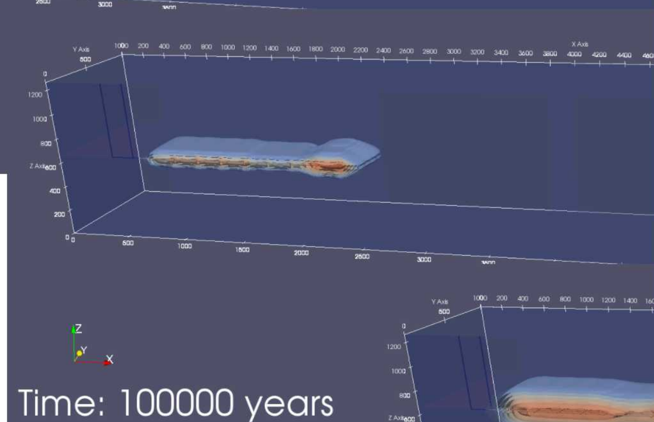
Sandia National Laboratories

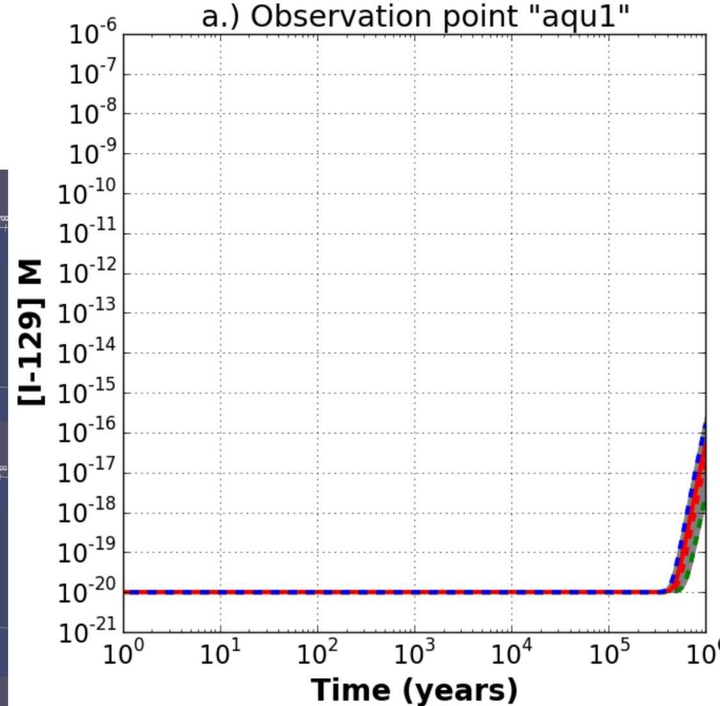


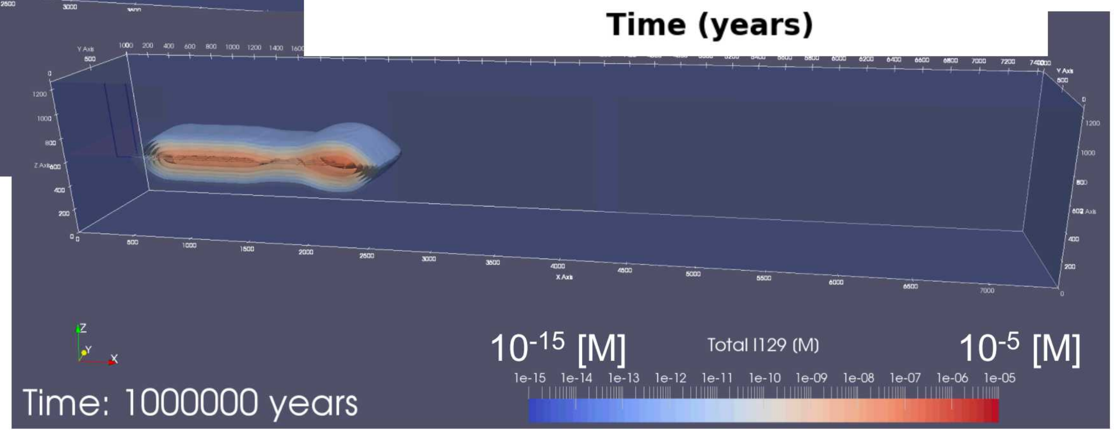
Undisturbed Halite	Disturbed Rock Zone (DRZ)	Crushed Salt Backfill	Waste Packages

Stein, E.R., S.D. Sevougian, G.E. Hammond, J.M. Frederick and P.E. Mariner, (2016) *Performance Assessment of a Generic Repository in Bedded Salt, AGU Fall Meeting, San Francisco CA. SAND2016-12457C*

I^{129} Concentration

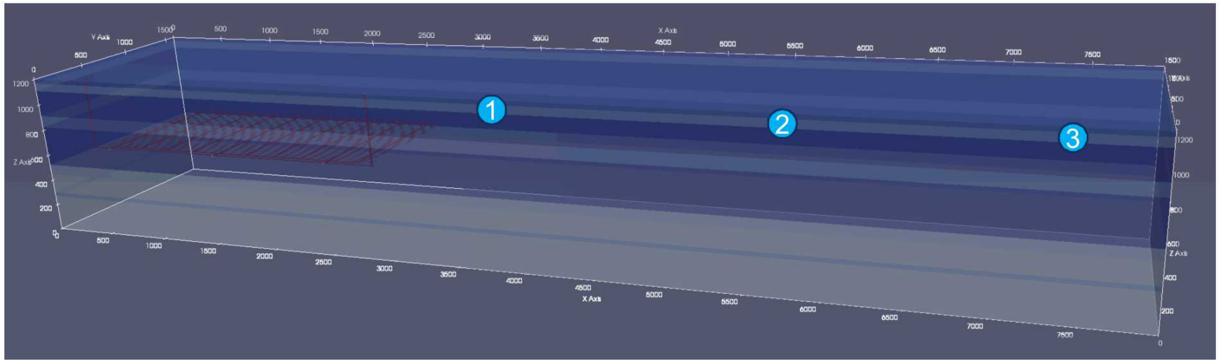






Stein, E.R., S.D. Sevougian, G.E. Hammond, J.M. Frederick and P.E. Mariner, (2016) *Performance Assessment of a Generic Repository in Bedded Salt, AGU Fall Meeting, San Francisco CA. SAND2016-12457C*

I^{129} Breakthrough in Argillite



Stein, ER., P.E. Mariner, G.E. Hammond, J.M. Frederick and S.D. Sevougian (2017) Generic Disposal System Analysis: Argillite Reference Case and Performance Assessment, Spent Fuel and Waste Science and Technology Working Group, May 23-25, Las Vegas, NV. SAND2017-5450 PE