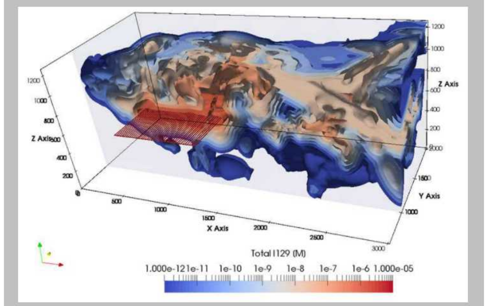
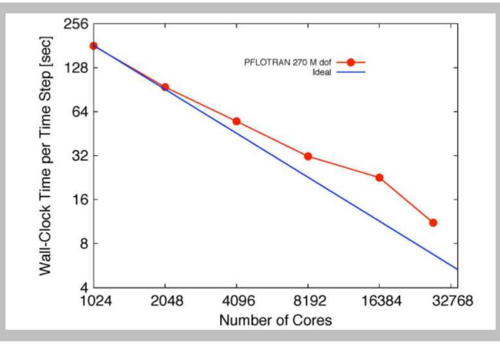
SAND2018-11088PE

$$\frac{\partial m_a}{\partial t} = -\nabla \cdot \left(\rho_l X_a^l \boldsymbol{q}_l + \rho_g X_a^g \boldsymbol{q}_g + \boldsymbol{J}_a^l + \boldsymbol{J}_a^g\right) + q_a^G,$$
$$\frac{\partial m_w}{\partial t} = -\nabla \cdot \left(\rho_l X_w^l \boldsymbol{q}_l + \rho_g X_w^g \boldsymbol{q}_g + \boldsymbol{J}_w^l + \boldsymbol{J}_w^g\right) + q_w^G,$$
$$\frac{\partial e}{\partial t} = -\nabla \cdot \left(\rho_l H_l \boldsymbol{q}_l + \rho_g H_g \boldsymbol{q}_g - \kappa_{\text{eff}} \nabla T\right) + q_e^G,$$





The Origins, Evolution and Applications of PFLOTRAN

Glenn Hammond

September 29, 2018

U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration

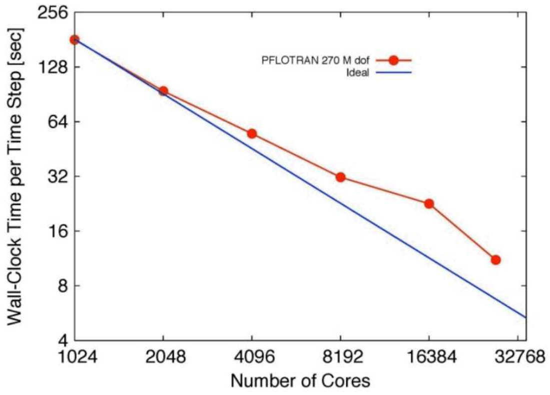
Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525. SAND NO. SAND2018-XXXX PE

Bio

- BS, Civil & Environmental Engineering, BYU, 1997
  - Gained programming experience developing GMS
- MS, Civil & Environmental Engineering, UIUC, 1999
  - Verification of the Kinetic Precipitation-Dissolution Reaction in the Finite Element Heat and Mass Transfer Code (FEHM)
- PhD, Civil & Environmental Engineering, UIUC, 2003
  - DOE Computational Science Graduate Fellow
  - Innovative Methods for Solving Multicomponent Biogeochemical Groundwater Transport on Supercomputers
- Sandia National Laboratories, Geohydrology, 2003-2005
- Pacific Northwest National Laboratory, Hydrology, 2005-2013
- Sandia National Laboratories, Applied Systems Analysis and Research, 2013-present

PFLOTRAN

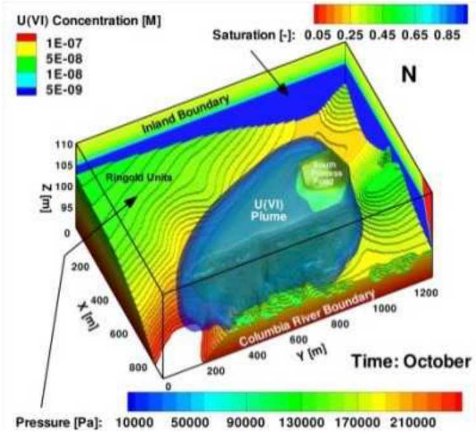
- Petascale reactive multiphase flow and transport code
- Open source license (GNU LGPL 2.0)
- Object-oriented Fortran 2003/2008
  - Pointers to procedures
  - Classes (extendable derived types with member procedures)



- 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
  - 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

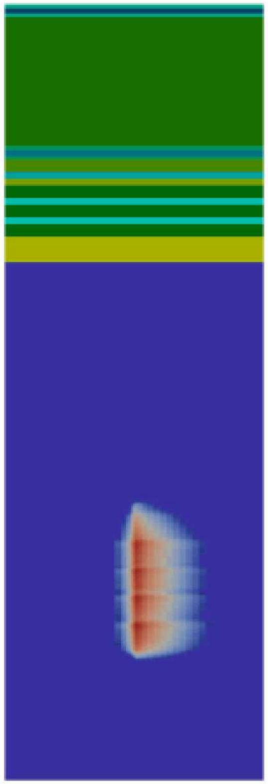


Hammond and Lichtner, WRR, 2010

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
  - Geophysics and flow/transport: sequential

Deep Borehole Waste Disposal

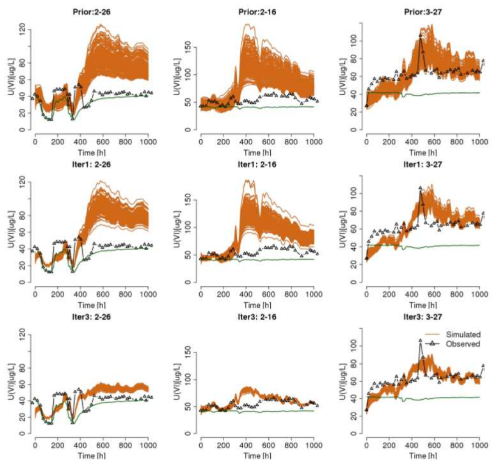


Emily Stein, SNL, 2015

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

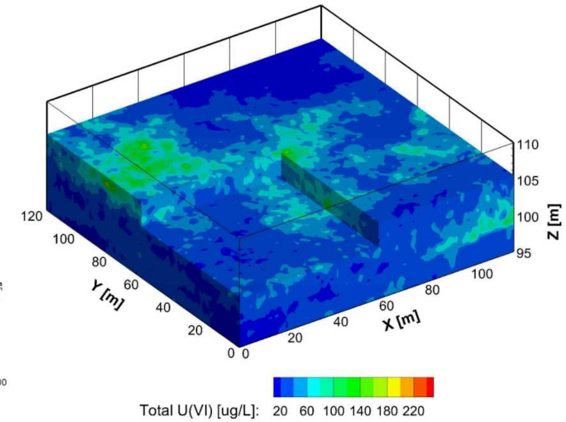


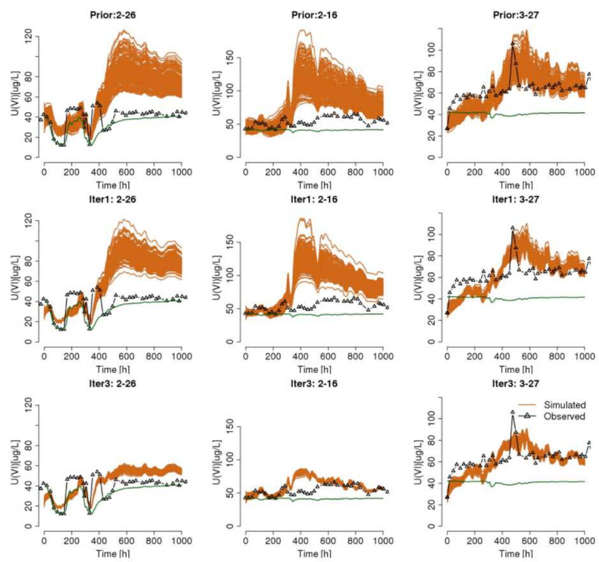
Xingyuan Chen, PNNL, 2011

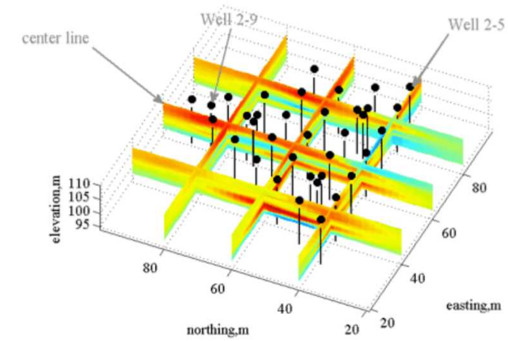
Benefits of Massively Parallel HPC

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

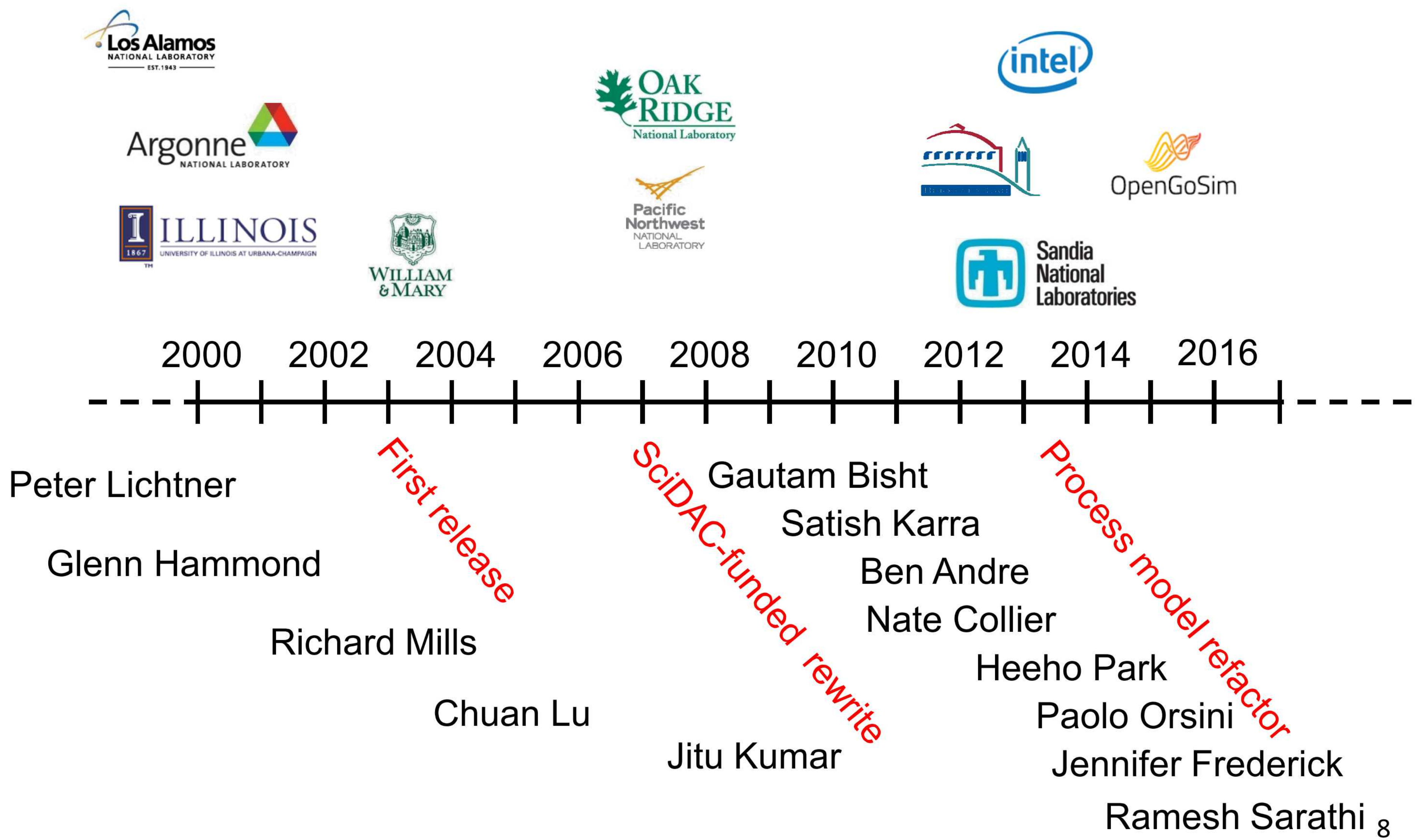
- Problem domain:
  - 120×120×15m
  - $\Delta x, \Delta y, \Delta z$ = 1,1,0.5 m
  - 432K grid cells
  - 15 chemical species
  - 6.48M dofs total
- 1-2 month simulation:
  - Δt = 1 hour
- Computing, e.g.
  - 128 cores
    (single realization)
  - 64,000 cores
    (500 realizations)
  - 1 hour wallclock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



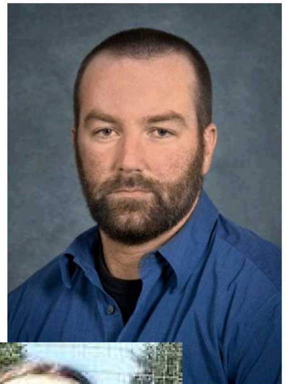




PFLOTRAN Development Timeline

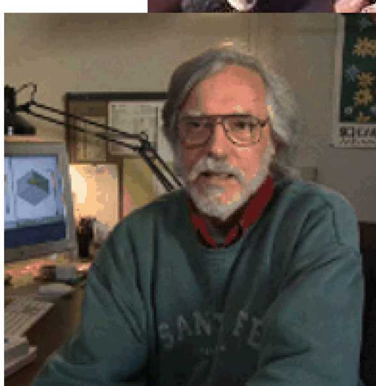
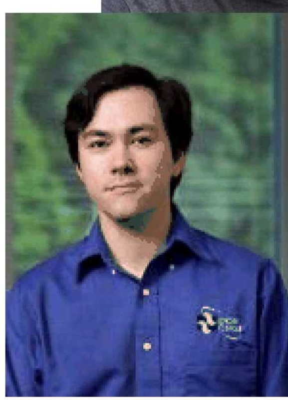


PFLOTRAN Developers



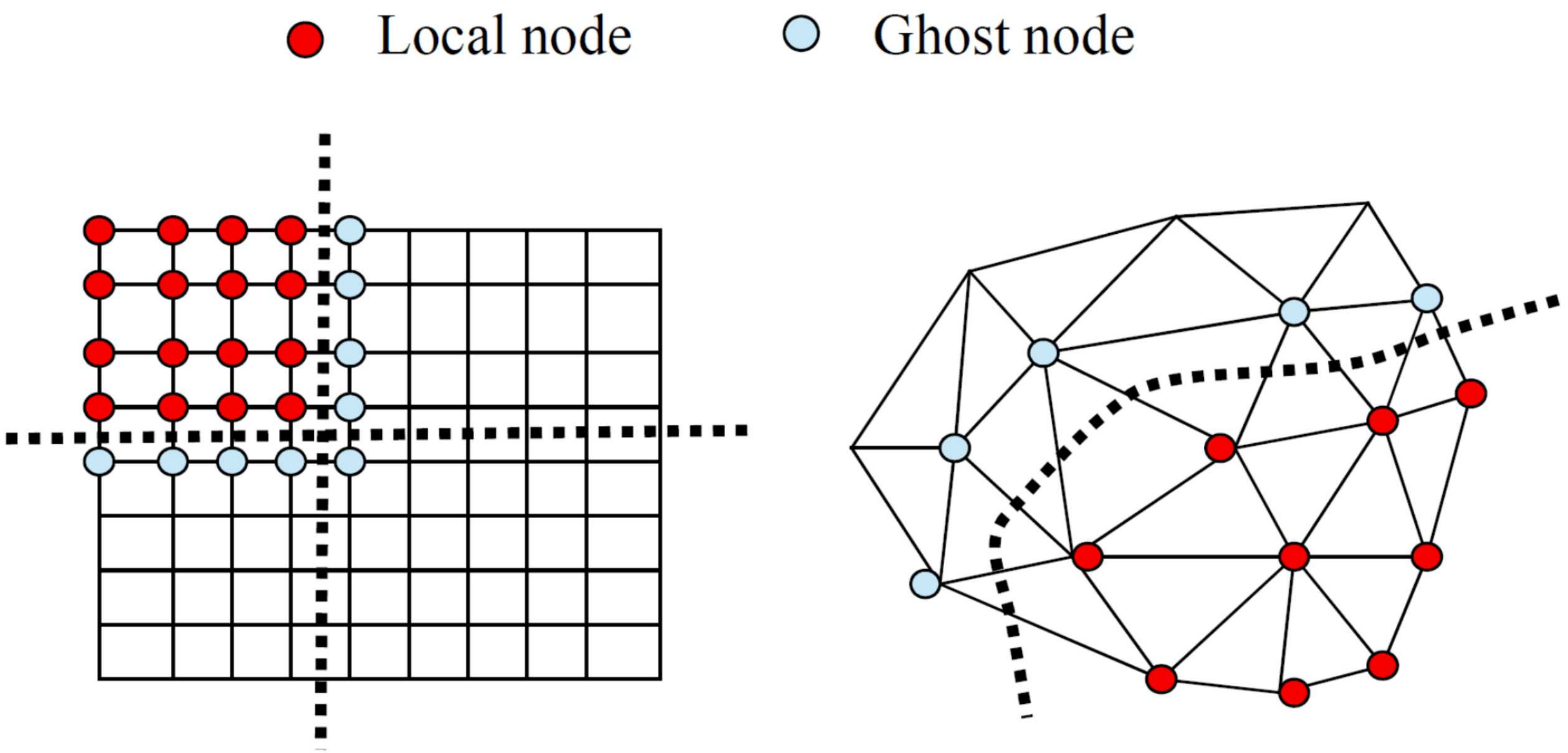




Approach to Parallelization

Domain Decomposition



Ghost node information used only in flux calculations.

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
      - FAQ (entries motivated by questions on mailing list)
- Travis CI: automated building and testing (regression and unit)
- Google Groups: pflotran-users and pflotran-dev mailing lists
- Google Analytics: tracks behavior on Bitbucket

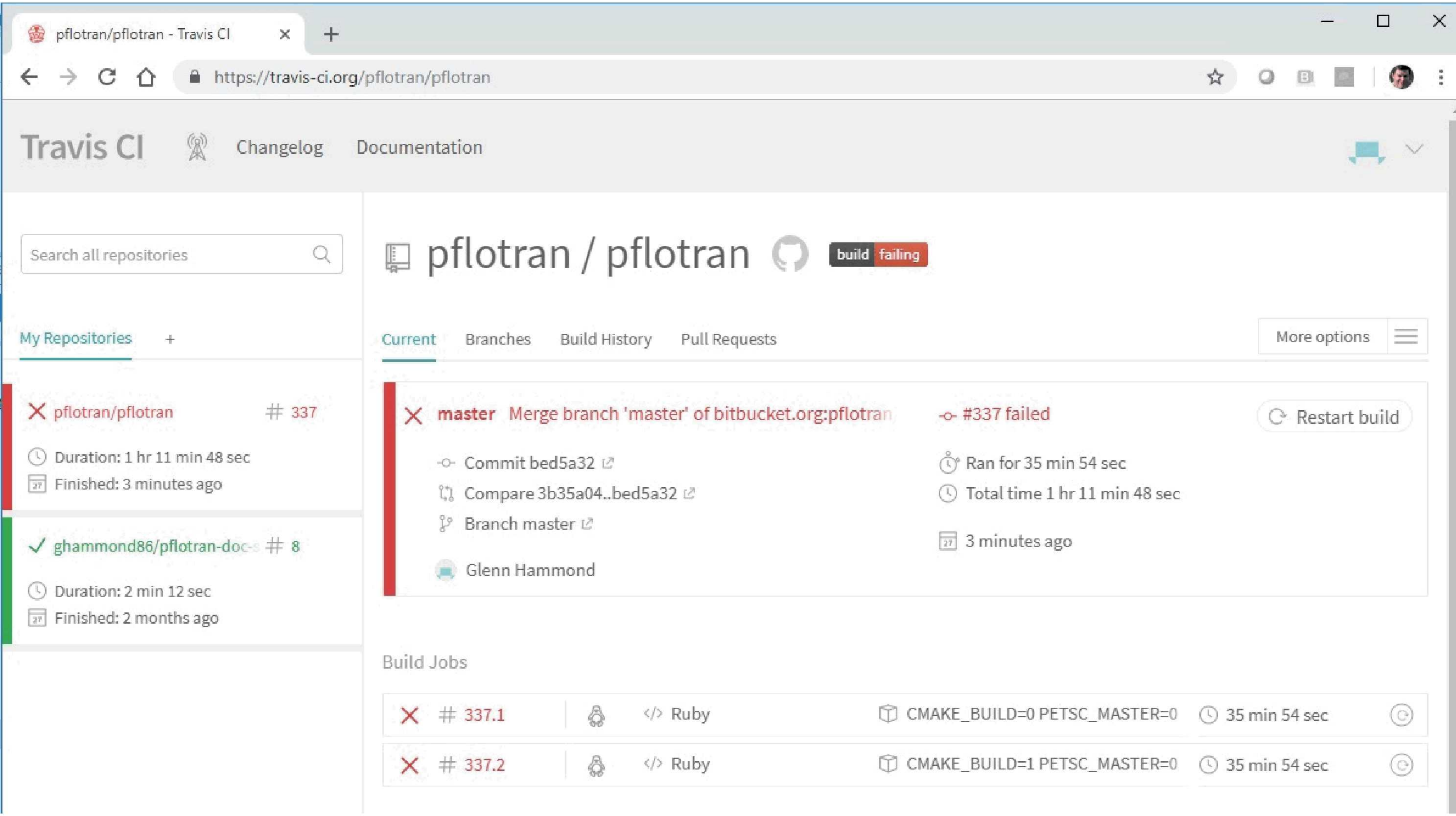
AUTOMATED BUILD-TEST

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



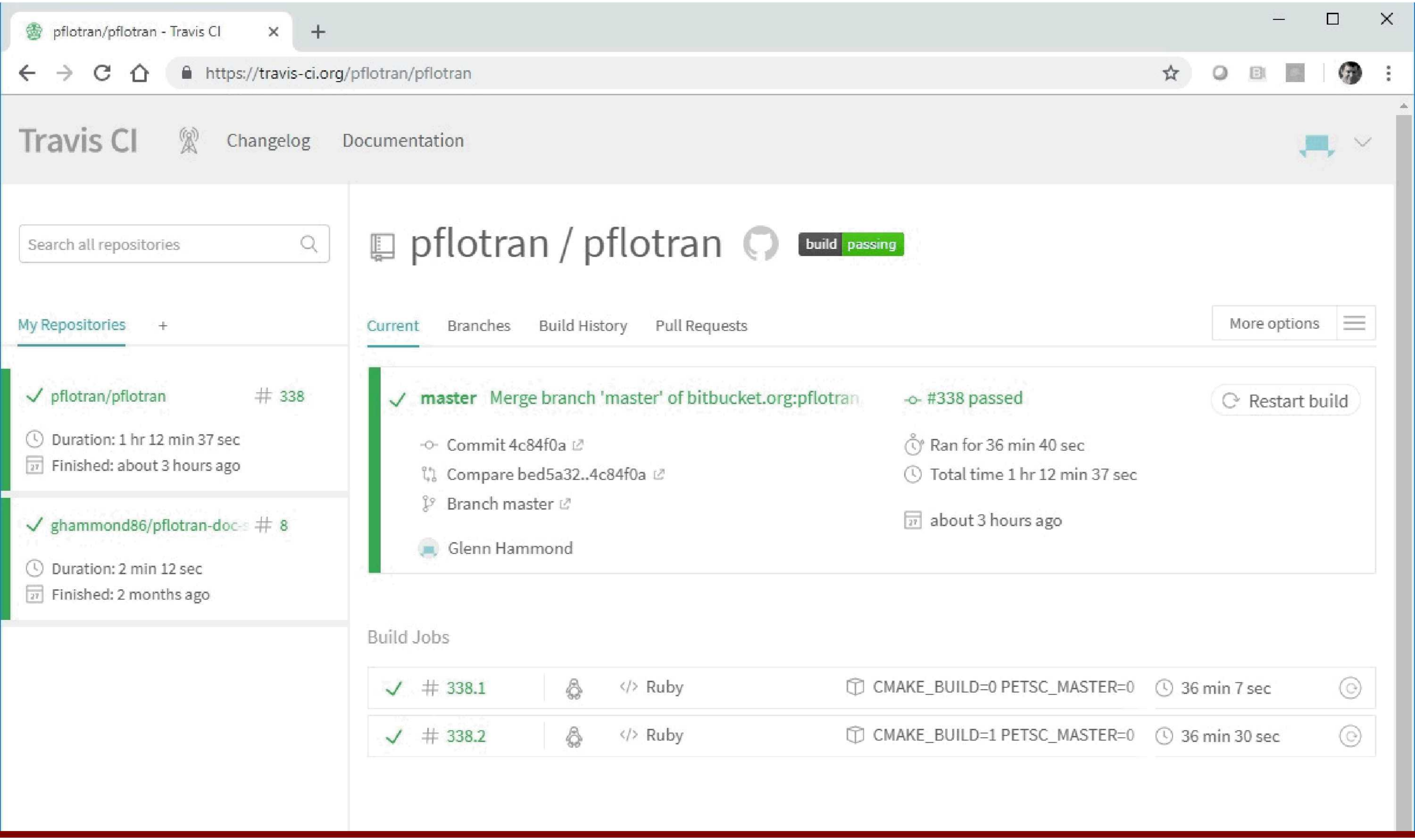
PFLOTRAN Unit/Regression Test Output

```
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.
```

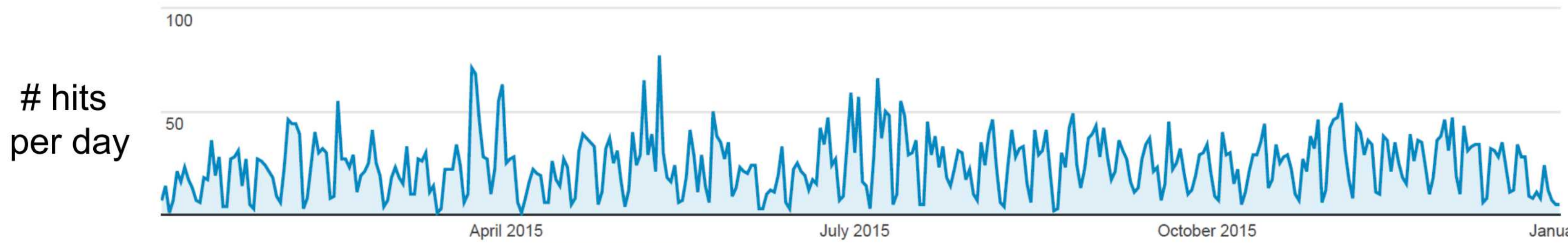
Travis CI: Build/Test Success

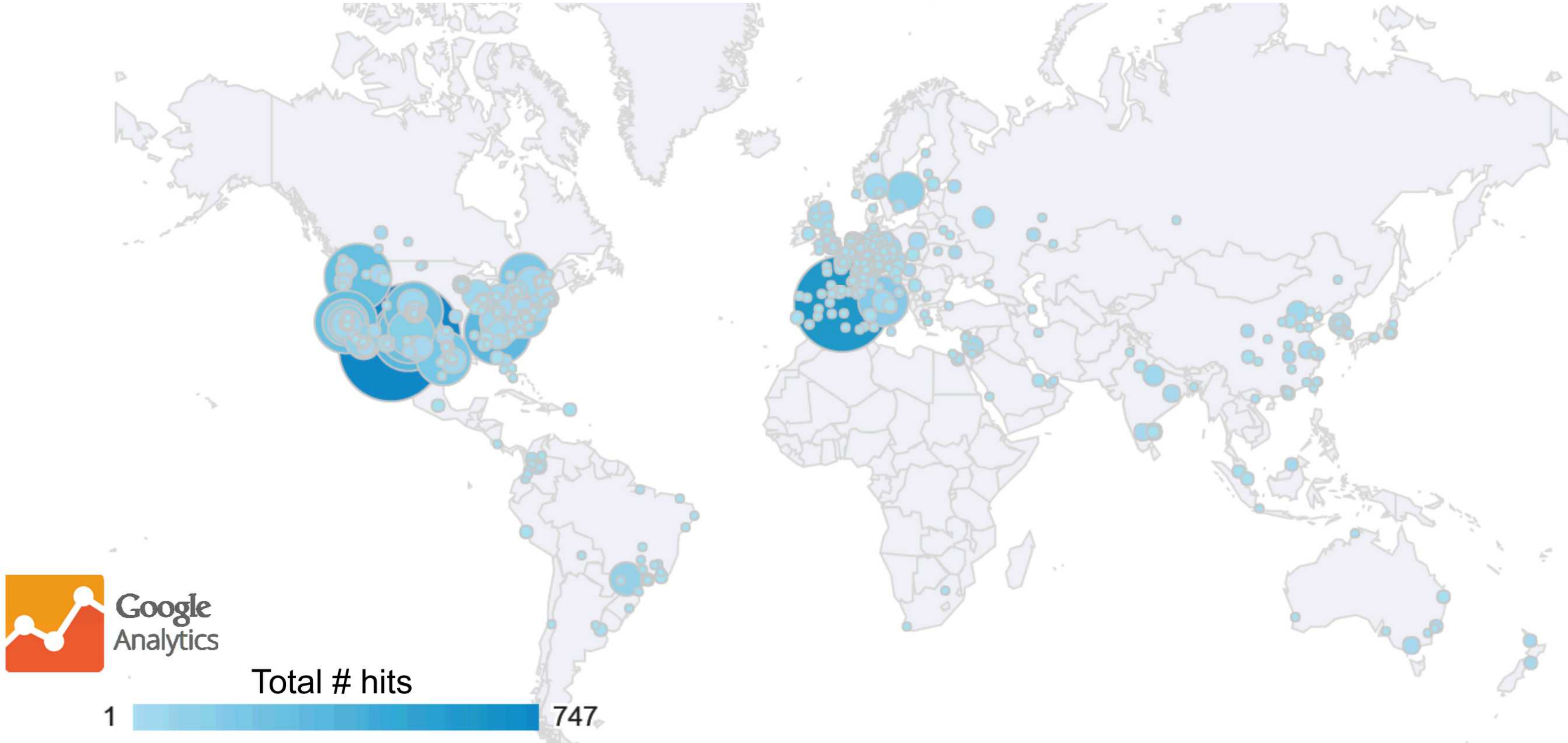


PFLOTRAN Unit/Regression Test Output

```
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.
```

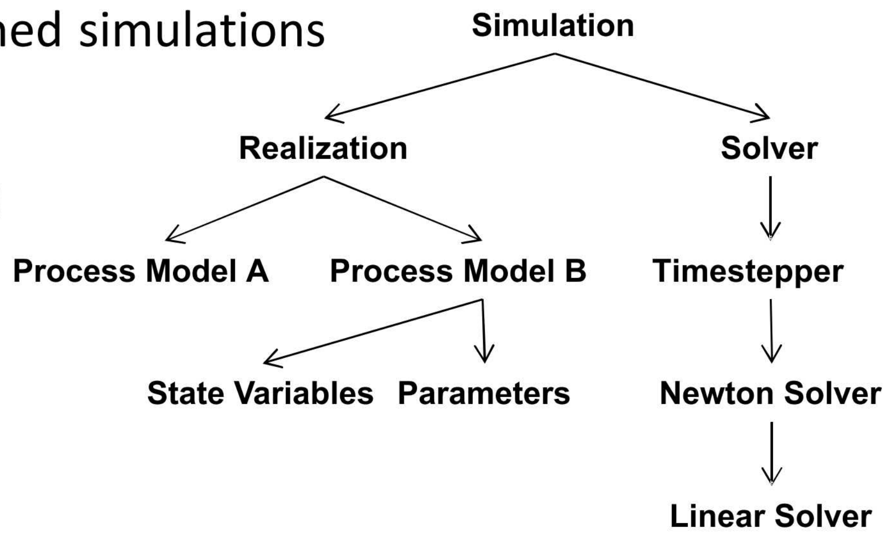
Hits on PFLOTRAN Bitbucket Site in 2015





Why Object-Oriented Fortran 2003/2008?

- Why Fortran?
  - Experienced domain scientists remain engaged
  - Commonality among all domain scientists
- Why object-oriented?
  - Modular data structures
    - Eases code development and debugging – data locality
    - Nesting of processes and data
  - Tree structure enables self-contained simulations
- Why Fortran 2003/2008?
  - Classes (extendable derived types)
    - Member functions
    - Inheritance
  - Pointers to procedures
    - E.g. swapping equations of state



CAPABILITIES

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)

Comparison of Gov. Flow Equations

GENERAL Mode (miscible air-water-energy)

Water Mass
$$\frac{\partial \phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_w^l \boldsymbol{q}_l + \rho_g X_w^g \boldsymbol{q}_g + \boldsymbol{J}_w^l + \boldsymbol{J}_w^g\right) + q_w$$

Air Mass
$$\frac{\partial \phi(s_l \rho_l X_a^l + s_g \rho_g X_a^g)}{\partial t} = -\nabla \cdot \left(\rho_l X_a^l \boldsymbol{q}_l + \rho_g X_a^g \boldsymbol{q}_g + \boldsymbol{J}_a^l + \boldsymbol{J}_a^g\right) + q_a$$

Energy
$$\frac{\partial \phi\left(s_l \rho_l U_l + s_g \rho_g U_g\right) + (1-\phi) C_p^{\mathrm{rock}} \rho_{\mathrm{rock}} T}{\partial t} = -\nabla \cdot \left(\rho_l H_l \boldsymbol{q}_l + \rho_g H_g \boldsymbol{q}_g - \kappa_{\mathrm{eff}} \nabla T\right) + q_e$$

RICHARDS Mode (variably saturated water)

Water Mass
$$\frac{\partial \phi(s_l \rho_l)}{\partial t} = -\nabla \cdot (\rho_l \boldsymbol{q}_l) + q_w^G$$

$$\boldsymbol{q}_\alpha = -\frac{k k_\alpha}{\mu_\alpha} \nabla (p_\alpha - \gamma_\alpha g z), \quad (\alpha = l,\, g)$$

$$\boldsymbol{J}_a^l = -\tau \phi s_l D_l \rho_l \boldsymbol{\nabla} X_a^l$$

$$\boldsymbol{J}_a^g = -\tau \phi s_g D_g^0 \left(\frac{T}{T_K}\right)^\theta \frac{p_0}{p_g} \rho_g \nabla X_a^g$$

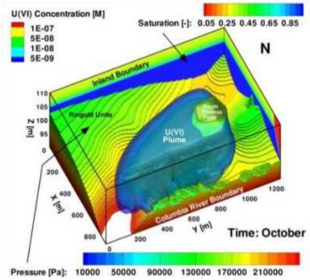
PFLOTRAN Reactive Transport

- Transport
  - Multicomponent
  - Mobile/immobile primary species
  - Advection (upwinding)
  - Hydrodynamic dispersion
- Reaction
  - Aqueous speciation
    - Ion activity models
  - General (A + B $\leftrightarrow$ 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

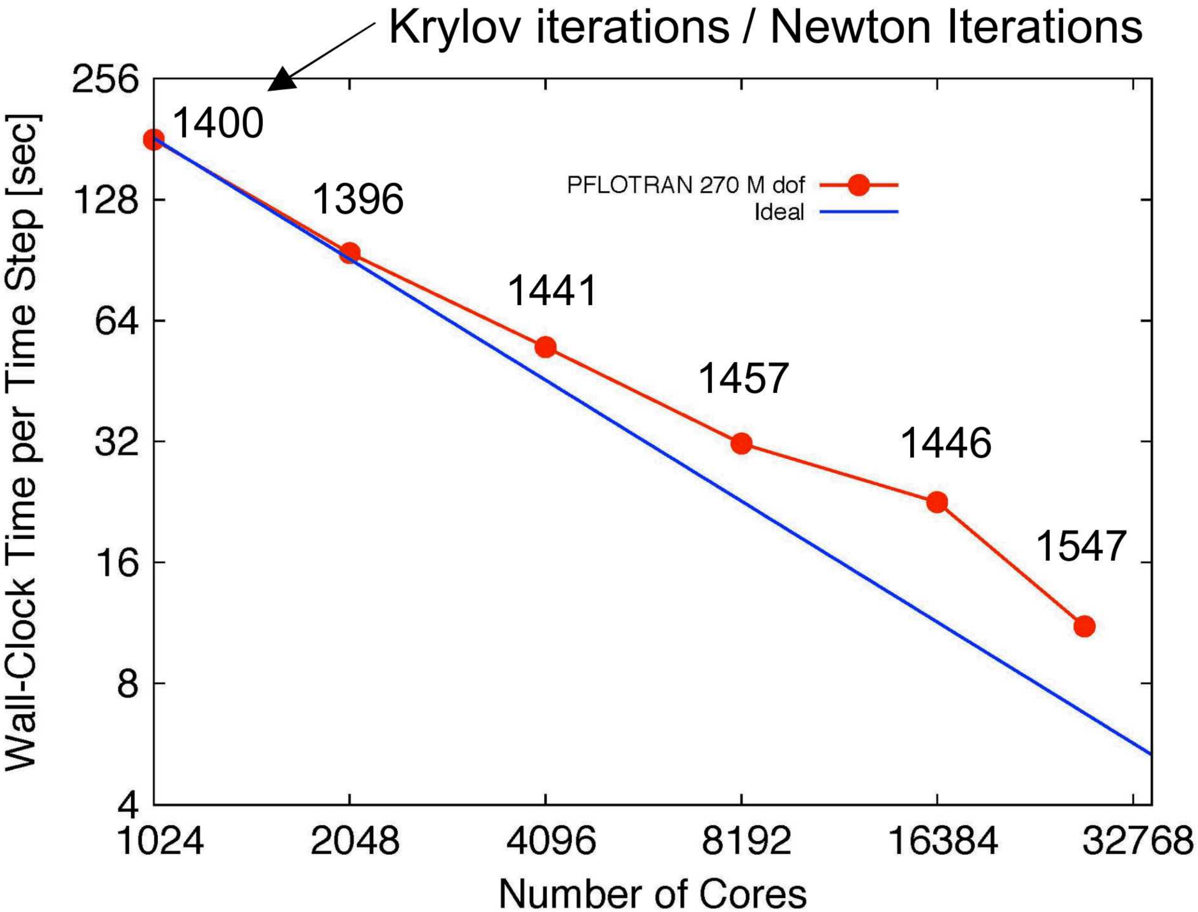
PARALLEL PERFORMANCE

PFLOTRAN Parallel Performance

Hanford 300 Area



Hammond and Lichtner, WRR, 2010



Overall 60% efficient

Science

(1-2% of overall time)

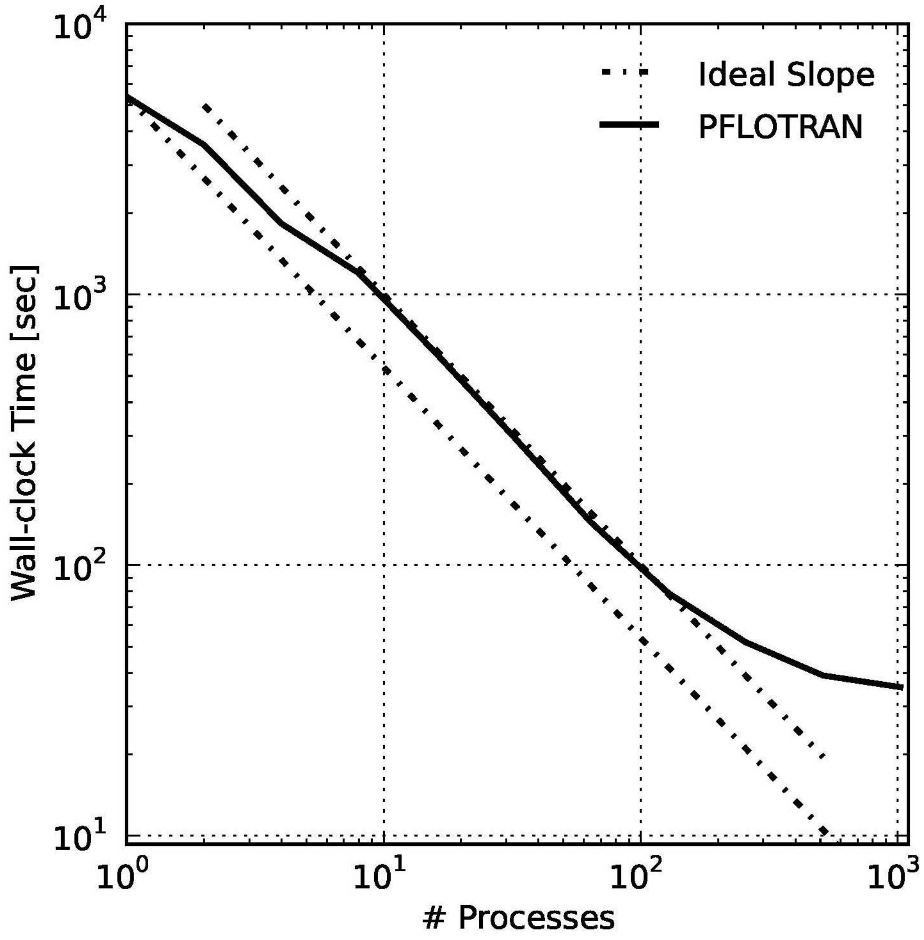
- 75% efficient (wall clock)

Solvers

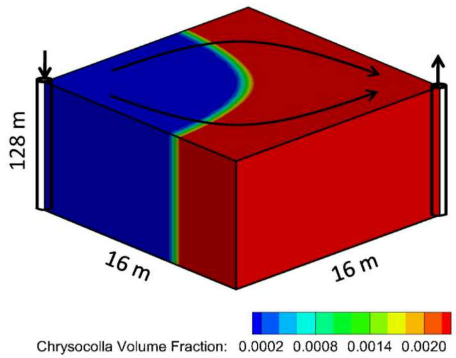
(96% of overall time)

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

PFLOTRAN Single Node Performance on Cray XK6 Interlagos Processor



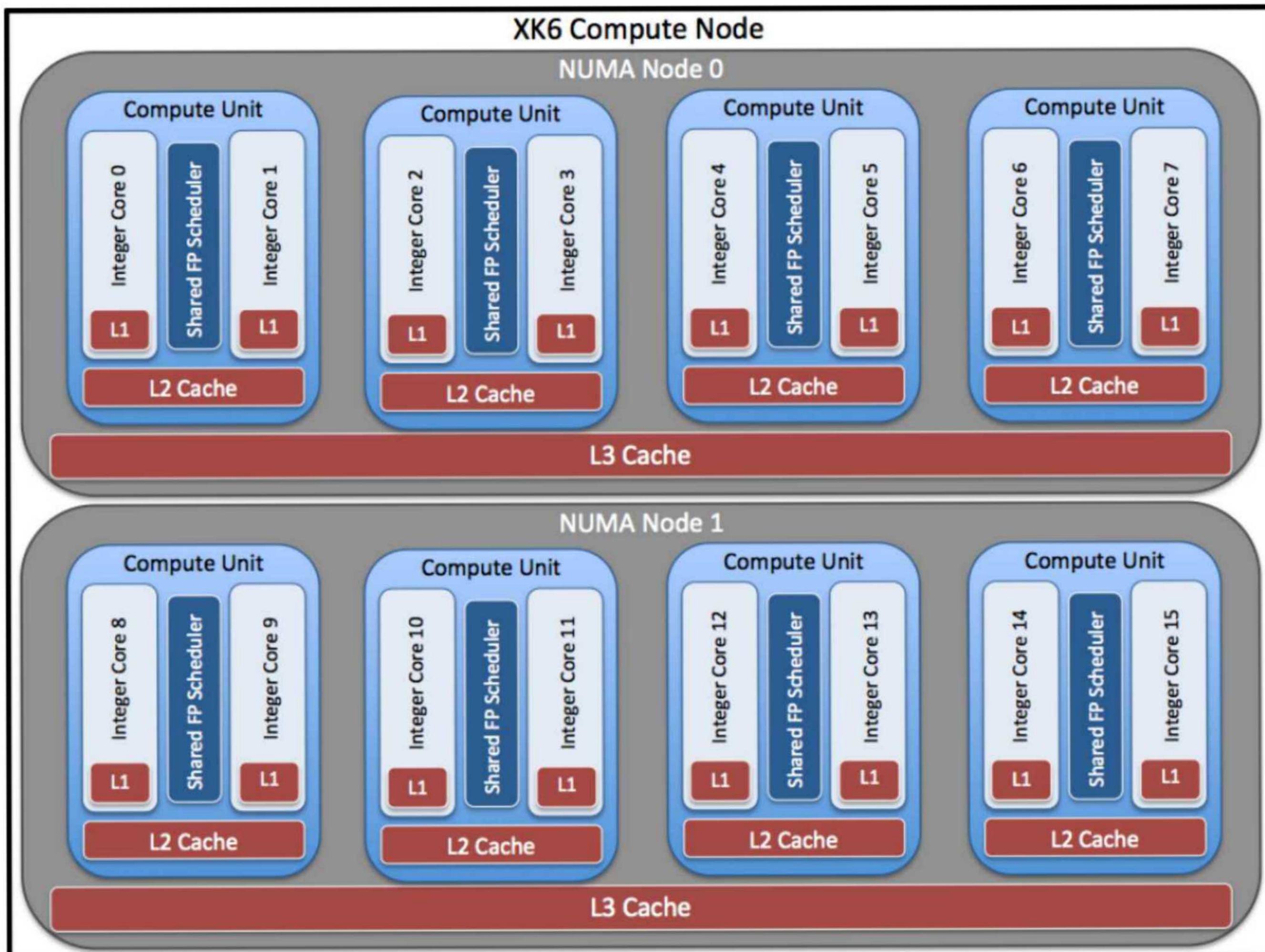
Copper Leaching



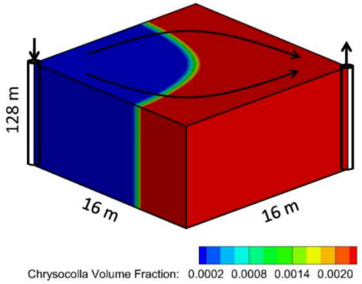
48K DOFs

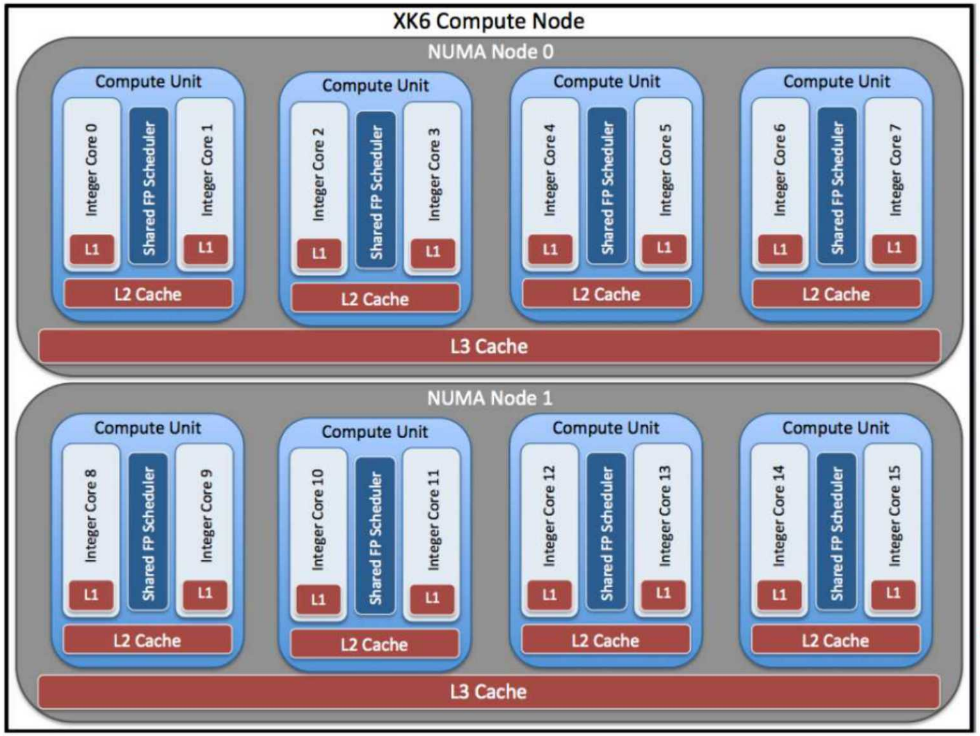
Hammond, G.E., P.C. Lichtner and R.T. Mills (2014) Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTRAN, Water Resources Research, 50, doi:10.1002/2012WR013483.

Memory Hierarchy on NUMA Node

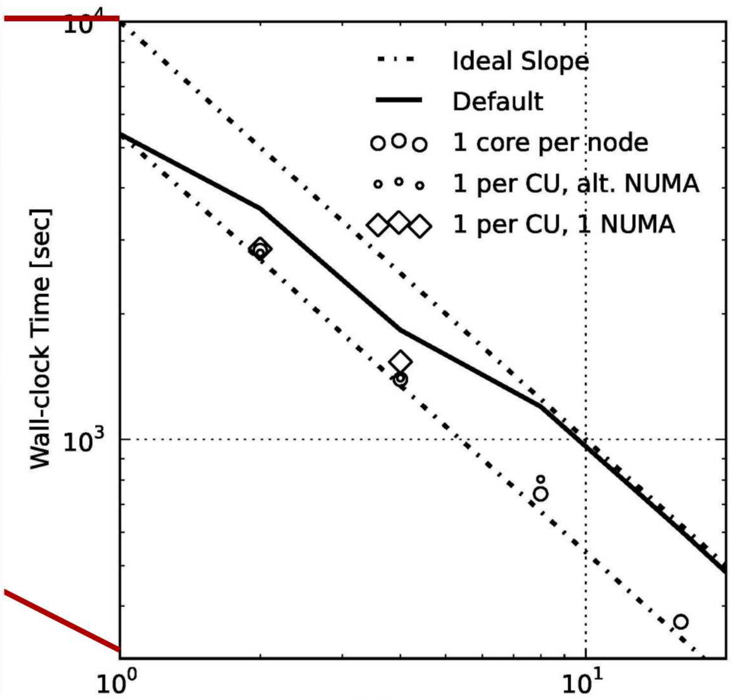


PFLOTRAN Single Node Performance on Cray XK6 Interlagos Processor





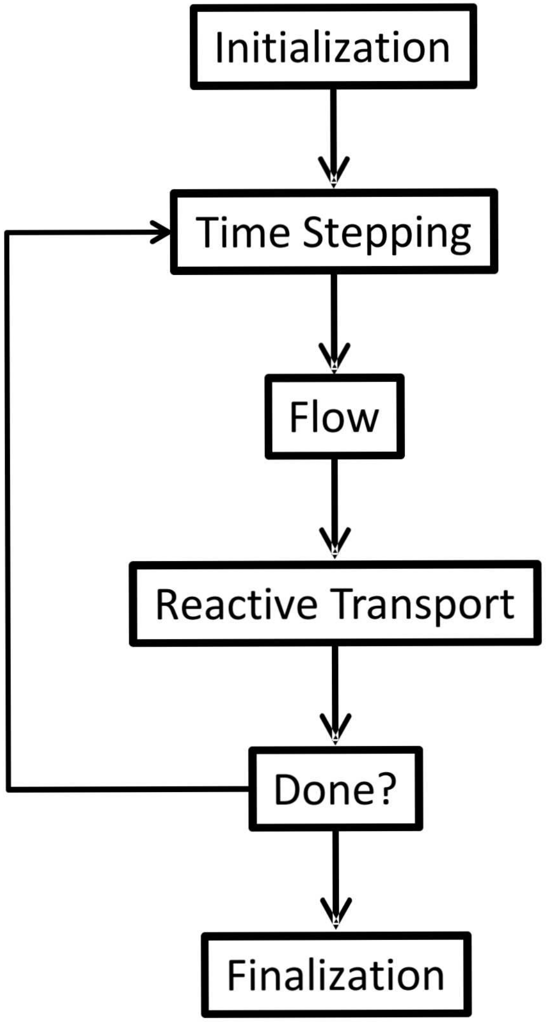
Processes



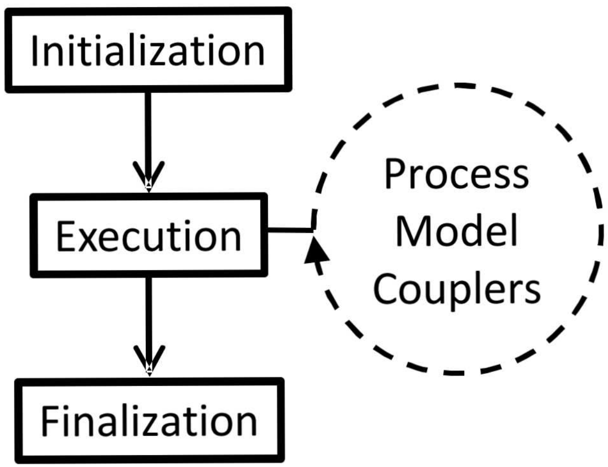
PROCESS MODEL COUPLING

Traditional Process Model Coupling

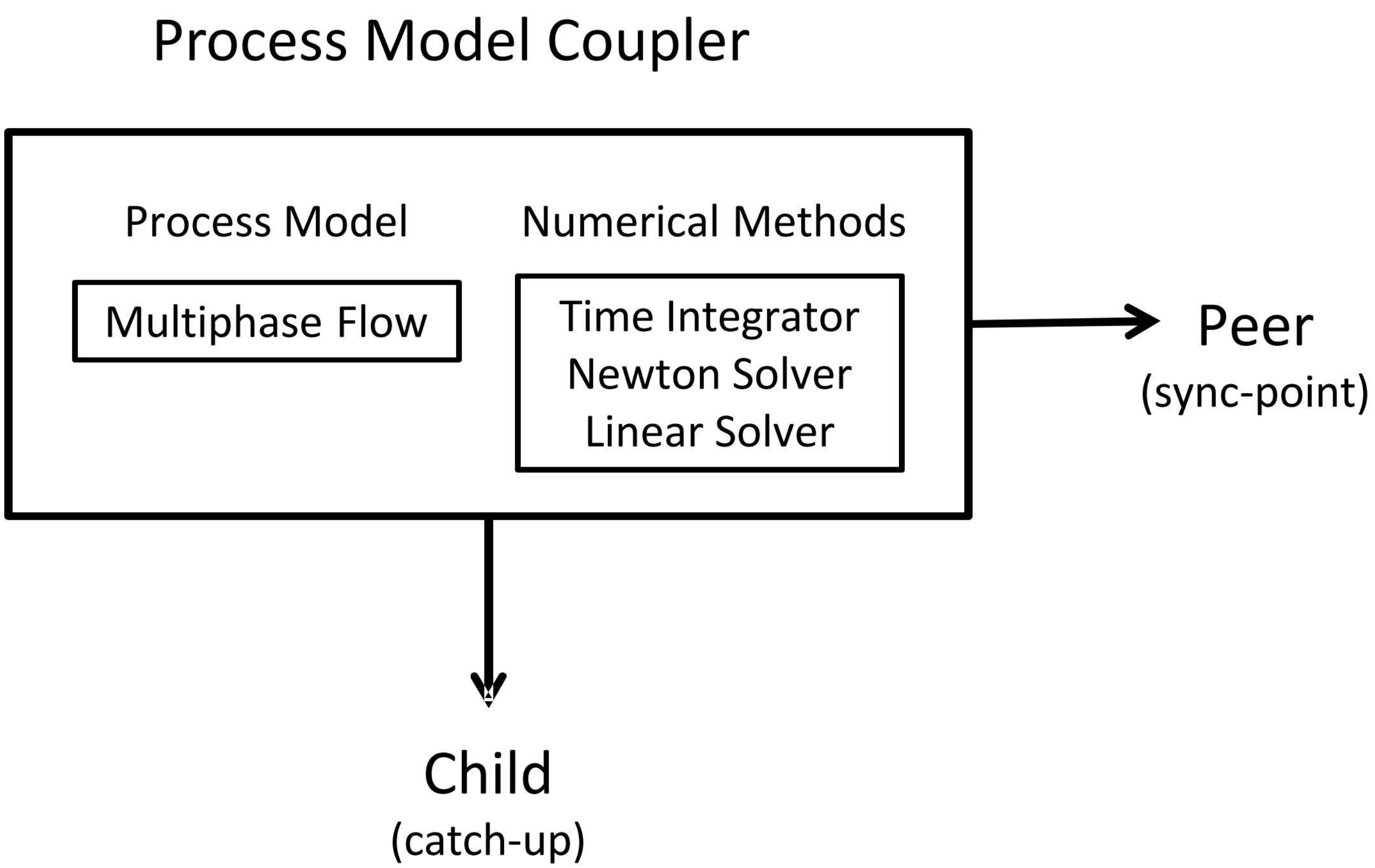
Traditional Time Stepping Loop



PFLOTRAN Workflow

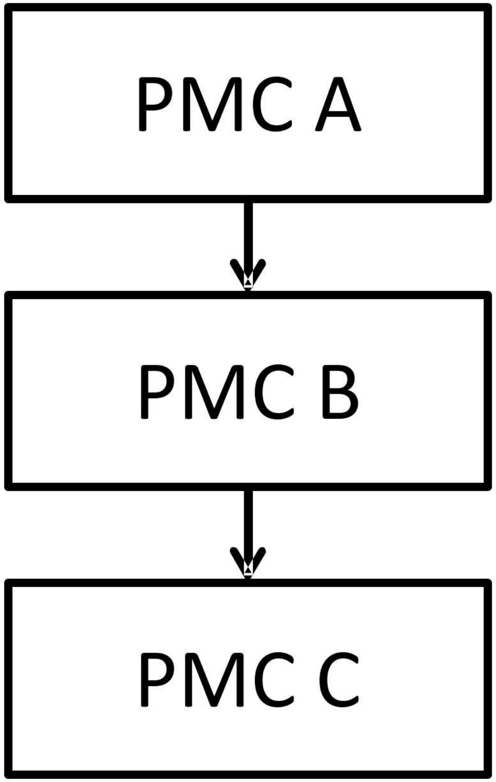


Process Model Coupling



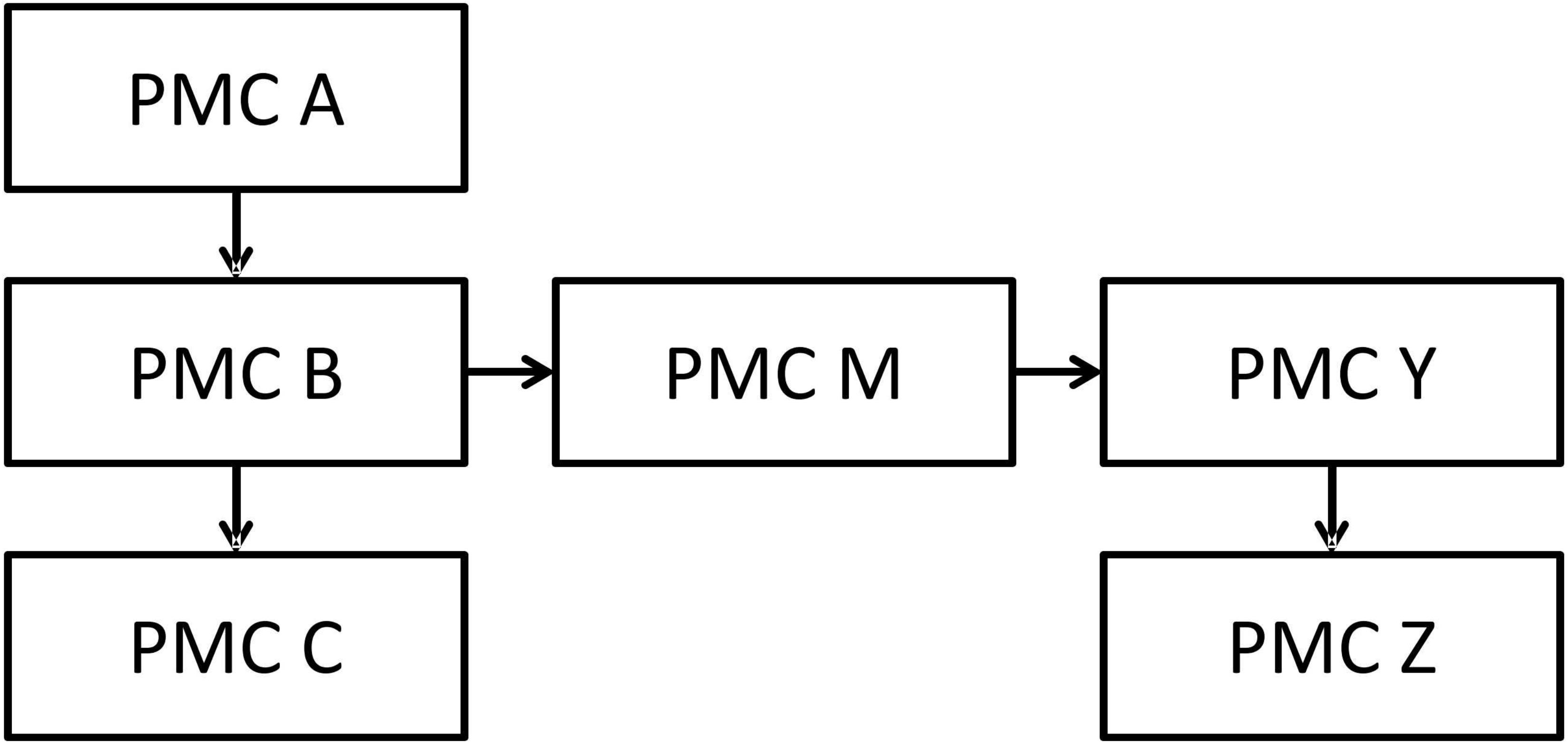
Hypothetical PMC Coupling

PMC = Process Model Coupler

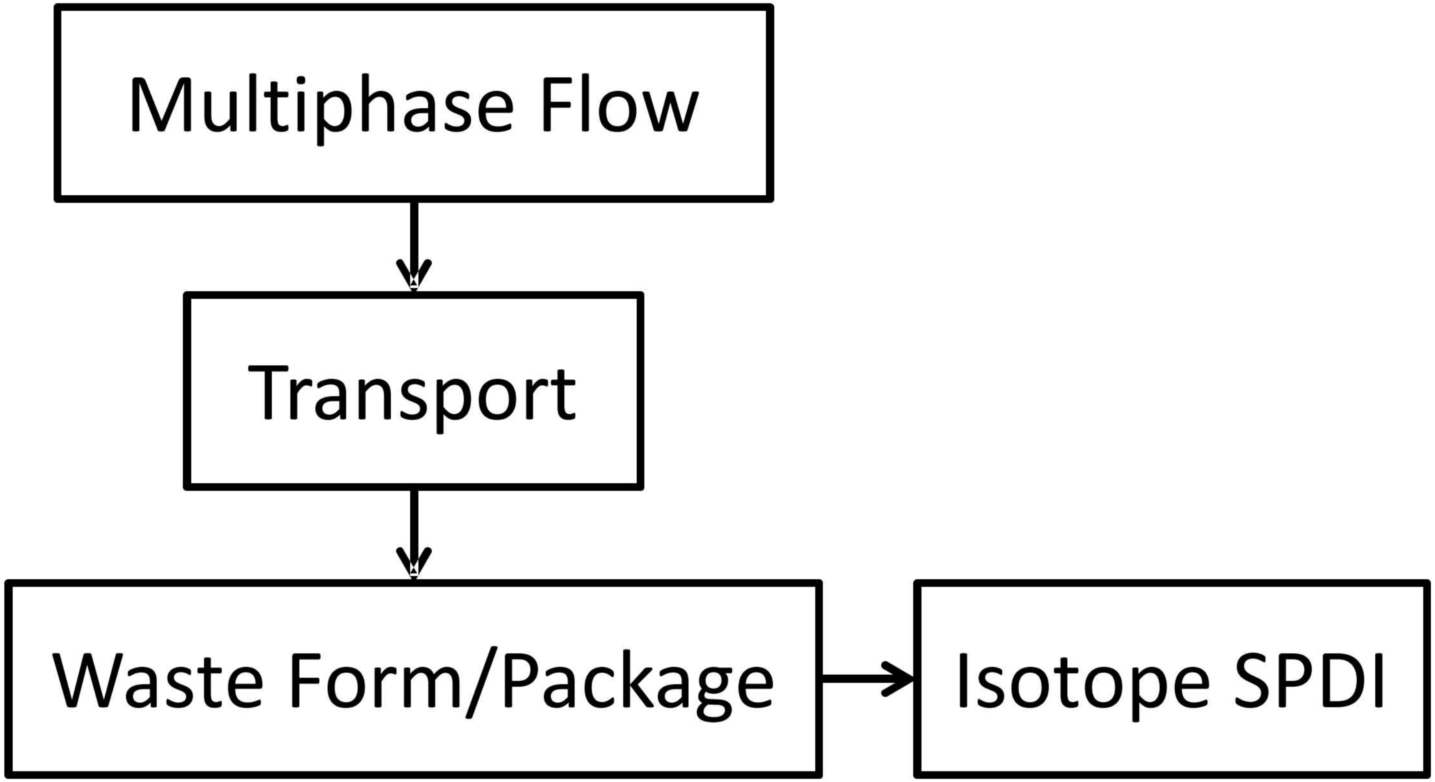


Hypothetical PMC Coupling

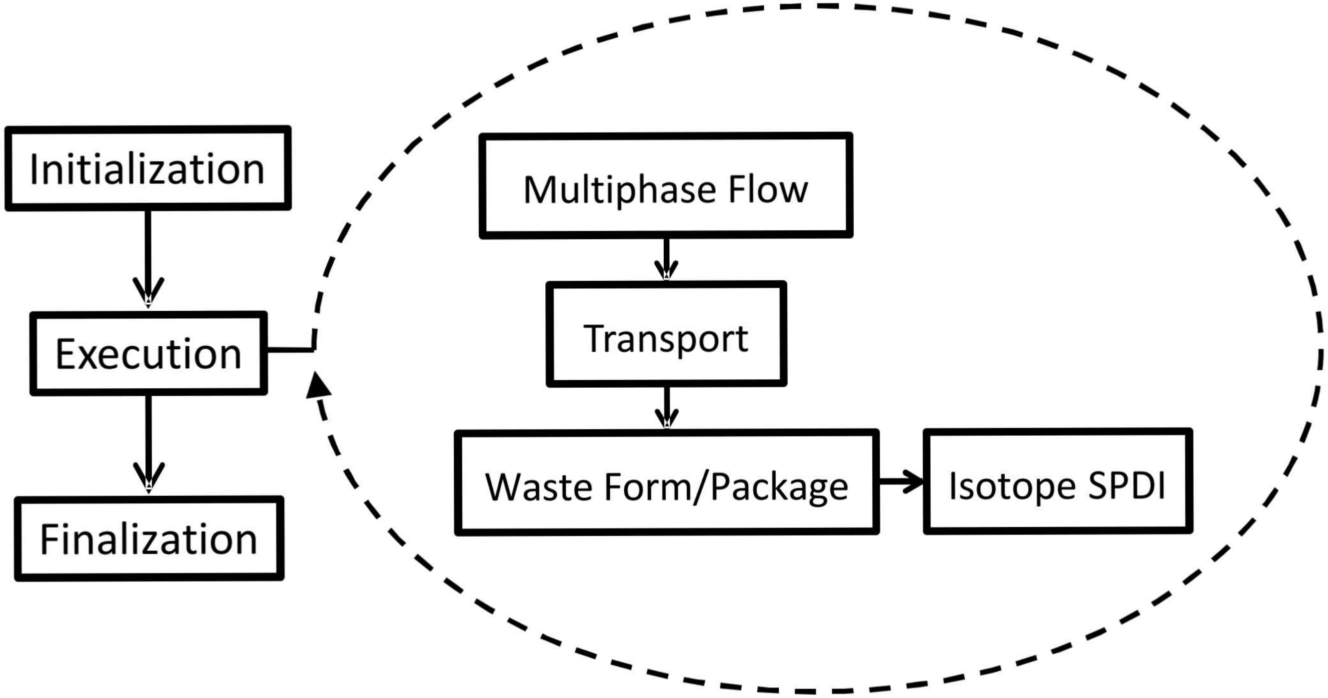
PMC = Process Model Coupler



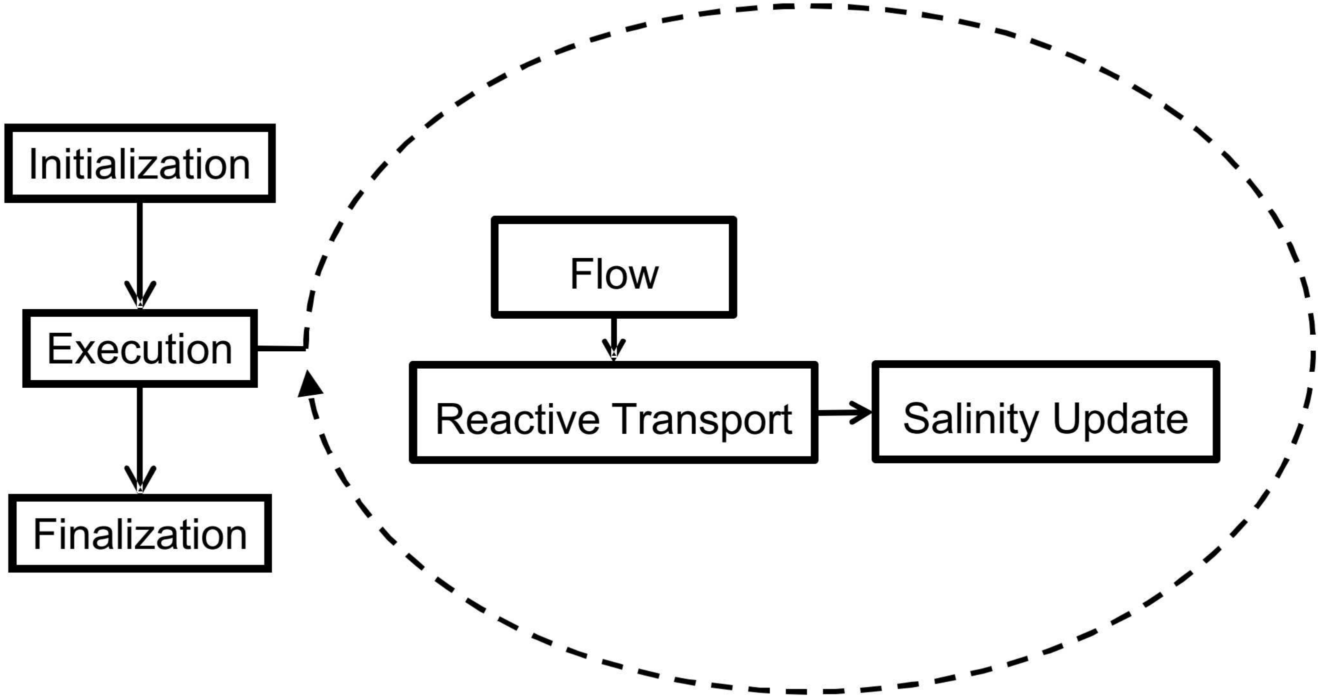
Radioactive Waste Process Models



PFLOTRAN Radioactive Waste Workflow



PFLOTRAN Salinity-Dependent Density Workflow



Flexible Process Model Coupling

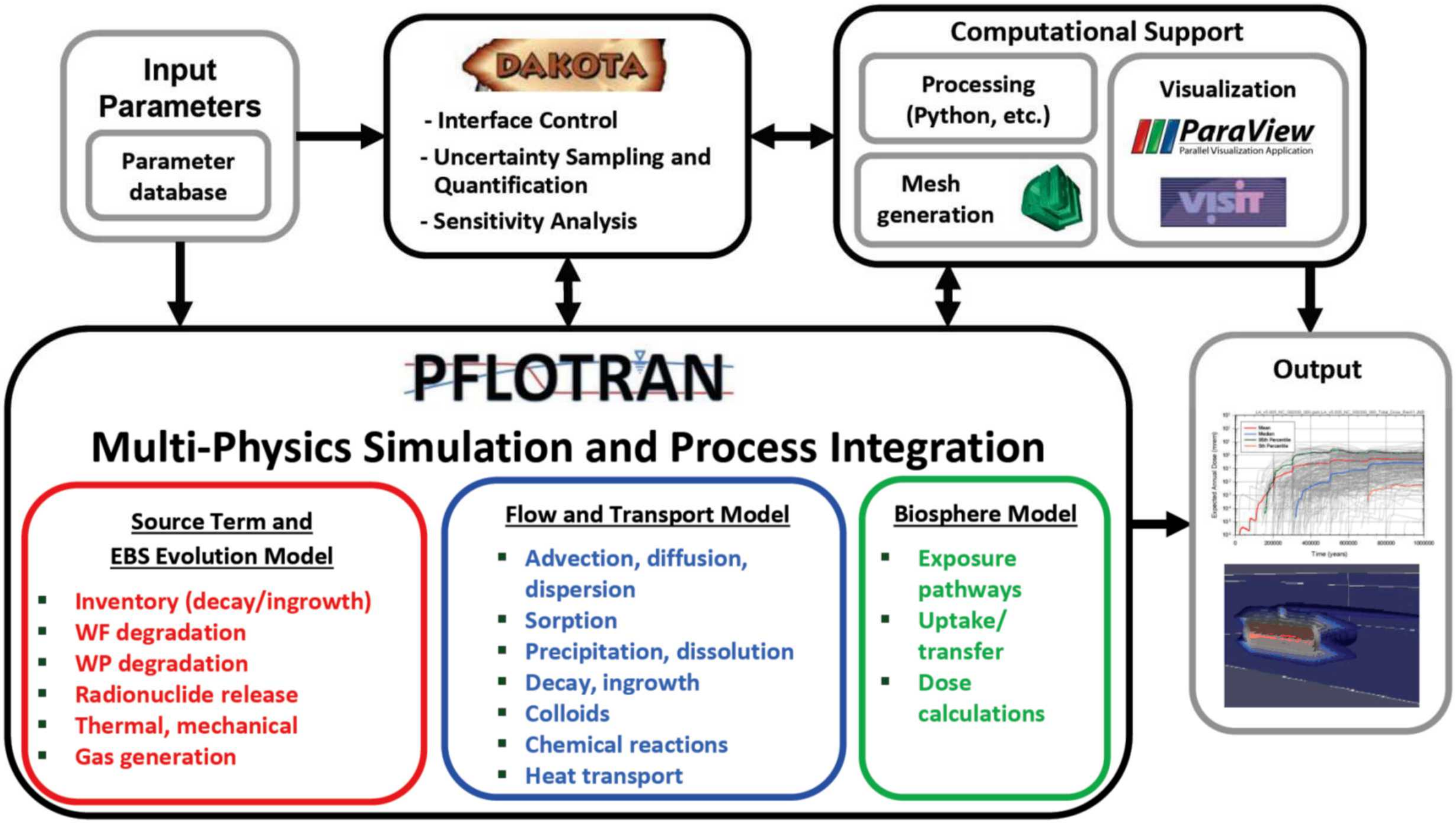
- Benefits
  - Customizable linkage between process models, e.g.
    - Flow
    - Transport
    - Reaction
    - Updates to material properties at select times
  - Flexible time stepping
    - Individual processes may run at their own time scale.
  - Modularity for incorporating new process models
    - Time stepping loops for existing process models are not impacted.

APPLICATIONS

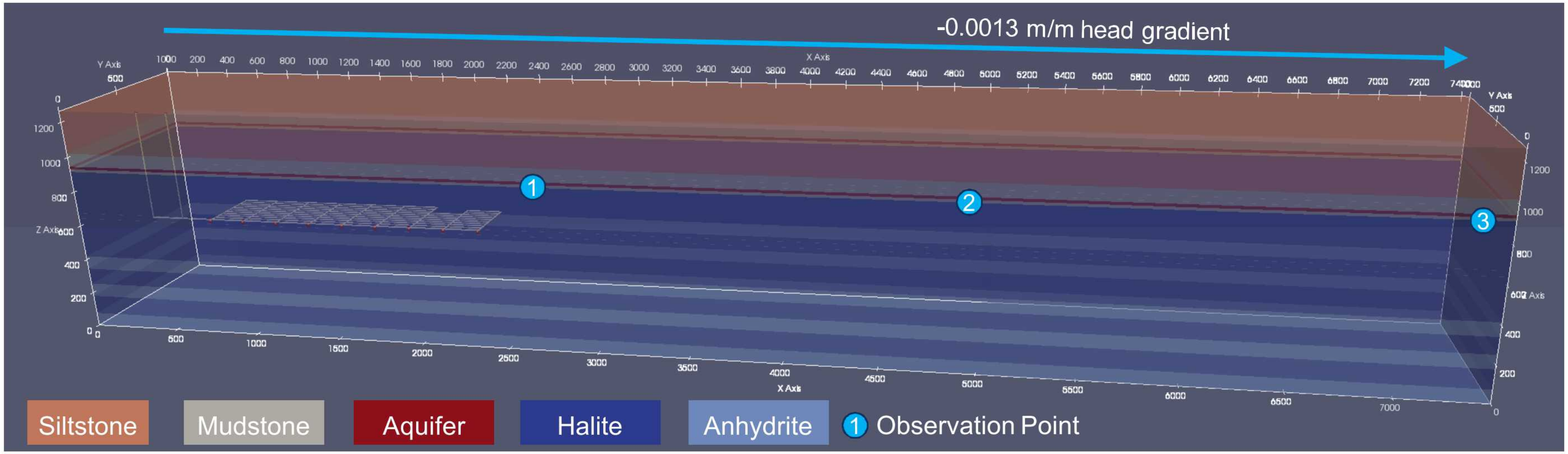
NUCLEAR WASTE REPOSITORY IN SALT FORMATION

GDSA Framework

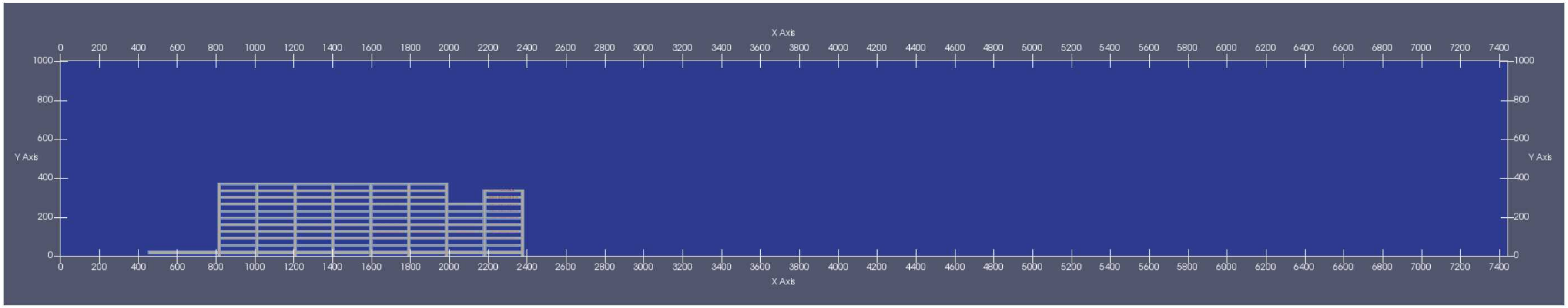
Geologic Disposal Safety Assessment – pa.sandia.gov



Generic Salt Repository

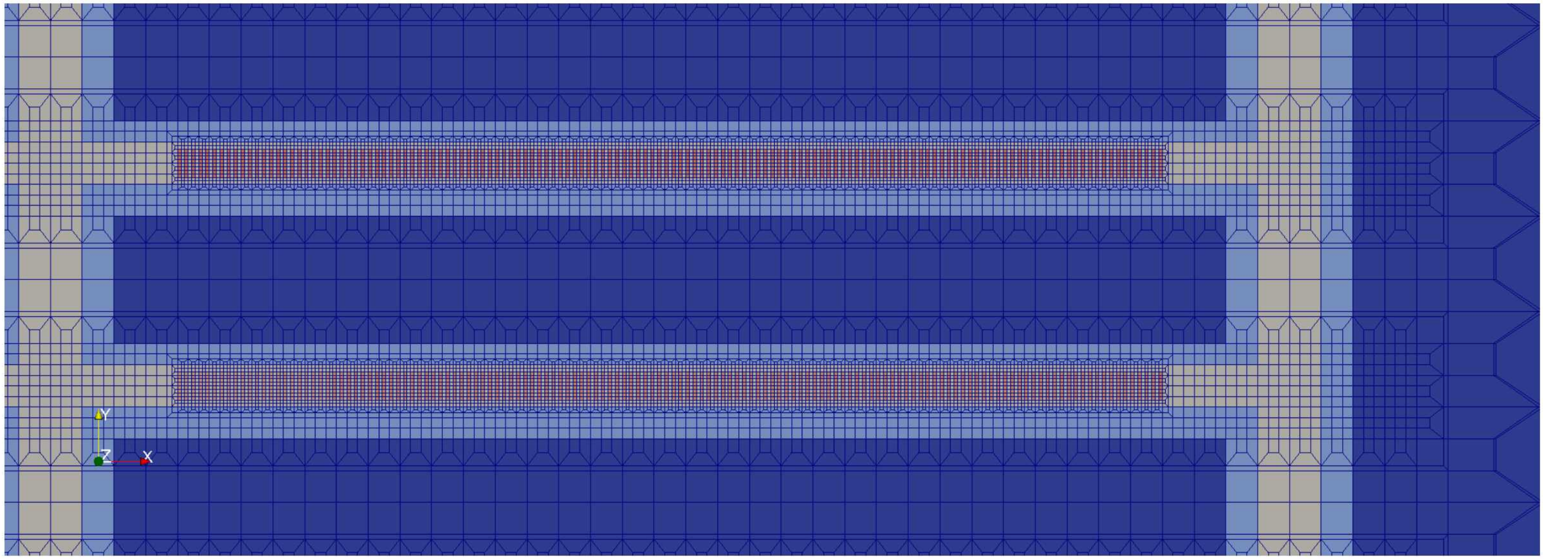


Horizontal Cross Section



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*

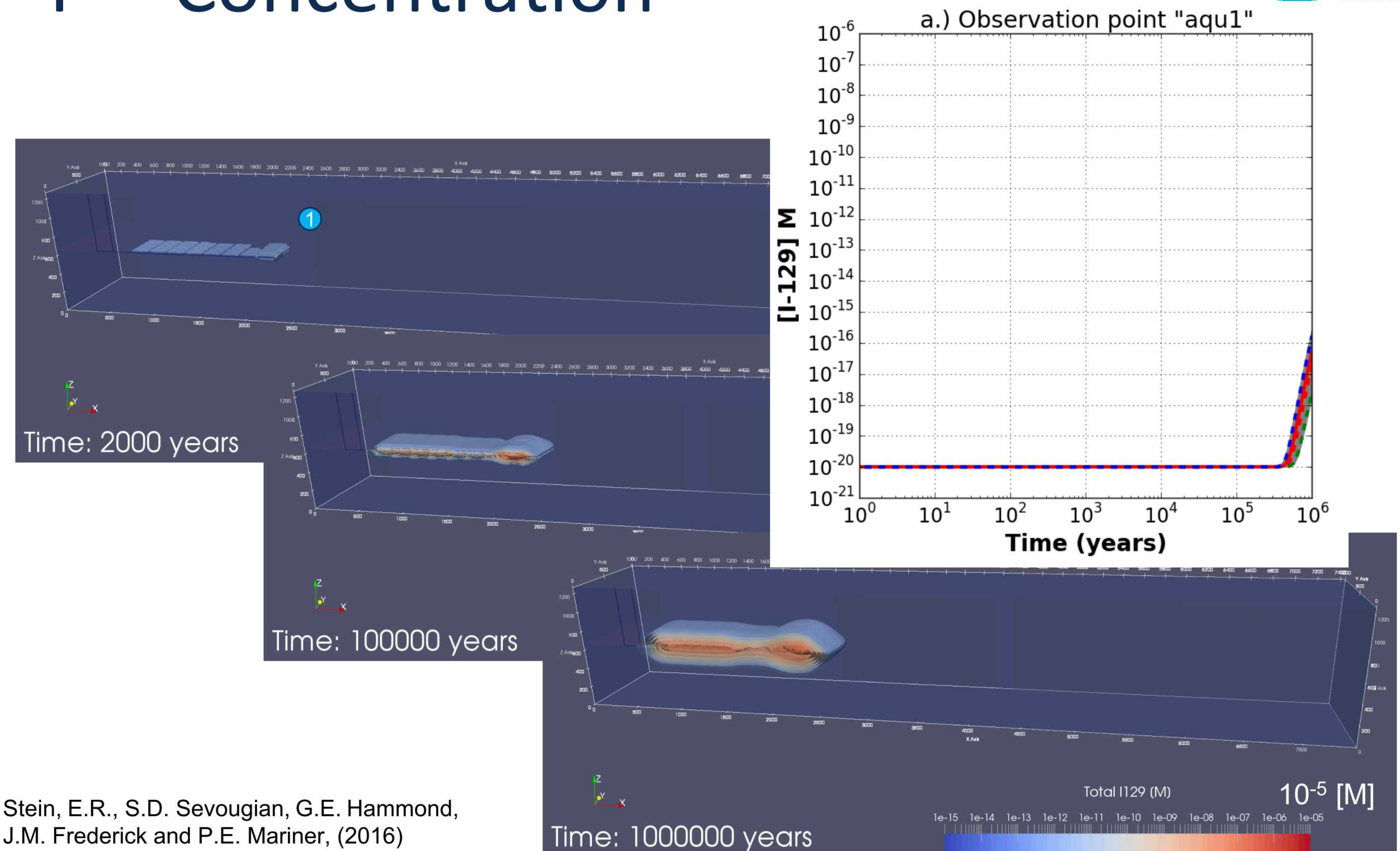
Grid Refinement in Repository Rooms



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

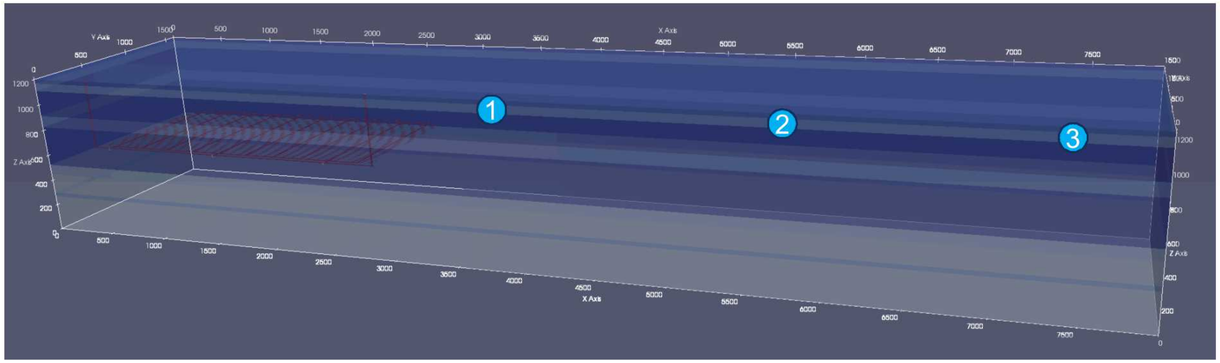
Stein, E.R., S.D. Sevougian, G.E. Hammond, J.M. Frederick and P.E. Mariner, (2016) *Performance Assessment of a Generic Repository in Bedded Salt, AGU Fall Meeting, San Francisco CA. SAND2016-12457C*

I^{129} Concentration

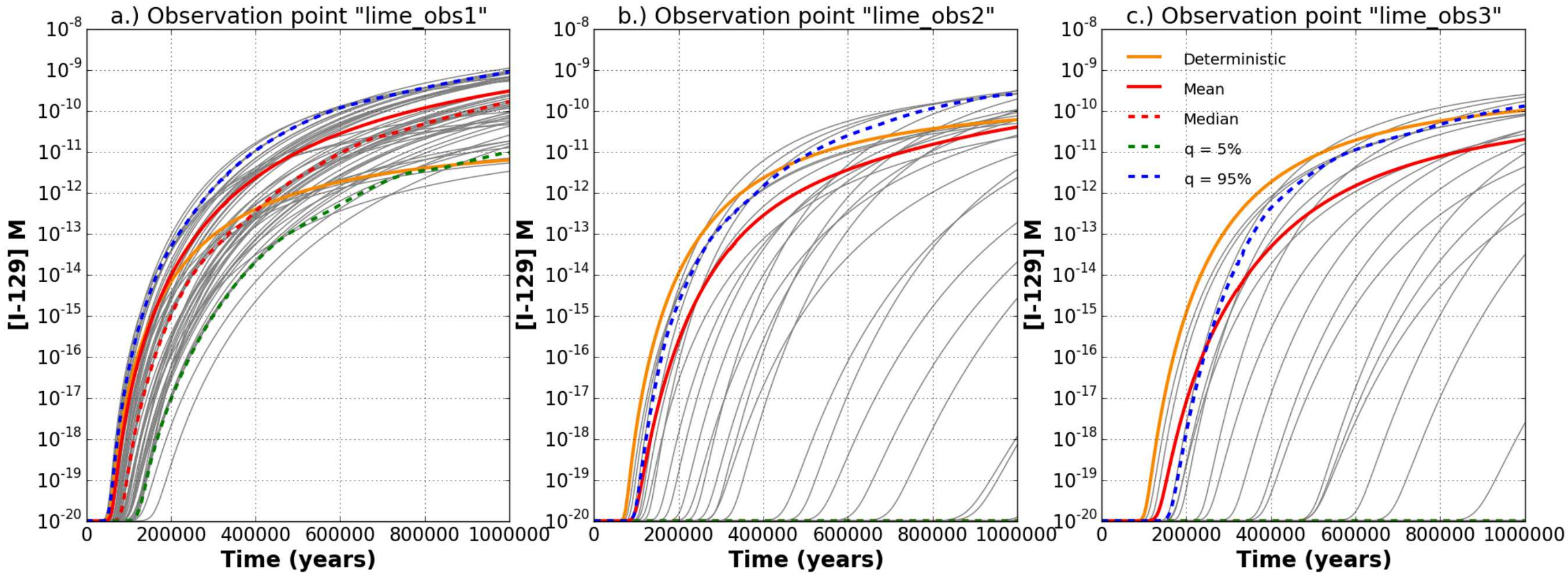


Stein, E.R., S.D. Sevougian, G.E. Hammond, J.M. Frederick and P.E. Mariner, (2016) *Performance Assessment of a Generic Repository in Bedded Salt, AGU Fall Meeting, San Francisco CA. SAND2016-12457C*

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

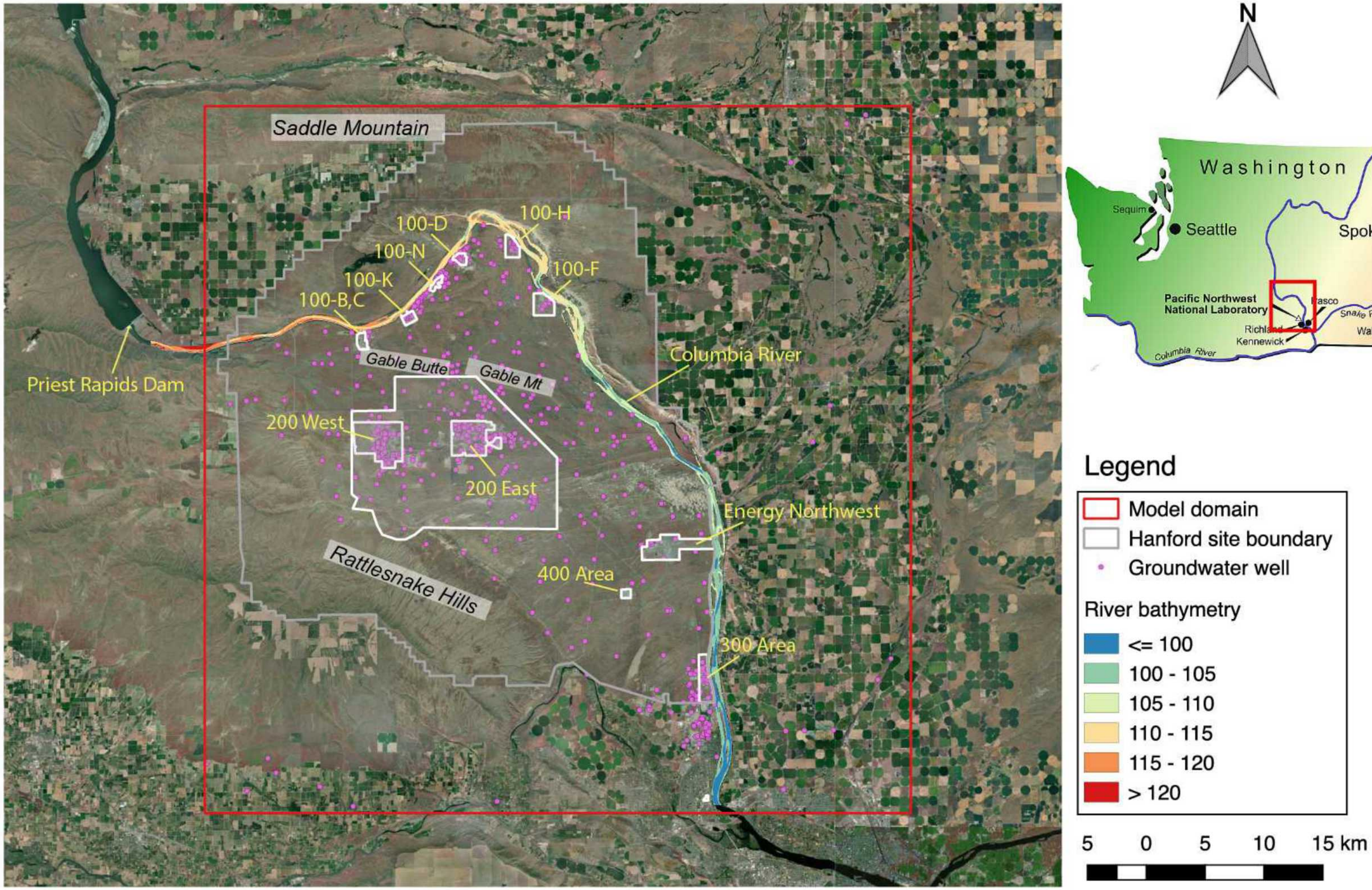


COLUMBIA RIVER GROUNDWATER – RIVER WATER EXCHANGE

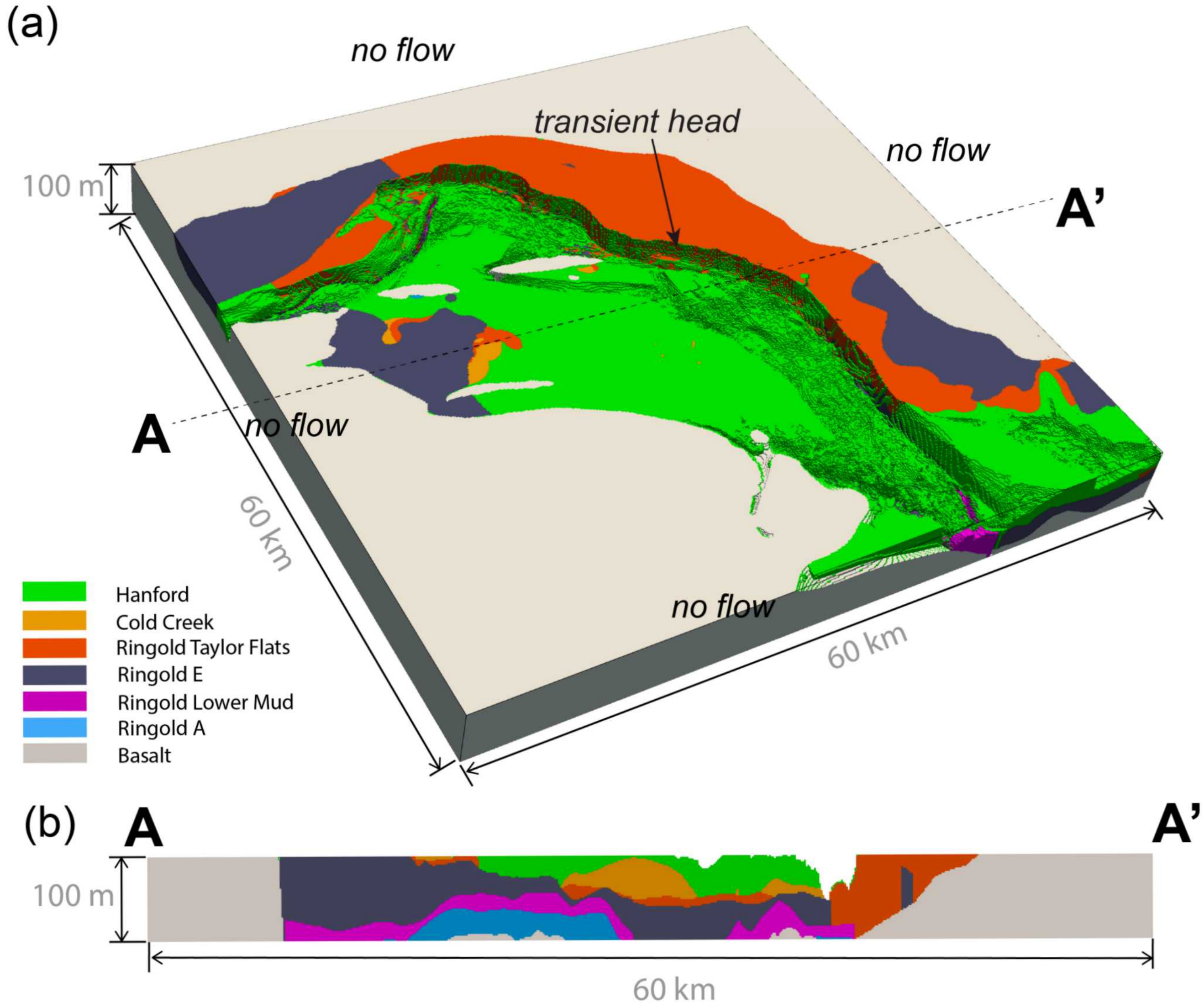
Groundwater-River Water Exchange Along Hanford Reach

Shuai, P., X. Chen, X. Song, G. Hammond, J. Zachara, P. Royer, H. Ren, W. Perkins (2018) Daily Dam Operations and Subsurface Hydrogeology Control Hydrologic Exchange Flows Hot Spots and Hot Moments in a Regulated River Reach, Manuscript in preparation for *Water Resources Research*.

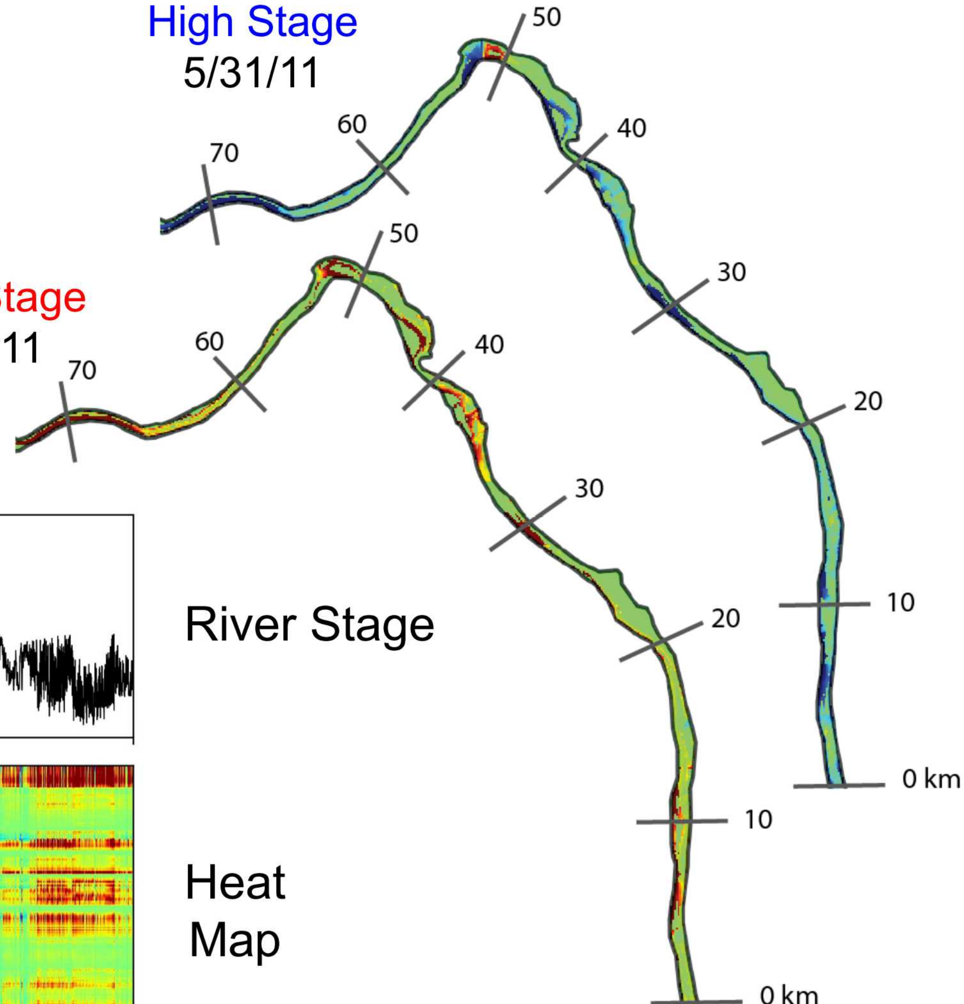
Hanford Reach



Geologic Units

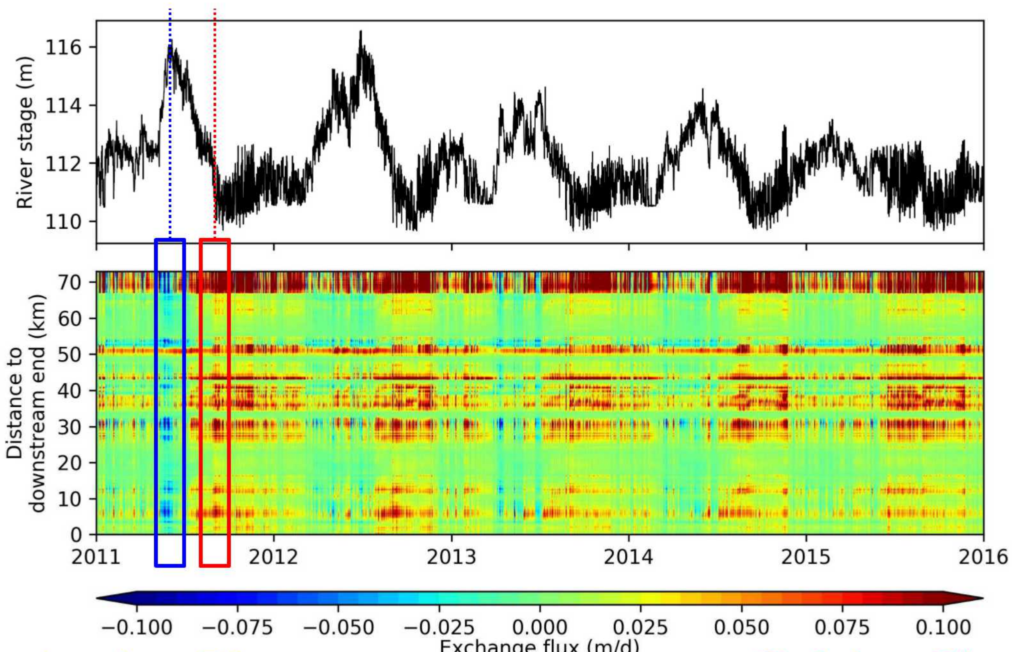


Exchange Flux Heat Map vs. River Stage



River Stage

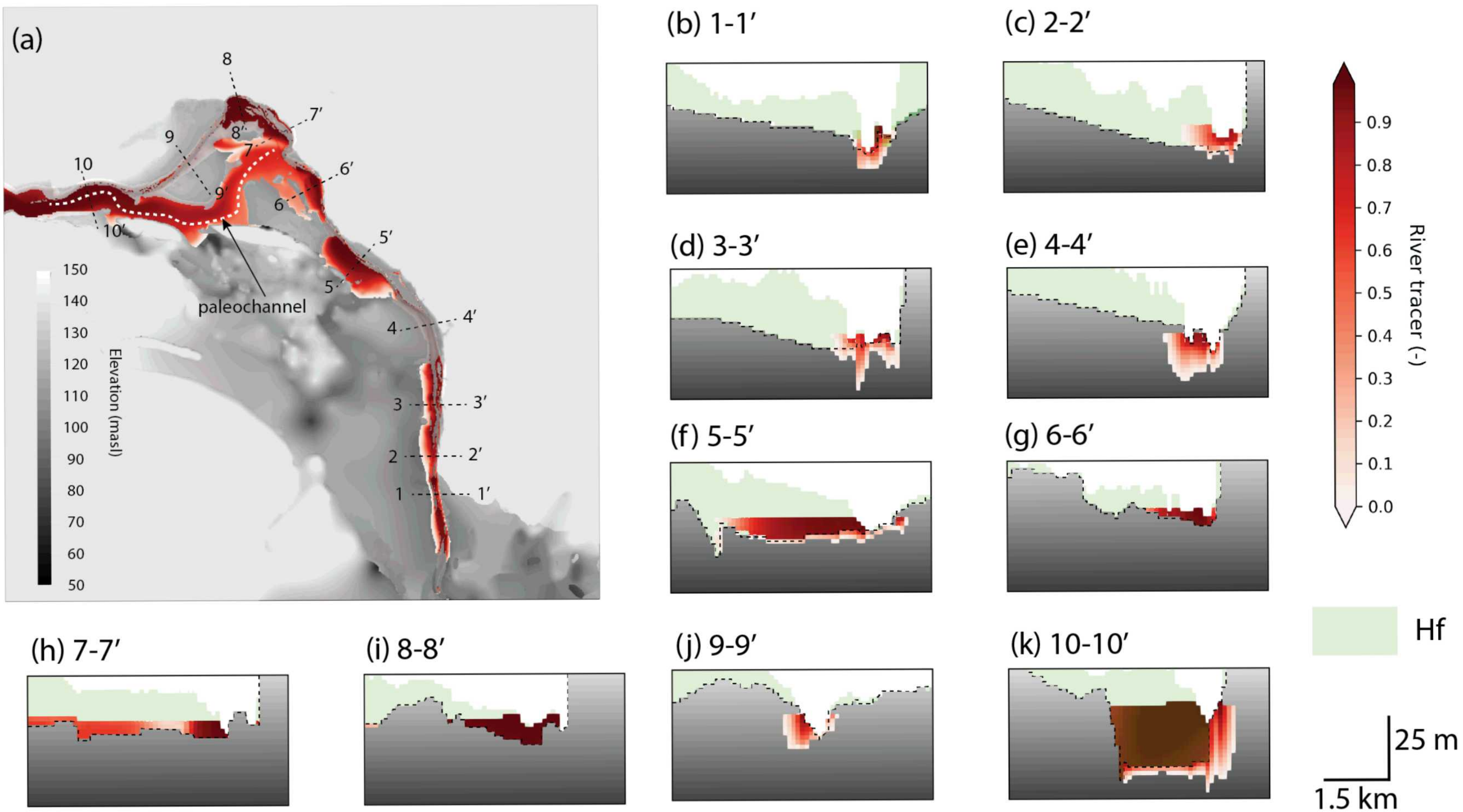
Heat Map



Losing River

Gaining River

River Tracer Intrusion



River Tracer and Existing Plumes